Supporting Information

Facile Synthesis of 5α-Functionalized Pyrroles *via* Multicomponent Reactions of Vicinal Tricarbonyl Compounds, Enamines, and Nucleophiles

Hua-li Wan, [a,#] Zhao-ping Shi, [a,#] and Qiang Sha [a,*]

[a] Jiangsu Key Laboratory of Pesticide Science and Department of Chemistry, College of Sciences, Nanjing Agricultural University, 1 Weigang Road, Xuanwu District, Nanjing 210095, P. R. China.

E-mail: qsha@njau.edu.cn

Table of Contents

General S2

General procedure for the synthesis of 1,3-dicarbonyl compounds S2

General procedure for the synthesis of enamines 2 S3

General procedure for the synthesis of nucleophilic substrates 3 S4

General procedure for the synthesis of vicinal tricarbonyl compounds 1 S4

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and H_2O S4-S5

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and alcohol S5

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and nucleophiles S5

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 18 and 19 S6

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 19 and 20 S6

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 19 and 21 S7

General procedure for gram-scale synthesis of 4aa S7

Characterization data of 1,3-dicarbonyl compounds S8-S9

Characterization data of enamines 2 S9-S16

Characterization data of pyrrole products 4-17 S16-S50

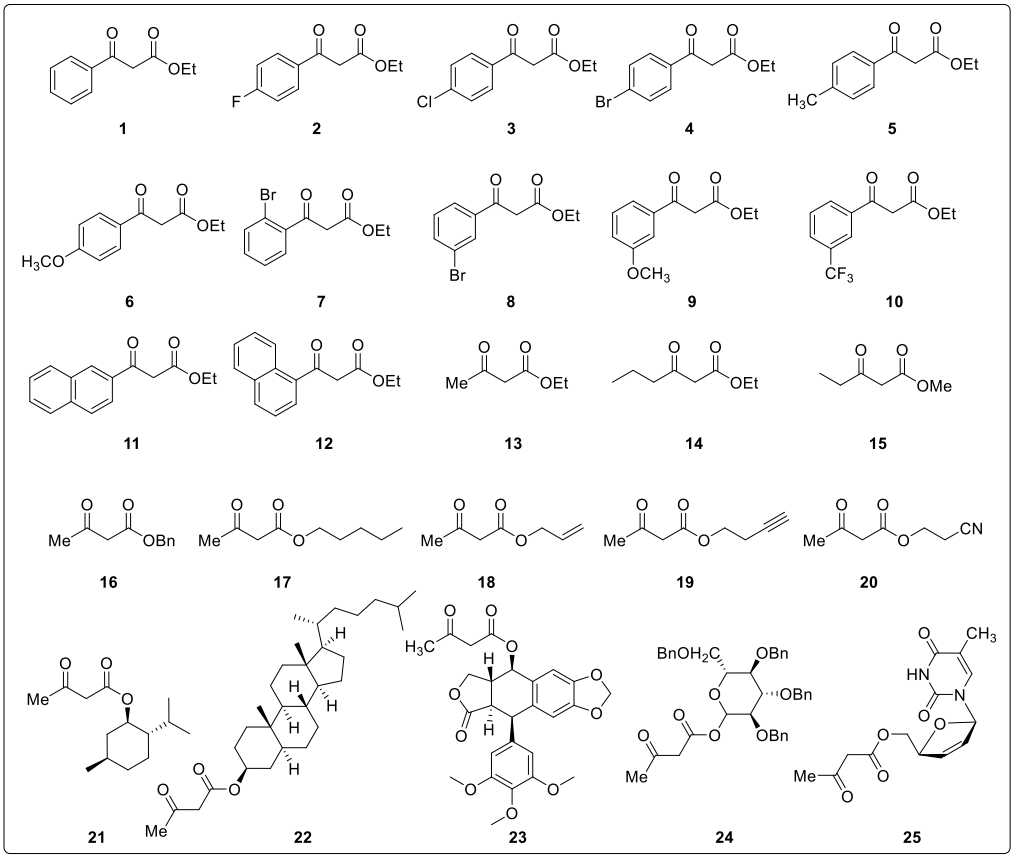
References S51

^1H and ^{13}C spectra of starting materials, pyrroles 4-17 S52-S144

Crystallographic data for compound 4ag S145-S160

General. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on a Bruker Avance III 400 MHz spectrometer or JNM-ECZ500R JEOL-500 MHz spectrometer. Chemical shifts are reported in ppm with the solvent signals as reference, and coupling constants (*J*) are given in Hertz (Hz). The peak information is described as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Analytical thin layer chromatography was performed on 0.25 mm extra hard silica gel plates with UV254 fluorescent indicator. High-resolution mass spectra (HRMS) were performed on a microTOF-ESI mass spectrometer using CsOAc as the standard. Melting points were obtained uncorrected from an Electrothermo Mel-Temp DLX 104 device. Unless otherwise noted, all reagents and solvents (AR grade) were obtained from commercial sources (aladdin, energy-chemical, J&K chemical) and used directly without purification. Unless otherwise noted, all reactions were performed under air atmosphere.

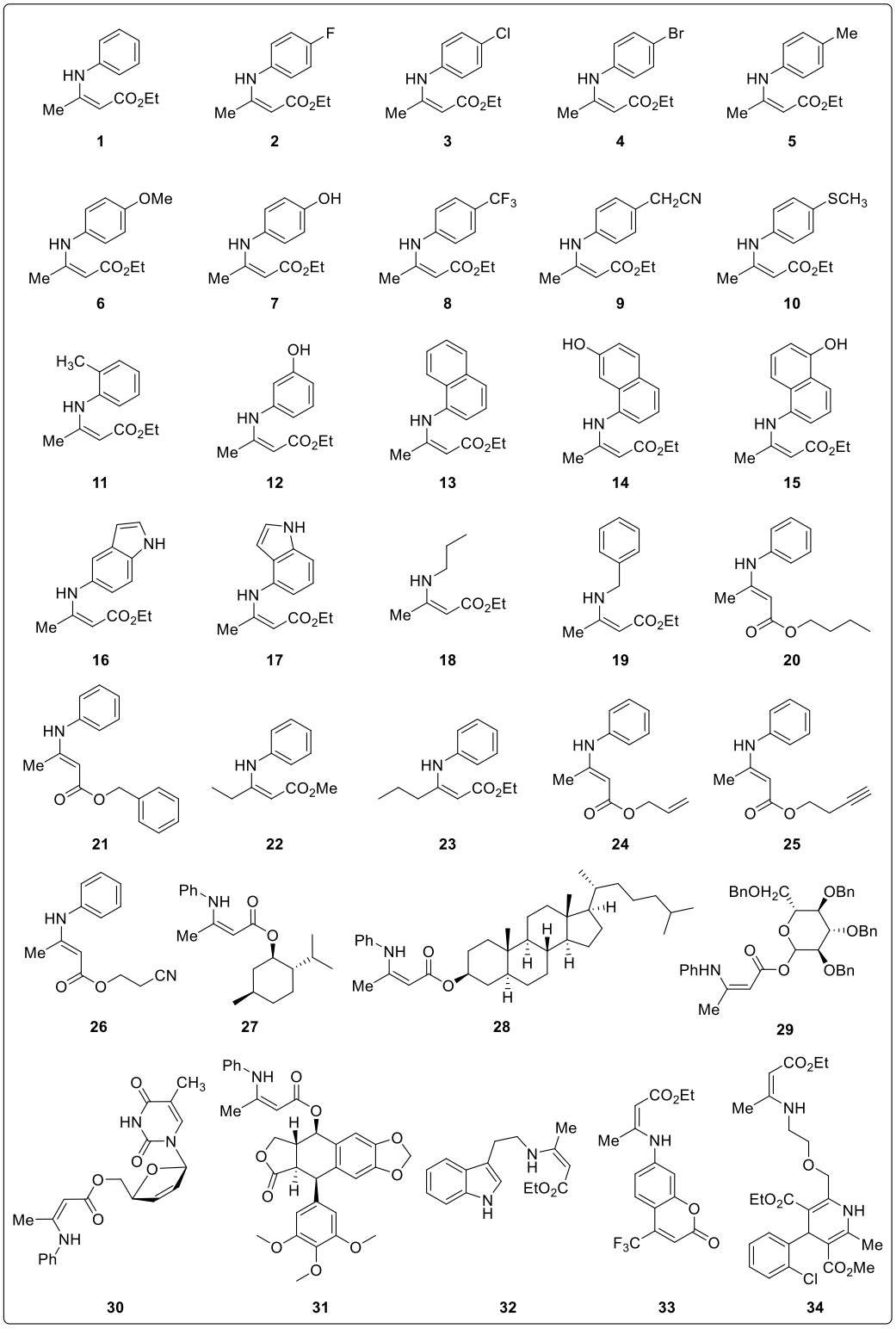
General procedure for the synthesis of 1,3-dicarbonyl compounds



1,3-Dicarbonyl compound **1**, **13**-**17** was purchased from chemical companies. 1,3-Dicarbonyl compounds **2**-**12** were synthesized from corresponding ketones and diethyl carbonate.[1] 1,3-Dicarbonyl compounds **18**-**25** were synthesized from corresponding alcohols and 2,2,6-trimethyl-4*H*-1,3-dioxin-4-one.[2]

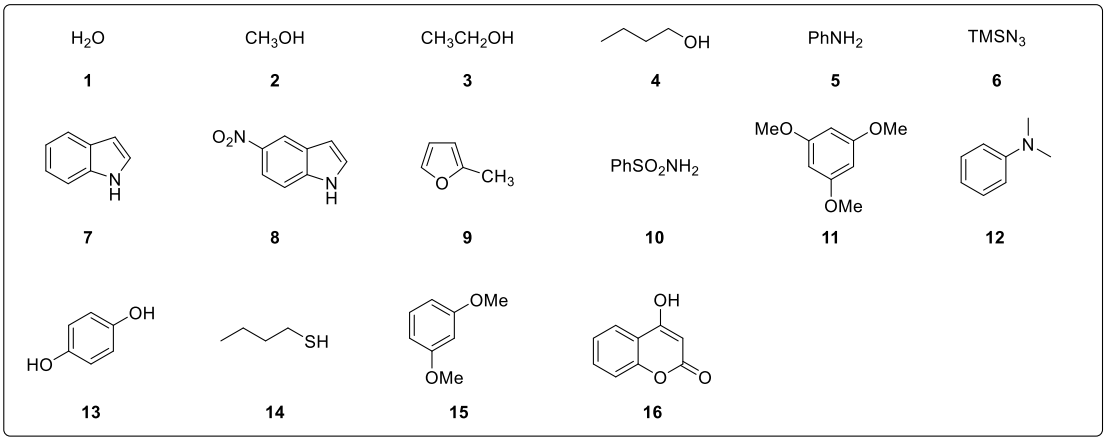
General procedure for the synthesis of enamines 2

The enamines **1-34** were synthesized by condensation reactions of amines with 1,3-dicarbonyl compounds according to literature procedure.[4]



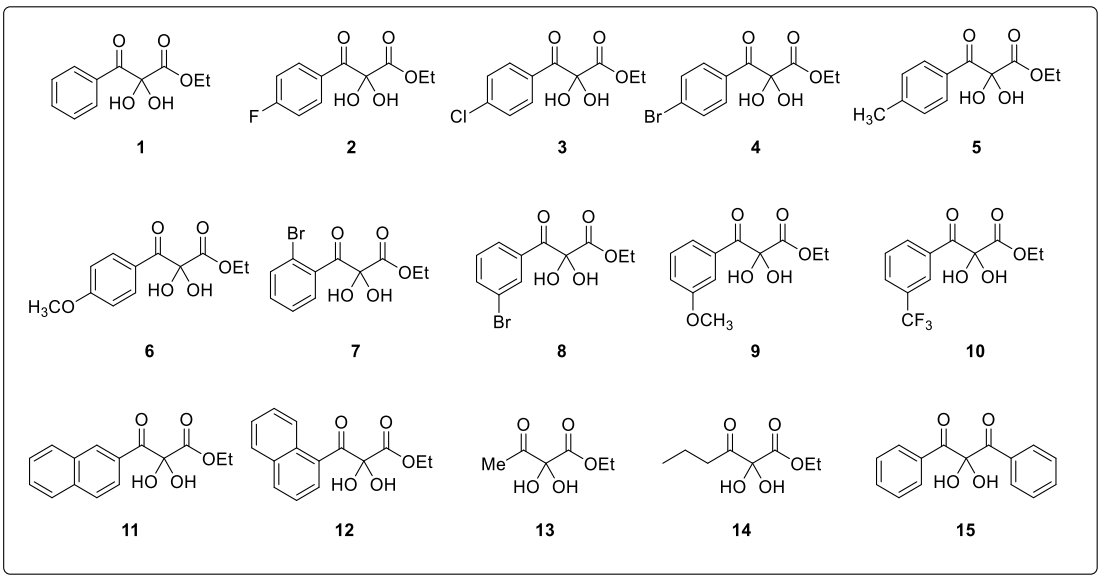
General procedure for the synthesis of nucleophilic substrates 3

All the nucleophilic substrates that used were purchased from chemical companies and used directly as received.

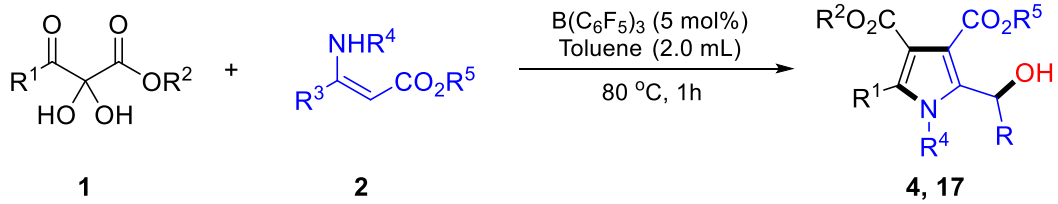


General procedure for the synthesis of vicinal tricarbonyl compounds 1

The vicinal tricarbonyl compounds were known compounds and were synthesized according to literature.[5-9]



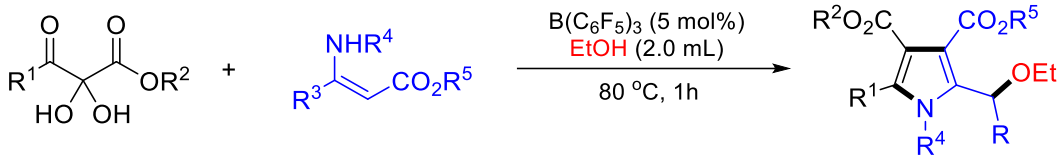
Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and H_2O



Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1**

(0.2 mmol), enamine **2** (0.24 mmol, 1.2 equiv.), toluene (2.0 mL) and $B(C_6F_5)_3$ (0.01 mmol, 5mol%). After being stirred for 1h at 80°C, the mixture was cooled down to room temperature and poured into 10% Na_2CO_3 solution (10 mL), and the resultant mixture was extracted with EtOAc (3×10 mL). The organic layers were combined, washed with brine (2×20 mL), dried over Na_2SO_4. At this time, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **4**, **17** as a solid or oil.

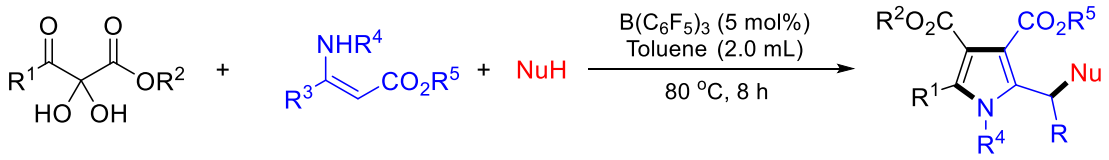
Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and alcohol



1 **2** **5**

Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1** (0.2 mmol), enamine **2** (0.24 mmol, 1.2 equiv.), ethanol (2.0 mL) and $B(C_6F_5)_3$ (0.01 mmol, 5 mol%). After being stirred for 1h at 80°C, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **5** as oil. MeOH (2.0 mL) was used for the synthesis of **5ab**. *n*-BuOH/toluene (1:1, 2.0 mL) was used for the synthesis of **5ac**.

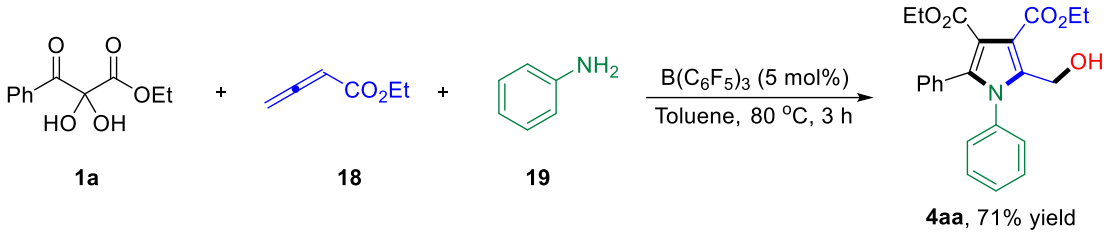
Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1, 2 and nucleophiles



1 **2** **3** **6-17**

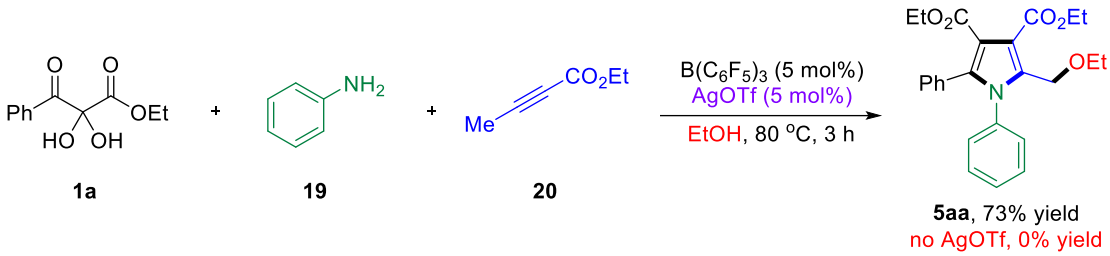
Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1** (0.2 mmol), enamine **2** (0.24 mmol, 1.2 equiv.), nucleophilic reagents **3** (0.6 mmol, 3.0 equiv.), toluene (2.0 mL) and $B(C_6F_5)_3$ (0.01 mmol, 5mol%). After being stirred for corresponding time at 80°C, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give pure products **6-17**.

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 18 and 19



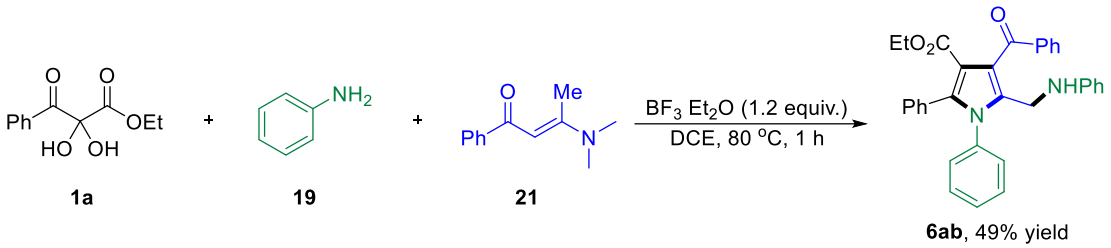
Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1a** (0.2 mmol), ethyl buta-2,3-dienoate **18** (0.24 mmol, 1.2 equiv.), aniline **19** (0.24 mmol, 1.2 equiv.), toluene (2.0 mL) and $B(C_6F_5)_3$ (0.01 mmol, 5mol%). After being stirred for 3h at 80°C, the mixture was cooled down to room temperature and poured into 10% Na_2CO_3 solution (10 mL), and the resultant mixture was extracted with EtOAc (3×10 mL). The organic layers were combined, washed with brine (2×20 mL), dried over Na_2SO_4. At this time, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **4aa** in 71% yield.

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 19 and 20



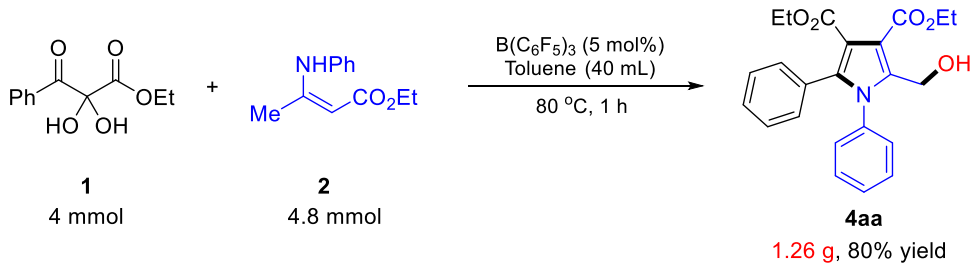
Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1a** (0.2 mmol), aniline **19** (0.24 mmol, 1.2 equiv.), ethyl but-2-ynoate **20** (0.24 mmol, 1.2 equiv.), ethanol (2.0 mL), AgOTf (0.01 mmol, 5mol%) and $B(C_6F_5)_3$ (0.01 mmol, 5mol%). After being stirred for 3h at 80°C, the mixture was cooled down to room temperature and poured into 10% Na_2CO_3 solution (10 mL), and the resultant mixture was extracted with EtOAc (3×10 mL). The organic layers were combined, washed with brine (2×20 mL), dried over Na_2SO_4. At this time, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **5aa** in 73% yield.

Procedure for $B(C_6F_5)_3$ catalyzed three component reactions of 1a, 19 and 21



Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with 2,3-diketoester **1a** (0.2 mmol), aniline **19** (0. 4 mmol, 2.0 equiv.), (*E*)-3-(dimethylamino)-1-phenylbut-2-en-1-one **21** (0.2 mmol, 1.0 equiv.), DCE (2.0 mL) and $BF_3{\cdot}Et_2O$ (0.24 mmol, 1.2 equiv.). After being stirred for 1h at 80°C, the mixture was cooled down to room temperature and poured into 10% Na_2CO_3 solution (10 mL), and the resultant mixture was extracted with EtOAc (3×10 mL). The organic layers were combined, washed with brine (2×20 mL), dried over Na_2SO_4. At this time, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **6ab** in 49% yield.

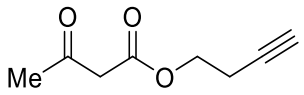
General procedure for gram-scale synthesis of 4a



Under air atmosphere, a Schlenk tube with a magnetic stir bar charged with ethyl 2,2-dihydroxy-3-oxo-3-phenylpropanoate **1a** (4 mmol, 0.896 g), ethyl (*Z*)-3-(phenylamino)but-2-enoate **2a** (0.24 mmol, 1.2 equiv.), toluene (40 mL) and $B(C_6F_5)_3$ (0.2 mmol, 102.4 mg, 5 mol%). After being stirred for 1h at 80°C, the mixture was cooled down to room temperature and poured into 10% Na_2CO_3 solution (100 mL), and the resultant mixture was extracted with EtOAc (3×50 mL). The organic layers were combined, washed with brine (2×100 mL), dried over Na_2SO_4. At this time, the solvent was removed from the reaction mixture under vacuum and the crude reaction mixture was purified by medium pressure chromatography to give **4**aa as colorless oil (1.26 g, 80% yield).

Characterization data of 1,3-dicarbonyl compounds

But-3-yn-1-yl 3-oxobutanoate (19) [3]

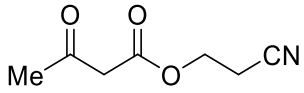


Light yellow oil;

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.24 (t, *J* = 6.8 Hz, 2H), 3.47 (s, 2H), 2.54 (td, *J* = 6.8 Hz, 2.6 Hz, 2H), 2.27 (s, 3H), 1.99 (t, *J* = 2.6 Hz, 1H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 200.4, 166.9, 79.8, 70.2, 63.0, 50.0, 30.3, 18.9.

2-Cyanoethyl 3-oxobutanoate (20) [2]

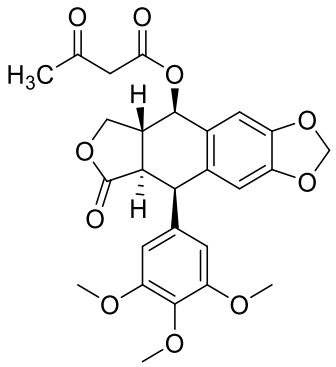


Light yellow oil, R_f = 0.28 (PE/EtOAc = 2:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.34 (t, *J* = 6.3 Hz, 2H), 3.52 (s, 2H), 2.73 (t, *J* = 6.3 Hz, 2H), 2.27 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 200.0, 166.6, 116.7, 59.5, 49.7, 30.4, 18.0.

(5*R*,5a*R*,8a*R*,9*R*)-8-Oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7] naphtho[2,3-*d*][1,3]dioxol-5-yl 3-oxobutanoate (23)



White solid, m.p. 133-135 °C, R_f = 0.14 (PE/EtOAc = 2:1);

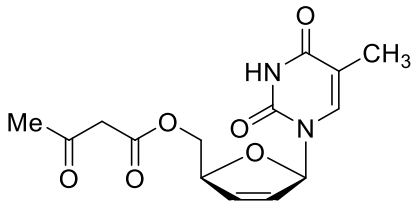
^{1}H NMR (500 MHz, $CDCl_3$) δ 6.83 (s, 1H), 6.51 (s, 1H), 6.35 (s, 2H), 5.96-5.93 (m, 3H), 4.58 (d, *J* = 2.0 Hz, 1H), 4.46-4.43 (m, 1H), 4.21-4.17 (m, 1H), 3.79-3.78 (m, 3H), 3.72 (s, 6H), 3.61 (d, *J* = 16.2 Hz, 1H), 3.57 (d, *J* = 16.2 Hz, 1H), 2.93-2.83 (m, 2H), 2.27 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.0, 173.6, 167.6, 152.7, 148.2, 147.6, 137.3, 134.8, 132.4,

127.9, 109.7, 108.2, 107.1, 101.6, 74.6, 71.3, 60.8, 56.2, 50.1, 45.5, 43.7, 38.6, 30.4;

HRMS (ESI) *m/z* calculated for $[C_{26}H_{26}O_{10}+Na]^+$ $[M+Na]^+$ 521.1418, found: 521.1424.

((2*S*,5*R*)-5-(5-Methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl 3-oxobutanoate (25)



White solid, m.p. 191-193 °C, R_f = 0.32 (EtOAc);

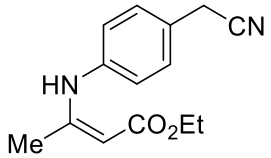
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.18 (s, 1H), 7.12 (s, 1H), 6.97 (d, *J* = 1.6 Hz, 1H), 6.28 (d, *J* = 5.9 Hz, 1H), 5.91 (d, *J* = 5.6 Hz, 1H), 5.02 (s, 1H), 4.42 (dd, *J* = 12.2 Hz, 4.8 Hz, 1H), 4.27 (dd, *J* = 12.1 Hz, 3.1 Hz, 1H), 3.51 (d, *J* = 15.8 Hz, 1H), 3.44 (d, *J* = 15.8 Hz, 1H), 2.25 (s, 3H), 1.89 (s, 3H);

^{13}C NMR (101 MHz, $CDCl_3$) δ 200.1, 166.8, 163.9, 150.9, 135.4, 133.2, 127.5, 111.3, 90.0, 84.0, 65.6, 49.9, 30.4, 12.6;

HRMS (ESI) *m/z* calculated for $[C_{14}H_{16}N_2O_6+H]^+$ $[M+H]^+$ 309.1081, found: 309.1082.

Characterization data of enamines 2

Ethyl (*Z*)-3-((4-(cyanomethyl)phenyl)amino)but-2-enoate (9)



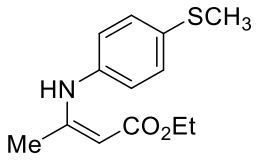
Light yellow solid, m.p. 112-114 °C, R_f = 0.11 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.4 (s, 1H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.05 (d, *J* = 8.4 Hz, 2H), 4.69 (s, 1H), 4.11 (q, *J* = 7.1 Hz, 2H), 3.70 (s, 2H), 1.98 (s, 3H), 1.25 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4, 158.4, 139.4, 128.8, 126.2, 124.6, 117.9, 87.0, 59.0, 23.1, 20.4, 14.7;

HRMS (ESI) *m/z* calculated for $[C_{14}H_{16}N_2O_2+H]^+$ $[M+H]^+$ 245.1285, found: 245.1287.

Ethyl (*Z*)-3-((4-(methylthio)phenyl)amino)but-2-enoate (10)



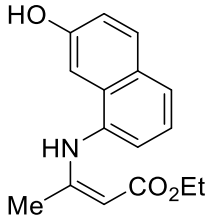
Light yellow solid, m.p. 137-139 °C, R_f = 0.56 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.30 (s, 1H), 7.19 (d, *J* = 8.6 Hz, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 4.66 (s, 1H), 4.12 (q, *J* = 7.1 Hz, 2H), 2.45 (s, 3H), 1.95 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 159.0, 136.7, 134.8, 127.6, 125.1, 86.1, 58.9, 20.4, 16.4, 14.7;

HRMS (ESI) *m/z* calculated for $[C_{13}H_{17}NO_2S+H]^+$ $[M+H]^+$ 252.1053, found: 252.1052.

Ethyl (*Z*)-3-((7-hydroxynaphthalen-1-yl)amino)but-2-enoate (14)



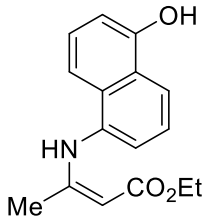
Light yellow solid, m.p. 173-175 °C, R_f = 0.21 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.37 (s, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.62 (d, *J* = 7.7 Hz, 1H), 7.38 (d, *J* = 1.8 Hz, 1H), 7.24-7.19 (m, 2H), 7.15 (dd, *J* = 8.8 Hz, 2.3 Hz, 1H), 6.46 (brs, 1H), 4.80 (s, 1H), 4.20 (q, *J* = 7.1 Hz, 2H), 1.82 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 171.5, 161.8, 155.8, 133.5, 132.0, 130.3, 129.4, 126.8, 124.4, 122.5, 119.0, 104.3, 84.9, 59.3, 20.2, 14.6;

HRMS (ESI) *m/z* calculated for $[C_{16}H_{17}NO_3+H]^+$ $[M+H]^+$ 272.1281, found: 272.1282.

Ethyl (*Z*)-3-((5-hydroxynaphthalen-1-yl)amino)but-2-enoate (15)



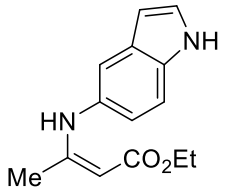
Light yellow solid, m.p. 187-188 °C, R_f = 0.15 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.38 (s, 1H), 8.14 (d, *J* = 8.4 Hz, 1H), 7.39-7.32 (m, 2H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.08-7.05 (m, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.70 (brs, 1H), 4.82 (s, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.83 (s, 3H), 1.34 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 171.5, 161.6, 152.6, 134.7, 131.9, 126.9, 125.8, 124.32, 124.26, 121.1, 114.5, 109.4, 85.2, 59.4, 20.2, 14.7;

HRMS (ESI) *m/z* calculated for $[C_{16}H_{17}NO_3+H]^+$ $[M+H]^+$ 272.1281, found: 272.1283.

Ethyl (*Z*)-3-((1H-indol-5-yl)amino)but-2-enoate (16)



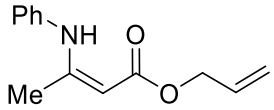
Light yellow solid, m.p. 163-164 °C, R_f = 0.12 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 8.35 (s, 1H), 7.36 (s, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.32 (t, *J* = 2.7 Hz, 1H), 6.93 (dd, *J* = 8.5 Hz, 1.9 Hz, 1H), 6.51 (t, *J* = 2.1 Hz, 1H), 4.66 (s, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 1.90 (s, 3H), 1.29 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 179.8, 161.1, 134.1, 131.7, 128.1, 125.5, 121.1, 117.9, 111.3, 102.8, 83.9, 58.7, 20.4, 14.8;

HRMS (ESI) *m/z* calculated for $[C_{14}H_{16}N_2O_2+H]^+$ $[M+H]^+$ 245.1285, found: 245.1283.

Allyl (*Z*)-3-(phenylamino)but-2-enoate (24)



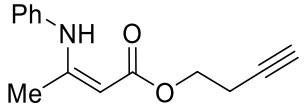
Colorless oil, R_f = 0.74 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.36 (brs, 1H), 7.34-7.31 (m, 2H), 7.17-7.14 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 2H), 6.02-5.94 (m, 1H), 5.34 (dq, *J* = 17.2 Hz, 1.6 Hz, 1H), 5.22 (dq, *J* = 10.5 Hz, 1.3 Hz, 1H), 4.74 (d, *J* = 0.4 Hz, 1H), 4.61 (dt, *J* = 5.6 Hz, 1.5 Hz, 2H), 2.00 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 159.5, 139.3, 133.4, 129.2, 125.2, 124.6, 117.4, 85.6, 63.7, 20.5;

HRMS (ESI) *m/z* calculated for $[C_{13}H_{15}NO_2+H]^+$ $[M+H]^+$ 218.1176, found: 218.1174.

But-3-yn-1-yl (*Z*)-3-(phenylamino)but-2-enoate (25)



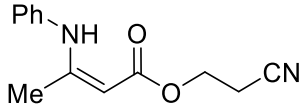
Colorless oil, R_f = 0.61 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.32 (s, 1H), 7.34-7.31 (m, 2H), 7.18-7.15 (m, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 4.72 (s, 1H), 4.21 (t, *J* = 6.9 Hz, 2H), 2.56 (td, *J* = 6.9 Hz, 2.7 Hz, 2H), 2.01 (t, *J* = 2.7 Hz, 1H), 1.99 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 159.7, 139.2, 129.2, 125.2, 124.7, 85.5, 80.8, 69.8, 60.8, 20.4, 19.4;

HRMS (ESI) *m/z* calculated for $[C_{14}H_{15}NO_2+H]^+$ $[M+H]^+$ 230.1176, found: 230.1175.

2-Cyanoethyl (*Z*)-3-(phenylamino)but-2-enoate (26)



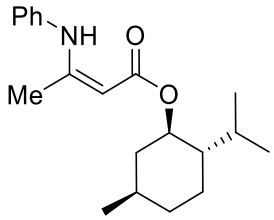
White solid, m.p. 103-105 ºC, R_f = 0.12 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.26 (s, 1H), 7.35-7.32 (m, 2H), 7.20-7.17 (m, 1H), 7.09 (d, *J* = 7.8 Hz, 2H), 4.72 (s, 1H), 4.29 (t, *J* = 6.4 Hz, 2H), 2.72 (t, *J* = 6.4 Hz, 2H), 1.99 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 169.4, 160.7, 138.9, 129.2, 125.6, 124.9, 117.5, 84.8, 57.3, 20.4, 18.5;

HRMS (ESI) *m/z* calculated for $[C_{13}H_{14}N_2O_2+H]^+$ $[M+H]^+$ 231.1128, found: 231.1126.

(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl (*Z*)-3-(phenylamino)but-2-enoate (27)



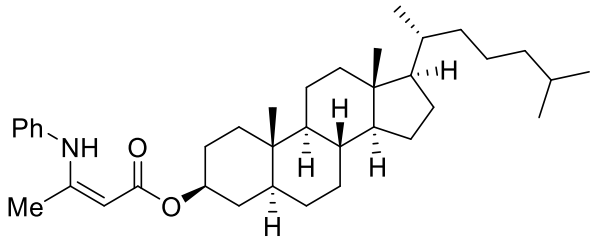
White solid, m.p. 187-189 ºC, R_f = 0.74 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.42 (s, 1H), 7.31-7.28 (m, 2H), 7.14-7.11 (m, 1H), 7.07 (d, *J* = 7.8 Hz, 2H), 4.70 (dd, *J* = 10.8 Hz, 4.2 Hz, 1H), 4.67 (s, 1H), 2.06-2.03 (m, 1H), 1.99 (s, 3H), 1.96-1.94 (m, 1H), 1.68-1.63 (m, 2H), 1.51-1.50 (m, 1H), 1.40-1.35 (m, 1H), 1.09-0.98 (m, 2H), 0.90-0.86 (m, 7H), 0.79 (d, *J* = 6.9 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.2, 158.8, 139.5, 129.1, 124.8, 124.3, 86.5, 72.3, 47.3, 41.6, 34.5, 31.6, 26.4, 23.7, 22.2, 20.9, 20.5, 16.6;

HRMS (ESI) *m/z* calculated for $[C_{20}H_{29}NO_2+H]^+$ $[M+H]^+$ 316.2271, found: 316.2276.

(3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl (*Z*)-3-(phenylamino)but-2-enoate (28)



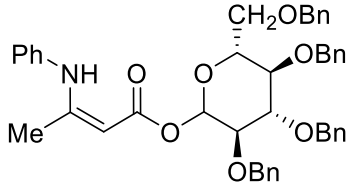
White solid, m.p. 201-203 °C, R_f = 0.77 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.43 (s, 1H), 7.33-7.30 (m, 2H), 7.15-7.12 (m, 1H), 7.08 (d, *J* = 7.7 Hz, 2H), 4.75-4.69 (m, 1H), 4.66 (s, 1H), 2.00 (s, 3H), 1.96 (dt, *J* = 12.7 Hz, 3.4 Hz, 1H), 1.85-1.78 (m, 2H), 1.74 (dt, *J* = 13.3 Hz, 3.4 Hz, 1H), 1.66-1.62 (m, 2H), 1.56-1.47 (m, 4H), 1.40-1.21 (m, 10H), 1.16-0.97 (m, 10H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.87 (d, *J* = 2.3 Hz, 3H), 0.85 (d, *J* = 2.3 Hz, 3H), 0.83 (s, 3H), 0.67-0.62 (m, 4H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 158.9, 139.5, 129.1, 124.9, 124.3, 86.6, 72.1, 56.5, 56.3, 54.3, 44.9, 42.7, 40.1, 39.6, 37.0, 36.3, 35.9, 35.61, 35.57, 34.6, 32.1, 28.8, 28.4, 28.1, 28.0, 24.3, 23.9, 22.9, 22.7, 21.3, 20.5, 18.8, 12.4, 12.2;

HRMS (ESI) *m/z* calculated for $[C_{37}H_{57}NO_2+H]^+$ $[M+H]^+$ 548.4462, found: 548.4466.

(3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl (*Z*)-3-(phenylamino)but-2-enoate (29)



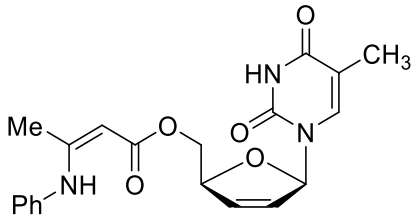
White solid, m.p. 183-185 °C, R_f = 0.20 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.45 (s, 1H), 7.42-7.29 (m, 2H), 7.22-7.18 (m, 2H), 7.13 (d, *J* = 7.6 Hz, 2H), 6.47 (d, *J* = 3.5 Hz, 1H), 5.05 (d, *J* = 10.9 Hz, 1H), 4.92-4.88 (m, 2H), 4.82-4.80 (m, 2H), 4.72 (d, *J* = 11.8 Hz, 1H), 4.67 (d, *J* = 12.2 Hz, 1H), 4.55 (d, *J* = 10.6 Hz, 1H), 4.51 (d, *J* = 12.1 Hz, 1H), 4.12-4.08 (m, 1H), 3.98 (d, *J* = 10.0 Hz, 1H), 3.85 (d, *J* = 9.7 Hz, 1H), 3.84-3.77 (m, 2H), 3.71 (dd, *J* = 10.8 Hz, 1.6 Hz, 1H), 2.03 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 168.6, 161.0, 139.1, 139.0, 138.4, 138.1, 138.0, 129.3, 128.58, 128.56, 128.5, 128.24, 128.19, 128.13, 128.08, 128.0, 127.90, 127.86, 127.8, 125.5, 124.8, 88.7, 85.4, 82.2, 79.0, 75.9, 75.4, 73.7, 72.9, 72.4, 68.3, 20.5;

HRMS (ESI) *m/z* calculated for $[C_{44}H_{45}NO_7+H]^+$ $[M+H]^+$ 700.3269, found: 700.3273.

((2*S*,5*R*)-5-(5-Methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl (*Z*)-3-(phenylamino)but-2-enoate (30)



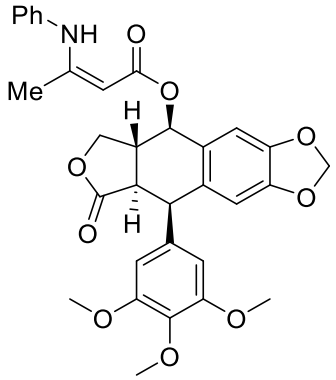
White solid, m.p. 235-237 °C,R_f = 0.55 (EtOAc);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.30 (s, 1H), 9.18 (s, 1H), 7.37 (s, 1H), 7.34-7.30 (m, 2H), 7.19-7.16 (m, 1H), 7.07 (d, *J* = 8.1 Hz, 2H), 7.01 (d, *J* = 1.6 Hz, 1H), 6.30 (d, *J* = 5.9 Hz, 1H), 5.84 (d, *J* = 4.9 Hz, 1H), 5.04 (s, 1H), 4.64 (s, 1H), 4.48 (dd, *J* = 12.5 Hz, 2.9 Hz, 1H), 4.25 (dd, *J* = 12.6 Hz, 2.2 Hz, 1H), 1.96 (s, 3H), 1.94 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 169.5, 164.1, 160.5, 151.0, 138.9, 136.2, 133.8, 129.3, 127.0, 125.6, 124.8, 110.9, 89.7, 85.1, 84.8, 62.8, 20.4, 12.6;

HRMS (ESI) *m/z* calculated for $[C_{20}H_{21}N_3O_5+H]^+$ $[M+H]^+$ 384.1554, found: 384.1557.

(5*R*,5a*R*,8a*R*,9*R*)-8-Oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-*d*][1,3]dioxol-5-yl (*Z*)-3-(phenylamino)but-2-enoate (31)



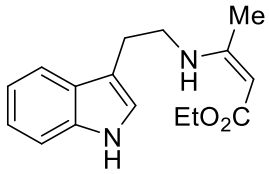
White solid, m.p. 193-195 °C, R_f = 0.53 (PE/EtOAc = 2:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.31 (s, 1H), 7.34-7.31 (m, 2H), 7.19-7.16 (m, 1H), 7.10-7.09 (m, 2H), 6.85 (s, 1H), 6.49 (s, 1H), 6.40 (s, 2H), 5.94-5.93 (m, 2H), 5.89 (d, *J* = 8.8 Hz, 1H), 4.73 (s, 1H), 4.57 (d, *J* = 3.9 Hz, 1H), 4.45-4.42 (m, 1H), 4.23-4.19 (m, 1H), 3.78 (s, 3H), 3.74 (s, 6H), 2.93-2.82 (m, 2H), 1.99 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 174.2, 170.3, 160.7, 152.6, 147.9, 147.6, 138.9, 135.3, 132.1, 129.8, 129.3, 125.7, 124.9, 109.6, 108.2, 107.4, 101.6, 84.8, 71.9, 71.7, 60.8, 56.2, 45.7, 43.9, 39.0, 20.4;

HRMS (ESI) *m/z* calculated for $[C_{32}H_{31}NO_9+H]^+$ $[M+H]^+$ 574.2072, found: 574.2076.

Ethyl (*Z*)-3-((2-(1*H*-indol-3-yl)ethyl)amino)but-2-enoate (32)



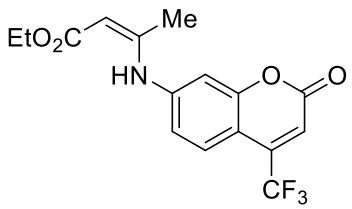
Colorless oil, R_f = 0.50 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (s, 1H), 8.22 (s, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.34-7.32 (m, 1H), 7.20-7.17 (m, 1H), 7.14-7.10 (m, 1H), 7.03 (d, *J* = 2.3 Hz, 1H), 4.43 (s, 1H), 4.09 (q, *J* = 7.1 Hz, 2H), 3.51 (q, *J* = 7.0 Hz, 2H), 3.00 (t, J = 7.1 Hz, 2H), 1.84 (d, *J* = 0.5 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.8, 162.0, 136.4, 127.2, 122.5, 122.1, 119.5, 118.5, 112.5, 111.4, 82.1, 58.4, 43.6, 26.6, 19.6, 14.8;

HRMS (ESI) *m/z* calculated for $[C_{16}H_{20}N_2O_2+H]^+$ $[M+H]^+$ 273.1598, found: 273.1603.

Ethyl (*Z*)-3-((2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)amino)but-2-enoate (33)



Yellow solid, m.p. 177-179 °C, R_f = 0.48 (PE/EtOAc = 10:1);

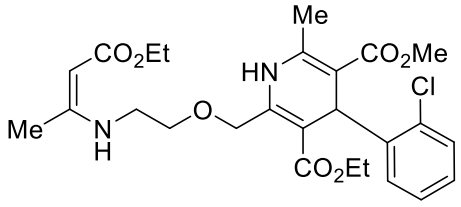
^{1}H NMR (500 MHz, $CDCl_3$) δ 10.90 (s, 1H), 7.60 (dd, *J* = 8.8 Hz, 1.7 Hz, 1H), 7.06 (d, *J* = 2.2 Hz, 1H), 6.97 (dd, *J* = 8.8 Hz, 2.3 Hz, 1H), 6.64 (s, 1H), 4.86 (s, 1H), 4.16 (q, *J* = 7.1 Hz, 2H), 2.22 (s, 3H), 1.28 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 159.2, 155.8, 155.6, 144.5, 141.4 (q, J = 32.7 Hz), 126.2 (q, J = 2.4 Hz), 122.7, 118.5, 113.2 (q, J = 5.7 Hz), 108.7, 108.2, 91.7, 59.6, 21.2, 14.5.

^{19}F NMR (470 MHz, $CDCl_3$) δ -64.60;

HRMS (ESI) *m/z* calculated for $[C_{16}H_{14}F_3NO_4+H]^+$ $[M+H]^+$ 342.0948, found: 342.0952.

3-Ethyl 5-methyl (*Z*)-4-(2-chlorophenyl)-2-((2-((4-ethoxy-4-oxobut-2-en-2-yl)amino)ethoxy) methyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (34)



Light yellow solid, m.p. 241-243 °C, R_f = 0.31 (PE/EtOAc = 3:1);

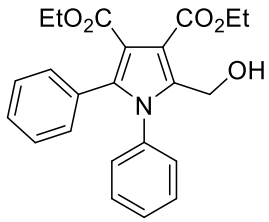
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.38 (dd, *J* = 7.8 Hz, 1.6 Hz, 1H), 7.21 (dd, *J* = 8,0 Hz, 1.3 Hz, 1H), 7.14-7.10 (m, 2H), 7.04-7.02 (m, 1H), 5.39 (s, 1H), 4.79 (d, *J* = 15.8 Hz, 1H), 4.71 (d, *J* = 15.8 Hz, 1H), 4.52 (s, 1H), 4.08-4.02 (m, 4H), 3.60 (s, 3H), 3.47 (q, *J* = 5.5 Hz, 2H), 2.36 (s, 3H), 1.94 (s, 3H), 1.22 (t, *J* = 7.2 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.9, 168.1, 167.3, 161.5, 145.9, 145.0, 144.7, 132.3, 131.6, 129.2, 127.4, 127.0, 103.9, 101.9, 83.5, 70.2, 68.0, 59.9, 58.6, 50.9, 42.3, 37.1, 19.5, 19.2, 14.7, 14.4;

HRMS (ESI) *m/z* calculated for $[C_{26}H_{33}ClN_2O_7+H]^+$ $[M+H]^+$ 521.2049, found: 521.2048.

Characterization data of pyrrole products 4-17

Diethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4aa)



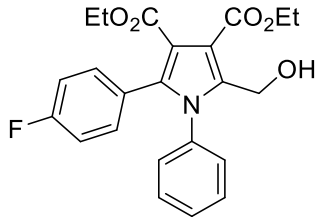
68.4 mg, 87% yield, white solid, m.p. 134-136 °C, R_f = 0.31 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.29 (m, 3H), 7.18-7.09 (m, 7H), 4.48 (d, *J* = 4.8 Hz, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.76 (t, *J* = 5.9 Hz, 1H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.6, 139.8, 136.1, 135.0, 130.6, 130.0, 129.2, 128.9, 128.5, 128.2, 127.8, 116.4, 113.4, 61.0, 55.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{23}NO_5+H]^+$ $[M+H]^+$ 394.1649, found: 394.1654.

Diethyl 2-(4-fluorophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ba)



55.9 mg, 68% yield, light yellow solid, m.p. 166-168 ºC, R_f = 0.26 (PE/EtOAc = 3:1);

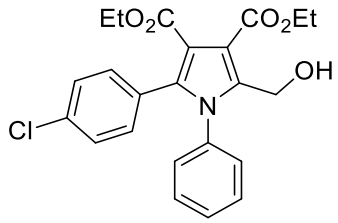
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.31 (m, 3H), 7.13-7.09 (m, 4H), 6.88-6.84 (m, 2H), 4.47 (d, *J* = 6.5 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.18 (q. *J* = 7.1 Hz, 2H), 3.74 (t, *J* = 6.9 Hz, 1H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.5, 162.5 (d, *J* = 247.1 Hz), 139.8, 135.9, 134.1, 132.6 (d, *J* = 8.3 Hz), 129.3, 129.0, 128.5, 126.0 (d, *J* = 3.4 Hz), 116.5, 115.0 (d, *J* = 21.6 Hz), 113.6, 61.1, 61.0, 55.2, 14.3, 14.1;

^{19}F NMR (470 MHz, $CDCl_3$) δ 112.56;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}FNO_5+H]^+$ $[M+H]^+$ 412.1555, found: 412.1563.

Diethyl 2-(4-chlorophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ca)



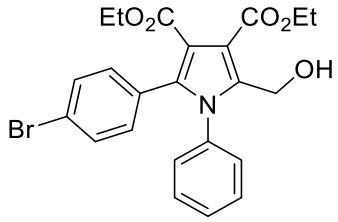
50.5 mg, 59% yield, light yellow solid, m.p. 162-164 ºC, R_f = 0.25 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.31 (m, 3H), 7.13 (d, *J* = 8.7 Hz, 2H), 7.10-7.08 (m, 2H), 7.06 (d, *J* = 8.7 Hz, 2H), 4.46 (d, *J* = 7.1 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.72 (t, *J* = 7.2 Hz, 1H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 165.4, 140.0, 135.9, 134.4, 133.7, 131.9, 129.4, 129.1, 128.47, 128.46, 128.2, 116.7, 113.7, 61.12, 61.08, 55.1, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}ClNO_5+H]^+$ $[M+H]^+$ 428.1259, found: 428.1267.

Diethyl 2-(4-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4da)



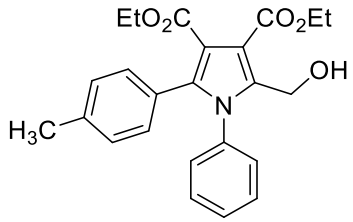
49.7 mg, 53% yield, light yellow solid, m.p. 180-182 °C, R_f = 0.28 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.34 (m, 3H), 7.30 (d, *J* = 8.7 Hz, 2H), 7.11-7.09 (m, 2H), 7.01 (d, *J* = 8.7 Hz,); 4.48 (d, *J* = 5.7 Hz, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 4.19 (q, *J* = 7.1 Hz, 2H), 3.72 (t, *J* = 6.5 Hz, 1H), 1.37 (t, *J* = 7.1 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.4, 140.0, 135.9, 133.7, 132.1, 131.1, 129.5, 129.1, 128.9, 128.5, 122.7, 116.7, 113.7, 61.2, 61.1, 55.2, 14.3, 14.2;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}BrNO_5+H]^+$ $[M+H]^+$ 472.0754, found: 472.0761.

Diethyl 2-(hydroxymethyl)-1-phenyl-5-(p-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ea)



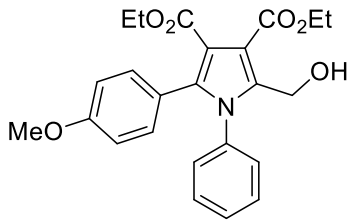
46.4 mg, 57% yield, light yellow solid, m.p. 151-152 °C, R_f = 0.31 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.30 (m, 3H), 7.13-7.10 (m, 2H), 7.02 (d, *J* = 8.2 Hz), 6.96 (d, *J* = 8.0 Hz, 2H), 4.48 (d, *J* = 6.7 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.77 (t, *J* = 7.0 Hz, 1H), 2.24 (s, 3H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.19 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.6, 139.7, 138.1, 136.2, 135.1, 130.4, 129.2, 128.8, 128.6, 128.5, 126.9, 116.2, 113.4, 61.00, 60.97, 55.2, 21.3, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5+H]^+$ $[M+H]^+$ 408.1805, found: 408.1808.

Diethyl 2-(hydroxymethyl)-5-(4-methoxyphenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4fa)



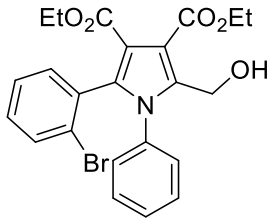
35.5 mg, 42% yield, colorless oil, R_f = 0.21 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31-7.30 (m, 3H), 7.10-7.08 (m, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 6.68 (d, *J* = 8.8 Hz, 2H), 4.46 (s, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.74 (brs, 1H), 3.71 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.19 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.7, 159.4, 139.5, 136.2, 135.1, 132.0, 129.2, 128.8, 128.5, 122.2, 116.0, 113.4, 113.3, 61.0, 55.3, 55.2, 14.3, 14.2;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_6+H]^+$ $[M+H]^+$ 424.1755, found: 424.1760.

Diethyl 2-(2-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ga)



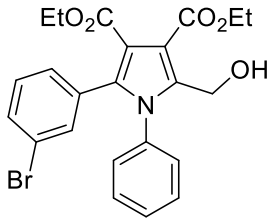
57.5 mg, 61% yield, light yellow solid, m.p. 171-173 °C, R_f = 0.25 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 8.0 Hz, 1.1 Hz, 1H), 7.25-7.20 (m, 4H), 7.14-7.07 (m, 2H), 7.04-7.01 (m, 2H), 4.39 (d, *J* = 6.7 Hz, 2H), 4.30 (q, *J* = 7.2 Hz, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 3.68 (t, *J* = 7.0 Hz, 1H), 1.31 (t, *J* = 7.2 Hz, 3H), 0.96 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 164.2, 139.6, 135.7, 133.4, 132.3, 132.2, 130.4, 129.0, 128.2, 126.6, 125.9, 116.1, 114.0, 61.2, 60.5, 55.2, 14.3, 13.9;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}BrNO_5+H]^+$ $[M+H]^+$ 472.0754, found: 472.0758.

Diethyl 2-(3-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ha)



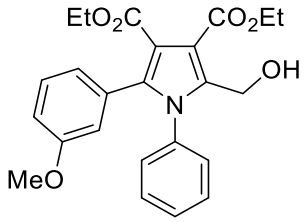
60.3 mg, 64% yield, light yellow solid, m.p. 177-179 °C, R_f = 0.29 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.34 (m, 1H), 7.33-7.31 (m, 1H), 7.12-7.10 (m, 2H), 7.03-6.98 (m, 2H), 4.48 (d, *J* = 6.2 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.20 (q, *J* = 7.3 Hz, 2H), 3.75 (t, *J* = 6.8 Hz, 1H), 1.36 (t, *J* = 7.3 Hz, 3H), 1.21 (t, *J* = 7.3 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.42, 165.40, 140.1, 135.8, 133.5, 133.1, 132.0, 131.3, 129.4, 129.3, 129.2, 129.1, 128.5, 121.8, 117.0, 113.7, 61.2, 61.1, 55.1, 14.3, 14.2;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}BrNO_5+Na]^+$ $[M+Na]^+$ 494.0574, found: 494.0588.

Diethyl 2-(hydroxymethyl)-5-(3-methoxyphenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ia)



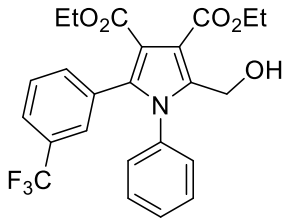
30.1 mg, 36% yield, colorless oil, R_f = 0.22 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.31 (m, 3H), 7.12-7.11 (m, 2H), 7.10-7.04 (m, 1H), 6.73-6.70 (m, 2H), 6.65-6.64 (m, 1H), 4.49 (d, *J* = 7.1 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.77 (q, *J* = 7.2 Hz, 1H), 3.58 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.19 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.5, 158.9, 139.9, 136.2, 134.5, 131.1, 129.3, 128.90, 128.89, 128.5, 123.0, 116.6, 115.5, 114.5, 113.3, 61.1, 61.0, 55.2, 55.1, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_6+H]^+$ $[M+H]^+$ 424.1755, found: 424.1757.

Diethyl 2-(hydroxymethyl)-1-phenyl-5-(3-(trifluoromethyl)phenyl)-1*H*-pyrrole-3,4-dicarboxylate (4ja)



70.1 mg, 76% yield, white solid, m.p. 152-154 °C, R_f = 0.33 (PE/EtOAc = 3:1);

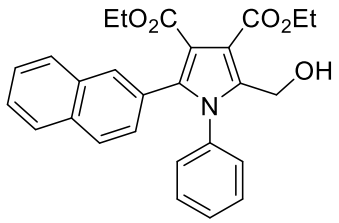
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45-7.42 (m, 2H), 7.34-7.33 (m, 3H), 7.29-7.27 (m, 2H), 7.11-7.09 (m, 2H), 4.49 (s, 2H), 4.35 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 3.73 (brs, 1H), 1.36 (t, *J* = 7.1 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.39, 165.37, 140.3, 135.7, 133.8 (q, *J* = 1.2 Hz), 133.1, 130.8, 130.3 (q, *J* = 32.4 Hz), 129.5, 129.2, 128.5, 128.4, 127.5 (q, *J* = 3.9 Hz), 124.9 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 270.7 Hz), 117.1, 113.8, 61.23, 61.15, 55.1, 14.3, 14.0;

^{19}F NMR (470 MHz, $CDCl_3$) δ -63.84;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{22}F_3NO_5+H]^+$ $[M+H]^+$ 462.1523, found: 462.1532.

Diethyl 2-(hydroxymethyl)-5-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ka)



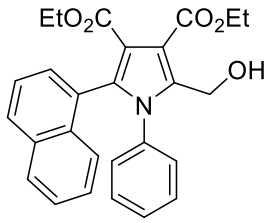
38.1 mg, 43% yield, white solid, m.p. 144-145 °C, R_f = 0.26 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 (d, *J* = 1.2 Hz, 1H), 7.74-7.69 (m, 2H), 7.59 (d, *J* = 8.6 Hz, 1H), 7.46-7.42 (m, 2H), 7.31-7.28 (m, 3H), 7.17-7.15 (m, 2H), 7.12 (dd, *J* = 8.5 Hz, 1.8 Hz, 1H), 4.54 (d, *J* = 6.3 Hz, 2H), 4.38 (q, *J* = 7.2 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 3.80 (t, J = 6.9 Hz, 1H), 1.39 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.6, 140.0, 136.1, 134.7, 132.74, 132.69, 130.4, 129.3, 128.9, 128.5, 128.2, 127.7, 127.6, 127.43, 127.38, 126.7, 126.3, 116.9, 113.5, 61.10, 61.05, 55.3, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{25}NO_5+H]^+$ $[M+H]^+$ 444.1805, found: 444.1809.

Diethyl 2-(hydroxymethyl)-5-(naphthalen-1-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4la)



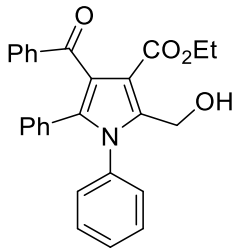
37.2 mg, 42% yield, colorless oil, R_f = 0.25 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (m, 2H), 7.67-7.65 (m, 1H), 7.40-7.38 (m, 2H), 7.28-7.25 (m, 2H), 7.23-7.14 (m, 2H), 7.12-7.09 (m, 1H), 6.98-6.92 (m, 2H), 4.52 (s, 2H), 4.39 (q, *J* = 7.2 Hz, 2H), 3.90-3.85 (m, 3H), 1.38 (t, *J* = 7.2 Hz, 3H), 0.72 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 164.8, 139.8, 136.0, 134.5, 133.4, 133.1, 130.1, 129.3, 128.9, 128.7, 128.2, 128.1, 126.5, 125.95, 125.92, 124.6, 117.3, 113.9, 61.1, 60.4, 55.4, 14.3, 13.6;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{25}NO_5+H]^+$ $[M+H]^+$ 444.1805, found: 444.1809.

Ethyl 4-benzoyl-2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3-carboxylate (4ma)



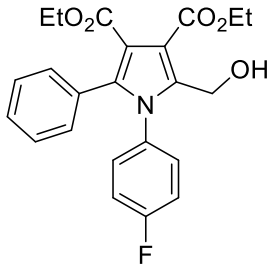
33.2 mg, 39% yield, white solid, m.p. 177-178 °C, R_f = 0.31 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89-7.87 (m, 2H), 7.51-7.48 (m, 1H), 7.41-7.38 (m, 2H), 7.36-7.35 (m, 3H), 7.19-7.17 (m, 2H), 7.10-7.06 (m, 5H), 4.59 (d, *J* = 6.2 Hz, 2H), 4.20 (t, *J* = 7.0 Hz, 1H), 3.95 (q, *J* = 7.2 Hz, 2H), 0.80 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 193.7, 165.6, 140.3, 139.0, 136.2, 134.4, 132.8, 130.6, 129.8, 129.4, 129.3, 128.9, 128.6, 128.4, 128.0, 127.9, 123.0, 113.8, 60.7, 55.5, 13.4;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{23}NO_4+H]^+$ $[M+H]^+$ 426.1700, found: 426.1710.

Diethyl 1-(4-fluorophenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ab)



50.2 mg, 61% yield, colorless oil, R_f = 0.27 (PE/EtOAc = 3:1);

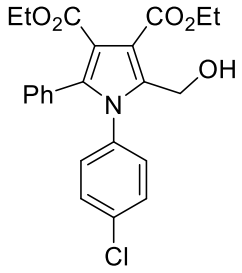
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20-7.15 (m, 3H), 7.12-7.08 (m, 4H), 7.01-6.97 (m, 2H), 4.47 (d, *J* = 6.8 Hz, 2H), 4.34 (q. *J* = 7.2 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.68 (t, *J* = 6.9 Hz, 1H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.4, 162.3 (d, *J* = 248.2 Hz), 139.7, 135.2, 132.1 (d, *J* = 3.3 Hz), 130.6, 130.3 (d, *J* = 8.7 Hz), 129.8, 128.4, 128.0, 116.5, 116.3 (d, *J* = 22.8 Hz), 113.6, 61.06, 61.04, 55.1, 14.3, 14.1;

^{19}F NMR (470 MHz, $CDCl_3$) δ 111.41;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}FNO_5+H]^+$ $[M+H]^+$ 412.1555, found: 412.1553.

Diethyl 1-(4-chlorophenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ac)



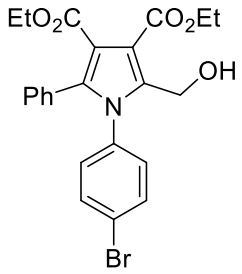
63.7 mg, 75% yield, colorless oil, R_f = 0.31 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (d, *J* = 8.8 Hz, 2H), 7.21-7.16 (m, 3H), 7.12-7.10 (m, 2H), 7.05 (d, *J* = 8.8 Hz, 2H), 4.46 (d, *J* = 6.2 Hz, 2H), 4.33 (q, *J* = 7.2 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.68 (t, *J* = 6.7 Hz, 1H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 165.4, 139.5, 135.0, 134.8, 134.7, 130.6, 129.8, 129.7, 129.5, 128.5, 128.0, 116.6, 113.8, 61.09, 61.07, 55.0, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}ClNO_5+H]^+$ $[M+H]^+$ 428.1259, found: 428.1262.

Diethyl 1-(4-bromophenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ad)



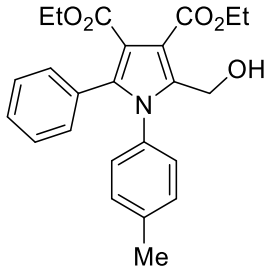
72.5 mg, 77% yield, colorless oil, R_f = 0.28 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, J = 8.7 Hz, 2H), 7.21-7.17 (m, 3H), 7.12-7.10 (m, 2H), 6.98 (d, J = 8.7 Hz, 2H), 4.46 (s, 2H), 4.34 (q, J = 7.2 Hz, 2H), 4.15 (q, J = 7.2 Hz, 2H), 3.66 (s, 1H), 1.34 (t, J = 7.2 Hz, 3H), 1.14 (t, J = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 165.4, 139.4, 135.2, 135.0, 132.5, 130.6, 130.0, 129.7, 128.5, 128.1, 122.9, 116.7, 113.9, 61.10, 61.07, 55.0, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}BrNO_5+H]^+$ $[M+H]^+$ 472.0754, found: 472.0757.

Diethyl 2-(hydroxymethyl)-5-phenyl-1-(*p*-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ae)



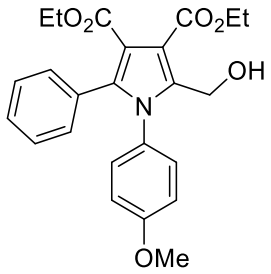
67.0 mg, 82% yield, colorless oil, R_f = 0.27 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18-7.12 (m, 5H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.97 (d, *J* = 8.2 Hz, 2H), 4.47 (d, *J* = 6.8 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.74 (t, *J* = 7.0 Hz, 1H), 2.31 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.6, 139.9, 138.9, 135.0, 133.5, 130.6, 130.1, 129.8, 128.2, 128.1, 127.8, 116.3, 113.2, 60.99, 60.98, 55.3, 21.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5+H]^+$ $[M+H]^+$ 408.1805, found: 408.1806.

Diethyl 2-(hydroxymethyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4af)



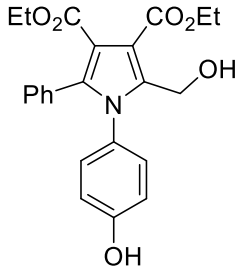
58.3 mg, 69% yield, colorless oil, R_f = 0.16 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.17-7.11 (m, 5H), 7.01 (d, *J* = 8.9 Hz, 2H), 6.78 (d, *J* = 8.9 Hz, 2H), 4.47 (d, *J* = 6.6 Hz, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.76 (brs, 1H), 3.74 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.6, 159.6, 140.0, 135.2, 130.6, 130.1, 129.6, 128.8, 128.1, 127.9, 116.2, 114.3, 113.1, 60.973, 60.966, 55.5, 55.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_6+H]^+$ $[M+H]^+$ 424.1755, found: 424.1752.

Diethyl 2-(hydroxymethyl)-1-(4-hydroxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ag)



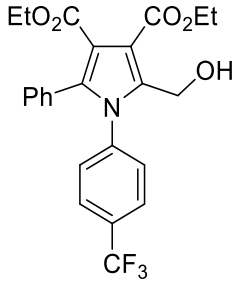
34.0 mg, 42% yield, white solid, m.p. 214-215 °C, R_f = 0.37 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (brs, 1H), 7.25-7.13 (m, 3H), 7.11-7.09 (m, 2H), 6.84 (d, *J* = 8.7 Hz, 2H), 6.59 (d, *J* = 8.7 Hz, 2H), 4.73 (s, 1H), 4.52 (s, 2H), 4.33 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.08, 166.07, 157.1, 139.4, 135.7, 130.5, 129.9, 129.6, 128.3, 127.9, 127.6, 116.01, 115.99, 113.2, 61.27, 61.21, 55.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{23}NO_6+H]^+$ $[M+H]^+$ 410.1598, found: 410.1600.

Diethyl 2-(hydroxymethyl)-5-phenyl-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrole-3,4-dicarboxylate (4ah)



56.5 mg, 61% yield, colorless oil, R_f = 0.33 (PE/EtOAc = 3:1);

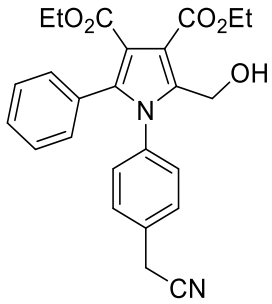
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.3 Hz, 2H), 7.26 (d, *J* = 8.3 Hz, 2H), 7.22-7.17 (m, 3H), 7.12-7.10 (m, 2H), 4.47 (d, *J* = 4.7 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.62 (t, *J* = 5.7 Hz, 1H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 165.3, 139.3, 135.0, 130.9 (q, *J* = 32.9 Hz), 130.6, 129.5, 129.0, 128.6, 128.1, 126.4 (q, *J* = 3.7 Hz), 123.5 (q, *J* = 270.8 Hz), 116.9, 114.3, 61.2, 61.1, 55.0, 14.3, 14.1;

^{19}F NMR (470 MHz, $CDCl_3$) δ 62.6;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{22}F_3NO_5+H]^+$ $[M+H]^+$ 462.1523, found: 462.1525.

Diethyl 1-(4-(cyanomethyl)phenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ai)



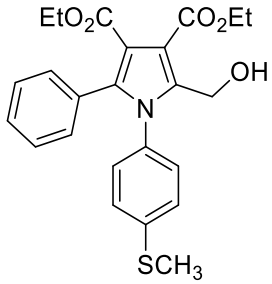
46.7 mg, 54% yield, white solid, m.p. 153-155 °C, R_f = 0.42 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.3 Hz, 2H), 7.20-7.17 (m, 3H), 7.14-7.09 (m, 4H), 4.46 (d, *J* = 2.5 Hz, 2H), 4.34 (q, *J* = 7.2 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.72 (s, 2H), 3.65 (brs, 1H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.4, 139.5, 136.1, 135.1, 130.8, 130.6, 129.7, 129.2, 128.8, 128.4, 128.0, 117.3, 116.6, 113.8, 61.09, 61.06, 55.1, 23.4, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{24}N_2O_5+H]^+$ $[M+H]^+$ 433.1758, found: 433.1763.

Diethyl 2-(hydroxymethyl)-1-(4-(methylthio)phenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4aj)



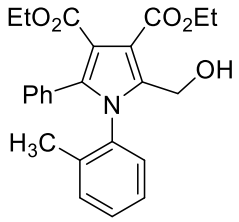
47.4 mg, 54% yield, light yellow solid, m.p. 144-146 °C, R_f = 0.24 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19-7.15 (m, 3H), 7.13-7.11 (m, 4H), 7.00 (d, *J* = 8.6 Hz, 2H), 4.47 (d, *J* = 6.1 Hz, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.70 (t, *J* = 6.8 Hz, 1H), 2.42 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 165.5, 140.1, 139.8, 135.0, 132.8, 130.6, 129.9, 128.7, 128.3, 127.9, 126.3, 116.4, 113.5, 61.0, 55.2, 15.4, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5S+H]^+$ $[M+H]^+$ 440.1526, found: 440.1533.

Diethyl 2-(hydroxymethyl)-5-phenyl-1-(o-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ak)



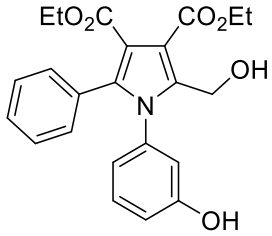
72.3 mg, 89% yield, colorless oil, R_f = 0.28 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24-7.21 (m, 1H), 7.17-7.12 (m, 8H), 4.36 (dd, *J* = 7.1 Hz, 1.2 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.20-4.13 (m, 2H), 3.93 (t, *J* = 7.2 Hz, 1H), 1.89 (s, 3H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 165.7, 140.0, 136.5, 135.3, 134.9, 131.1, 130.1, 130.0, 129.6, 129.5, 128.3, 127.8, 126.7, 116.5, 113.1, 61.0, 55.3, 17.6, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5+H]^+$ $[M+H]^+$ 408.1805, found: 408.1803.

Diethyl 2-(hydroxymethyl)-1-(3-hydroxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4al)



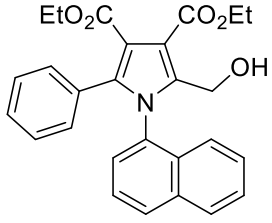
21.3 mg, 26% yield, brown solid, m.p. 190-192 ºC, R_f = 0.44 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 (brs, 1H), 7.19-7.14 (m, 3H), 7.12-7.10 (m, 2H), 7.08-7.05 (m, 1H), 6.76-6.73 (m, 1H), 6.63 (t, *J* = 2.0 Hz, 1H), 6.50-6.48 (m ,1H), 4.61 (d, *J* = 12.6 Hz, 1H), 4.39-4.32 (m, 4H), 4.16 (q, *J* = 7.2 Hz, 2H), 1.35 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.1, 165.9, 157.0, 139.1, 136.7, 135.3, 130.4, 130.0, 129.8, 128.4, 127.9, 120.1, 116.4, 116.1, 115.8, 113.5, 61.3, 61.2, 55.1, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{23}NO_6+H]^+$ $[M+H]^+$ 410.1598, found: 410.1603.

Diethyl 2-(hydroxymethyl)-1-(naphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4am)



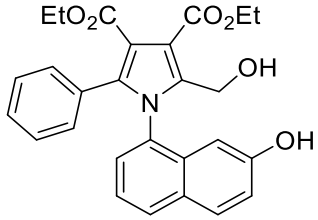
47.5 mg, 54% yield, colorless oil, R_f = 0.22 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84-7.81 (m, 2H), 7.48-7.46 (m, 2H), 7.40-7.37 (m, 1H), 7.33-7.32 (m, 2H), 7.06-7.03 (m, 3H), 7.00-6.97 (m, 2H), 4.43-4.36 (m, 3H), 4.21-4.16 (m, 3H), 3.91 (t, *J* = 6.8 Hz, 1H), 1.39 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.7, 141.1, 136.1, 133.8, 132.6, 131.2, 129.9, 128.3, 128.2, 127.9, 127.7, 127.4, 127.0, 125.0, 122.5, 116.6, 113.2, 61.12, 61.06, 55.5, 14.3, 14.11, 14.08;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{25}NO_5+H]^+$ $[M+H]^+$ 444.1805, found: 444.1798.

Diethyl 2-(hydroxymethyl)-1-(7-hydroxynaphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4an)



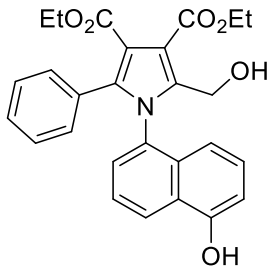
41.4 mg, 45% yield, yellow solid, m.p. 213-215 °C, R_f = 0.14 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.5 Hz, 1H), 7.65 (d, *J* = 8.9 Hz, 1H), 7.17-7.12 (m, 2H), 7.06-7.00 (m, 4H), 7.00-6.95 (m, 2H), 6.66 (d, *J* = 2.0 Hz, 1H), 4.42-4.29 (m, 5H), 4.22-4.16 (m, 2H), 1.37 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.4, 165.9, 156.2, 140.7, 136.2, 132.7, 131.0, 130.2, 129.90, 129.85, 129.7, 129.0, 128.3, 127.8, 127.7, 122.2, 119.5, 116.5, 113.1, 104.3, 61.3, 55.5, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{25}NO_6+H]^+$ $[M+H]^+$ 460.1755, found: 460.1764.

Diethyl 2-(hydroxymethyl)-1-(5-hydroxynaphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ao)



46.0 mg, 50% yield, light yellow solid, m.p. 232-234 °C, R_f = 0.64 (PE/EtOAc = 1:1);

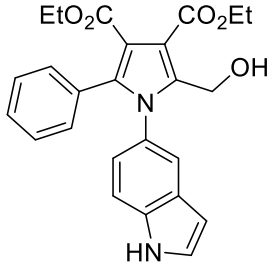
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.2 Hz, 1H), 7.64 (brs, 1H), 7.25-7.18 (m, 2H), 7.05-

7.00 (m, 4H), 6.98-6.94 (m, 2H), 6.74 (d, *J* = 8.5 Hz, 1H), 6.30 (d, *J* = 7.5 Hz, 1H), 4.70 (t, *J* = 6.4 Hz, 1H), 4.41-4.36 (m, 4H), 4.20 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.2, 166.1, 152.6, 140.7, 136.4, 132.4, 131.9, 129.9, 129.8, 128.4, 128.3, 127.7, 127.6, 125.2, 124.4, 123.6, 116.4, 113.6, 113.1, 109.2, 61.34, 61.25, 55.4, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{25}NO_6+H]^+$ $[M+H]^+$ 460.1755, found: 460.1759.

Diethyl 2-(hydroxymethyl)-1-(1*H*-indol-5-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ap)



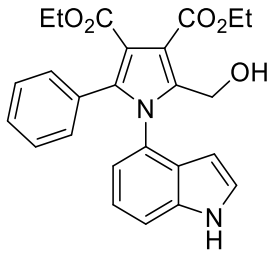
34.6 mg, 40% yield, white solid, m.p. 204-206 °C, R_f = 0.39 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.33 (d, *J* = 1.7 Hz, 1H), 7.16-7.13 (m, 3H), 7.09-7.05 (m, 4H), 6.72 (dd, *J* = 8.5 Hz, 1.9 Hz, 1H), 6.42 (t, *J* = 2.1 Hz, 1H), 4.56-4.47 (m, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.19 (q, *J* = 7.2 Hz, 2H), 4.14 (s, 1H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.17 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.3, 166.0, 140.6, 135.6, 135.4, 130.4, 130.3, 128.1, 128.0, 127.8, 127.7, 126.3, 121.9, 120.6, 116.0, 112.7, 111.6, 102.9, 61.08, 61.04, 55.4, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{24}N_2O_5+H]^+$ $[M+H]^+$ 433.1758, found: 433.1763.

Diethyl 2-(hydroxymethyl)-1-(1*H*-indol-4-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4aq)



25.1 mg, 29% yield, white solid, m.p. 195-197 °C, R_f = 0.43 (PE/EtOAc = 1:1);

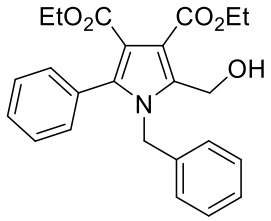
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (s, 1H), 7.25 (d, *J* = 8.2 Hz, 1H), 7.09-7.07 (m, 2H), 7.06-7.03 (m, 2H), 7.01-6.97 (m, 3H), 6.76 (dd, *J* = 7.5 Hz, 0.6 Hz, 1H), 6.19 (t, *J* = 2.1 Hz, 1H). 4.49 (dd, *J* = 13.7 Hz, 6.5 Hz, 1H), 4.39-4.34 (m, 3H), 4.20 (q, *J* = 7.1 Hz, 1.6 Hz, 2H), 4.10-4.07 (m, 4H), 1.37

(t, *J* = 7.2 Hz, 3H), 1.18 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.3, 165.9, 140.8, 136.6, 135.4, 130.3, 129.9, 128.0, 127.6, 126.6, 126.1, 120.3, 116.4, 112.9, 112.3, 99.8, 61.10, 61.04, 55.5, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{24}N_2O_5+H]^+$ $[M+H]^+$ 433.1758, found: 433.1759.

Diethyl 1-benzyl-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ar)



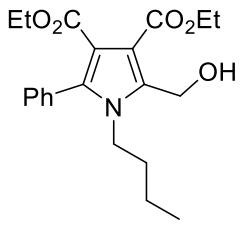
68.8 mg, 85% yield, Colorless oil, R_f = 0.18 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.28 (m, 3H), 7.26-7.21 (m, 5H), 6.85 (d, *J* = 7.1 Hz, 2H), 5.09 (s, 2H), 4.58 (s, 2H), 4.31 (q, *J* = 7.2 Hz, 2H), 4.08 (q, *J* = 7.2 Hz, 2H), 3.63 (brs, 1H), 1.33 (t, *J* = 7.2 Hz, 3H), 3.02 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.3, 138.2, 137.0, 136.4, 130.5, 130.2, 128.99, 128.97, 128.3, 127.7, 125.7, 115.9, 113.9, 61.0, 60.7, 55.0, 48.1, 14.3, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5+H]^+$ $[M+H]^+$ 408.1805, found: 408.1803.

Diethyl 1-butyl-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4as)



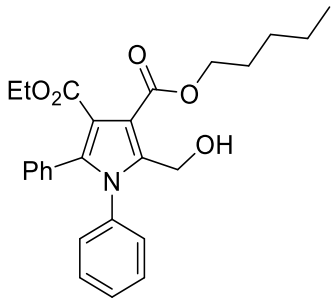
42.9 mg, 58% yield, Colorless oil, R_f = 0.22 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41-7.39 (m, 3H), 7.32-7.30 (m, 2H), 4.71 (s, 2H), 4.29 (q, *J* = 7.2 Hz, 2H), 4.04 (q, *J* = 7.2 Hz, 2H), 3.81-3.78 (m, 2H), 0.80 (brs, 1H), 1.52-1.46 (m, 2H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.14-1.08 (m, 2H), 1.03 (t, *J* = 7.2 Hz, 3H), 0.72 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.4, 138.0, 135.6, 130.7, 130.6, 128.9, 128.3, 115.7, 113.3, 60.9, 60.5, 54.9, 44.4, 33.6, 19.7, 14.3, 14.0, 13.5;

HRMS (ESI) *m/z* calculated for $[C_{21}H_{27}NO_5+H]^+$ $[M+H]^+$ 374.1962, found: 374.1970.

3-Ethyl 4-pentyl 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4at)



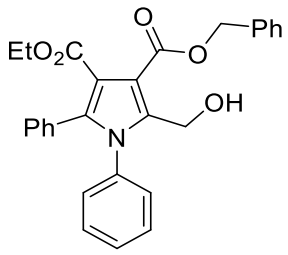
62.9 mg, 72% yield, Colorless oil, R_f = 0.41 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31-7.29 (m, 3H), 7.18-7.09 (m, 7H), 4.48 (d, *J* = 6.9 Hz, 2H), 4.28 (t, *J* = 6.8 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.79 (t, *J* = 7.1 Hz, 1H), 1.75-1.69 (m, 2H), 1.42-1.31 (m, 4H), 1.13 (t, *J* = 7.2 Hz, 3H), 0.91 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.7, 139.9, 136.1, 134.9, 130.5, 130.0, 129.2, 128.7, 128.5, 128.2, 127.9, 116.5, 113.3, 65.2, 61.0, 55.3, 28.5, 28.2, 22.5, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{26}H_{29}NO_5+H]^+$ $[M+H]^+$ 436.2118, found: 436.2122.

3-Benzyl 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4au)



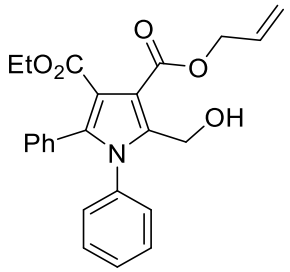
48.7 mg, 54% yield, Colorless oil, R_f = 0.30 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 7.1 Hz, 2H), 7.38-7.35 (m, 2H), 7.33-7.30 (m, 4H), 7.18-7.09 (m, 7H), 5.33 (s, 2H), 4.50 (d, *J* = 6.9 Hz, 2H), 3.92 (q, *J* = 7.2 Hz, 2H), 3.71 (t, *J* = 7.1 Hz, 1H), 0.98 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.3, 140.2, 136.1, 135.8, 134.8, 130.5, 129.9, 129.3, 128.9, 128.7, 128.5, 12.41, 128.39, 128.2, 127.9, 116.7, 112.9, 66.9, 61.1, 55.2, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{28}H_{25}NO_5+H]^+$ $[M+H]^+$ 456.1805, found: 456.1816.

3-Allyl 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4av)



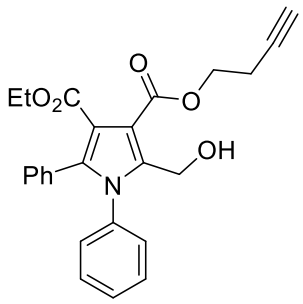
58.1 mg, 72% yield, white solid, m.p. 143-145 °C, R_f = 0.36 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.31 (m, 3H), 7.21-7.17 (m, 3H), 7.16-7.10 (m, 4H), 6.05-5.97 (m, 1H), 5.42 (dq, *J* = 17.2 Hz, 1.5 Hz, 1H), 5.28 (dq, *J* = 10.5 Hz, 1.2 Hz, 1H), 4.81 (dt, *J* = 5.7 Hz, 1.4 Hz, 2H), 4.50 (s, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.70 (s, 1H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.2, 140.0, 136.1, 135.1, 132.1, 130.6, 129.9, 129.3, 128.9, 128.5, 128.3, 127.9, 118.6, 116.5, 113.1, 65.7, 61.1, 55.2, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{23}NO_5+H]^+$ $[M+H]^+$ 406.1649, found: 406.1656.

3-(But-3-yn-1-yl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4aw)



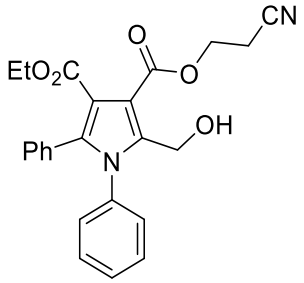
66.0 mg, 79% yield, Colorless oil, R_f = 0.29 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.28 (m, 3H), 7.19-7.14 (m, 3H), 7.14-7.10 (m, 4H), 4.49 (s, 2H), 4.40 (t, *J* = 6.8 Hz, 2H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.92-2.76 (m, 1H), 2.63 (td, *J* = 6.7, 2.7 Hz, 2H), 2.04-2.02 (m, 1H), 1.13 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 164.8, 139.7, 136.1, 135.3, 130.6, 130.0, 129.2, 128.9, 128.53, 128.3, 127.9, 116.6, 112.9, 80.3, 70.3, 62.6, 61.1, 55.1, 19.1, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{23}NO_5+H]^+$ $[M+H]^+$ 418.1649, found: 418.1651.

3-(2-Cyanoethyl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4ax)



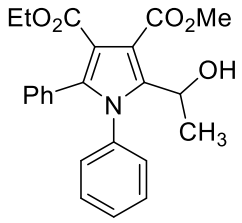
62.6 mg, 75% yield, white solid, m.p. 187-188 °C, R_f = 0.66 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.29 (m, 3H), 7.22-7.16 (m, 2H), 7.16-7.15 (m, 1H), 7.14-7.09 (m, 4H), 4.51-4.49 (m, 4H), 4.17 (q, *J* = 7.1 Hz, 2H), 3.46 (s, 1H), 2.81 (t, *J* = 6.3 Hz, 2H), 1.08 (t, *J* = 7.1 Hz, 3H).;

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.4, 164.7, 140.3, 135.9, 135.9, 130.6, 129.9, 129.3, 129.0, 128.5, 128.4, 127.8, 117.1, 116.4, 112.3, 61.2, 59.2, 55.0, 18.1, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{22}N_2O_5+H]^+$ $[M+H]^+$ 419.1601, found: 419.1610.

3-Ethyl 4-methyl 5-(1-hydroxyethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4ay)



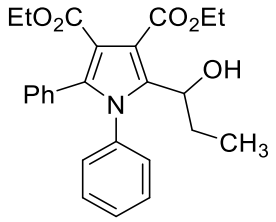
12.6 mg, 16% yield, Colorless oil, R_f = 0.33 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.28 (m, 3H), 7.18-7.12 (m, 4H), 7.10-7.08 (m, 2H), 6.99-6.97 (m, 1H), 5.50 (d, *J* = 8.1 Hz, 1H), 4.53 (t, *J* = 6.4 Hz, 1H), 4.19-4.14 (m, 2H), 3.88 (s, 3H), 1.44 (d, *J* = 6.8 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 167.1, 166.1, 145.0, 136.3, 134.3, 130.5, 129.9, 129.5, 129.20, 129.19, 128.9, 128.4, 128.2, 127.9, 117.1, 110.2, 63.5, 61.1, 52.3, 23.5, 14.2;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{23}NO_5+H]^+$ $[M+H]^+$ 394.1649, found: 394.1652.

Diethyl 2-(1-hydroxypropyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4az)



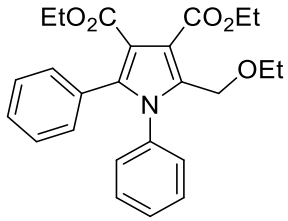
16.9 mg, 20% yield, Colorless oil, R_f = 0.51 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.29 (m, 2H), 7.27-7.24 (m, 1H), 7.23-7.21 (m, 1H), 7.16-7.08 (m, 5H), 6.93-6.91 (m, 1H), 5.33 (d, *J* = 11.2 Hz, 1H), 4.38 (q, *J* = 7.2 Hz, 2H), 4.26-4.21 (m, 1H), 4.18-4.11 (m, 2H), 1.91-1.82 (m, 1H), 1.69-1.61 (m, 1H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H), 0.78 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.7, 166.2, 144.2, 136.5, 134.2, 130.5, 130.0, 129.4, 129.1, 129.0, 128.7, 128.1, 127.8, 117.3, 110.7, 68.9, 61.3, 61.0, 30.4, 14.2, 14.1, 10.9;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{27}NO_5+H]^+$ $[M+H]^+$ 422.1962, found: 422.1972.

Diethyl 2-(ethoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5aa)



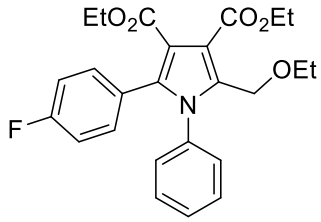
63.2 mg, 75% yield, light yellow oil, R_f = 0.14 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28-7.25 (m, 3H), 7.16-7.12 (m, 7H), 4.44 (s, 2H), 4.33 (q, *J* = 7.2 Hz, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 3.39 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.12 (t, *J* = 7.2 Hz, 3H), 1.09 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 164.7, 136.7, 136.5, 134.4, 130.6, 130.3, 128.7, 128.6, 128.1, 127.7, 65.5, 61.2, 60.7, 60.6, 15.2, 14.3, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{27}NO_5+H]^+$ $[M+H]^+$ 422.1962, found: 422.1972.

Diethyl 2-(ethoxymethyl)-5-(4-fluorophenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ba)



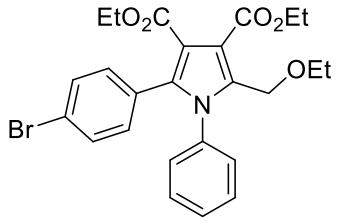
74.5 mg, 85% yield, light yellow oil, R_f = 0.16 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.27 (m, 3H), 7.14-7.10 (m, 4H), 6.85-6.82 (m, 2H), 4.42 (s, 2H), 4.33 (q, *J* = 7.2 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 3.37 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H), 1.08 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.3, 164.7, 162.4 (d, *J* = 246.9 Hz), 136.5, 135.6, 134.4, 132.6 (d, *J* = 8.2 Hz), 128.9, 128.74, 128.71, 126.4 (d, *J* = 3.5 Hz), 115.8, 115.6, 114.9 (d, *J* = 21.5 Hz), 65.6, 61.2, 60.72, 60.68, 15.1, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{26}FNO_5+H]^+$ $[M+H]^+$ 440.1868, found: 440.1875.

Diethyl 2-(4-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ca)



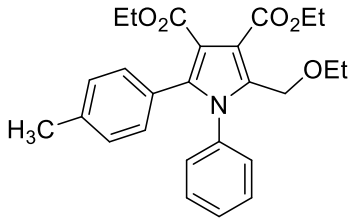
85.7 mg, 86% yield, light yellow oil, m.p. 131-132 °C, R_f = 0.14 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.26 (m, 5H), 7.15-7.13 (m, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 4.42 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 4.15 (q, *J* = 7.2 Hz, 2H), 3.37 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H), 1.08 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.3, 164.5, 136.4, 135.2, 134.7, 132.2, 131.0, 129.3, 129.0, 128.8, 128.7, 122.6, 116.1, 115.7, 65.6, 61.2, 60.8, 60.7, 15.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{26}BrNO_5+H]^+$ $[M+H]^+$ 500.1067, found: 500.1075.

Diethyl 2-(ethoxymethyl)-1-phenyl-5-(*p*-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (5da)



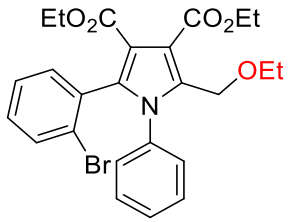
69.1 mg, 79% yield, light yellow oil, R_f = 0.16 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28-7.26 (m, 3H), 7.16-7.15 (m, 2H), 7.01 (d, *J* = 8.2 Hz, 2H), 6.94 (d, *J* = 7.9 Hz, 2H), 4.44 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 3.38 (q, *J* = 7.0 Hz, 2H), 2.22 (s, 3H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H), 1.09 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 164.7, 137.9, 136.8, 136.7, 134.3, 130.5, 128.8, 128.7, 128.53, 128.48, 127.3, 115.7, 115.4, 65.5, 61.2, 60.7, 60.6, 21.3, 15.2, 14.4, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{26}H_{29}NO_5+H]^+$ $[M+H]^+$ 436.2118, found: 436.2125.

Diethyl 2-(2-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ea)



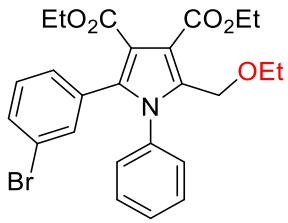
90.2 mg, 90% yield, light yellow oil, R_f = 0.11 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (dd, *J* = 7.9 Hz, 0.9 Hz, 1H), 7.20-7.18 (m, 5H), 7.10-7.04 (m, 2H), 7.01-6.98 (m, 1H), 4.42 (d, *J* = 11.9 Hz, 1H), 4.31-4.26 (m, 3H), 4.05-3.95 (m, 2H), 3.33-3.26 (m, 2H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.01 (t, *J* = 7.0 Hz, 3H), 0.94 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 163.9, 136.9, 136.2, 133.7, 133.1, 132.7, 132.2, 130.1, 128.8, 128.6, 128.4, 126.6, 125.7, 116.3, 115.3, 65.4, 61.3, 60.8, 60.2, 15.1, 14.3, 13.9;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{26}BrNO_5+H]^+$ $[M+H]^+$ 500.1067, found: 500.1075.

Diethyl 2-(3-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5fa)



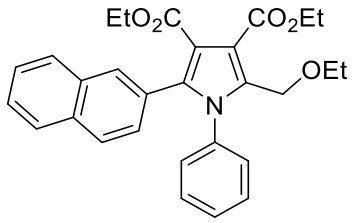
85.3 mg, 85% yield, light yellow oil, R_f = 0.14 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.31 (m, 1H), 7.31-7.27 (m, 4H), 7.16-7.14 (m, 2H), 7.01-6.97 (m, 2H), 4.43 (s, 2H), 4.32 (q, *J* = 7.2 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.37 (q, *J* = 7.0 Hz, 2H), 1.34 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.08 (t, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2, 164.5, 136.3, 134.8, 134.6, 133.6, 132.3, 131.1, 129.22, 129.19, 129.0, 128.9, 128.7, 121.7, 116.4, 115.6, 65.6, 61.1, 60.9, 60.7, 15.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{25}H_{26}BrNO_5+H]^+$ $[M+H]^+$ 500.1067, found: 500.1076.

Diethyl 2-(ethoxymethyl)-5-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ga)



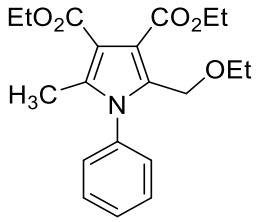
66.8 mg, 71% yield, light yellow oil, R_f = 0.14 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.71-7.67 (m, 2H), 7.58 (d, J = 8.5 Hz, 1H), 7.41-7.40 (m, 2H), 7.25-7.20 (m, 4H), 7.16 (dd, J = 8.5 Hz, 1.6 Hz, 1H), 4.50 (s, 2H), 4.36 (q, J = 7.2 Hz, 2H), 4.14 (q, J = 7.2 Hz, 2H), 3.43 (q, J = 7.0 Hz, 2H), 1.37 (t, J = 7.2 Hz, 3H), 1.13 (t, J = 7.0 Hz, 3H), 1.10 (t, J = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 164.6, 136.7, 136.2, 134.7, 132.73, 132.67, 130.4, 128.9, 128.74, 128.65, 128.2, 127.79, 127.77, 127.6, 127.2, 126.5, 126.2, 116.4, 115.5, 65.6, 61.2, 60.8, 60.6, 15.2, 14.4, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{29}H_{29}NO_5+H]^+$ $[M+H]^+$ 472.2118, found: 472.2125.

Diethyl 2-(ethoxymethyl)-5-methyl-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ha)



45.3 mg, 63% yield, colorless oil, R_f = 0.12 (PE/EtOAc = 10:1);

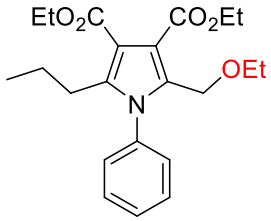
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.44 (m, 3H), 7.25-7.22 (m, 2H), 4.32-4.24 (m, 6H), 3.27 (q, *J* = 7.0 Hz, 2H), 2.16 (s, 3H), 1.32 (t, *J* = 7.1 Hz, 3H), 1.30 (t, *J* = 7.2 Hz, 3H), 1.02 (t, *J* = 7.0 Hz,

3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 165.2, 136.4, 136.3, 132.5, 129.3, 129.2, 128.4, 116.4, 112.4, 65.1, 61.2, 60.7, 60.2, 15.1, 14.4, 14.3, 12.0;

HRMS (ESI) *m/z* calculated for $[C_{20}H_{25}NO_5+H]^+$ $[M+H]^+$ 360.1805, found: 360.1812.

Diethyl 2-(ethoxymethyl)-1-phenyl-5-propyl-1*H*-pyrrole-3,4-dicarboxylate (5ia)



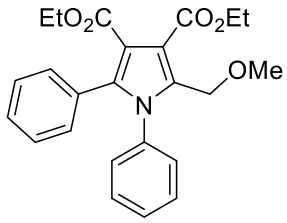
36.4 mg, 47% yield, colorless oil, R_f = 0.18 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47-7.46 (m, 3H), 7.26-7.24 (m, 2H), 4.31 (q, *J* = 7.2 Hz, 2H), 4.27 (q, *J* = 7.2 Hz, 2H), 4.25 (s, 2H), 3.25 (q, *J* = 7.0 Hz, 2H), 2.56-2.53 (m, 2H), 1.35-1.29 (m, 8H), 1.02 (t, *J* = 7.0 Hz, 3H), 0.72 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 165.2, 140.6, 136.3, 132.4, 129.3, 129.1, 128.8, 116.4, 112.3, 65.2, 61.2, 60.7, 60.2, 27.4, 23.2, 15.1, 14.36, 14.35, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{22}H_{29}NO_5+Na]^+$ $[M+Na]^+$ 410.1943, found: 410.1943.

Diethyl 2-(methoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5ab)



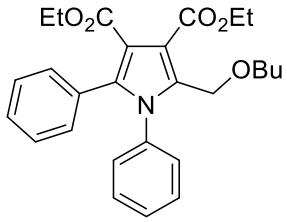
54.2 mg, 67% yield, light yellow oil, R_f = 0.11 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29-7.26 (m, 3H), 7.17-7.12 (m, 7H), 4.40 (s, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.25 (s, 3H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.13 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 164.7, 136.6, 136.5, 134.1, 130.6, 130.3, 128.8, 128.70, 128.65, 128.1, 127.8, 115.9, 115.6, 63.0, 60.8, 60.7, 57.8, 14.4, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{24}H_{25}NO_5+H]^+$ $[M+H]^+$ 408.1805, found: 408.1814.

Diethyl 2-(butoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5ac)



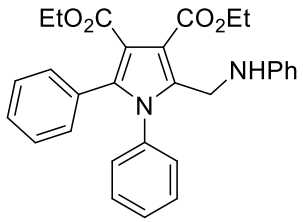
51.5 mg, 57% yield, light yellow oil, R_f = 0.11 (PE/EtOAc = 10:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28-7.25 (m, 3H), 7.17-7.12 (m, 7H), 4.43 (s, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 4.14 (q, *J* = 7.1 Hz, 2H), 3.33 (t, *J* = 6.5 Hz, 2H), 1.49-1.43 (m, 2H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.30-1.24 (m, 2H), 1.12 (t, *J* = 7.1 Hz, 3H), 0.85 (t, *J* = 7.4 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.5, 164.7, 136.7, 136.5, 134.4, 130.6, 130.3, 128.8, 128.7, 128.6, 128.1, 127.7, 115.9, 115.5, 70.1, 61.5, 60.7, 60.6, 31.8, 19.4, 14.4, 14.05, 13.98;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{31}NO_5+H]^+$ $[M+H]^+$ 450.2275, found: 450.2289.

Diethyl 1,2-diphenyl-5-((phenylamino)methyl)-1*H*-pyrrole-3,4-dicarboxylate (6aa)



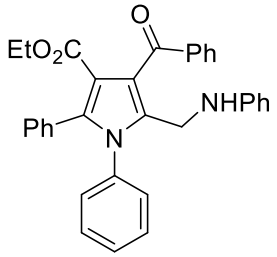
50.9 mg, 54% yield, light yellow oil, R_f = 0.60 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.27 (m ,3H), 7.18-7.06 (m, 9H), 6.70-6.66 (m, 1H), 6.44-6.42 (m, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 4.29 (s, 2H), 4.23 (brs, 1H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.16 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 164.8, 147.7, 136.6, 136.5, 135.5, 130.7, 130.2, 129.23, 129.18, 128.9, 128.5, 128.1, 127.8, 118.1, 116.4, 114.2, 113.8, 60.9, 60.7, 39.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{29}H_{28}N_2O_4+Na]^+$ $[M+Na]^+$ 491.1947, found: 491.1956.

Ethyl 4-benzoyl-1,2-diphenyl-5-((phenylamino)methyl)-1H-pyrrole-3-carboxylate (6ab)



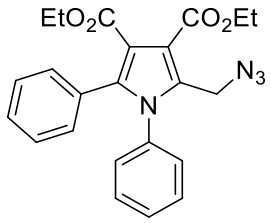
49.2 mg, 49% yield, light yellow solid, m.p. 178-180 ºC, R_f = 0.66 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93-7.91 (m, 2H), 7.54-7.51 (m, 1H), 7.45-7.42 (m, 2H), 7.31-7.30 (m, 3H), 7.25-7.23 (m, 1H), 7.20-7.18 (m, 6H), 7.01-6.98 (m, 2H), 6.64 (t, *J* = 7.3 Hz, 1H), 6.35 (d, *J* = 7.8 Hz, 2H), 4.15 (s, 2H), 3.61 (q, *J* = 7.2 Hz, 2H), 0.67 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 193.8, 163.9, 147.4, 139.5, 136.6, 135.2, 132.6, 131.5, 130.2, 129.5, 129.3, 129.1, 128.84, 128.80, 128.41, 128.40, 127.6, 127.5, 126.2, 123.7, 118.1, 113.9, 60.2, 39.1, 13.4;

HRMS (ESI) *m/z* calculated for $[C_{29}H_{28}N_2O_4+Na]^+$ $[M+Na]^+$ 523.1992, found: 523.1988.

Diethyl 2-(azidomethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (7aa)



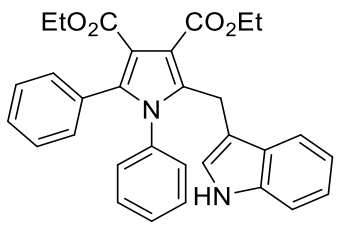
10.6 mg, 13% yield, colorless oil, R_f = 0.63 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.31 (m, 3H), 7.19-7.11 (m, 7H), 4.41 (brs, 2H), 4.36 (q, *J* = 7.2 Hz, 2H), 4.18 (q, *J* = 7.2 Hz, 2H), 1.36 (t, *J* = 7.2 Hz, 3H), 1.15 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 164.0, 136.4, 136.0, 132.4, 130.5, 129.9, 129.3, 129.2, 128.6, 128.3, 127.9, 116.7, 114.9, 61.0, 60.8, 44.0, 14.3, 14.1.;

HRMS (ESI) *m/z* calculated for $[C_{23}H_{22}N_4O_4+H]^+$ $[M+H]^+$ 419.1714, found: 419.1714.

Diethyl 2-((1*H*-indol-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (8aa)



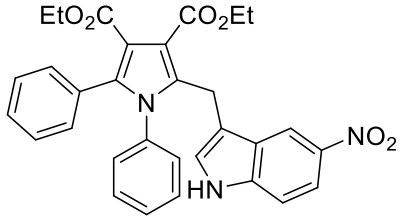
52.2 mg, 53% yield, light yellow solid, m.p. 177-179 °C, R_f = 0.82 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.92 (brs, 1H), 7.26-7.17 (m, 3H), 7.13-7.09 (m, 8H), 6.98-6.95 (m, 1H), 6.85 (d, *J* = 7.6 Hz, 2H), 6.55 (d, *J* = 2.0 Hz, 1H), 4.29 (q, *J* = 7.1 Hz, 2H), 4.24 (s, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.25 (t, *J* = 7.1 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 165.2, 138.2, 136.9, 136.0, 135.5, 130.6, 130.5, 128.8, 128.8, 128.4, 127.8, 127.6, 126.9, 122.7, 121.8, 119.2, 118.9, 115.9, 113.3, 113.0, 110.9, 60.8, 60.4, 21.7, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{28}N_2O_4+H]^+$ $[M+H]^+$ 493.2122, found: 493.2118.

Diethyl 2-((5-nitro-1*H*-indol-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (8ab)



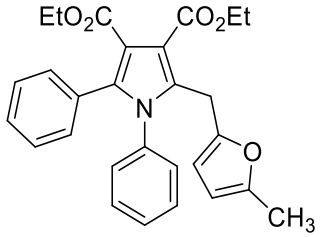
77.5 mg, 72% yield, yellow solid, m.p. 230-231 °C, R_f = 0.58 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.09 (s), 7.98 (d, *J* = 2.1 Hz, 1H), 7.94 (d, *J* = 8.9 Hz, 2.2 Hz, 1H), 7.24 (d, *J* = 8.9 Hz, 1H), 7.21-7.17 (m, 1H), 7.14-7.05 (m, 7H), 6.86-6.84 (m, 2H), 4.31 (q, *J* = 7.1 Hz, 2H), 4.27 (s, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 1.27 (t, *J* = 7.1 Hz, 3H), 1.14 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.3, 165.1, 141.3, 138.9, 138.1, 136.4, 135.6, 130.5, 130.2, 129.1, 128.9, 128.7, 128.1, 127.8, 126.21, 126.17, 117.3, 116.1, 116.0, 115.6, 112.6, 111.1, 61.0, 60.7, 21.2, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{27}N_3O_6+H]^+$ $[M+H]^+$ 538.1973, found: 538.1979.

Diethyl 2-((5-methylfuran-2-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (9aa)



26.1 mg, 29% yield, colorless oil, R_f = 0.64 (PE/EtOAc = 3:1);

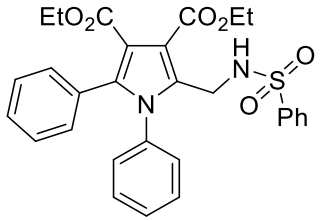
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27-7.23 (m, 3H), 7.14-7.11 (m, 5H), 7.01-7.00 (m, 2H), 5.73-5.72 (m, 1H), 5.63 (d, *J* = 2.8 Hz, 1H), 4.29 (q, *J* = 7.7 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 4.06 (s, 2H),

2.14 (s, 3H), 1.31 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 164.6, 150.6, 149.8, 136.7, 135.5, 135.4, 130.5, 130.4, 129.0, 128.9, 128.7, 127.9, 127.7, 116.1, 113.2, 107.0, 106.1, 60.8, 60.4, 24.9, 14.3, 14.1, 13.6;

HRMS (ESI) *m/z* calculated for $[C_{28}H_{27}NO_5+H]^+$ $[M+H]^+$ 458.1962, found: 458.1970.

Diethyl 1,2-diphenyl-5-(phenylsulfonamidomethyl)-1*H*-pyrrole-3,4-dicarboxylate (10aa)



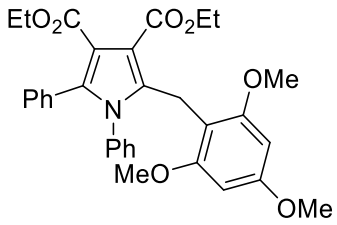
36.9 mg, 35% yield, white solid, m.p. 265-267 °C, R_f = 0.78 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73-7.71 (m, 2H), 7.55-7.52 (m, 1H), 7.46-7.43 (m, 2H), 7.32-7.26 (m, 3H), 7.17-7.12 (m, 3H), 7.07-7.05 (m, 2H), 7.01-6.99 (m, 2H), 5.96 (t, *J* = 6.7 Hz, 1H), 4.26 (q, *J* = 7.2 Hz, 2H), 4.14 (q, *J* = 7.2 Hz, 2H), 4.05 (d, *J* = 6.7 Hz, 2H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.14 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6, 164.9, 139.8, 135.5, 135.3, 134.2, 132.7, 130.5, 129.8, 129.3, 129.15, 129.10, 128.6, 128.3, 127.9, 127.1, 116.7, 113.9, 61.04, 60.97, 38.4, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{29}H_{28}N_2O_6S+H]^+$ $[M+H]^+$ 533.1741, found: 533.1747.

Diethyl 1,2-diphenyl-5-(2,4,6-trimethoxybenzyl)-1*H*-pyrrole-3,4-dicarboxylate (11aa)



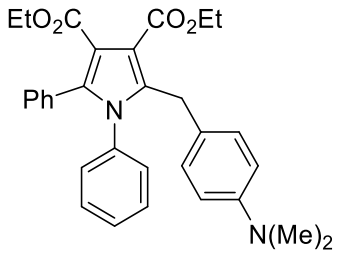
50.3 mg, 46% yield, colorless oil, R_f = 0.28 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.18-7.08 (m, 8H), 6.85 (d, *J* = 7.0 Hz, 2H), 5.89 (s, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 4.08 (q, *J* = 7.2 Hz, 2H), 4.01 (s, 2H), 3.73 (s, 3H), 3.51 (s, 6H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.2, 165.1, 160.0, 159.0, 137.2, 136.73, 136.67, 131.1, 129.3, 128.3, 128.0, 127.6, 127.3, 114.5, 113.9, 106.7, 100.0, 89.9, 60.4, 60.1, 55.6, 55.3, 19.6, 14.3, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{32}H_{33}NO_7+H]^+$ $[M+H]^+$ 544.2330, found: 544.2335.

Diethyl 2-(4-(dimethylamino)benzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (12aa)



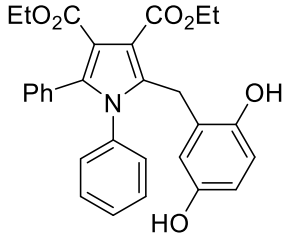
35.7 mg, 36% yield, colorless oil, R_f = 0.47 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.10 (m, 8H), 6.83 (d, *J* = 7.1 Hz, 2H), 6.69 (d, *J* = 8.7 Hz, 2H), 6.52 (d, *J* = 8.6 Hz, 2H), 4.30 (q, *J* = 7.1 Hz, 2H), 4.17 (q, *J* = 7.2 Hz, 2H), 4.04 (s, 2H), 2.85 (s, 6H), 1.30 (t, *J* = 7.1 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.1, 165.1, 149.2, 138.6, 136.9, 135.5, 130.6, 130.5, 129.10, 129.09, 128.8, 128.5, 127.8, 127.6, 115.8, 113.1, 112.8, 60.7, 60.4, 40.9, 30.4, 14.4, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{32}N_2O_4+H]^+$ $[M+H]^+$ 497.2435, found: 497.2442.

Diethyl 2-(2,5-dihydroxybenzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (13aa)



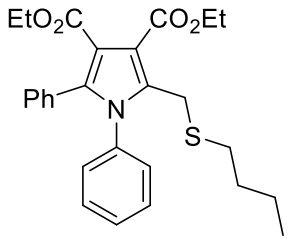
51.0 mg, 53% yield, colorless oil, R_f = 0.63 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.32-7.29 (m, 1H), 7.25-7.22 (m, 2H), 7.13-7.08 (m, 3H), 7.03-7.01 (m, 2H), 6.87 (d, *J* = 7.2 Hz, 2H), 6.59 (d, *J* = 8.6 Hz, 1H), 6.45 (dd, *J* = 8.6 Hz, 2.9 Hz, 1H), 5.27 (d, *J* = 2.7 Hz, 1H), 4.91 (s, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 4.03 (s, 2H), 1.32 (t, *J* = 7.2 Hz, 3H), 1.10 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 167.6, 165.7, 149.0, 148.2, 137.1, 136.7, 136.5, 130.4, 130.0, 129.4, 129.2, 129.1, 128.1, 127.7, 122.8, 117.5, 117.0, 115.4, 115.0, 112.1, 61.6, 60.8, 27.3, 14.2, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{29}H_{27}NO_6+H]^+$ $[M+H]^+$ 486.1911, found: 486.1922.

Diethyl 2-((butylthio)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (14aa)



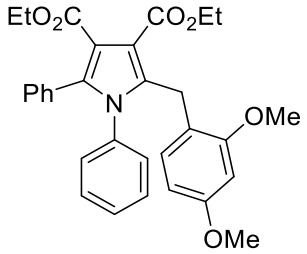
58.2 mg, 63% yield, colorless oil, R_f = 0.69 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.28 (m, 3H), 7.18-7.12 (m, 7H), 4.31 (q, *J* = 7.1 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.87 (s, 2H), 2.42 (t, *J* = 7.4 Hz, 2H), 1.41-1.25 (m, 7H), 1.12 (t, *J* = 7.2 Hz, 3H), 0.83 (t, *J* = 7.3 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 164.6, 136.4, 136.2, 135.9, 130.5, 130.3, 129.1, 129.0, 128.9, 128.0, 127.7, 116.2, 113.2, 60.8, 60.5, 32.2, 31.6, 25.8, 22.0, 14.4, 14.1, 13.7;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{31}NO_4S+H]^+$ $[M+H]^+$ 466.2047, found: 466.2054.

Diethyl 2-(2,4-dimethoxybenzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (15aa)



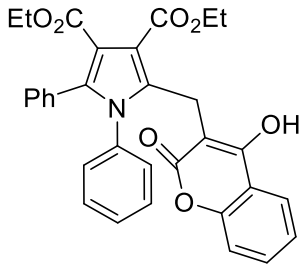
47.4 mg, 46% yield, colorless oil, R_f = 0.40 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.20-7.17 (m, 1H), 7.12-7.11 (m, 7H), 6.82 (d, *J* = 7.7 Hz, 2H), 6.74 (d, *J* = 8.3 Hz, 1H), 6.31 (dd, *J* = 8.4 Hz, 2.4 Hz, 1H), 6.24 (d, *J* = 2.3 Hz, 1H), 4.25 (q, *J* = 7.1 Hz, 2H), 4.18 (q, *J* = 7.1 Hz, 1H), 4.01 (s, 2H), 3.73 (s, 3H), 3.52 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 3H), 1.15 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.0, 165.0, 159.2, 157.5, 137.9, 136.8, 135.7, 130.6, 129.7, 128.8, 128.7, 128.3, 127.8, 127.6, 119.5, 115.7, 113.9, 103.7, 97.9, 60.7, 60.3, 55.4, 55.1, 24.5, 14.3, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{31}NO_6+H]^+$ $[M+H]^+$ 514.2224, found: 514.2224.

Diethyl 2-((4-hydroxy-2-oxo-2*H*-chromen-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (16aa)



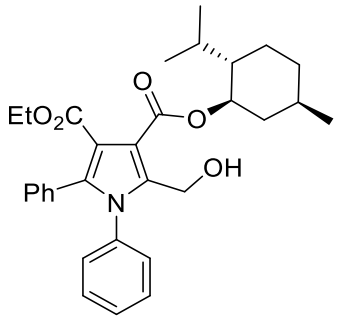
43.4 mg, 40% yield, white solid, m.p. 213-215 ºC, R_f = 0.49 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 11.55 (s, 1H), 7.89 (dd, *J* = 7.9 Hz, 1.4 Hz, 1H), 7.47-7.44 (m, 1H), 7.36-7.33 (m, 1H), 7.27-7.23 (m, 3H), 7.17 (d, *J* = 8.3 Hz, 1H), 7.14-7.08 (m, 3H), 7.06-7.04 (m, 2H), 6.92 (d, *J* = 7.4 Hz, 2H), 4.48 (q, *J* = 7.2 Hz, 2H), 4.12 (q, *J* = 7.2 Hz, 2H), 4.07 (s, 2H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.07 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 164.8, 162.7, 162.4, 152.5, 138.3, 137.3, 136.0, 131.8, 130.6, 130.0, 129.6, 129.4, 129.0, 128.3, 127.6, 123.8, 123.7, 116.6, 116.2, 114.4, 112.5, 100.2, 62.6, 60.7, 20.4, 14.1, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{32}H_{27}NO_7+H]^+$ $[M+H]^+$ 538.1860, found: 538.1866.

3-Ethyl 4-((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17aa)



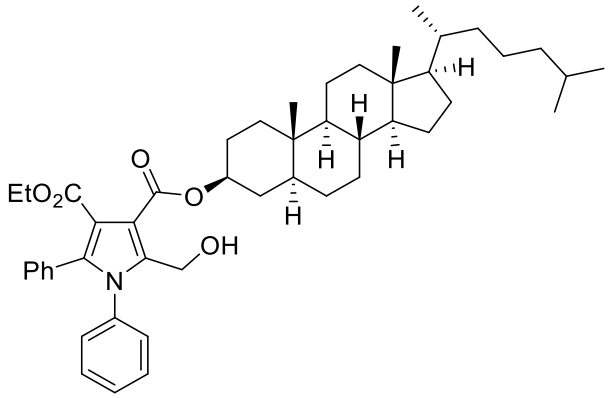
56.4 mg, 56% yield, colorless oil, R_f = 0.61 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32-7.31 (m, 3H), 7.20-7.15 (m, 3H), 7.14-7.10 (m, 4H), 4.94 (td, *J* = 10.9 Hz, 4.4 Hz, 1H), 4.54 (d, *J* = 13.6 Hz, 1H), 4.48 (d, *J* = 13.6 Hz, 1H), 4.23-4.11 (m, 2H), 3.91 (brs, 1H), 2.18-2.15 (m, 1H), 2.06-2.00 (m, 1H), 1.72 (d, *J* = 11.5 Hz, 2H), 1.58-1.50 (m, 1H), 1.46-1.40 (m, 1H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.13-1.06 (m, 2H), 0.94-0.91 (m, 6H), 0.89-0.86 (m, 1H), 0.80 (d, *J* = 7.0 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 166.2, 165.0, 140.0, 136.1, 134.0, 130.3, 130.0, 129.3, 128.9, 128.5, 128.1, 127.9, 117.0, 113.1, 75.0, 61.2, 55.4, 47.3, 41.0, 34.3, 31.6, 25.9, 23.1, 22.1, 21.1, 16.1, 14.1;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{37}NO_5+H]^+$ $[M+H]^+$ 504.2744, found: 504.2744.

3-((3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ab)



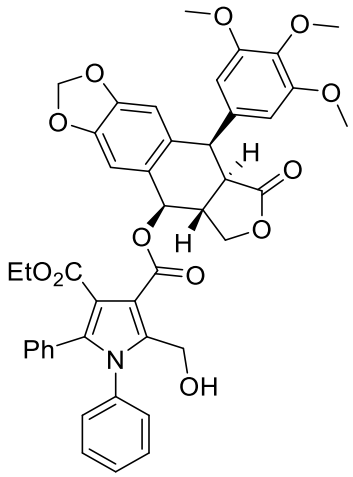
106.9 mg, 73% yield, colorless oil, R_f = 0.61 (PE/EtOAc = 3:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31-7.29 (m, 3H), 7.18-7.15 (m, 3H), 7.14-7.09 (m, 4H), 4.97-4.90 (m, 1H), 4.48 (s, 2H), 4.18 (q, *J* = 7.1 Hz, 2H), 3.84 (brs, 1H), 1.98-1.95 (m, 2H), 1.83-1.73 (m, 3H), 1.68-1.65 (m, 1H), 1.61-1.47 (m, 5H), 1.36-1.30 (m, 6H), 1.28-1.22 (m, 4H), 1.19-1.15 (m, 3H), 1.15-1.07 (m, 6H), 1.05-0.98 (m, 3H), 0.90 (d, *J* = 6.5 Hz, 3H), 0.86 (d, *J* = 2.4 Hz, 3H), 0.85 (d, *J* = 2.4 Hz, 3H), .0.84 (s, 3H), 0.70-0.67 (m, 1H), 0.65 (s, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 165.0, 139.7, 136.2, 134.6, 130.5, 130.0, 129.2, 128.8, 128.5, 128.2, 127.9, 116.6, 113.7, 74.7, 61.1, 56.5, 56.3, 55.3, 54.3, 44.8, 42.7, 40.1, 39.6, 36.9, 36.3, 35.9, 35.6, 35.6, 34.1, 32.1, 28.7, 28.4, 28.1, 27.6, 24.3, 23.9, 23.0, 22.7, 21.3, 18.8, 14.1, 12.4, 12.2;

HRMS (ESI) *m/z* calculated for $[C_{48}H_{65}NO_5+H]^+$ $[M+H]^+$ 736.4936, found: 736.4929.

3-Ethyl 4-((5*R*,5a*R*,8a*R*,9*R*)-8-oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7]naphtho[2,3-*d*][1,3]dioxol-5-yl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ac)



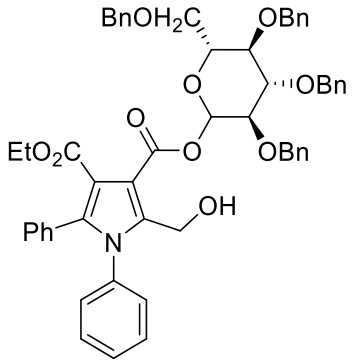
107.8 mg, 71% yield, white solid, m.p. 246-248 ºC,R_f = 0.38 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.29 (m, 3H), 7.18-7.13 (m, 3H), 7.08-7.07 (m, 3H), 6.95 (s, 1H), 6.52 (s, 1H), 6.40 (s, 2H), 6.12 (d, *J* = 8.5 Hz, 1H), 5.94-5.92 (m, 3H), 4.60 (d, *J* = 3.7 Hz, 1H), 4.56-4.52 (m, 3H), 4.30-4.25 (m, 1H), 3.97-3.92 (m, 1H), 3.85-3.82 (m, 1H), 3.77 (s, 3H), 3.76 (s, 6H), 3.71-3.70 (m, 2H), 0.94 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 174.0, 165.8, 165.3, 152.7, 148.1, 147.6, 140.3, 135.9, 135.6, 135.1, 132.5, 130.5, 129.9, 129.3, 129.1, 128.52, 128.49, 128.4, 127.9, 116.5, 112.3, 109.9, 108.1, 107.3, 101.6, 74.3, 71.7, 60.9, 60.8, 56.3, 56.2, 55.1, 45.6, 43.9, 38.7, 13.8;

HRMS (ESI) *m/z* calculated for $[C_{43}H_{39}NO_{12}+H]^+$ $[M+H]^+$ 762.2545, found: 762.2548.

3-Ethyl 4-((3*R*,4*S*,5*R*,6*R*)-3,4,5-tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ad)



145.2 mg, 82% yield, white solid, m.p. 231-233 ºC, R_f = 0.76 (PE/EtOAc = 1:1);

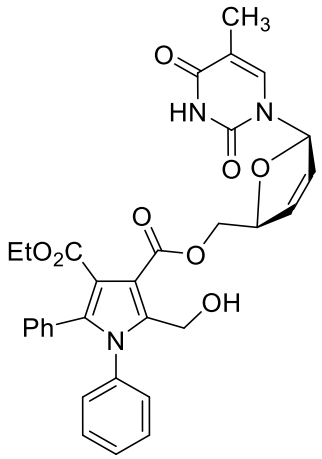
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37-7.27 (m, 23H), 7.20-7.15 (m, 7H), 5.02 (d, *J* = 10.9 Hz, 1H), 4.89 (d, *J* = 4.4 Hz, 1H), 4.87 (d, *J* = 4.5 Hz, 1H), 4.79 (d, *J* = 11.2 Hz, 1H), 4.73 (d, *J* = 14.5 Hz, 1H), 4.65 (d, *J* = 12.1 Hz, 1H), 4.54 (d, *J* = 10.9 Hz, 1H), 4.49 (d, *J* = 12.1 Hz, 1H), 4.39 (d, *J* = 9.3

Hz, 1H), 4.23-4.17 (m, 2H), 4.10-4.06 (m, 1H), 3.98 (d, *J* = 9.9 Hz, 2H), 3.85-3.79 (m, 4H), 3.71-3.70 (m, 1H), 0.99 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.9, 163.1, 140.4, 138.8, 138.5, 138.0, 137.5, 136.1, 135.1, 130.4, 130.1, 129.3, 129.0, 128.7, 128.52, 128.51, 128.38, 128.35, 128.2, 128.13, 128.10, 128.02, 127.97, 127.85, 127.82, 127.75, 127.71, 117.3, 112.3, 90.8, 82.3, 78.7, 76.9, 75.9, 75.1, 73.7, 73.4, 73.2, 68.1, 61.4, 55.2, 13.9;

HRMS (ESI) *m/z* calculated for $[C_{55}H_{53}NO_{10}+H]^+$ $[M+H]^+$ 888.3742, found: 888.3735.

3-Ethyl 4-(((2*S*,5*R*)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ae)



58.3 mg, 51% yield, white solid, m.p. 283-285 °C, R_f = 0.38 (EtOAc);

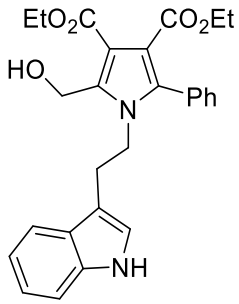
^{1}H NMR (500 MHz, $CDCl_3$) δ 9.32 (s, 1H), 7.30-7.28 (m, 3H), 7.16-7.12 (m, 4H), 7.07-7.05 (m, 3H), 7.01 (s, 1H), 6.41 (d, *J* = 5.9 Hz, 1H), 5.83 (d, *J* = 5.2 Hz, 1H), 5.08 (s, 1H), 4.64 (d, *J* = 12.1 Hz, 1H), 4.49-4.46 (m, 1H), 4.43-4.39 (m, 2H), 4.13-4.03 (m, 3H), 3.55 (t, *J* = 6.8 Hz, 1H), 1.63 (s, 3H), 1.00 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2, 165.1, 164.1, 151.0, 139.9, 136.2, 135.8, 134.0, 130.6, 129.9, 129.3, 129.0, 128.5, 128.4, 127.8, 126.8, 116.0, 113.0, 111.3, 89.7, 84.2, 65.1, 60.9, 60.5, 54.8, 14.0, 11.7;

HRMS (ESI) *m/z* calculated for $[C_{31}H_{29}N_3O_8+Na]^+$ $[M+Na]^+$ 594.1847, found: 594.1852.

Diethyl 1-(2-(1*H*-indol-3-yl)ethyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate

(17af)



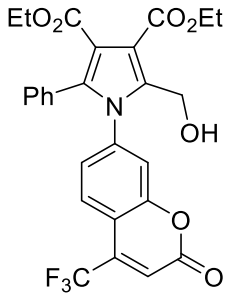
43.4 mg, 47% yield, colorless oil, R_f = 0.34 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (s, 1H), 7.45-7.42 (m, 1H), 7.39-7.36 (m, 2H), 7.26-7.25 (m, 3H), 7.13-7.10 (m, 1H), 6.94-6.91 (m, 1H), 6.83 (d, *J* = 7.9 Hz, 1H), 6.73 (d, *J* = 2.0 Hz, 1H), 4.68 (s, 2H), 4.32 (q, *J* = 7.1 Hz, 2H), 4.09-4.05 (m, 4H), 3.68 (brs, 1H), 2.93-2.90 (m, 2H), 1.34 (t, *J* = 7.1 Hz, 3H), 1.04 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 165.4, 138.0, 136.2, 135.9, 130.8, 130.6, 128.9, 128.5, 126.9, 122.4, 122.1, 119.5, 118.2, 115.7, 113.4, 111.3, 111.2, 60.9, 60.6, 54.8, 45.5, 27.5, 14.3, 14.0;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{28}N_2O_5+H]^+$ $[M+H]^+$ 461.2071, found: 461.2075.

Diethyl 2-(hydroxymethyl)-1-(2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (17ag)



66.9 mg, 63% yield, white solid, m.p. 201-203 °C, R_f = 0.79 (PE/EtOAc = 1:1);

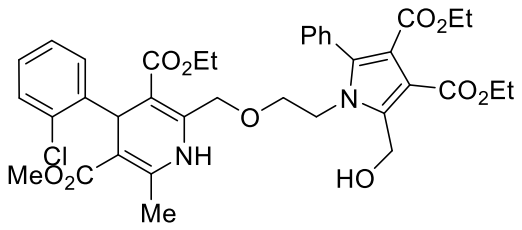
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.5 Hz, 1H), 7.25-7.18 (m, 4H), 7.17-7.13 (m, 3H), 6.80 (s, 1H), 4.50 (s, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.51 (s, 1H), 1.35 (t, *J* = 7.1 Hz, 3H), 1.14 (t, *J* = 7.1 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 165.0, 158.0, 154.2, 140.8 (q, *J* = 33.0 Hz), 140.2, 139.0, 135.1, 130.6, 129.2, 128.9, 128.3, 126.1 (q, *J* = 2.2 Hz), 125.2, 117.8, 117.2, 117.1 (q, *J* = 6.0 Hz), 114.8, 113.6, 61.23, 61.15, 54.8, 14.3, 14.1;

^{19}F NMR (470 MHz, $CDCl_3$) δ -64.67;

HRMS (ESI) *m/z* calculated for $[C_{27}H_{22}F_3NO_7+H]^+$ $[M+H]^+$ 530.1421, found: 530.1426.

3-Ethyl 5-methyl 2-((2-(3,4-bis(ethoxycarbonyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrol-1-yl)ethoxy)methyl)-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (17ah)



124.0 mg, 88% yield, white solid; m.p. 259-261 ºC, R_f = 0.36 (PE/EtOAc = 1:1);

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34-7.30 (m, 5H), 7.20 (d, *J* = 8.0 Hz, 1H), 7.13-7.10 (m, 1H), 7.03-7.00 (m, 2H), 5.45 (s, 1H), 5.37 (d, *J* = 4.0 Hz, 1H), 4.73 (s, 1H), 4.73 (d, *J* = 15.9 Hz, 0.5 H), 4.63 (d, *J* = 5.6 Hz, 1H), 4.55 (d, *J* = 15.9 Hz, 0.5 H), 4.11-4.07 (m, 1H), 4.04-3.97 (m, 3H), 3.68-3.61 (m, 3H), 3.583 (s, 1.5 H), 3.581 (s, 1.5 H), 3.25-.3.17 (m, 2H), 2.551 (s, 1.5 H), 2.546 (s, 1.5 H), 2.28 (s, 3H), 1.16-1.12 (m, 6H), 0.71 (t, *J* = 7.2 Hz, 3H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 173.1, 168.1, 168.0, 167.18, 167.17, 165.5, 165.4, 145.8, 145.7, 144.87, 144.86, 144.14, 144.13, 137.88, 137.87, 132.38, 132.36, 131.5, 129.3, 128.9, 127.5, 127.2, 127.0, 104.03, 104.0, 101.8, 101.7, 96.5, 85.0, 70.6, 70.5, 68.1, 68.0, 62.44, 62.42, 60.0, 58.9, 50.9, 42.1, 37.2, 19.34, 19.32, 14.5, 14.3, 13.4, 12.8;

HRMS (ESI) *m/z* calculated for $[C_{37}H_{41}ClN_2O_{10}+H]^+$ $[M+H]^+$ 709.2522, found: 709.2510.

References

[1] N. Jha, R. P. Singh, P. Saxena, M. Kapur. *Org. Lett*., **2021**, *23*, 8694-8698.

[2] P. F. Yuan, Q. B. Zhang, X. L. Jin, W. L. Lei, L. Z. Zhu, Q. Liu. *Green Chem.*, **2018**, *20*, 5464-5468.

[3] J. Qian, R. Wani, C. Klomsiri, L. B. Poole, A. W. Tsang, C. M. Furdui. *Chem. Commun.*, **2012**, *48*, 4091-4093.

[4] W. Huang, C. L. Zhu, M. K. Li, Y. Yu, W. Q. Wu, Z. C. Tu, H. F. Jiang, *Adv. Synth. Catal*., **2018**, *360*, 3117-3123.

[5] Q. Sha, H. Arman, M. P. Doyle, *Chem. Commun*. **2016**, *52*, 108-111.

[6] Q. Sha, J. K. Wang, M. P. Doyle, *J. Org. Chem*. **2018**, *83(18)*, 11288-11297.

[7] H. Dahn, L. H. Dao, R. Hunma, *Helv. Chim. Acta*. **1982**, *65(8)*, 2458-2463.

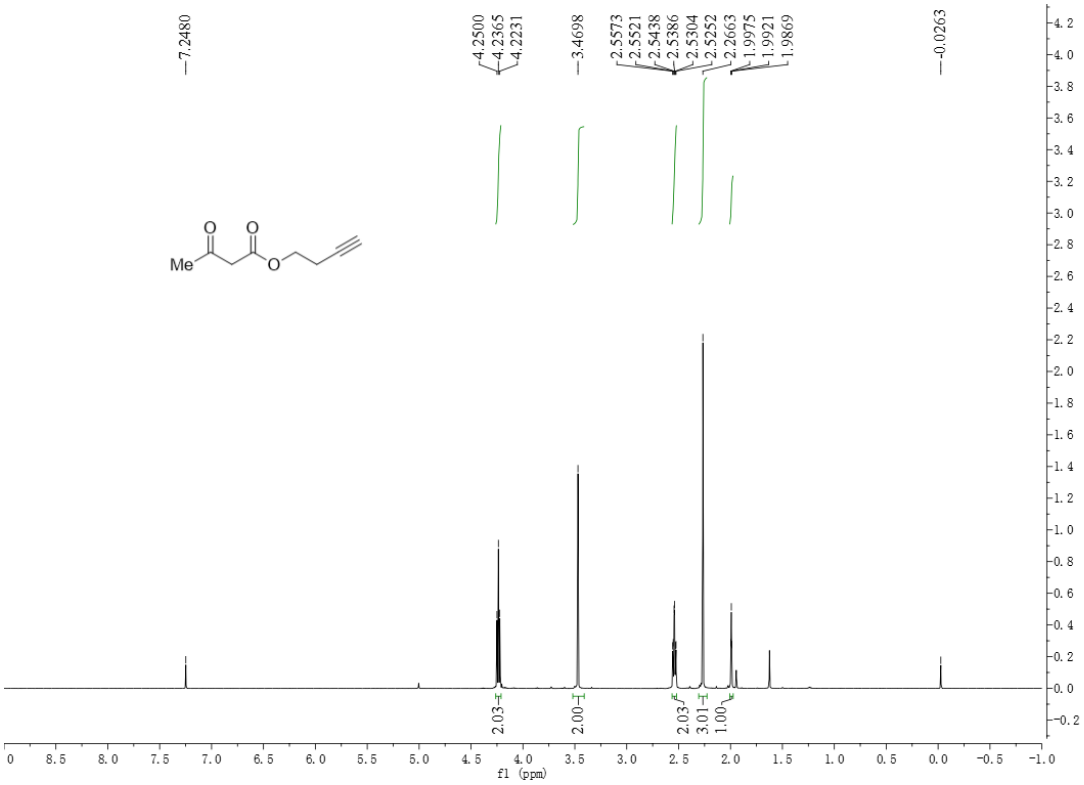
[8] H. Asahara, N. Nishiwaki, *J. Org. Chem*. **2014**, *79(23)*, 11735-11739.

[9] S. P. Stanforth, B. Tarbit, M. D. Watson, *Tetrahedron*, **2004**, *60(40)*, 8893-8897.

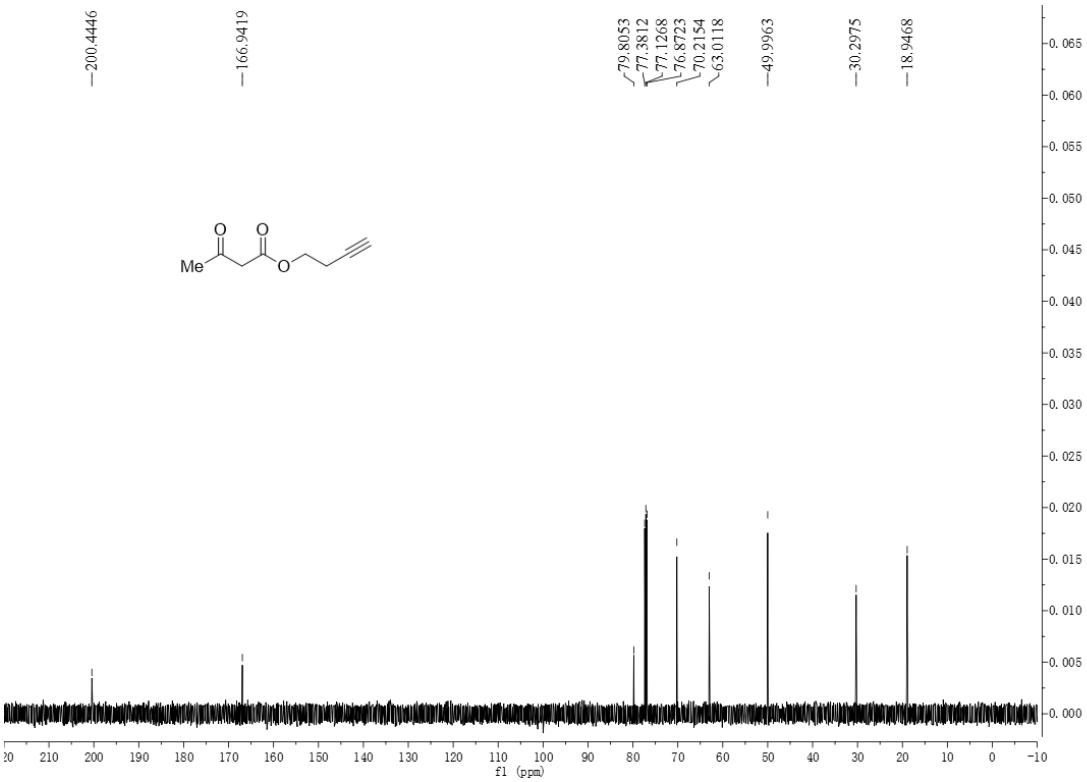
^{1}H and ^{13}C spectra of starting materials, pyrroles 4-17

But-3-yn-1-yl 3-oxobutanoate (19)

^{1}H NMR (500 MHz, $CDCl_3$)

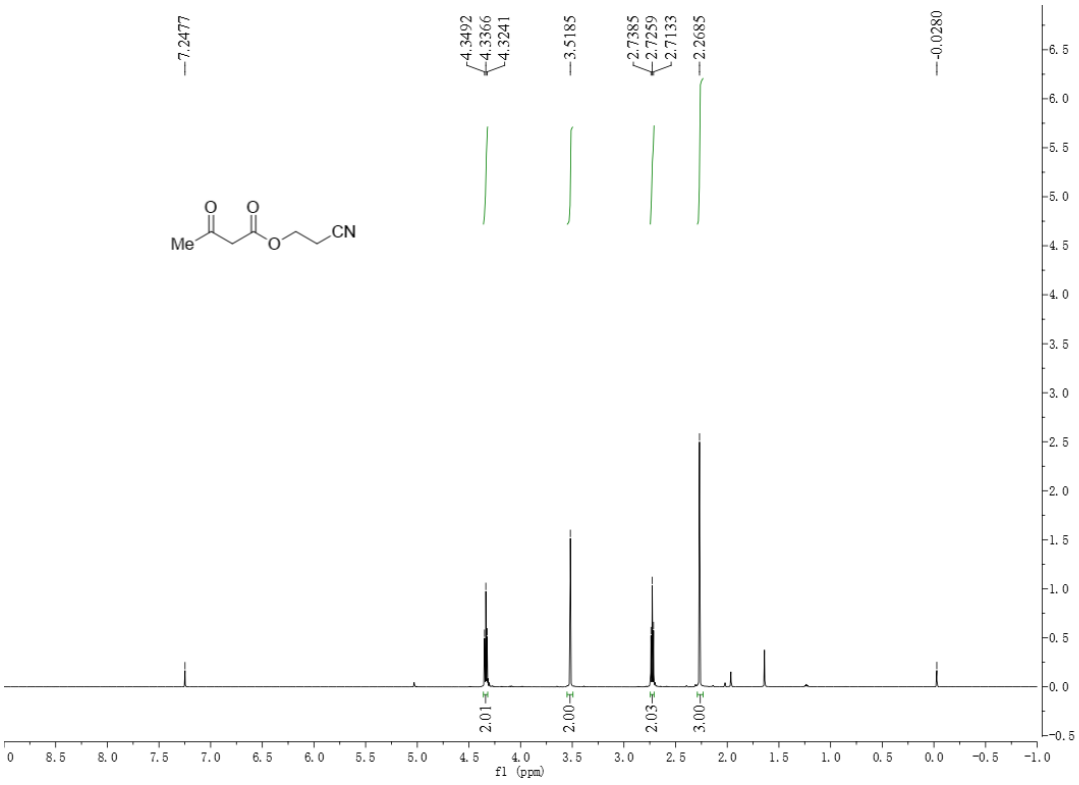


^{13}C NMR (125 MHz, $CDCl_3$)

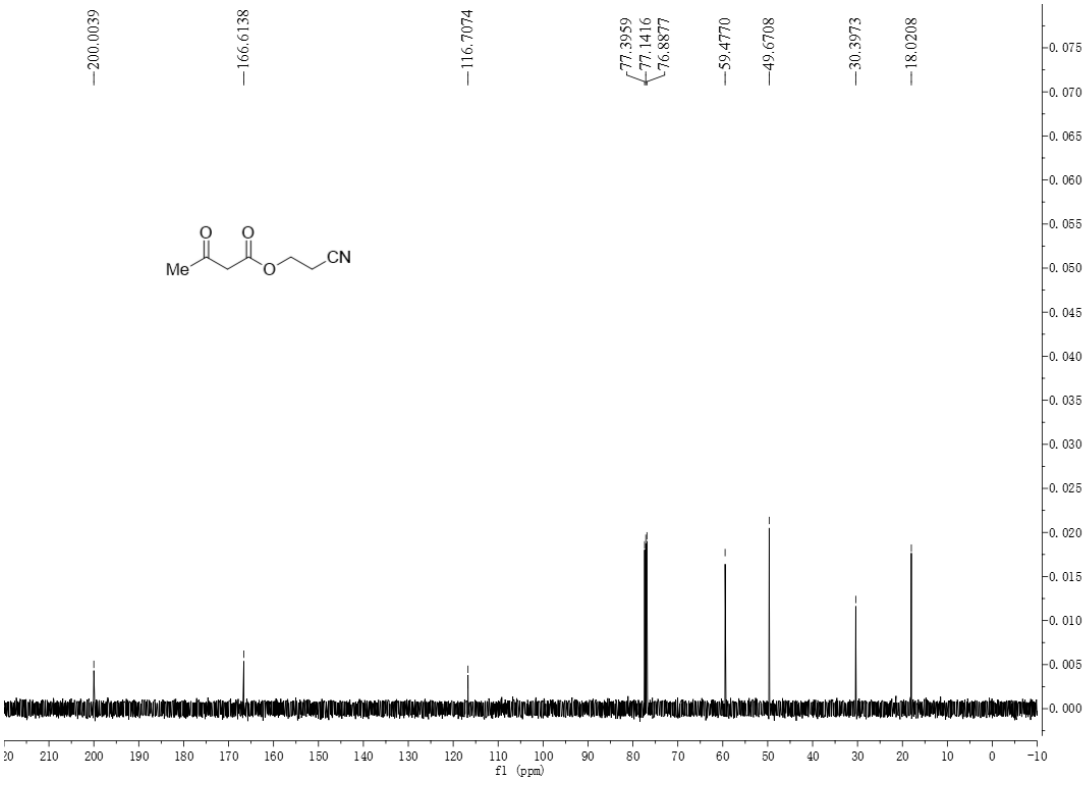


2-Cyanoethyl 3-oxobutanoate (20)

^{1}H NMR (500 MHz, $CDCl_3$)

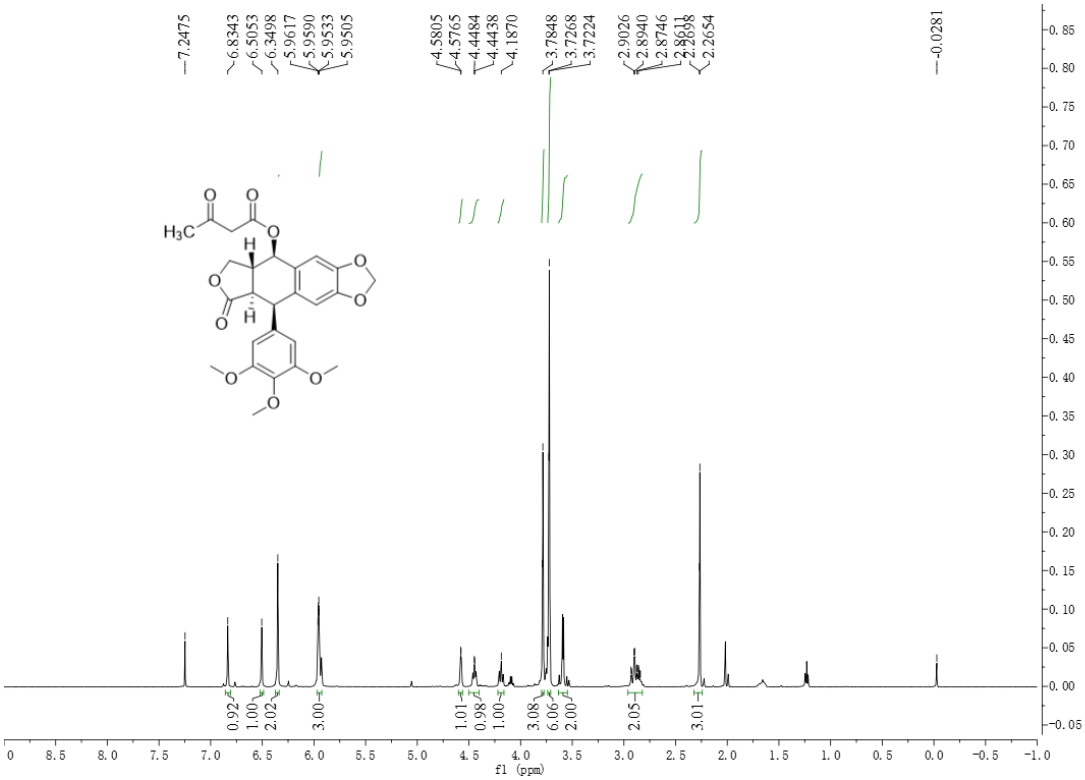


^{13}C NMR (125 MHz, $CDCl_3$)

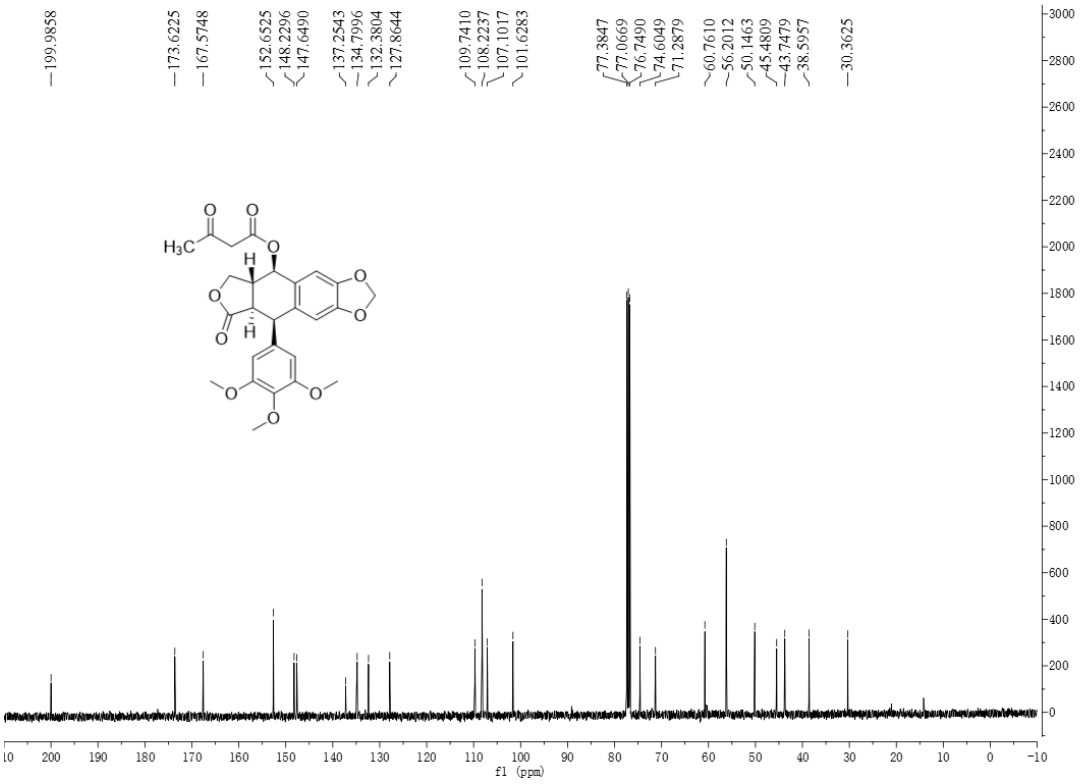


(5*R*,5a*R*,8a*R*,9*R*)-8-oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7] naphtho[2,3-*d*][1,3]dioxol-5-yl 3-oxobutanoate (23)

^{1}H NMR (500 MHz, $CDCl_3$)

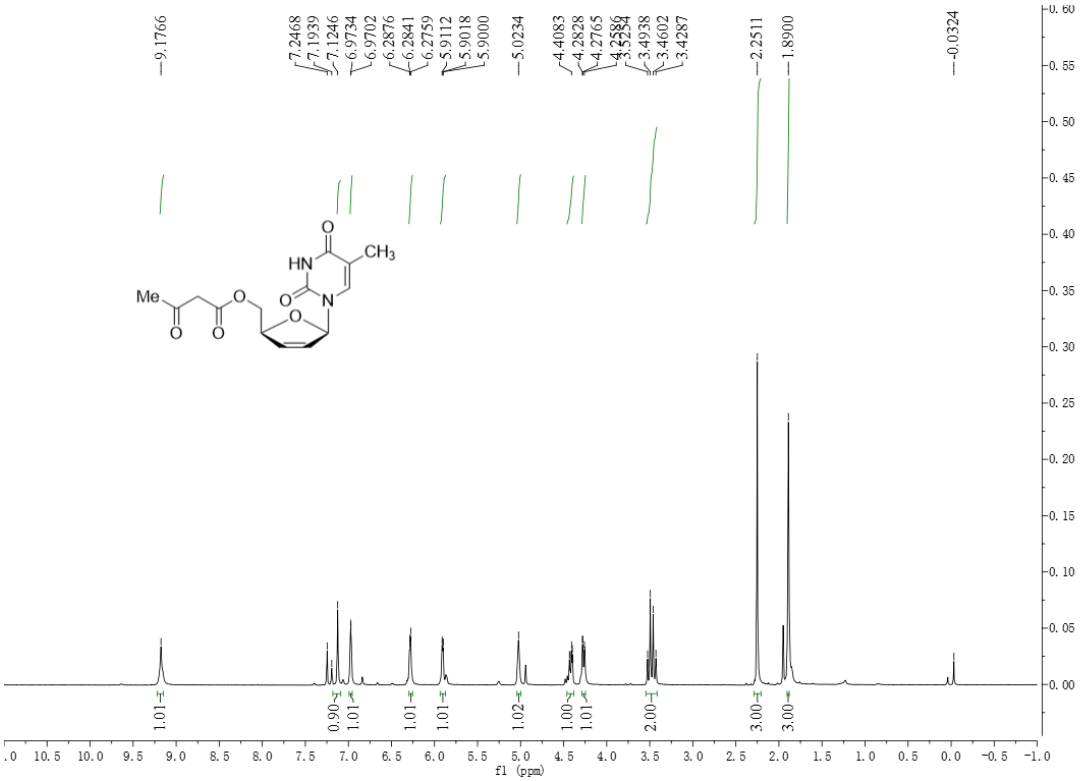


^{13}C NMR (101 MHz, $CDCl_3$)

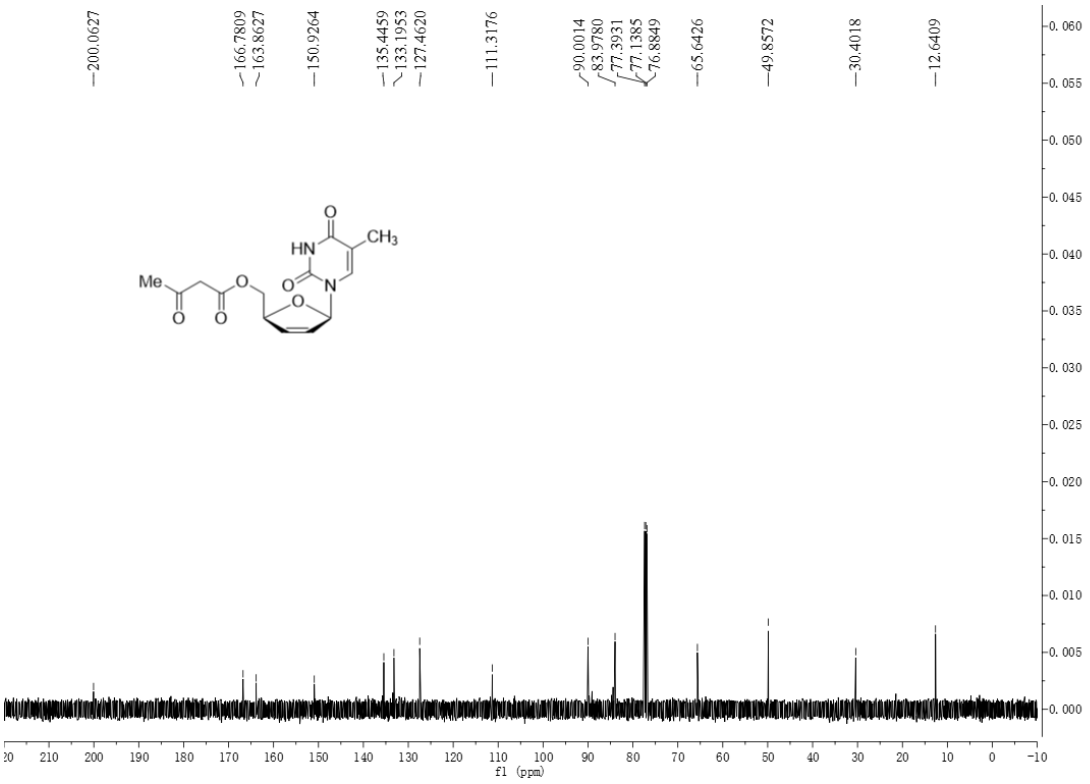


((2*S*,5*R*)-5-(5-Methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl 3-oxobutanoate (25)

^{1}H NMR (500 MHz, $CDCl_3$)

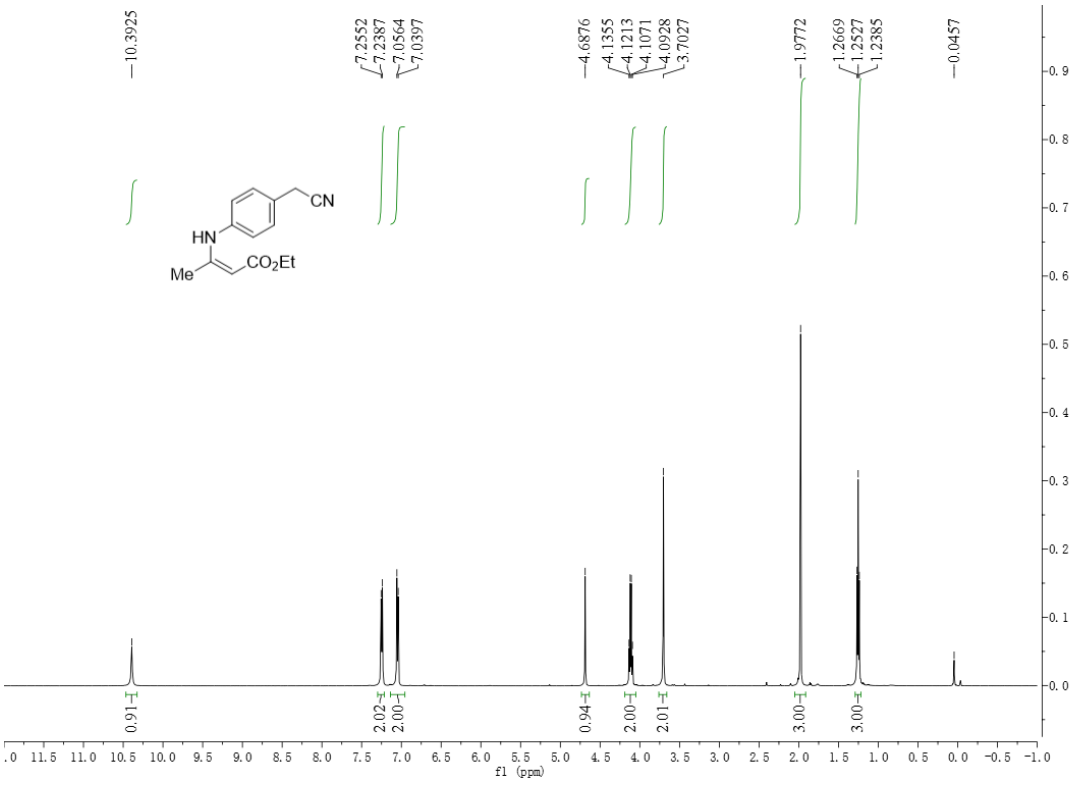


^{13}C NMR (101 MHz, $CDCl_3$)

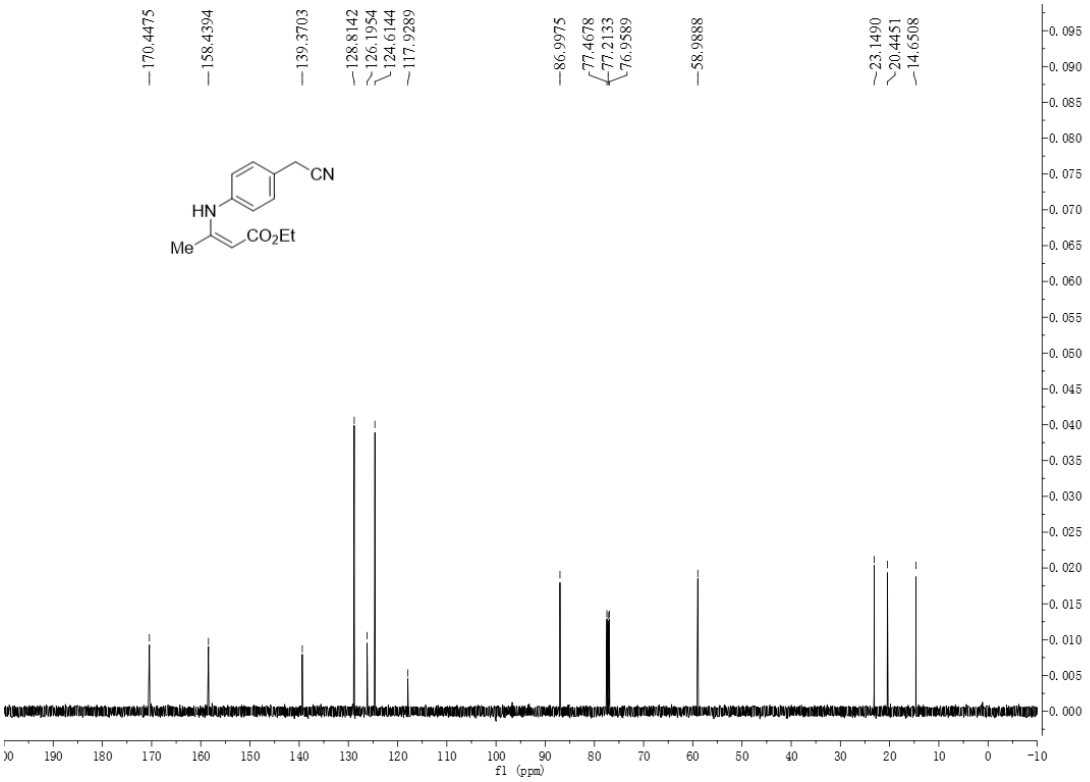


Ethyl (*Z*)-3-((4-(cyanomethyl)phenyl)amino)but-2-enoate (9)

^{1}H NMR (500 MHz, $CDCl_3$)

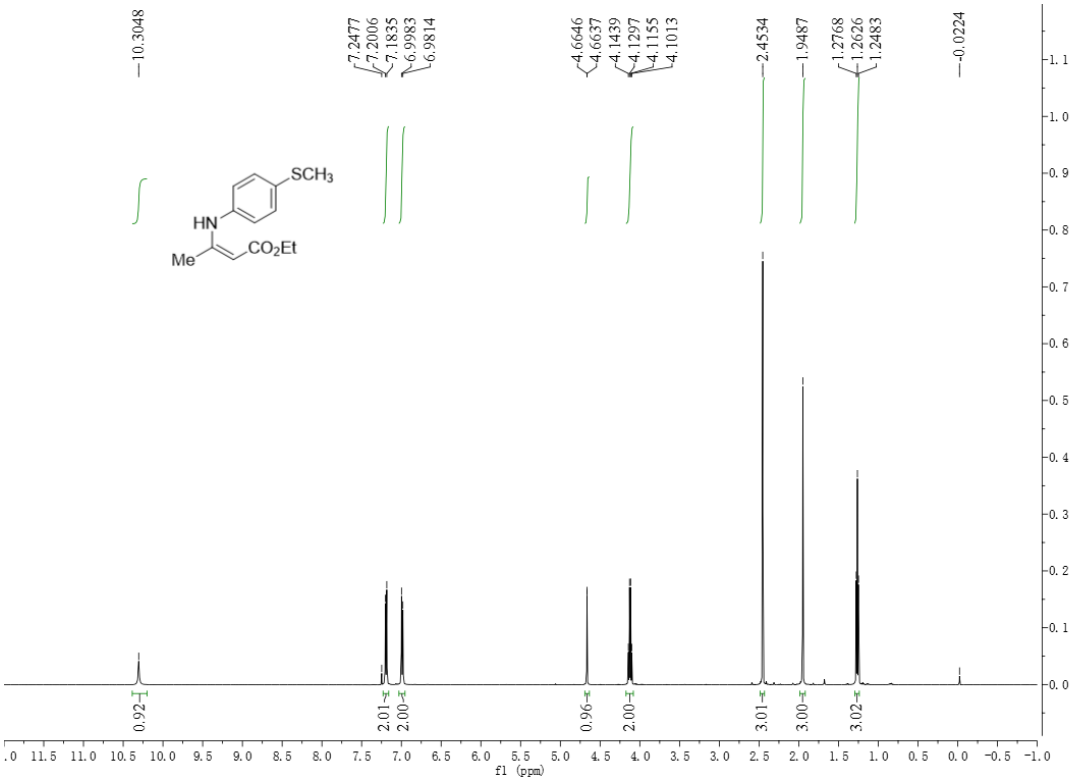


^{13}C NMR (125 MHz, $CDCl_3$)

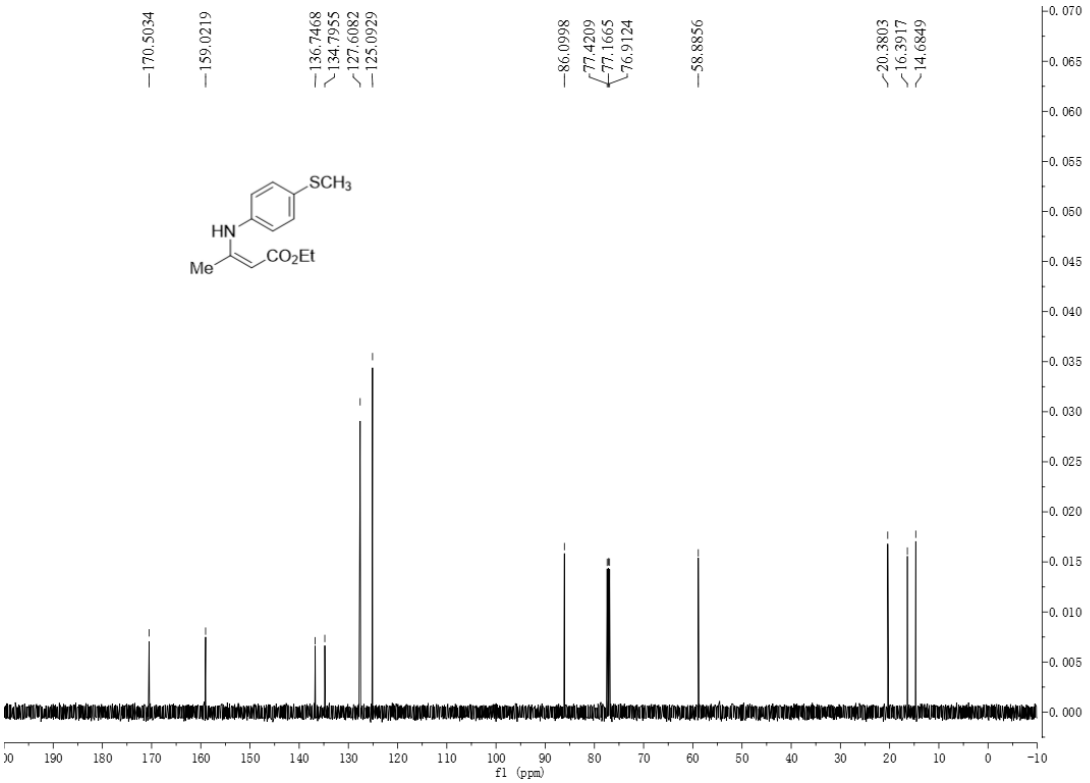


Ethyl (*Z*)-3-((4-(methylthio)phenyl)amino)but-2-enoate (10)

^{1}H NMR (500 MHz, $CDCl_3$)

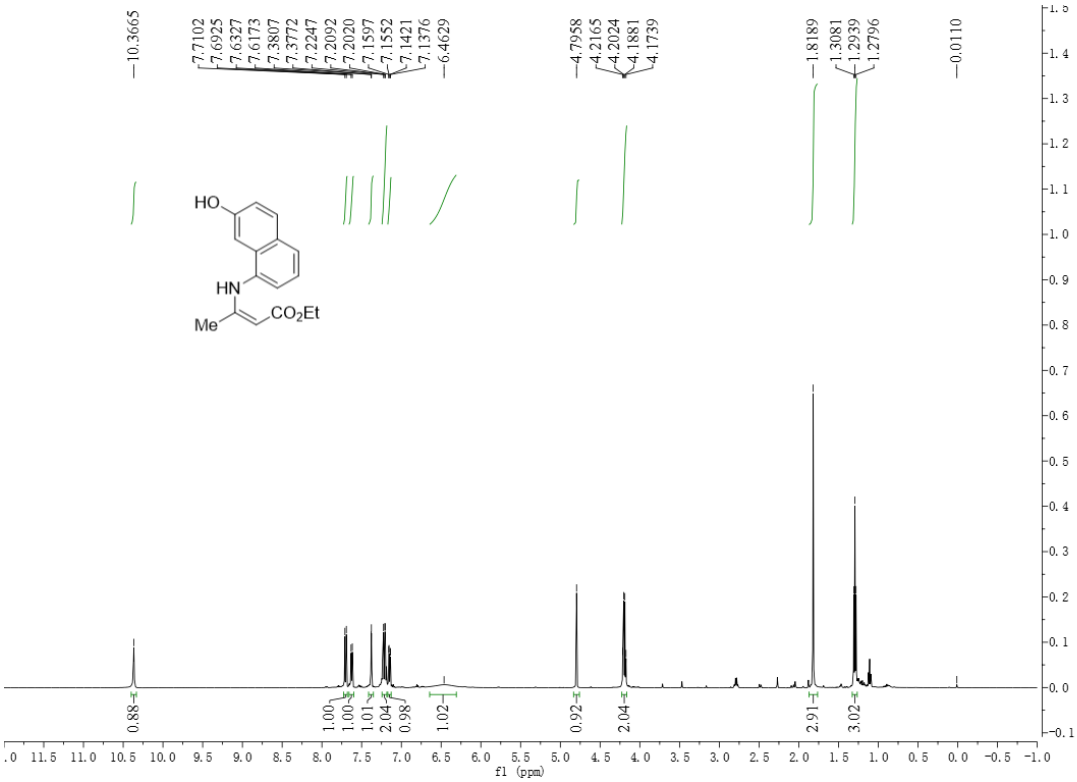


^{13}C NMR (125 MHz, $CDCl_3$)

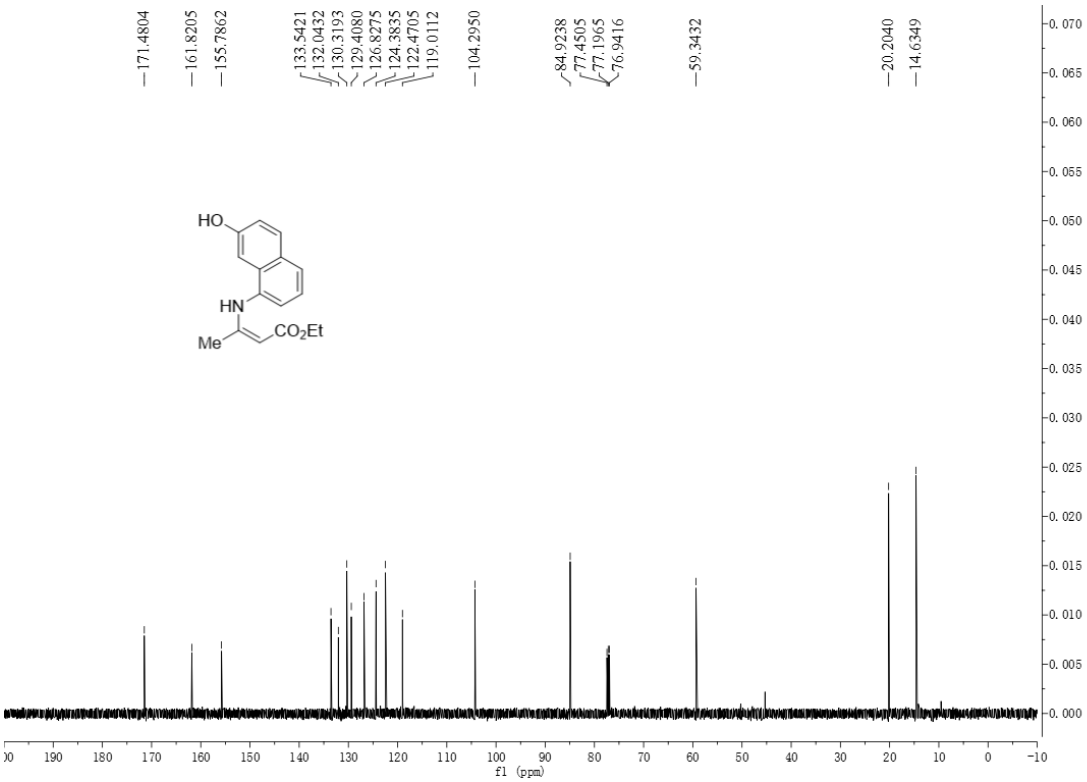


Ethyl (*Z*)-3-((7-hydroxynaphthalen-1-yl)amino)but-2-enoate (14)

^{1}H NMR (500 MHz, $CDCl_3$)

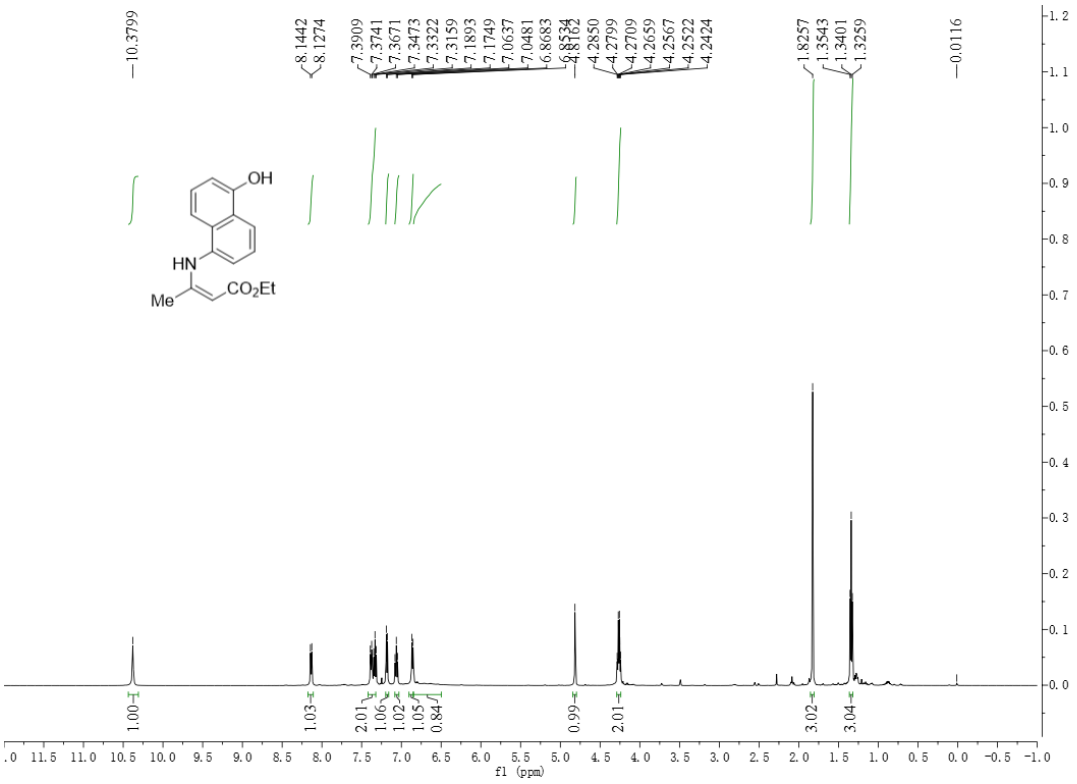


^{13}C NMR (125 MHz, $CDCl_3$)

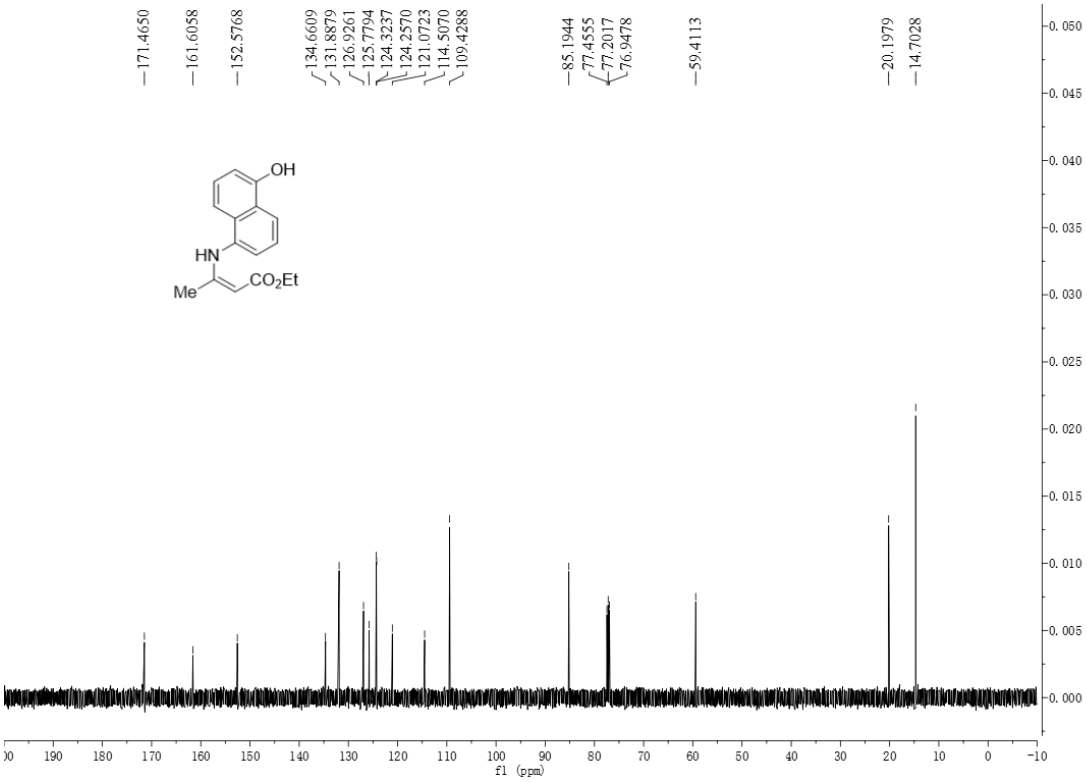


Ethyl (*Z*)-3-((5-hydroxynaphthalen-1-yl)amino)but-2-enoate (15)

^{1}H NMR (500 MHz, $CDCl_3$)

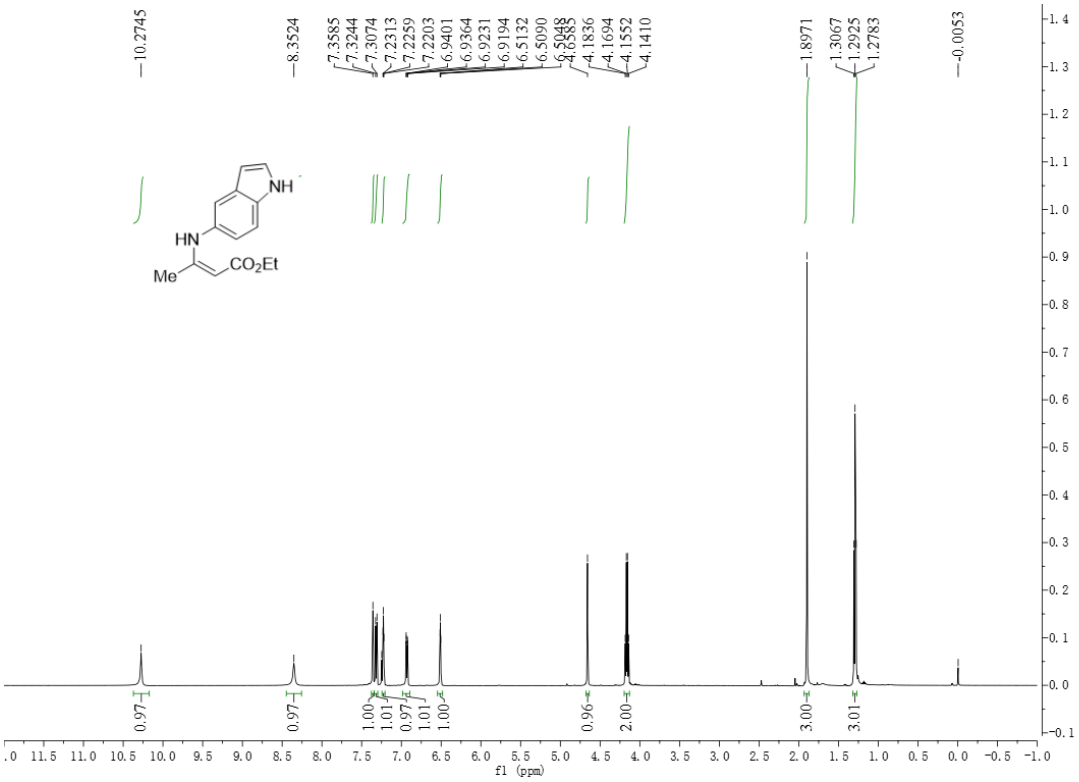


^{13}C NMR (125 MHz, $CDCl_3$)

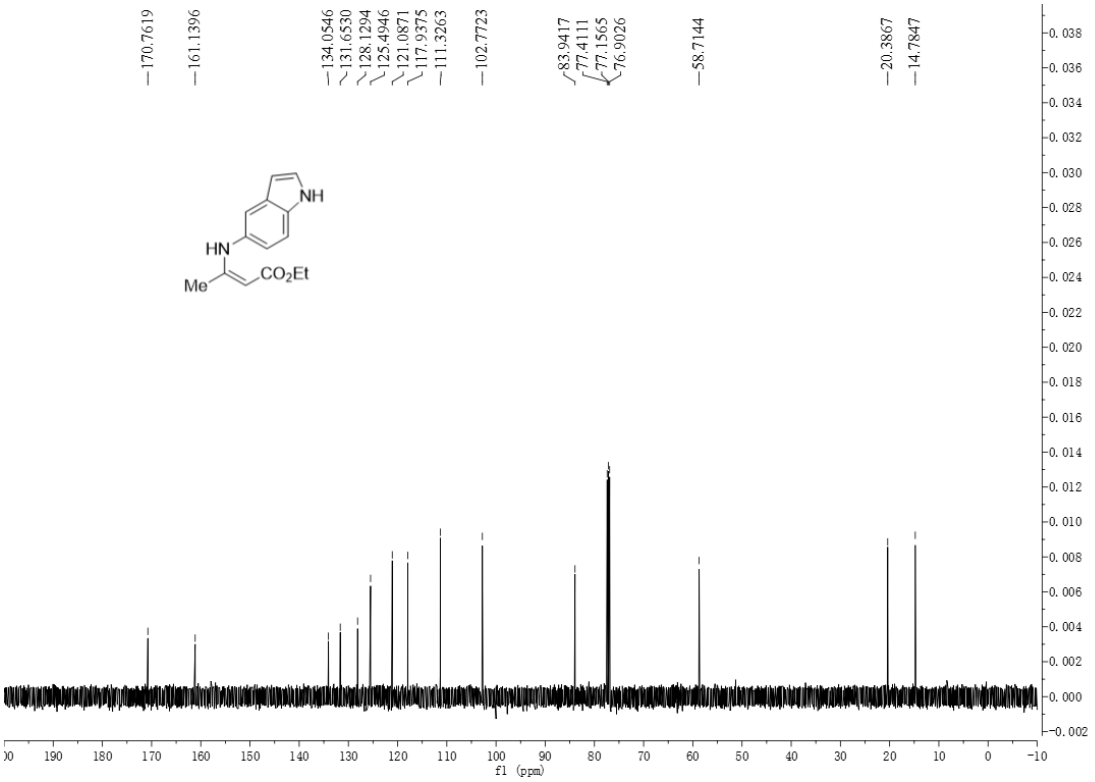


Ethyl (*Z*)-3-((1H-indol-5-yl)amino)but-2-enoate (16)

^{1}H NMR (500 MHz, $CDCl_3$)

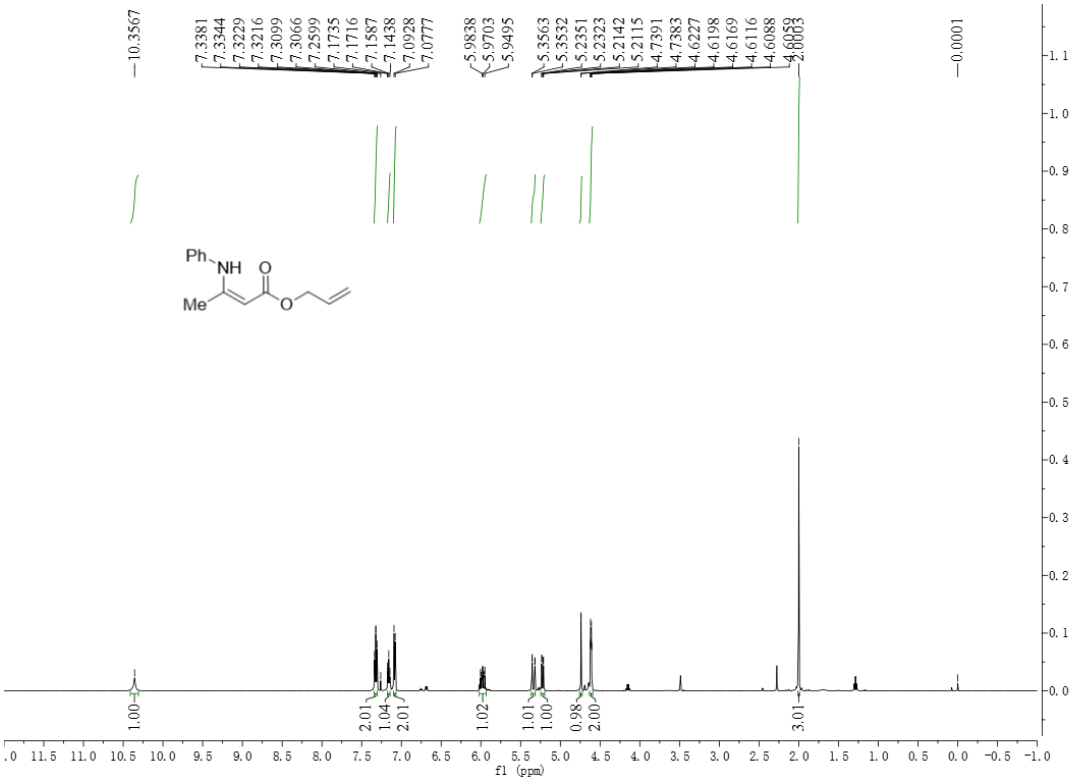


^{13}C NMR (125 MHz, $CDCl_3$)

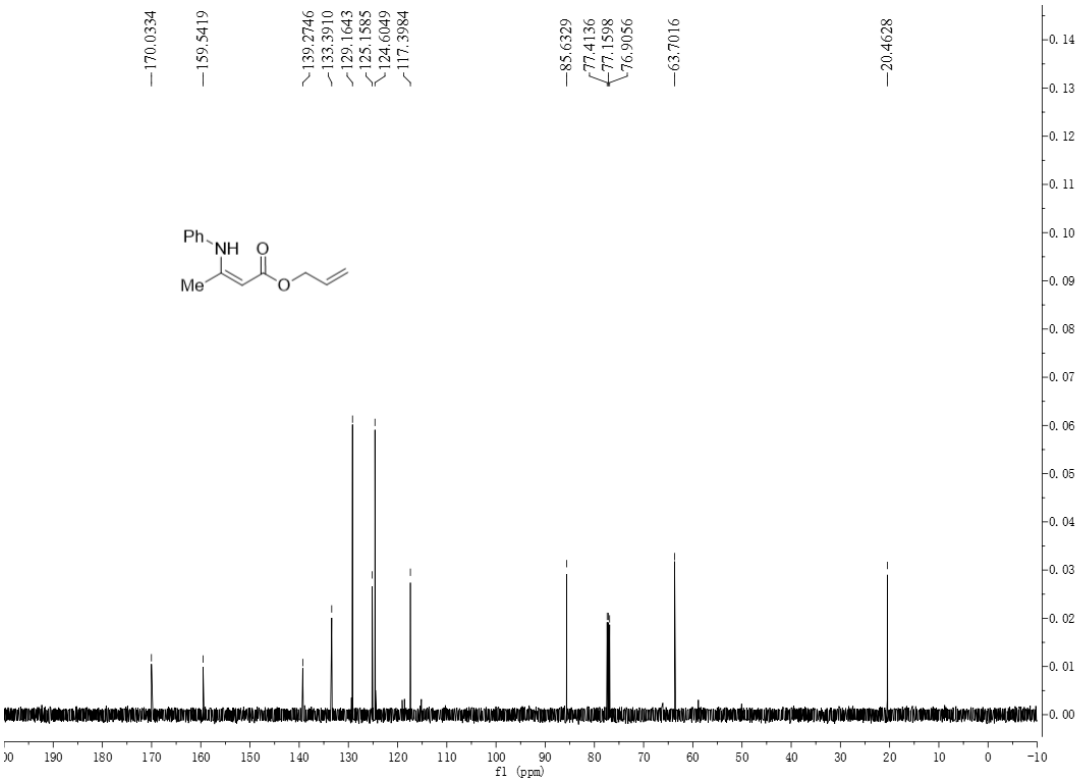


Allyl (*Z*)-3-(phenylamino)but-2-enoate (24)

^{1}H NMR (500 MHz, $CDCl_3$)

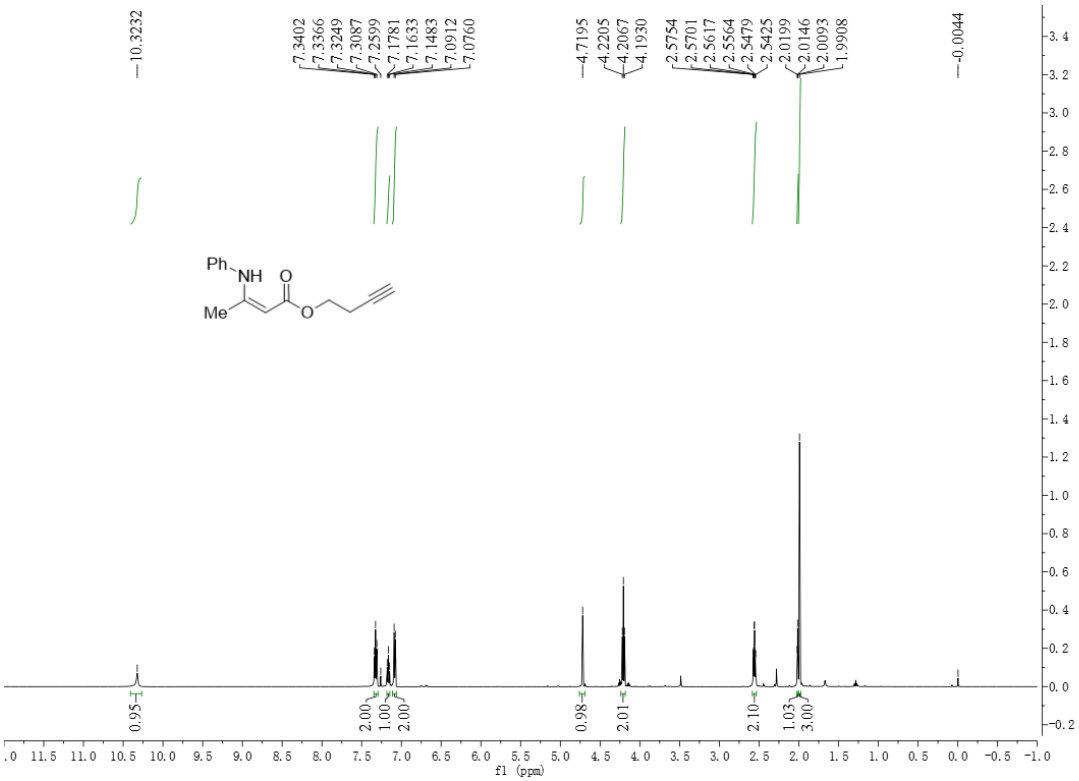


^{13}C NMR (125 MHz, $CDCl_3$)

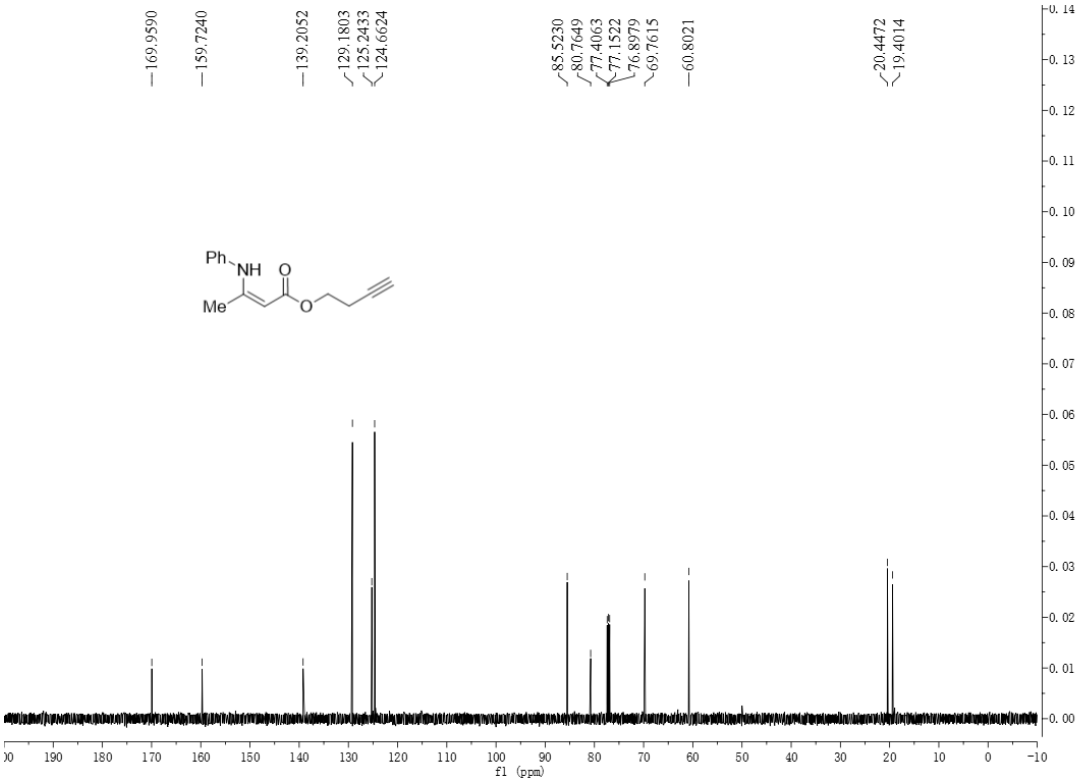


But-3-yn-1-yl (*Z*)-3-(phenylamino)but-2-enoate (25)

^{1}H NMR (500 MHz, $CDCl_3$)

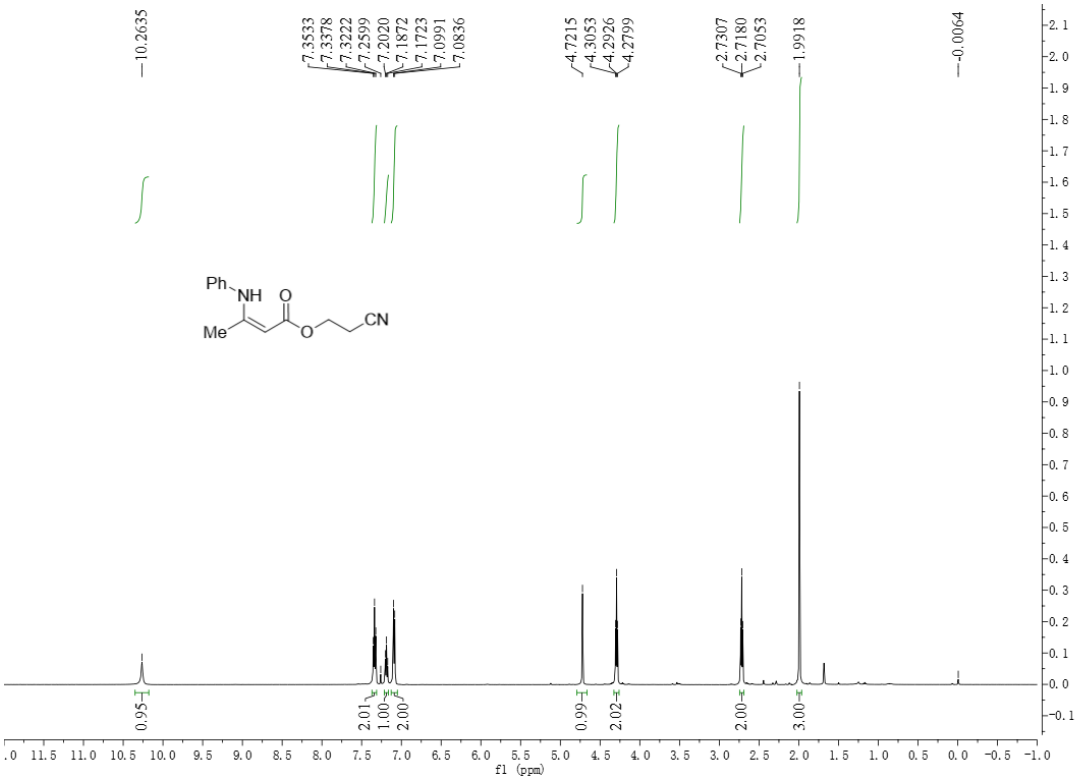


^{13}C NMR (125 MHz, $CDCl_3$)

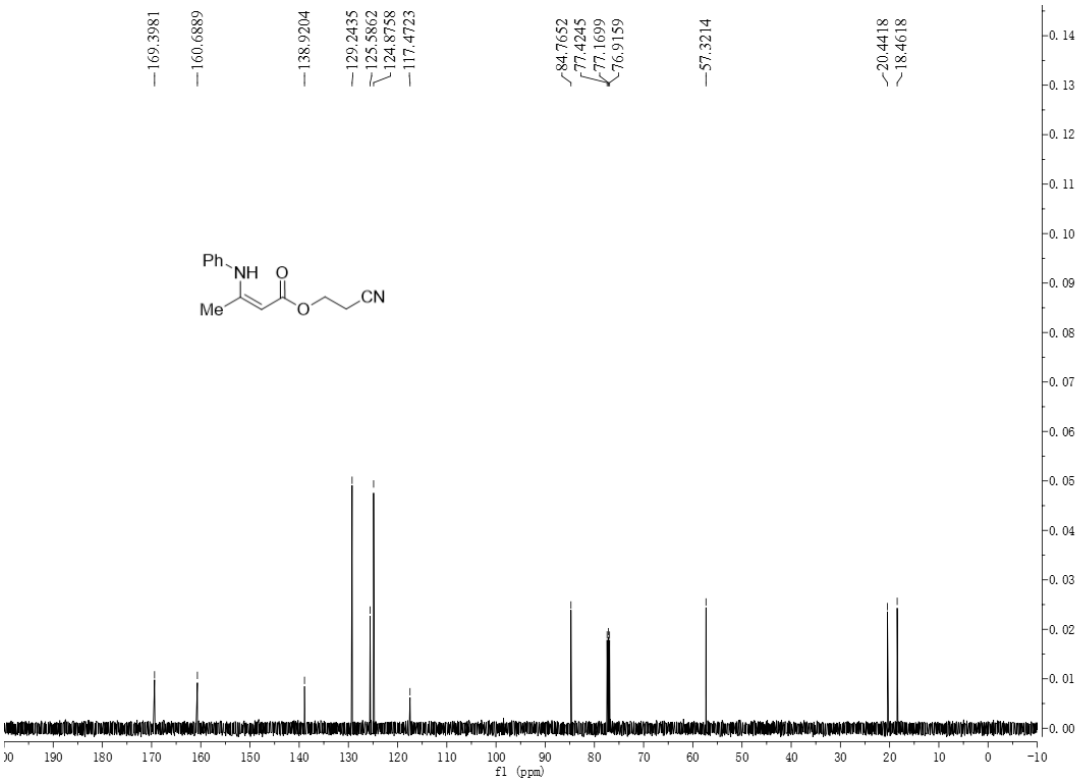


2-Cyanoethyl (*Z*)-3-(phenylamino)but-2-enoate (26)

^{1}H NMR (500 MHz, $CDCl_3$)

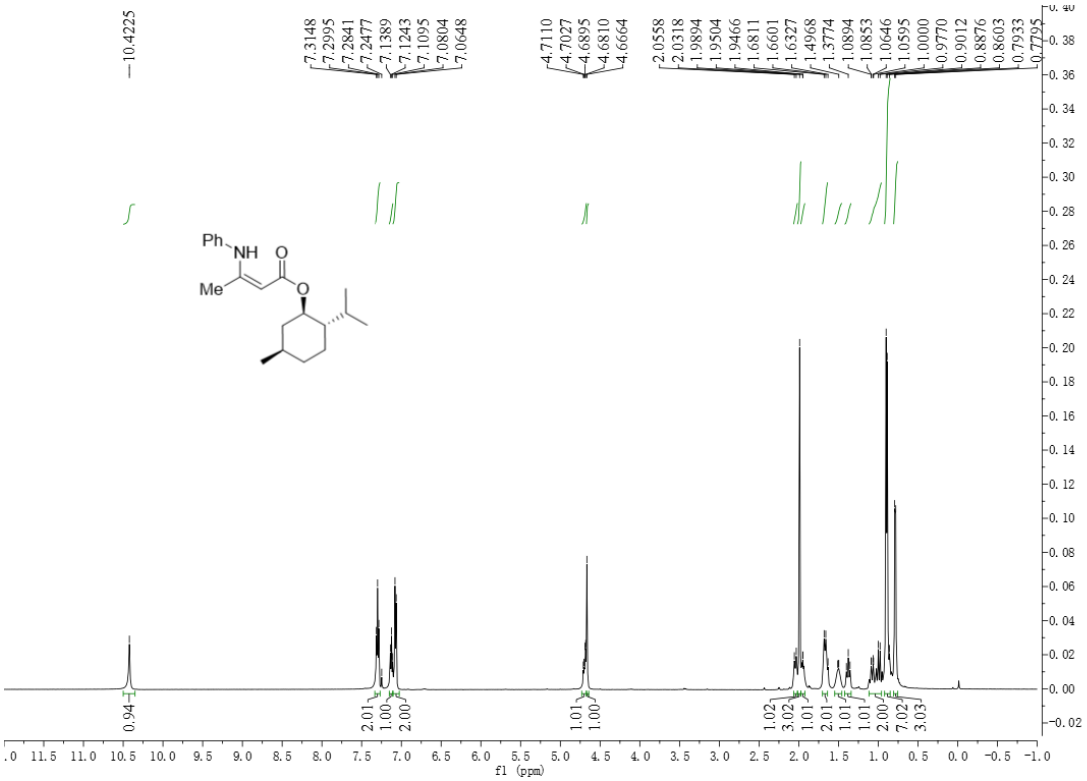


^{13}C NMR (125 MHz, $CDCl_3$)

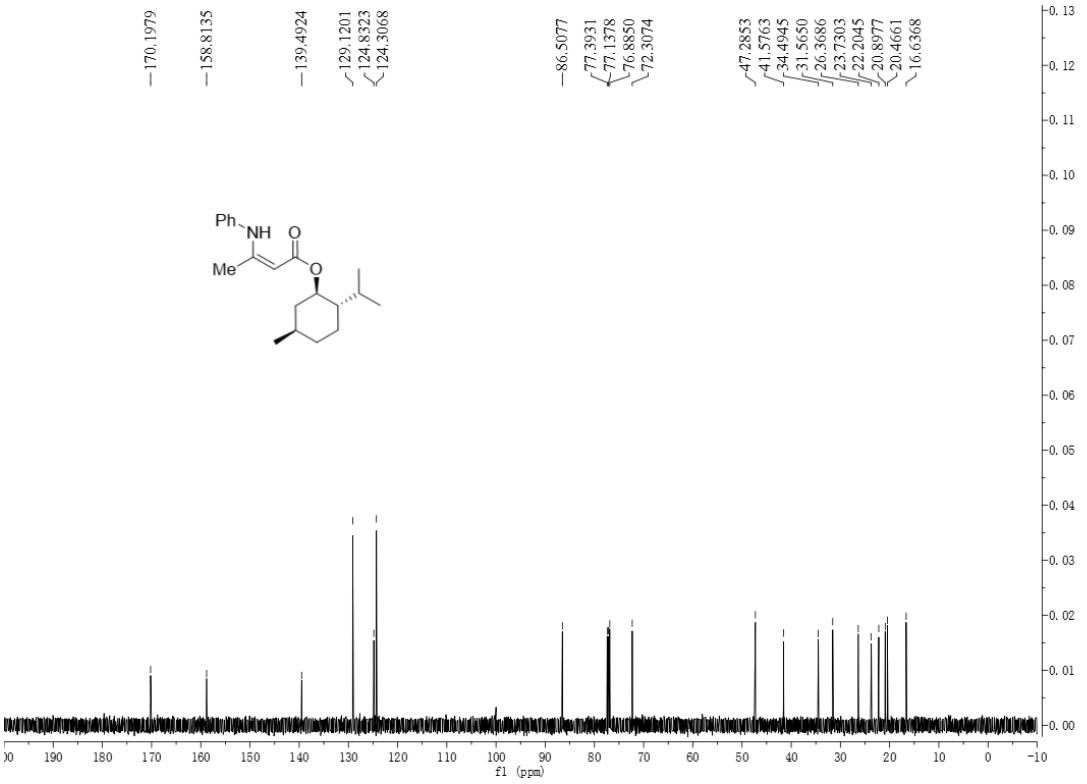


(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl (*Z*)-3-(phenylamino)but-2-enoate (27)

^{1}H NMR (500 MHz, $CDCl_3$)

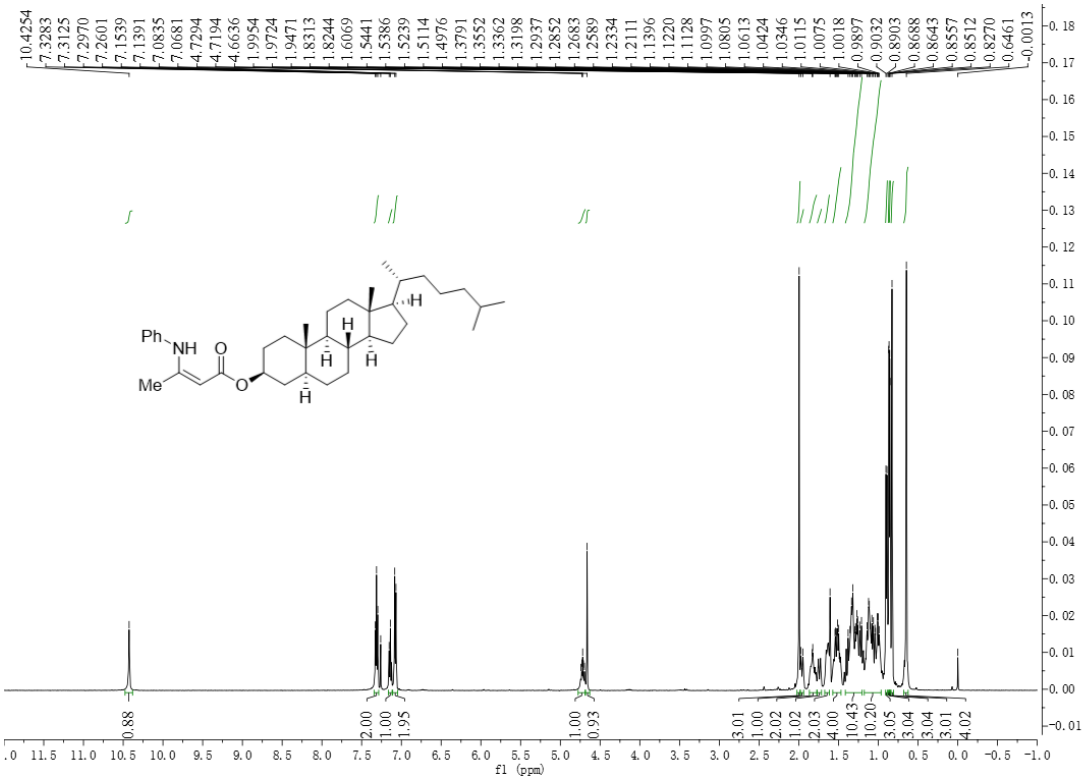


^{13}C NMR (125 MHz, $CDCl_3$)

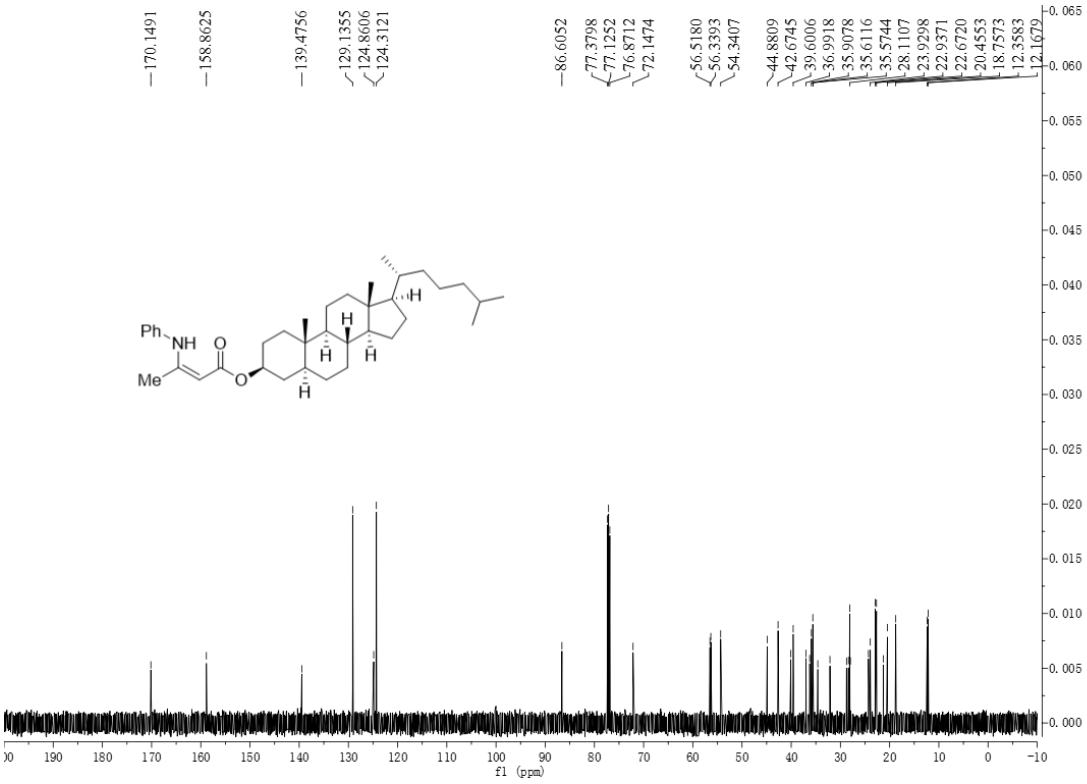


(3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl (*Z*)-3-(phenylamino)but-2-enoate (28)

^{1}H NMR (500 MHz, $CDCl_3$)

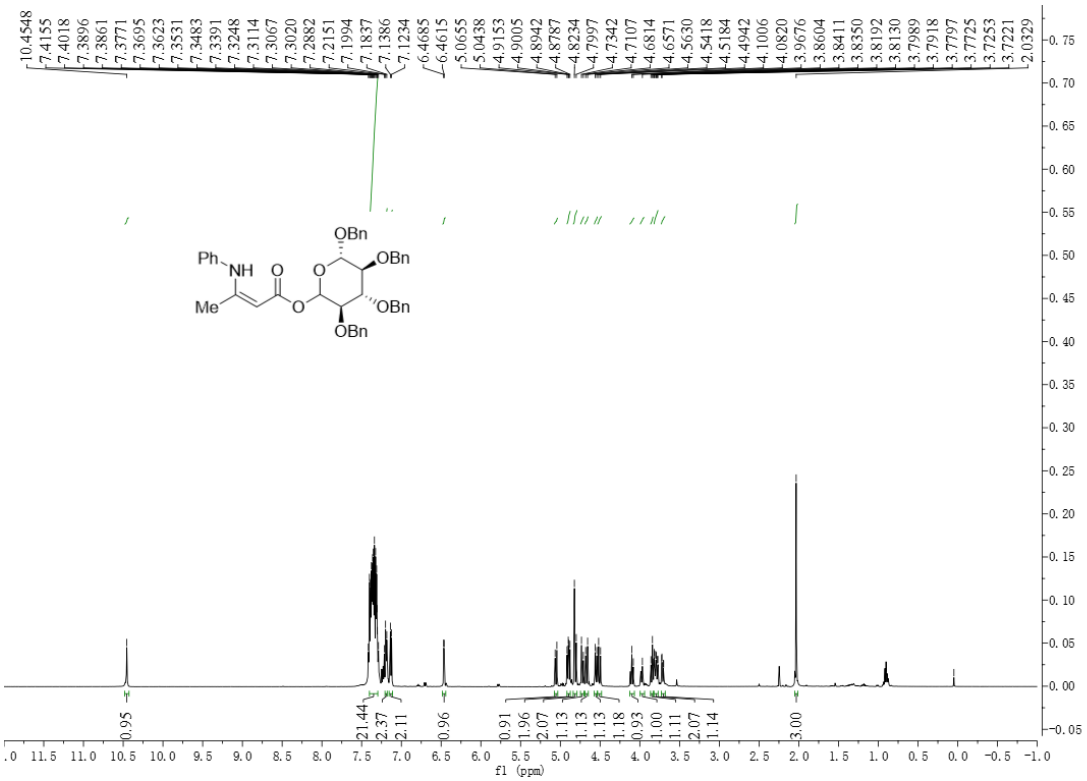


^{13}C NMR (125 MHz, $CDCl_3$)

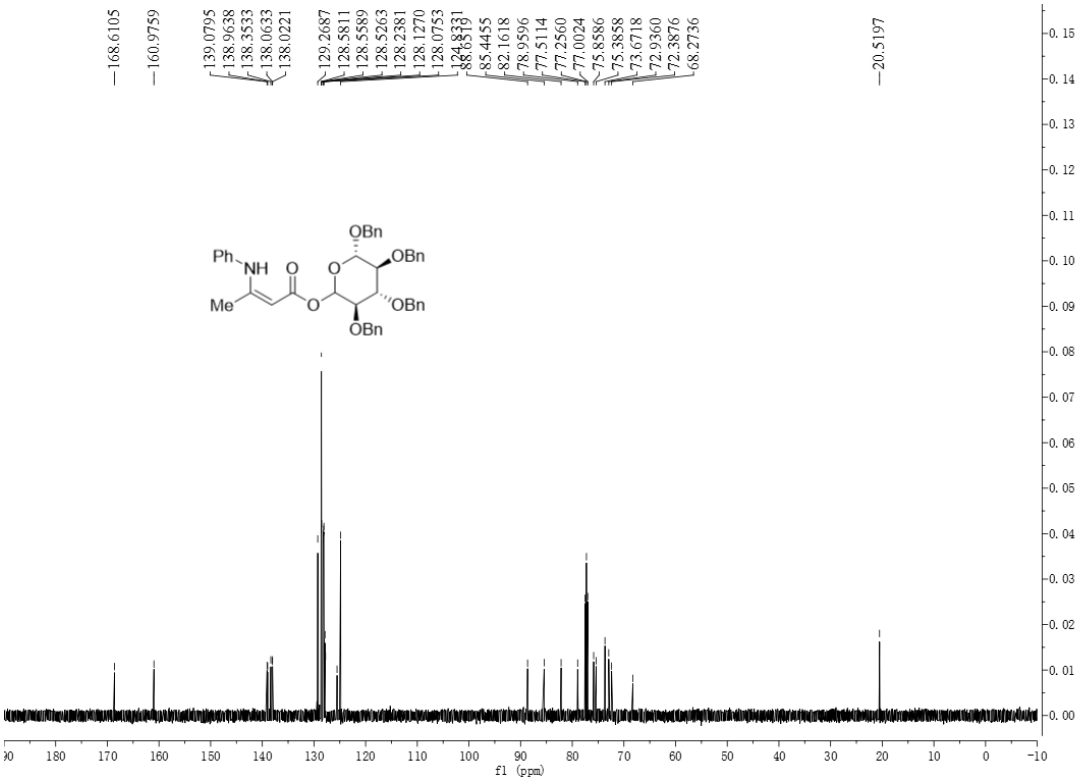


(3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl (*Z*)-3-(phenylamino)but-2-enoate (29)

^{1}H NMR (500 MHz, $CDCl_3$)

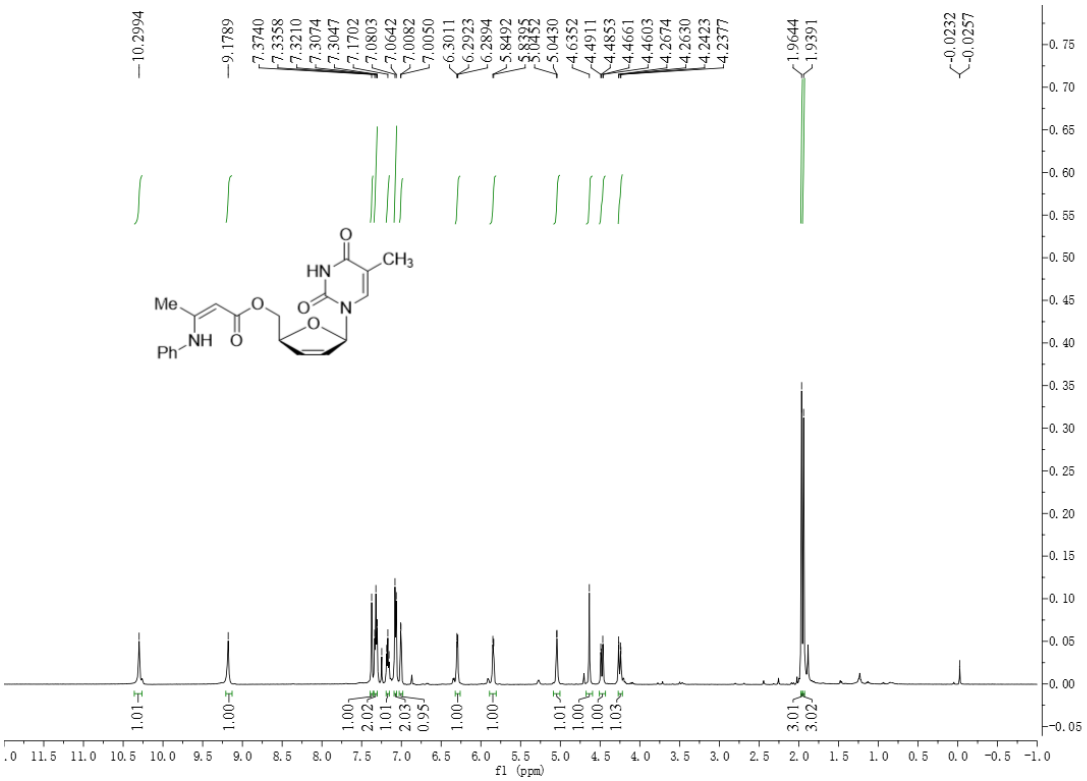


^{13}C NMR (125 MHz, $CDCl_3$)

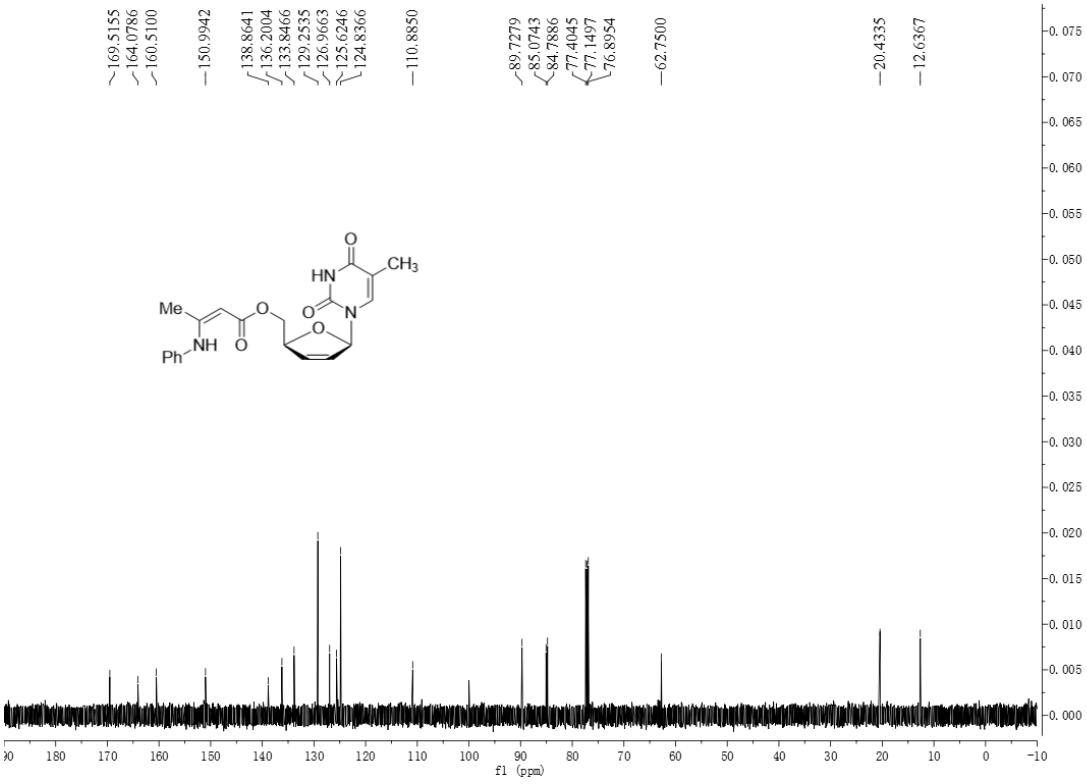


((2*S*,5*R*)-5-(5-Methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl (*Z*)-3-(phenylamino)but-2-enoate (30)

^{1}H NMR (500 MHz, $CDCl_3$)

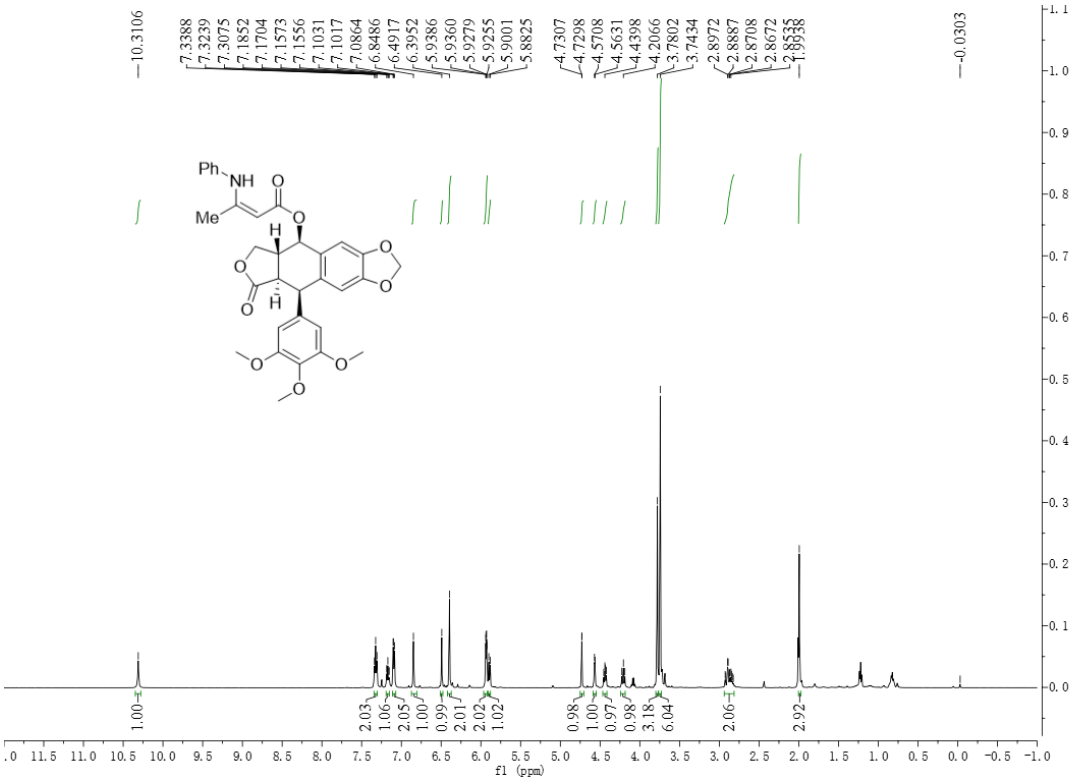


^{13}C NMR (125 MHz, $CDCl_3$)

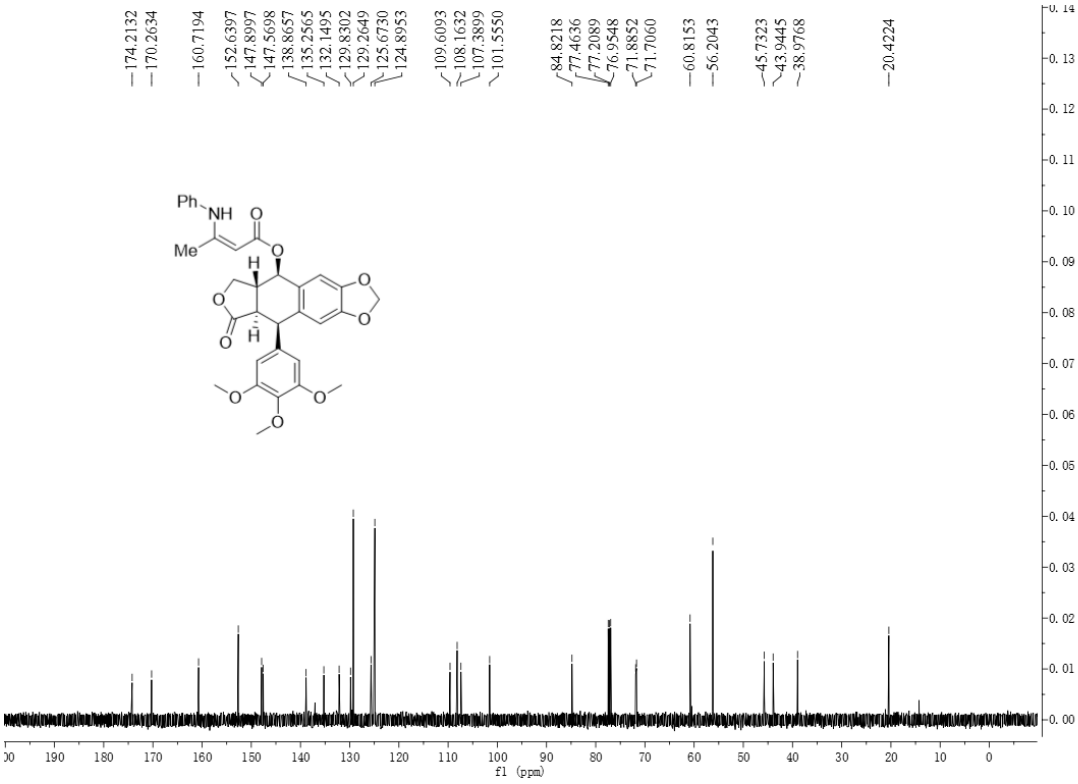


(5*R*,5a*R*,8a*R*,9*R*)-8-oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro[3',4':6,7] naphtho[2,3-*d*][1,3]dioxol-5-yl (*Z*)-3-(phenylamino)but-2-enoate (31)

^{1}H NMR (500 MHz, $CDCl_3$)

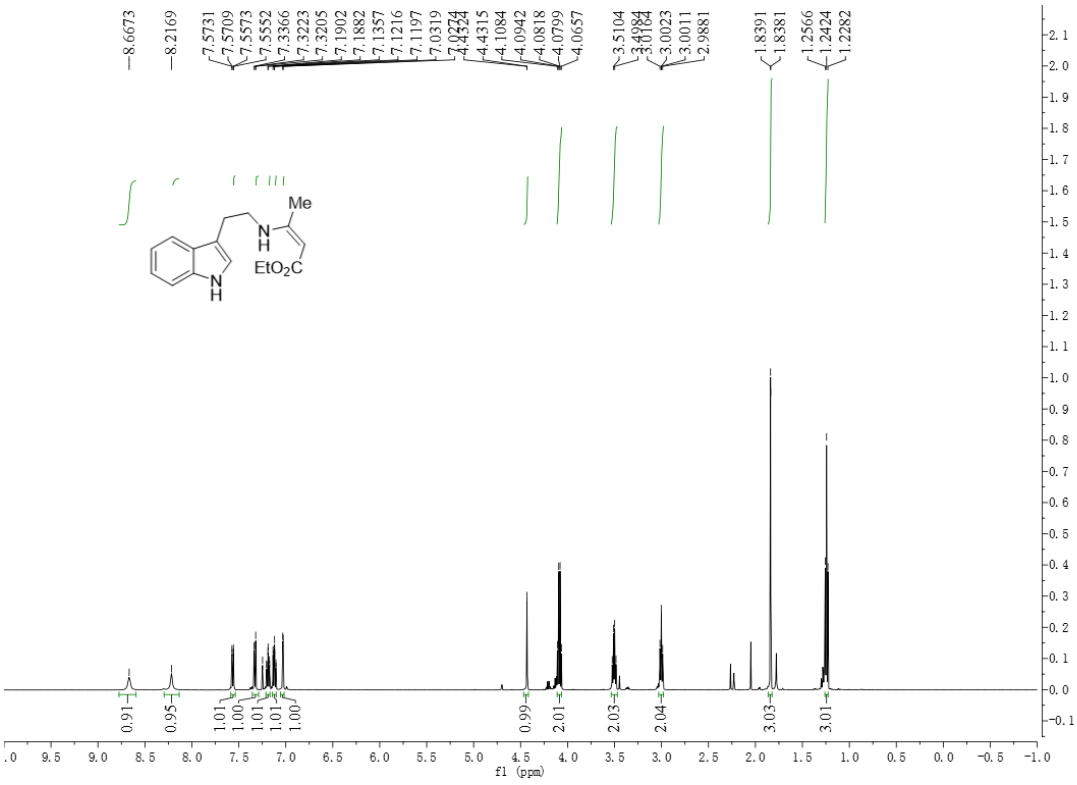


^{13}C NMR (125 MHz, $CDCl_3$)

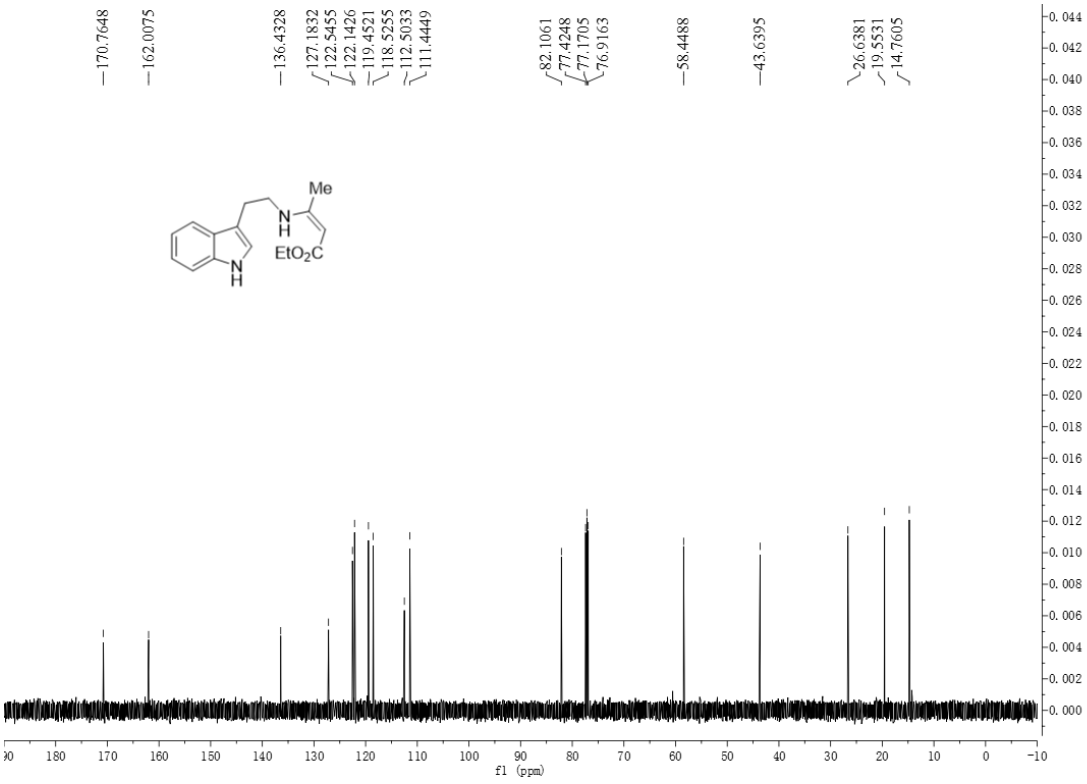


Ethyl (*Z*)-3-((2-(1*H*-indol-3-yl)ethyl)amino)but-2-enoate (32)

^{1}H NMR (500 MHz, $CDCl_3$)

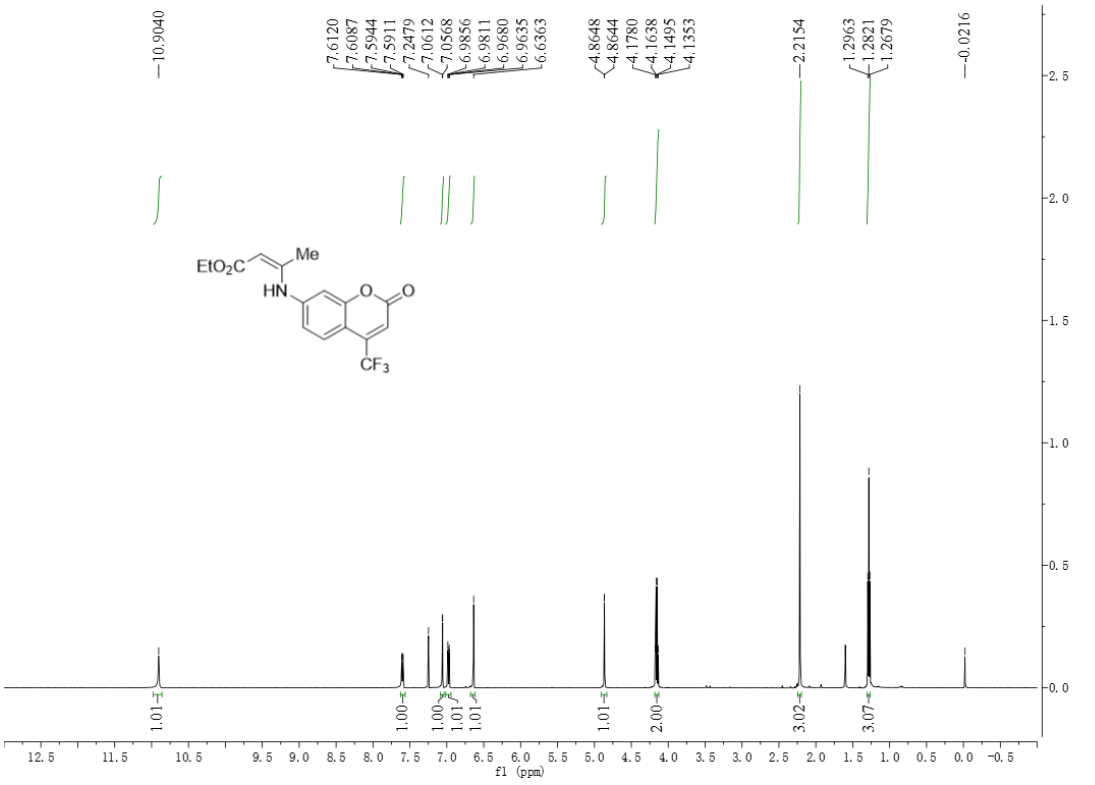


^{13}C NMR (125 MHz, $CDCl_3$)

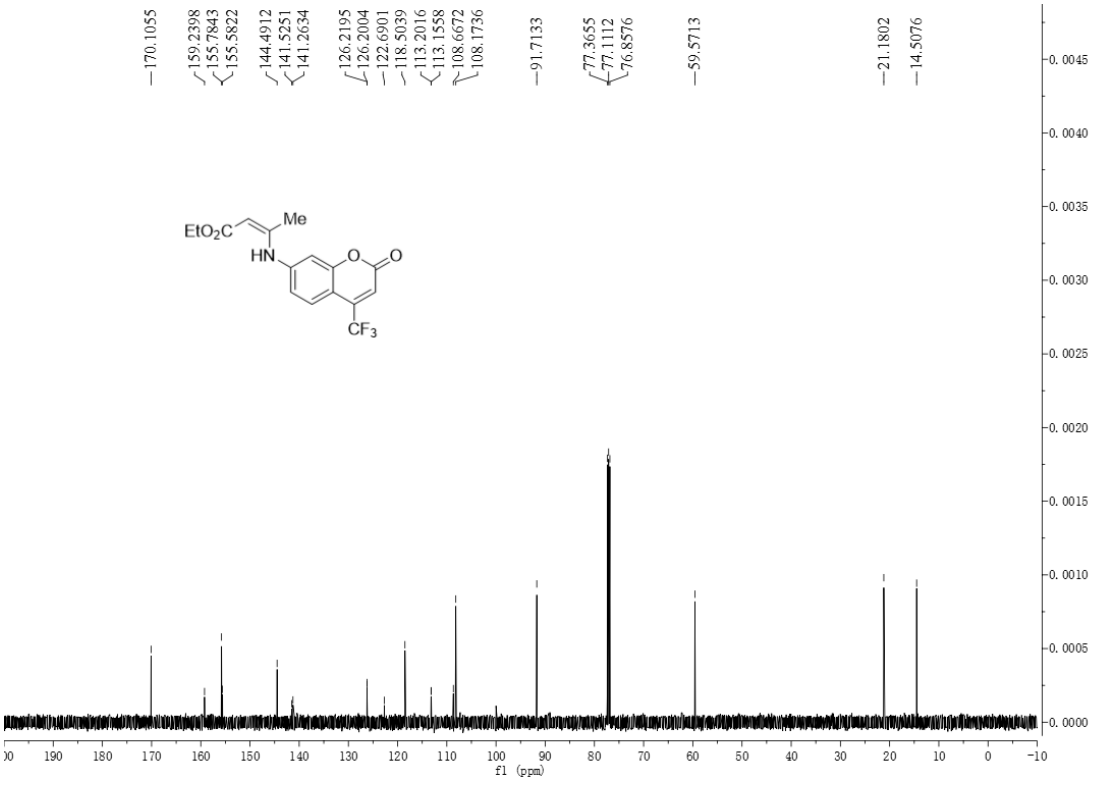


Ethyl (*Z*)-3-((2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)amino)but-2-enoate (33)

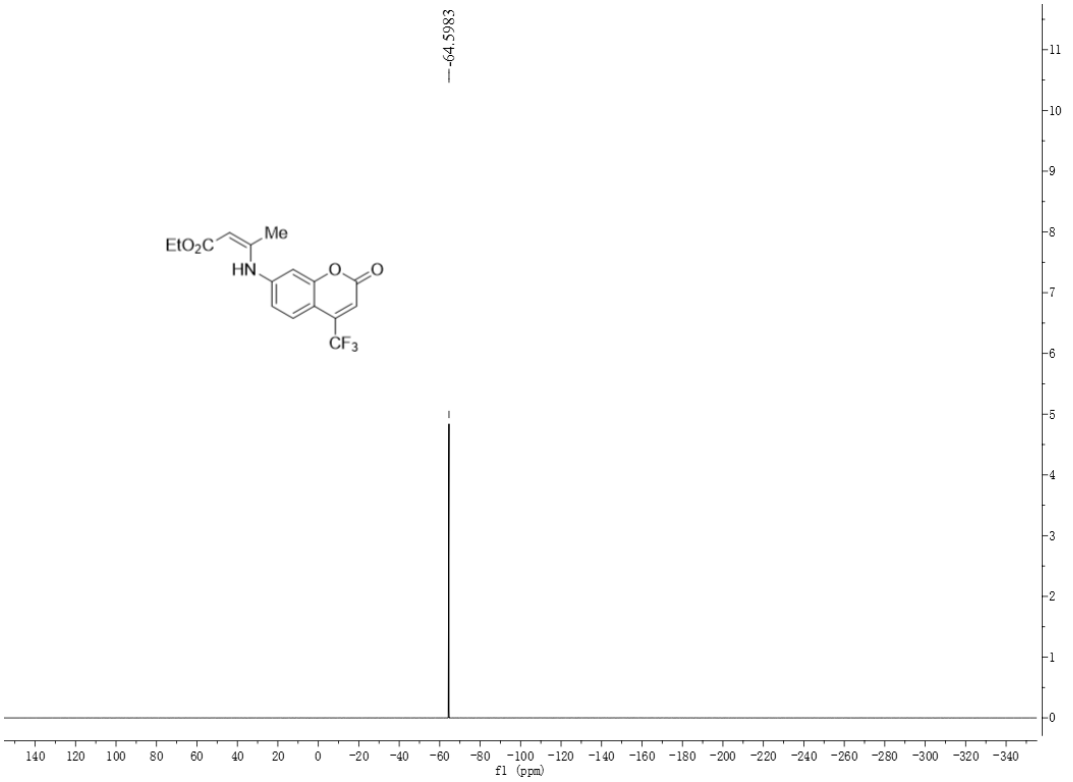
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)

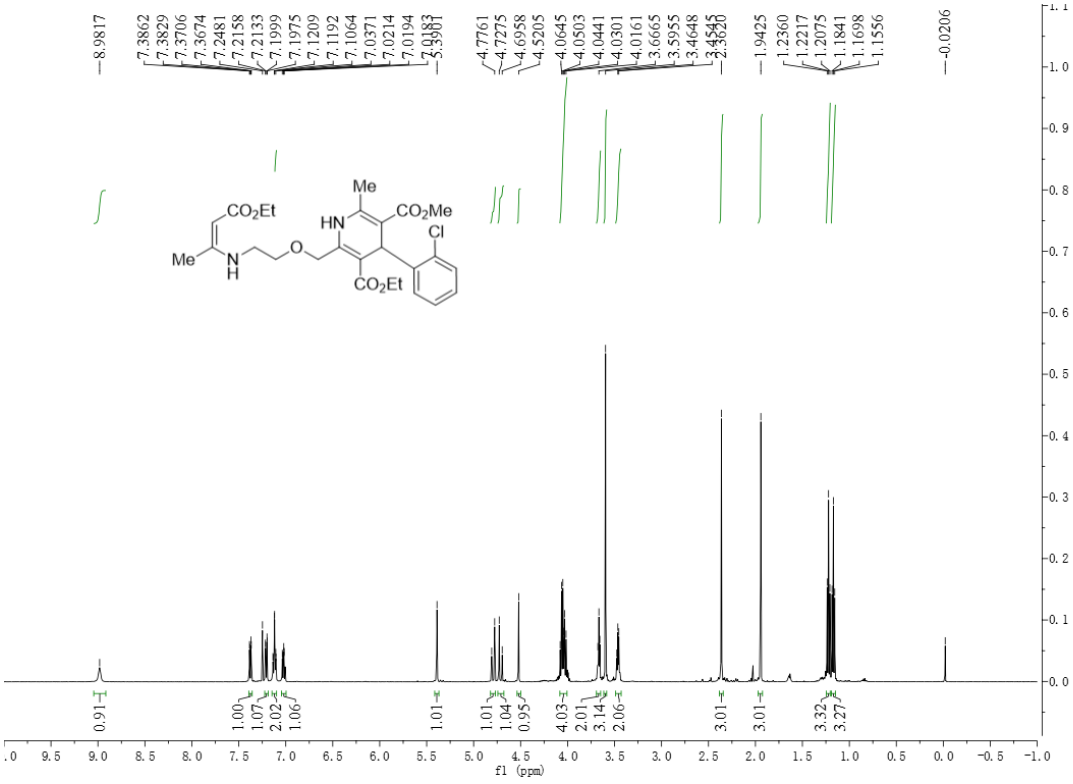


^{19}F NMR (470 MHz, $CDCl_3$)

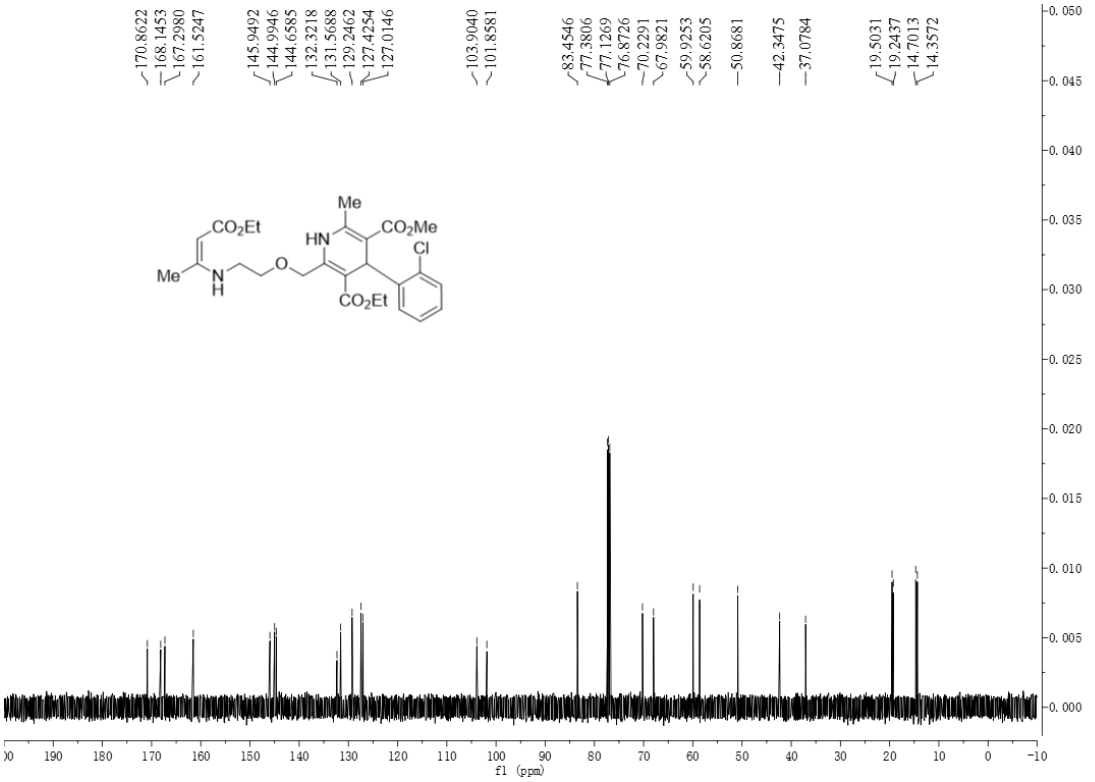


3-Ethyl 5-methyl (*Z*)-4-(2-chlorophenyl)-2-((2-((4-ethoxy-4-oxobut-2-en-2-yl)amino)ethoxy) methyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (34)

^{1}H NMR (500 MHz, $CDCl_3$)

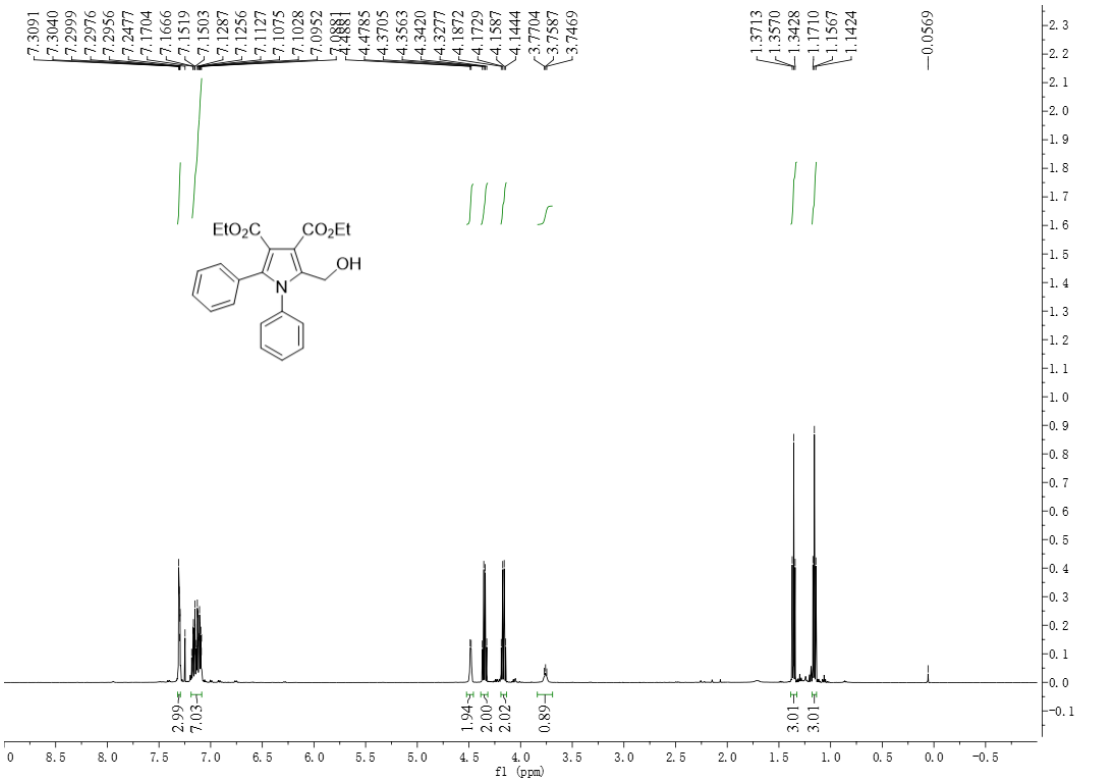


^{13}C NMR (125 MHz, $CDCl_3$)

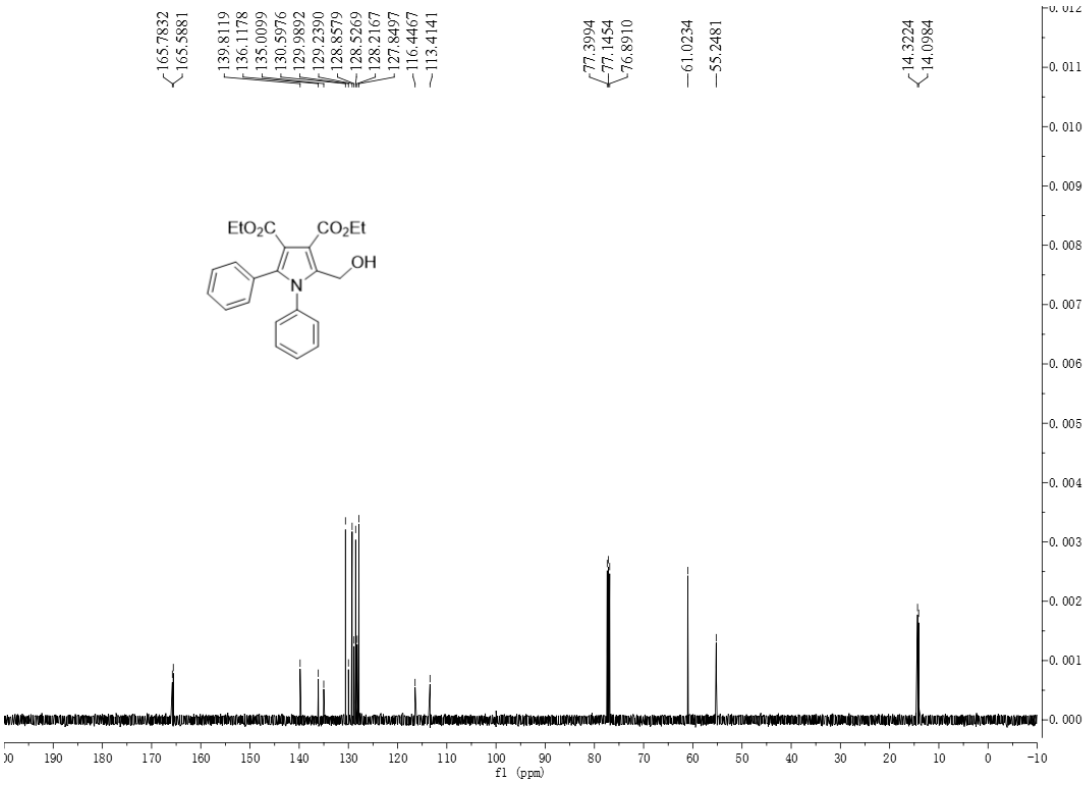


Diethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4aa)

^{1}H NMR (500 MHz, $CDCl_3$)

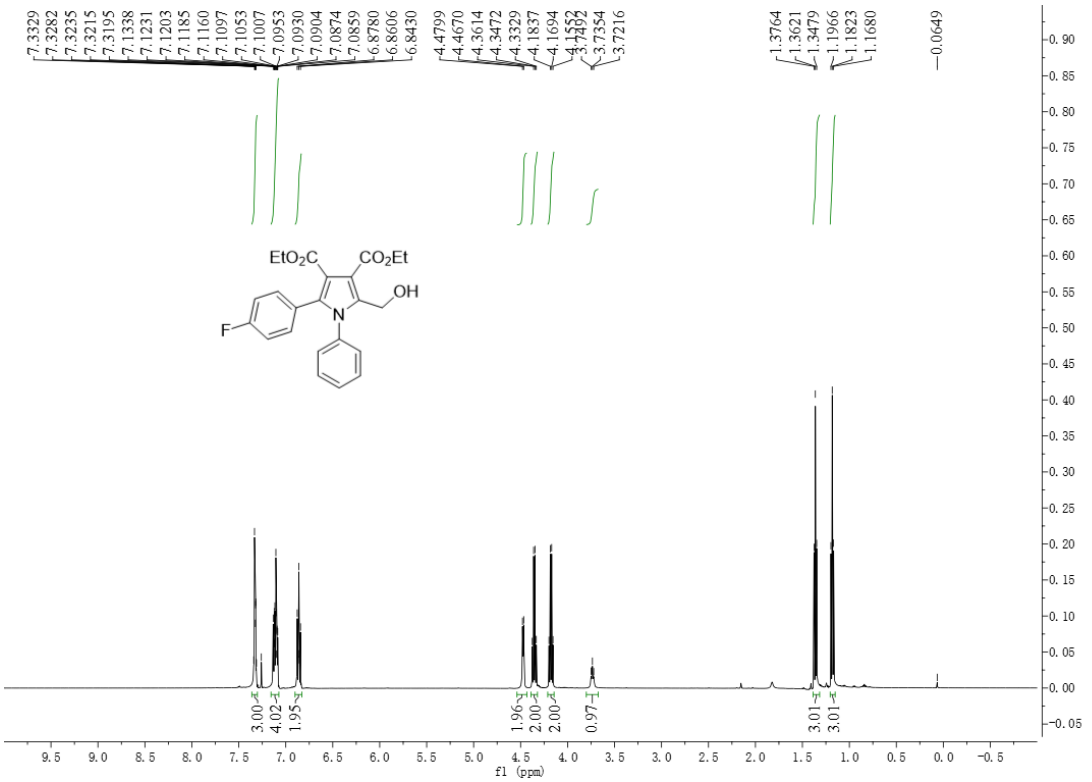


^{13}C NMR (125 MHz, $CDCl_3$)

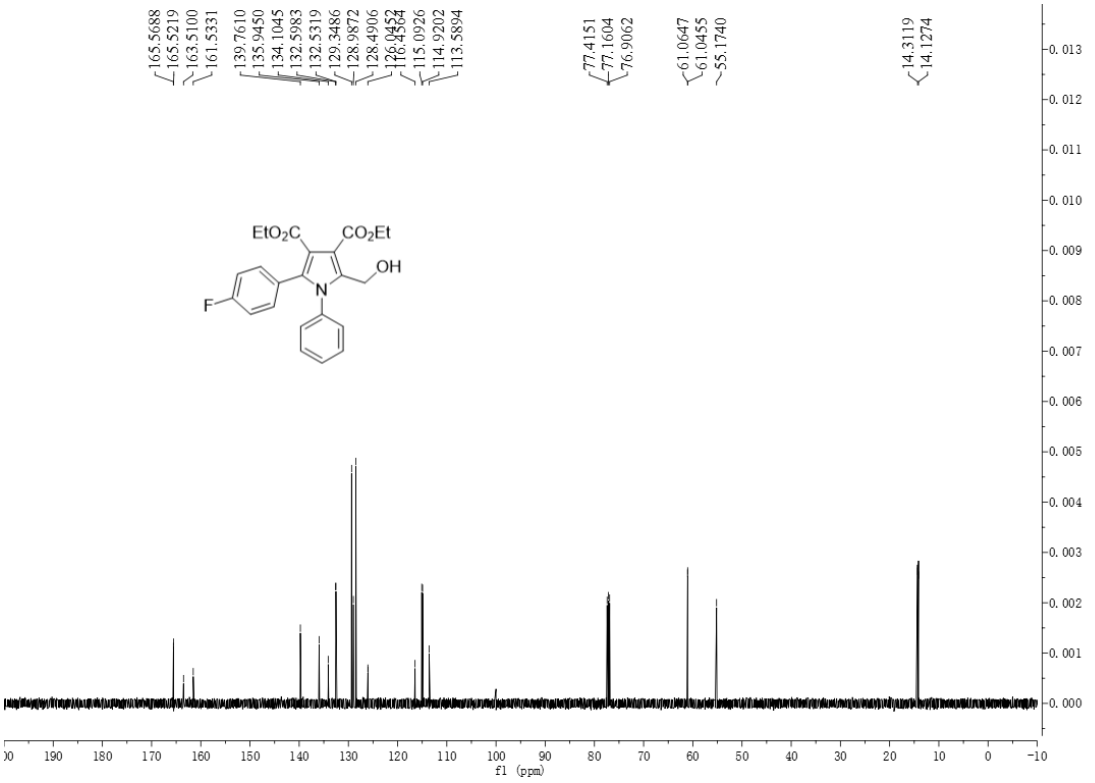


Diethyl 2-(4-fluorophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ba)

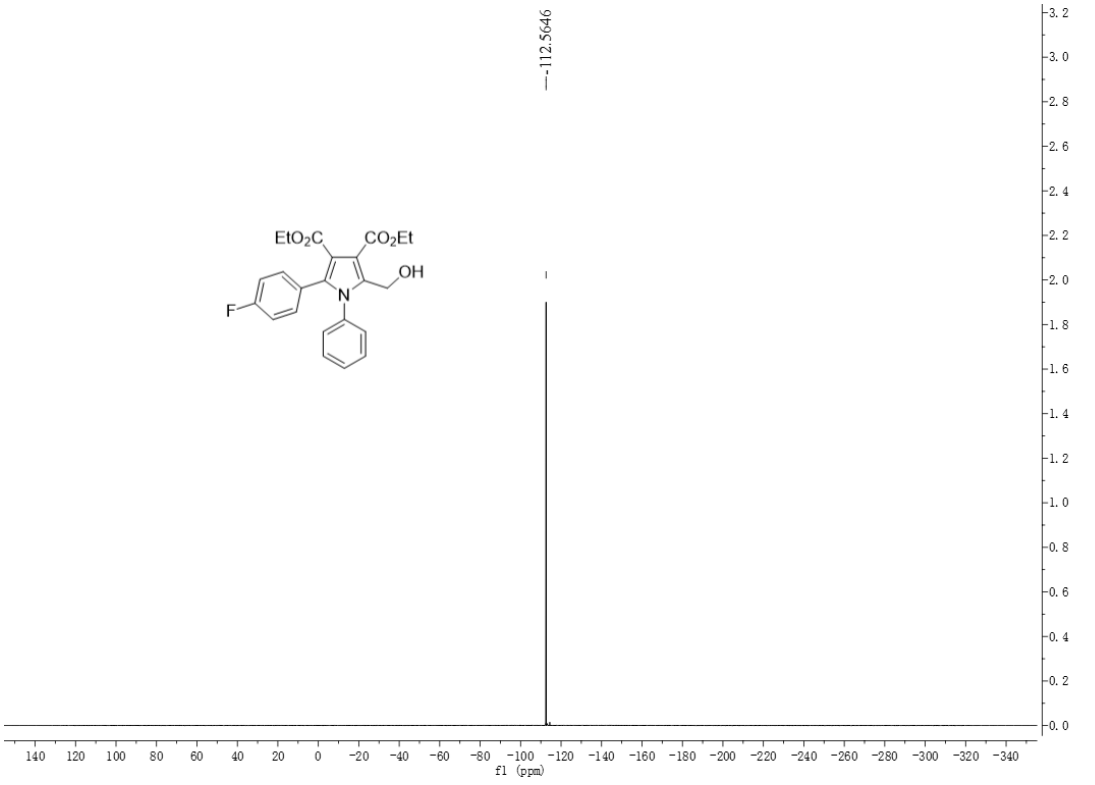
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)

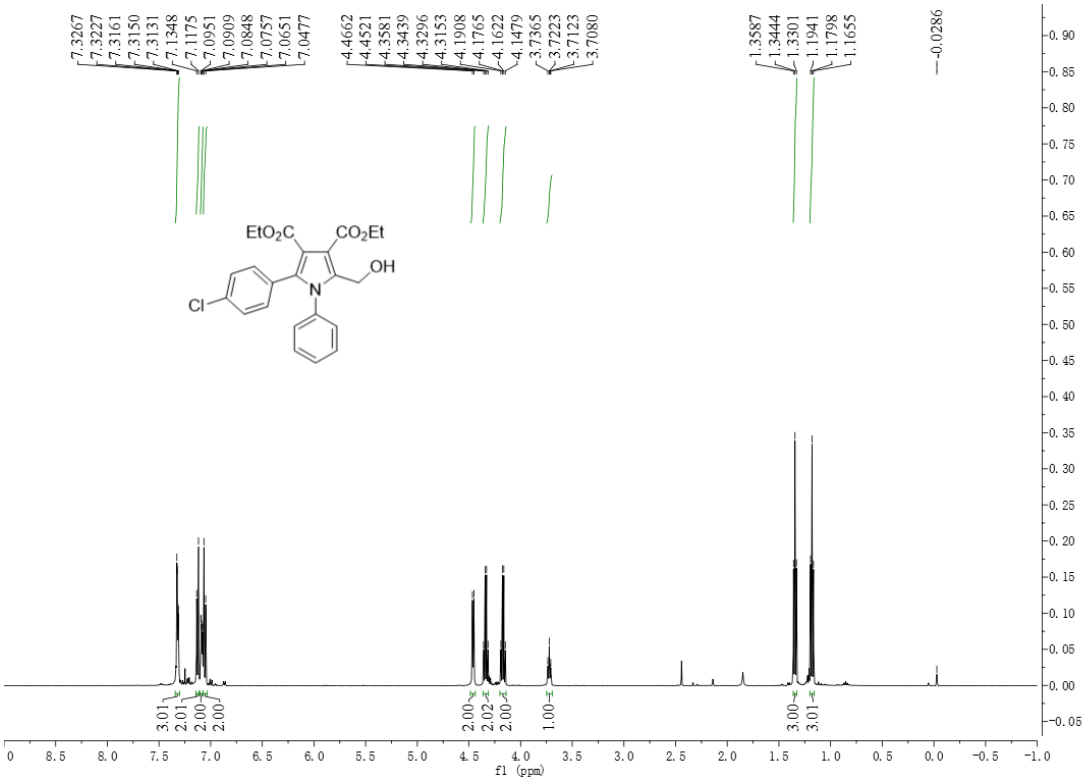


^{19}F NMR (470 MHz, $CDCl_3$)

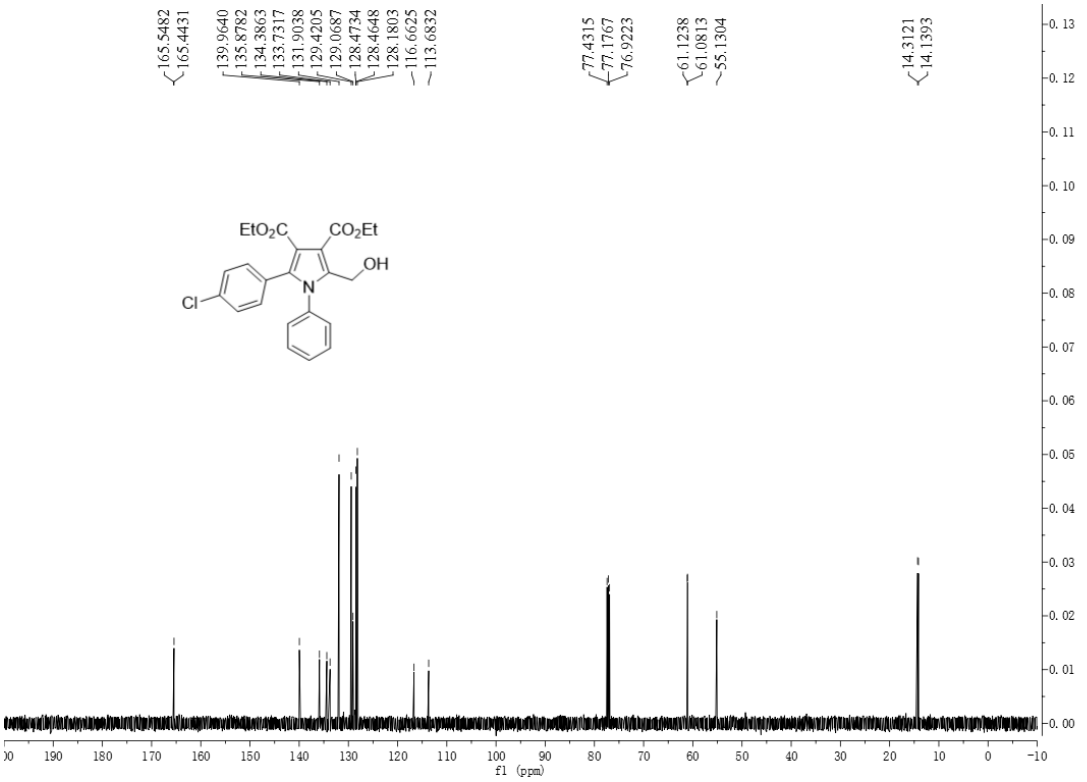


Diethyl 2-(4-chlorophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ca)

^{1}H NMR (500 MHz, $CDCl_3$)

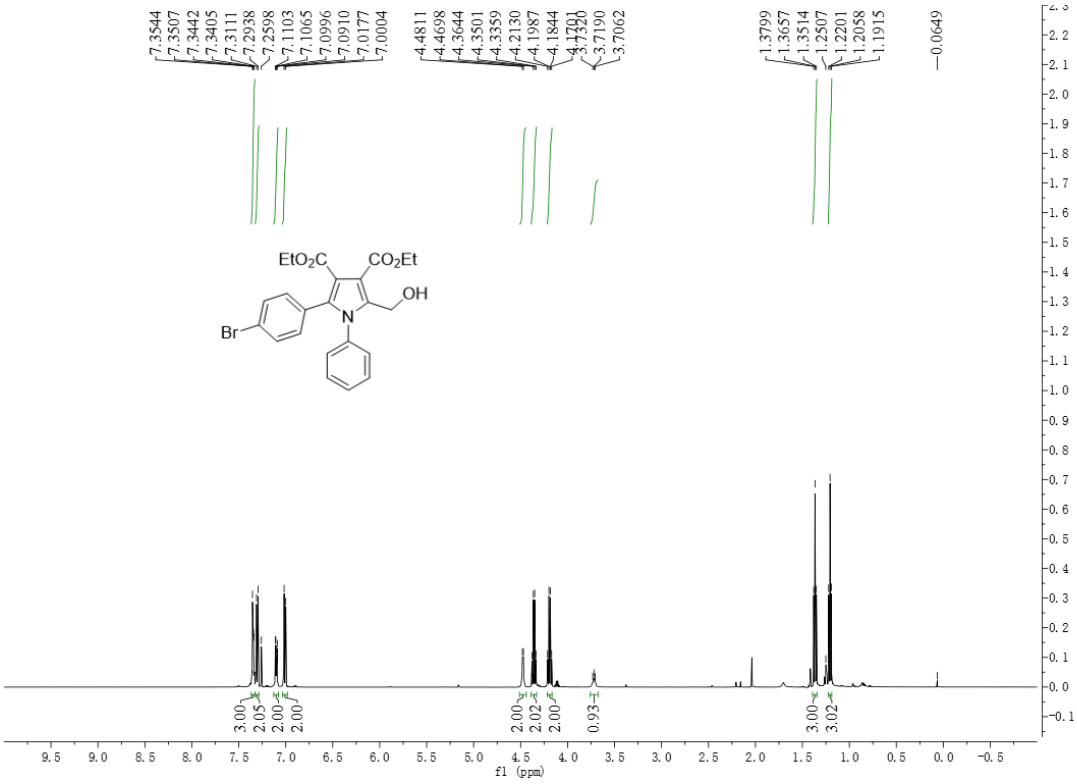


^{13}C NMR (125 MHz, $CDCl_3$)

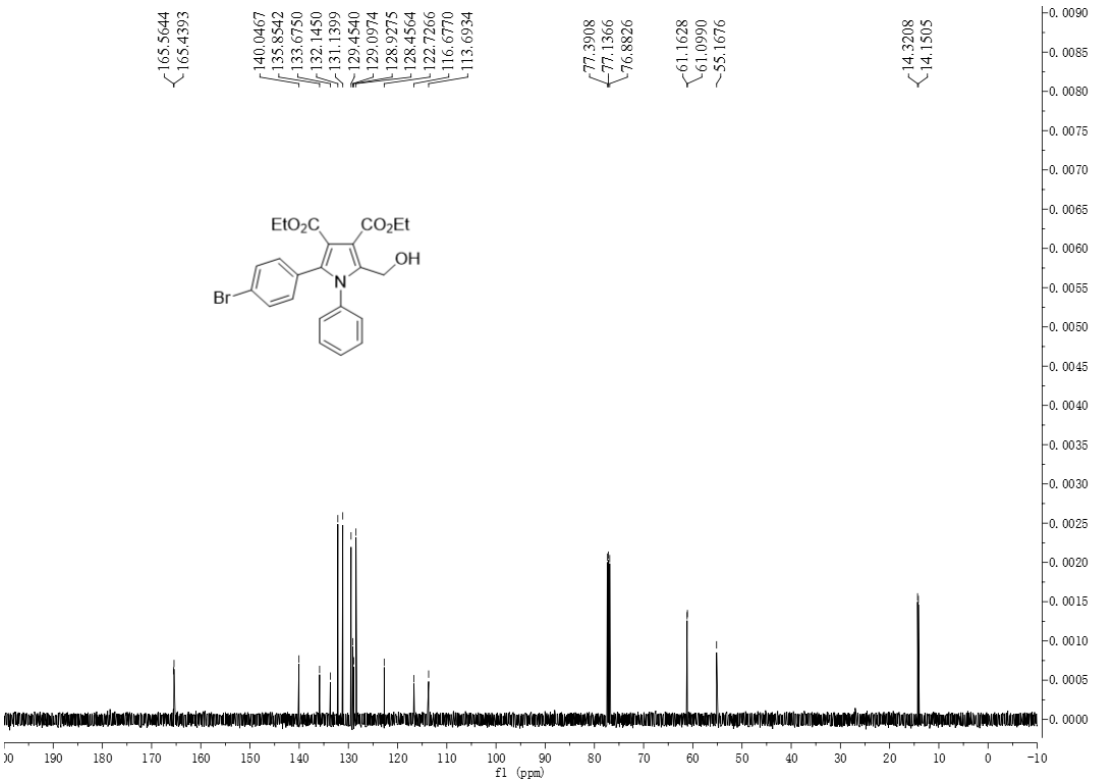


Diethyl 2-(4-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4da)

^{1}H NMR (500 MHz, $CDCl_3$)

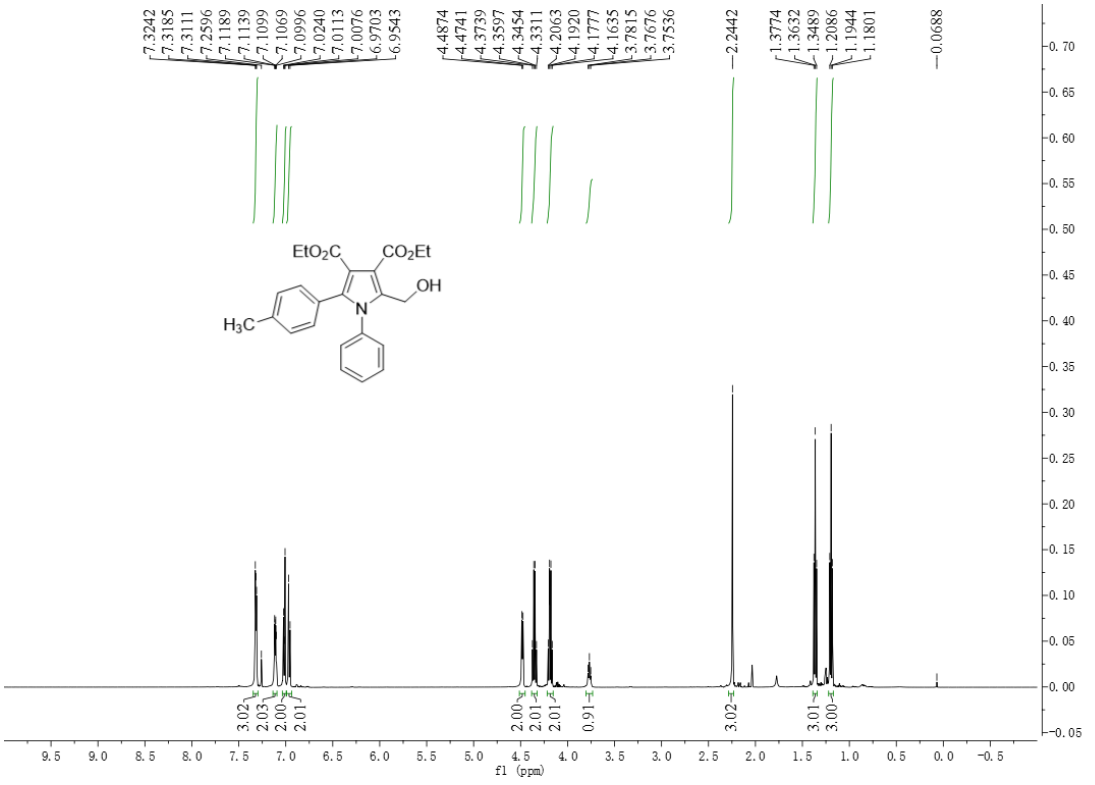


^{13}C NMR (125 MHz, $CDCl_3$)

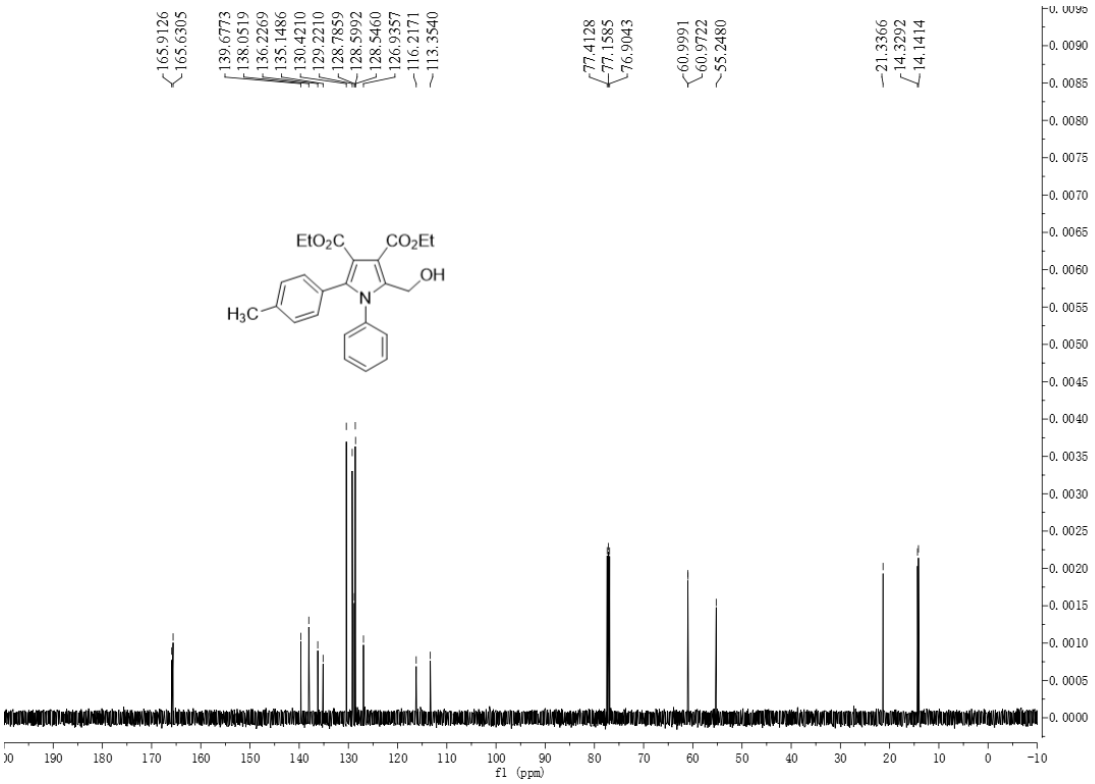


Diethyl 2-(hydroxymethyl)-1-phenyl-5-(p-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ea)

^{1}H NMR (500 MHz, $CDCl_3$)

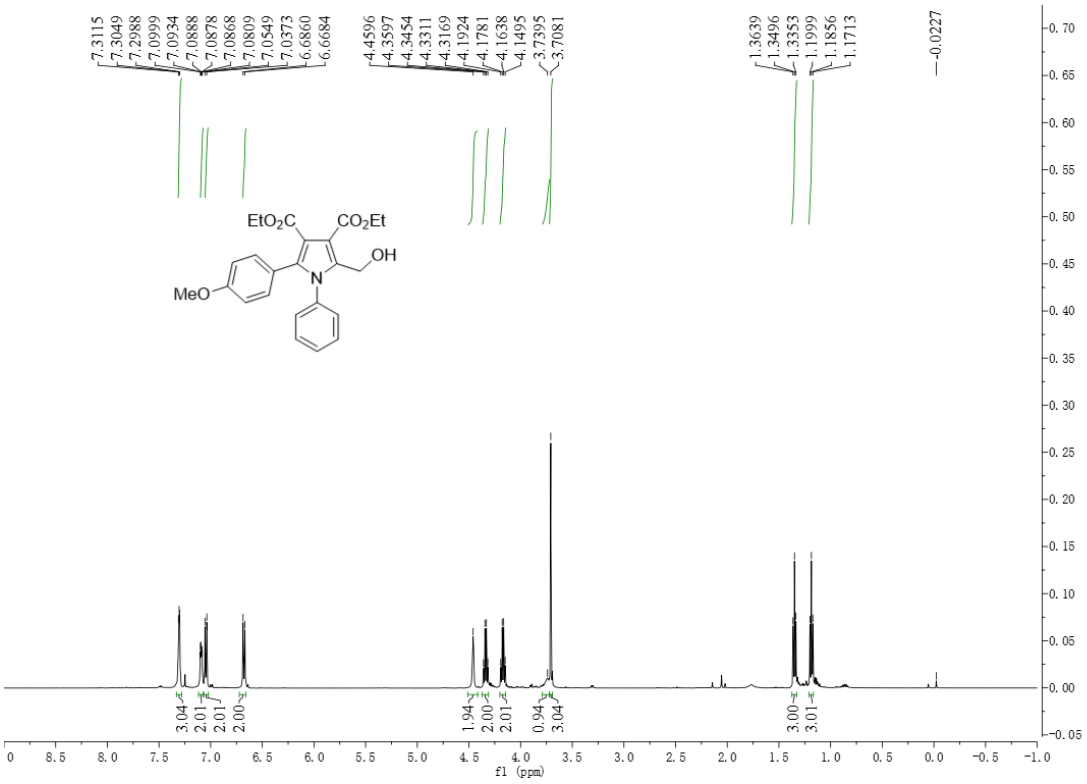


^{13}C NMR (125 MHz, $CDCl_3$)

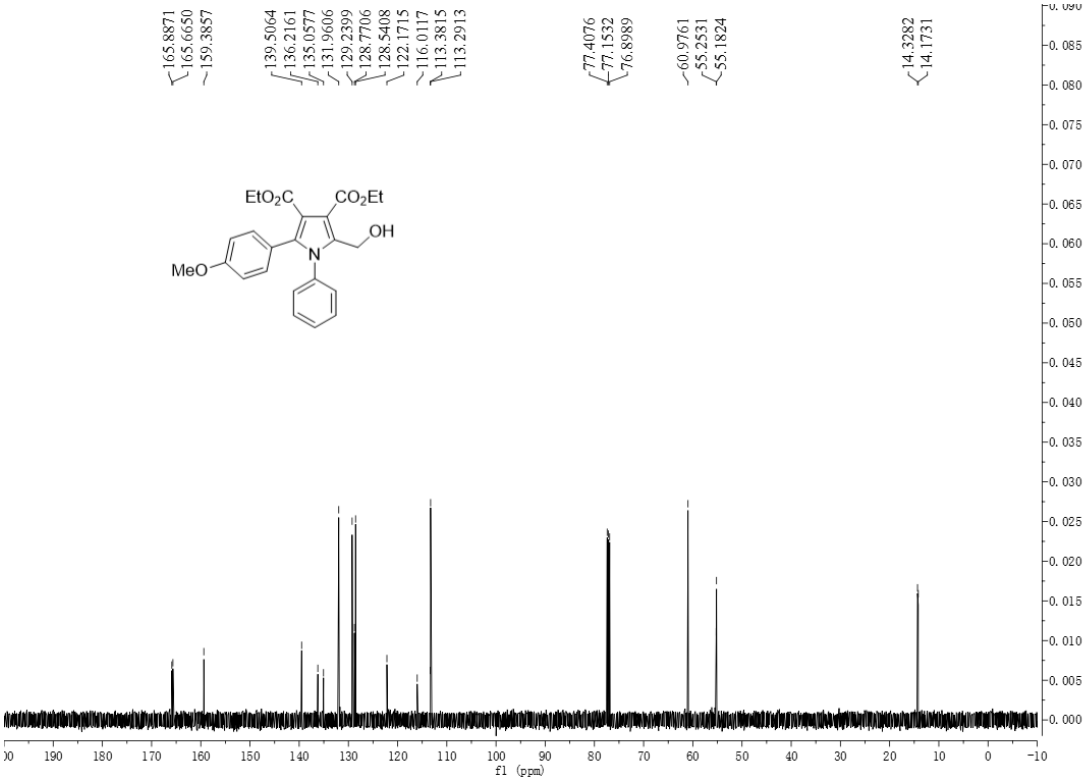


Diethyl 2-(hydroxymethyl)-5-(4-methoxyphenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4fa)

^{1}H NMR (500 MHz, $CDCl_3$)

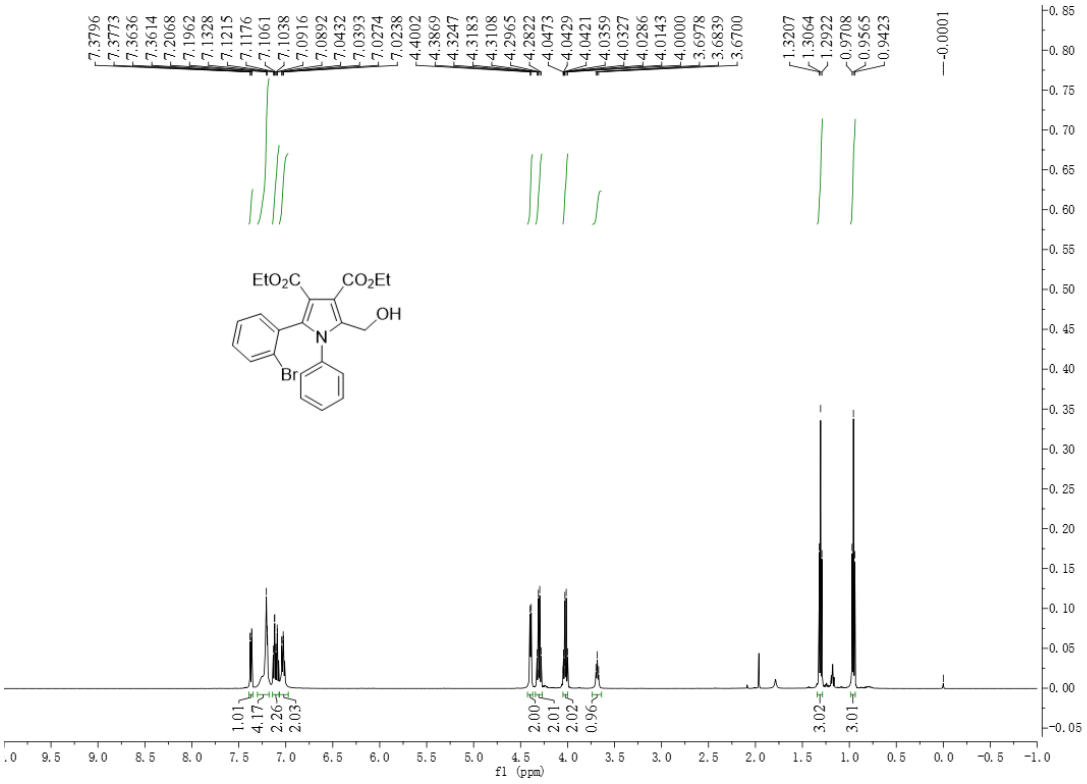


^{13}C NMR (125 MHz, $CDCl_3$)

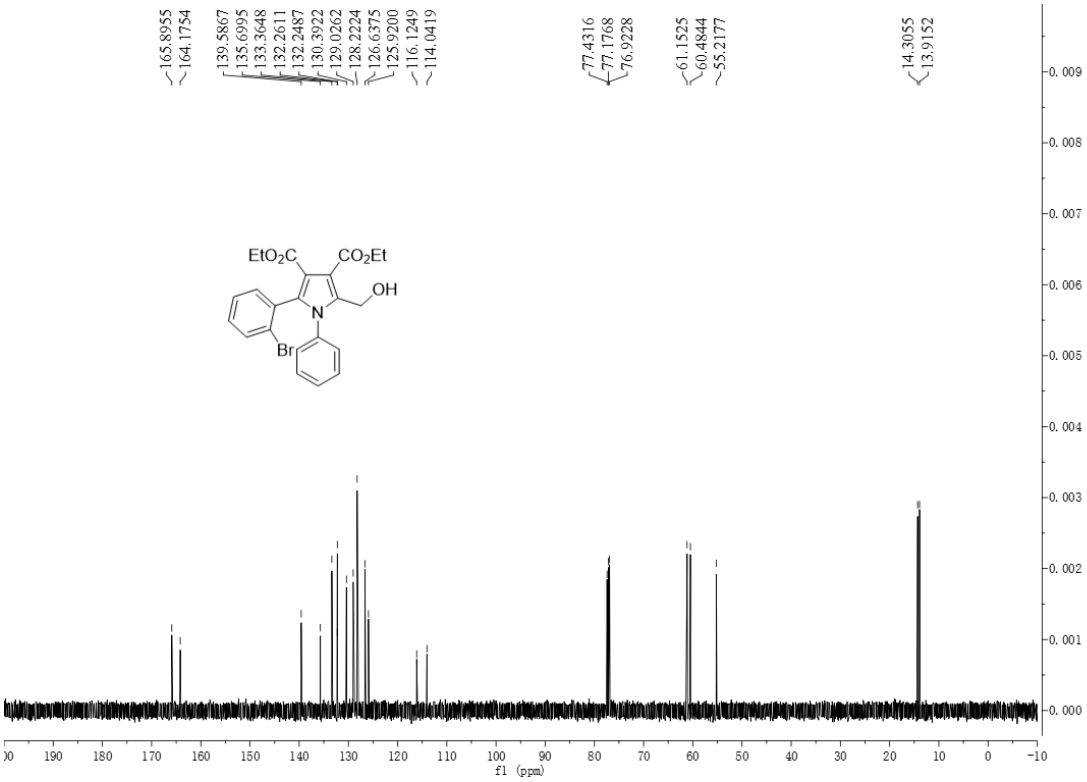


Diethyl 2-(2-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ga)

^{1}H NMR (500 MHz, $CDCl_3$)

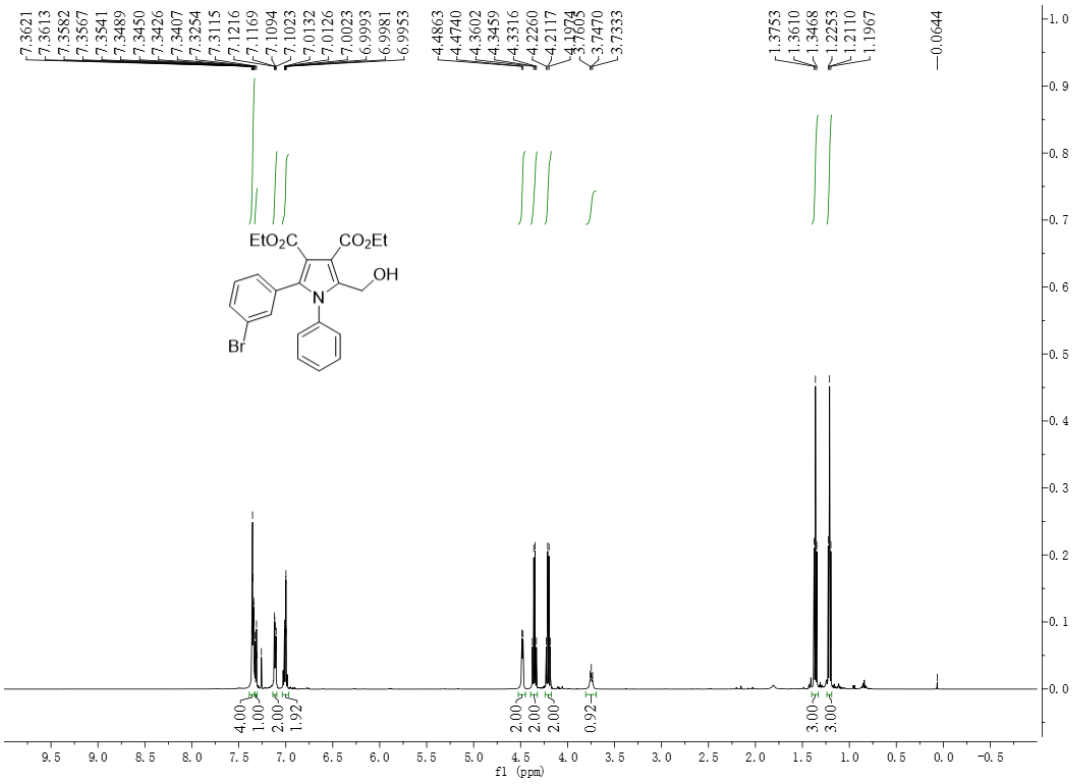


^{13}C NMR (125 MHz, $CDCl_3$)

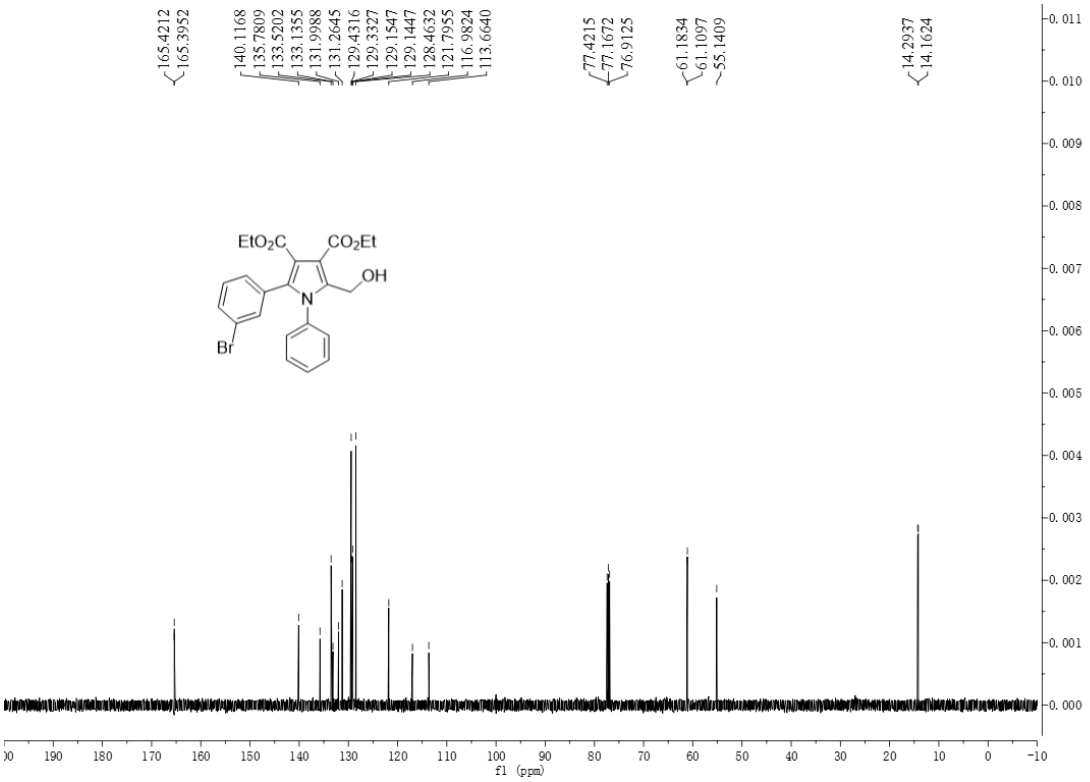


Diethyl 2-(3-bromophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ha)

^{1}H NMR (500 MHz, $CDCl_3$)

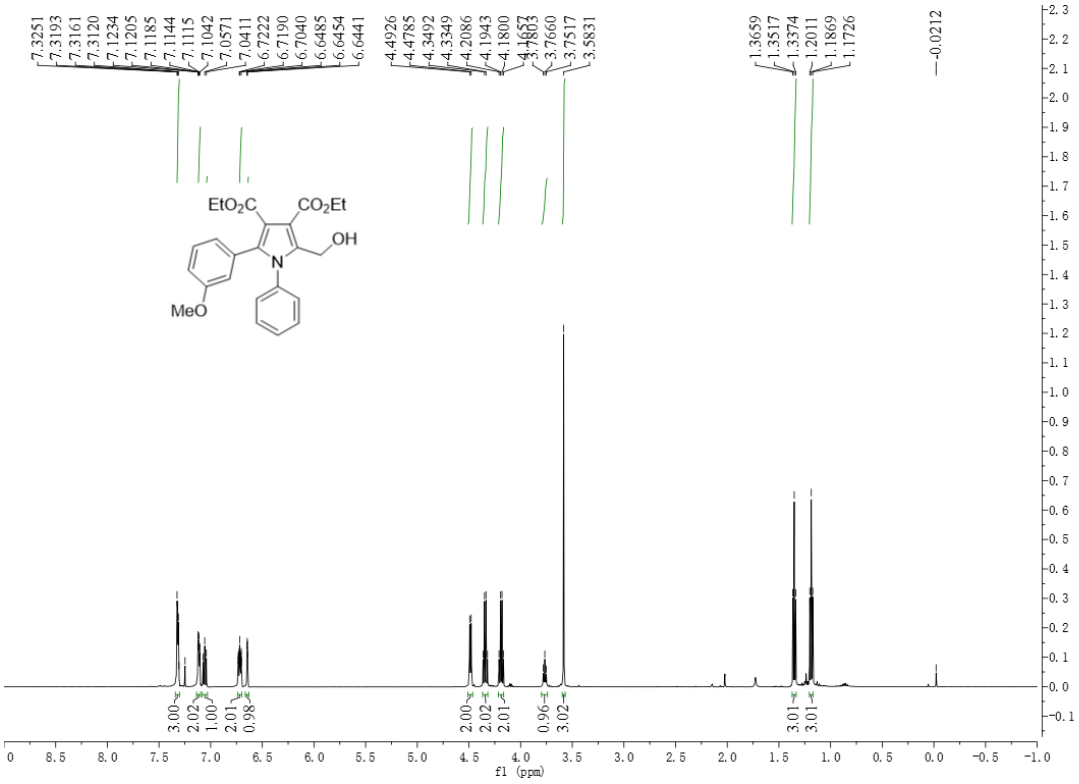


^{13}C NMR (125 MHz, $CDCl_3$)

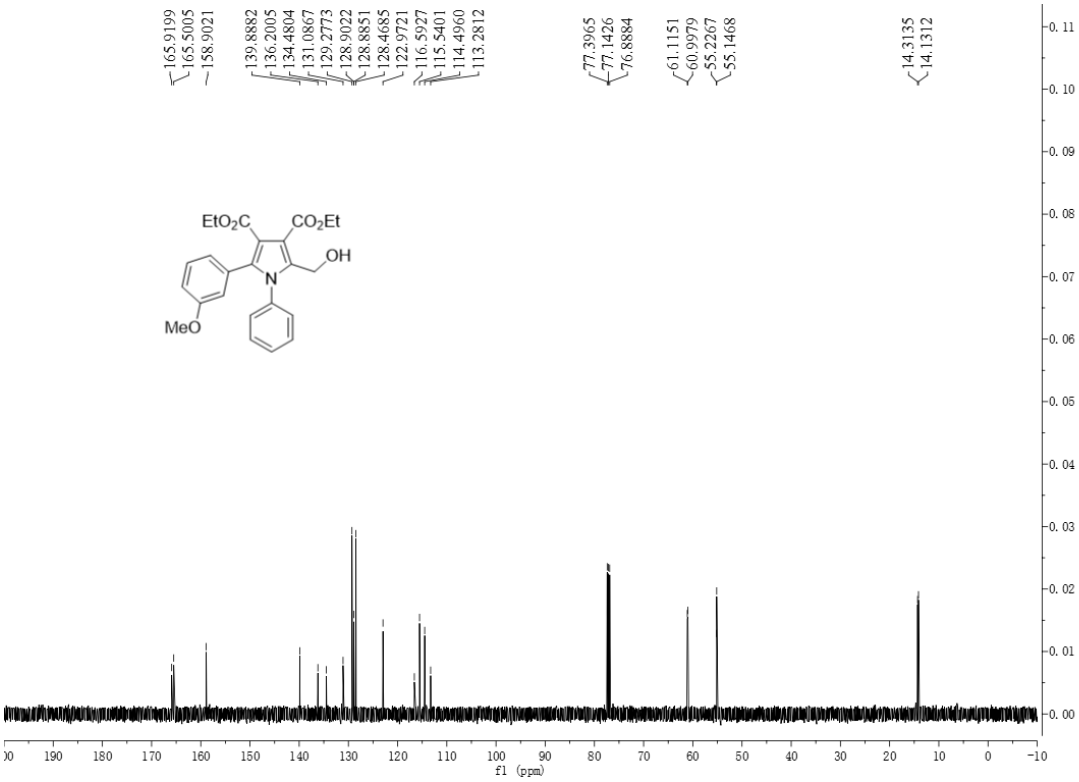


Diethyl 2-(hydroxymethyl)-5-(3-methoxyphenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ia)

^{1}H NMR (500 MHz, $CDCl_3$)

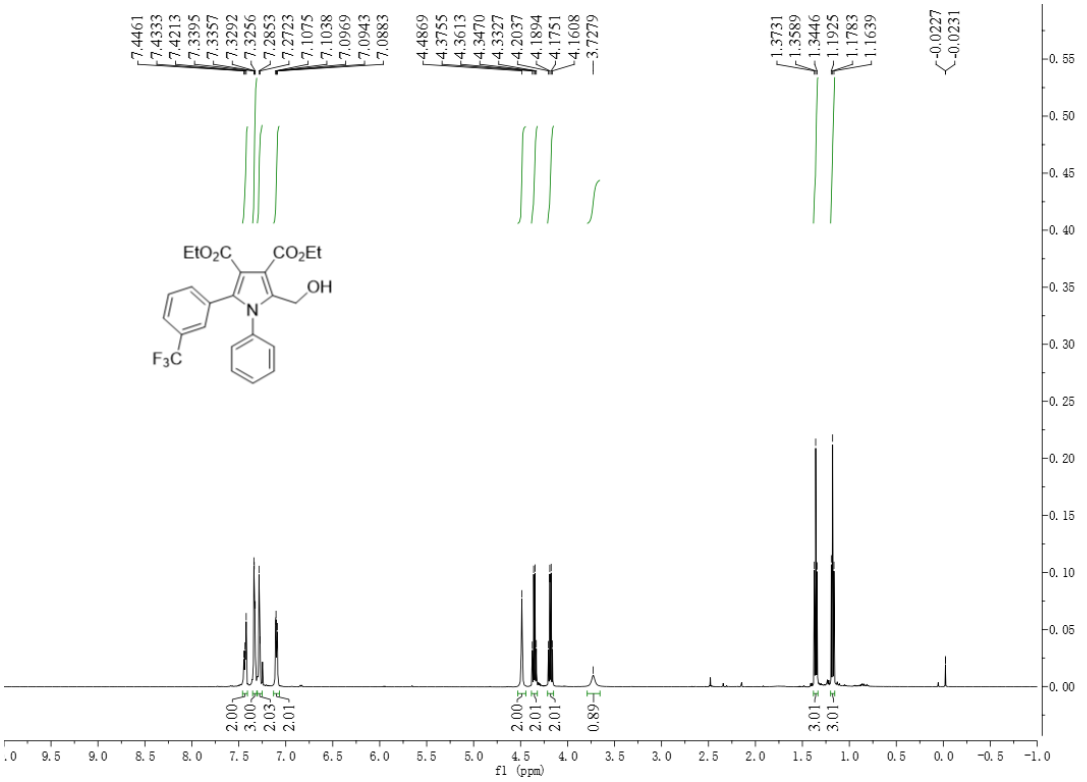


^{13}C NMR (125 MHz, $CDCl_3$)

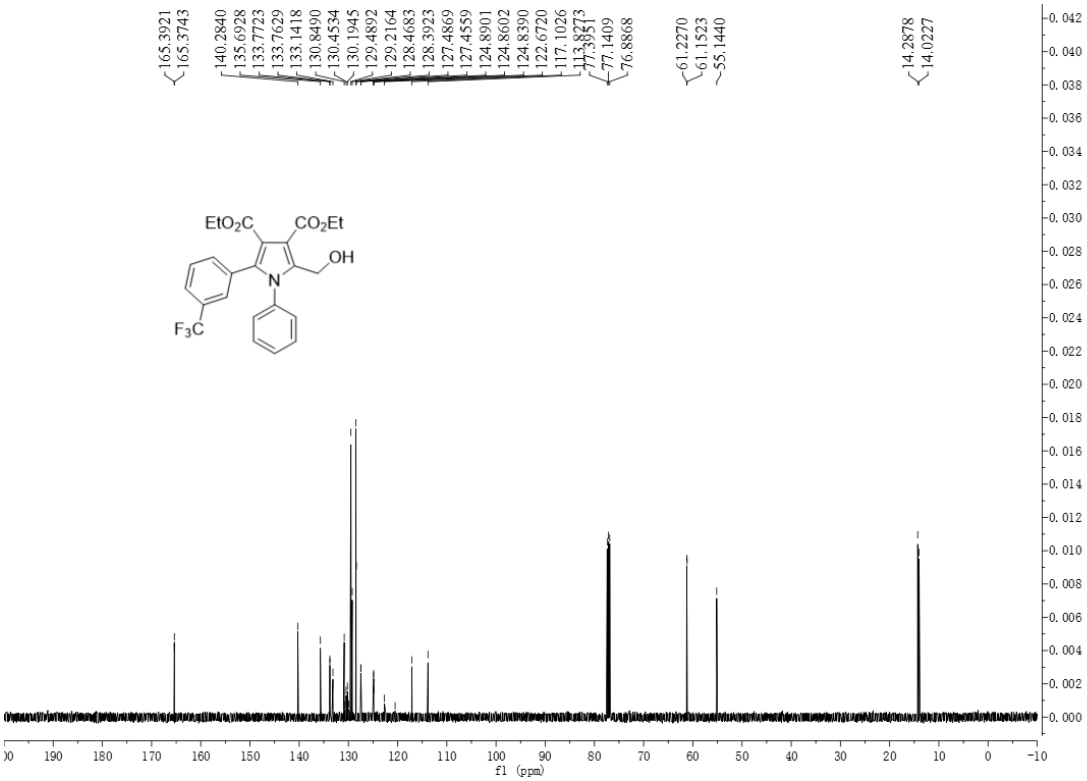


Diethyl 2-(hydroxymethyl)-1-phenyl-5-(3-(trifluoromethyl)phenyl)-1*H*-pyrrole-3,4-dicarboxylate (4ja)

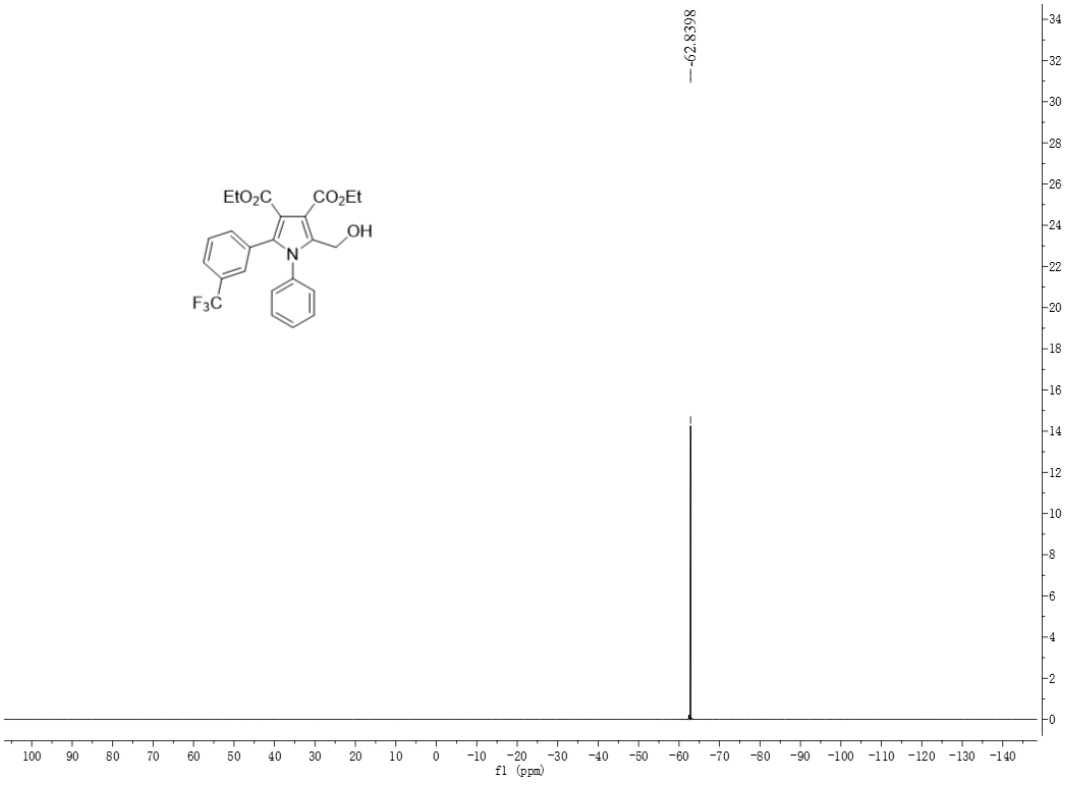
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)

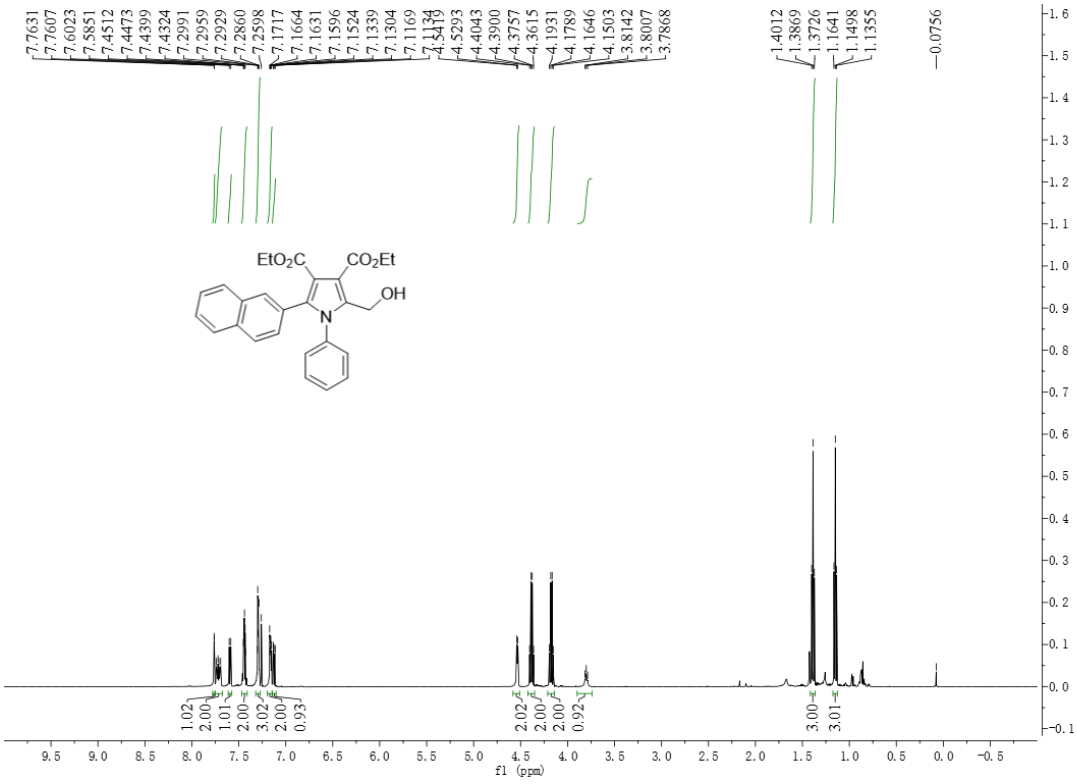


^{19}F NMR (470 MHz, $CDCl_3$)

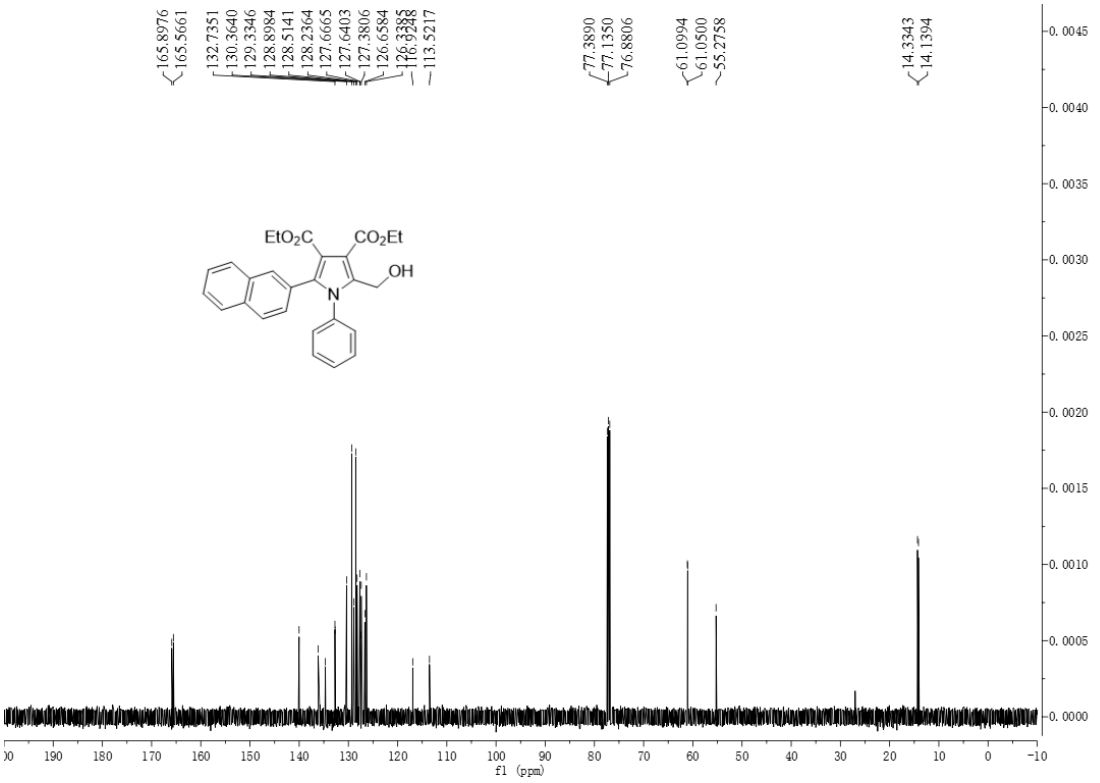


Diethyl 2-(hydroxymethyl)-5-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ka)

^{1}H NMR (500 MHz, $CDCl_3$)

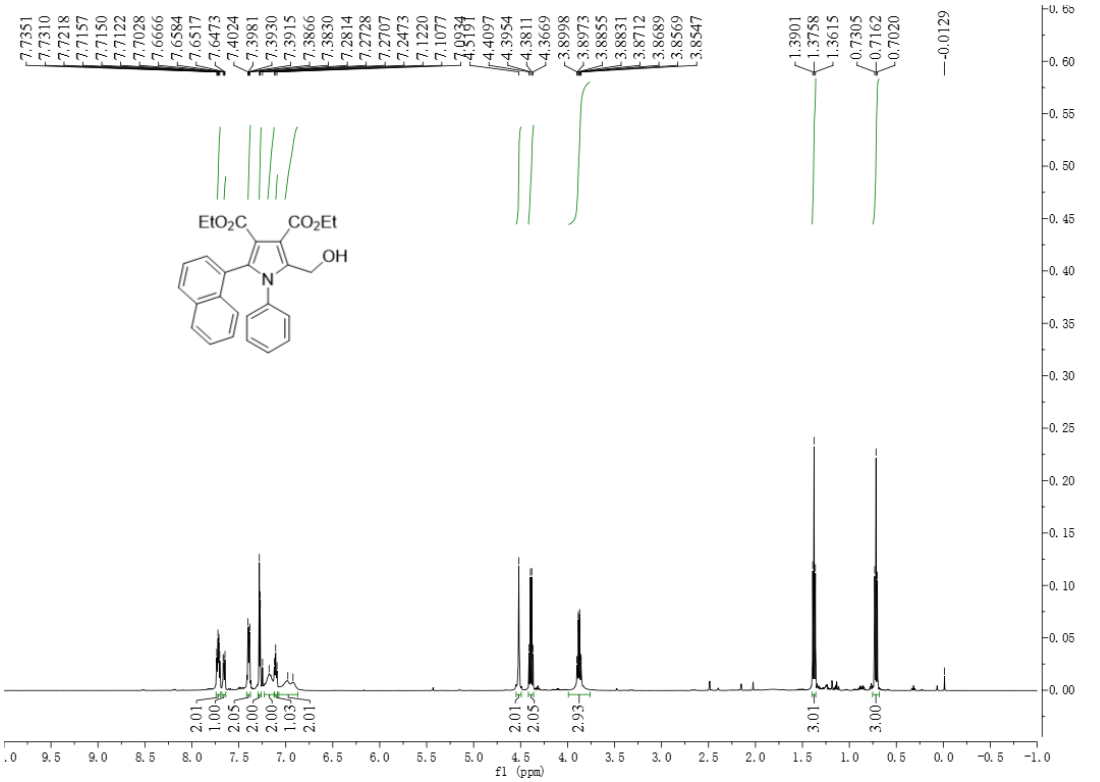


^{13}C NMR (125 MHz, $CDCl_3$)

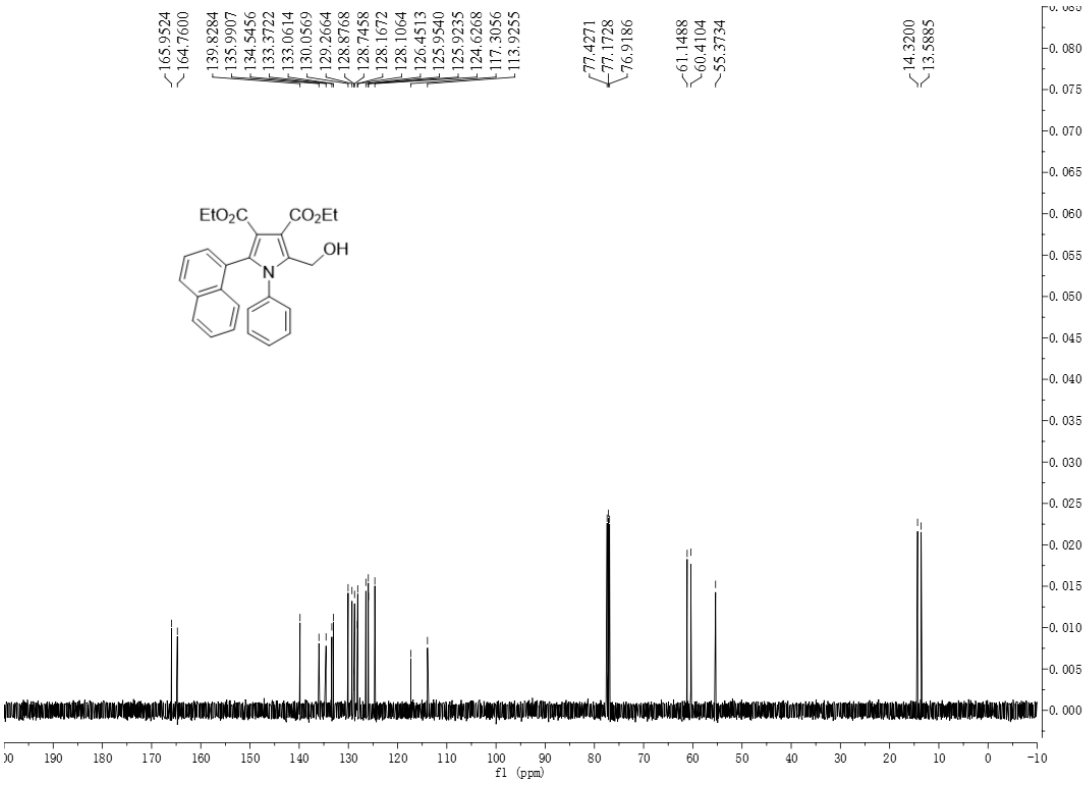


Diethyl 2-(hydroxymethyl)-5-(naphthalen-1-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4la)

^{1}H NMR (500 MHz, $CDCl_3$)

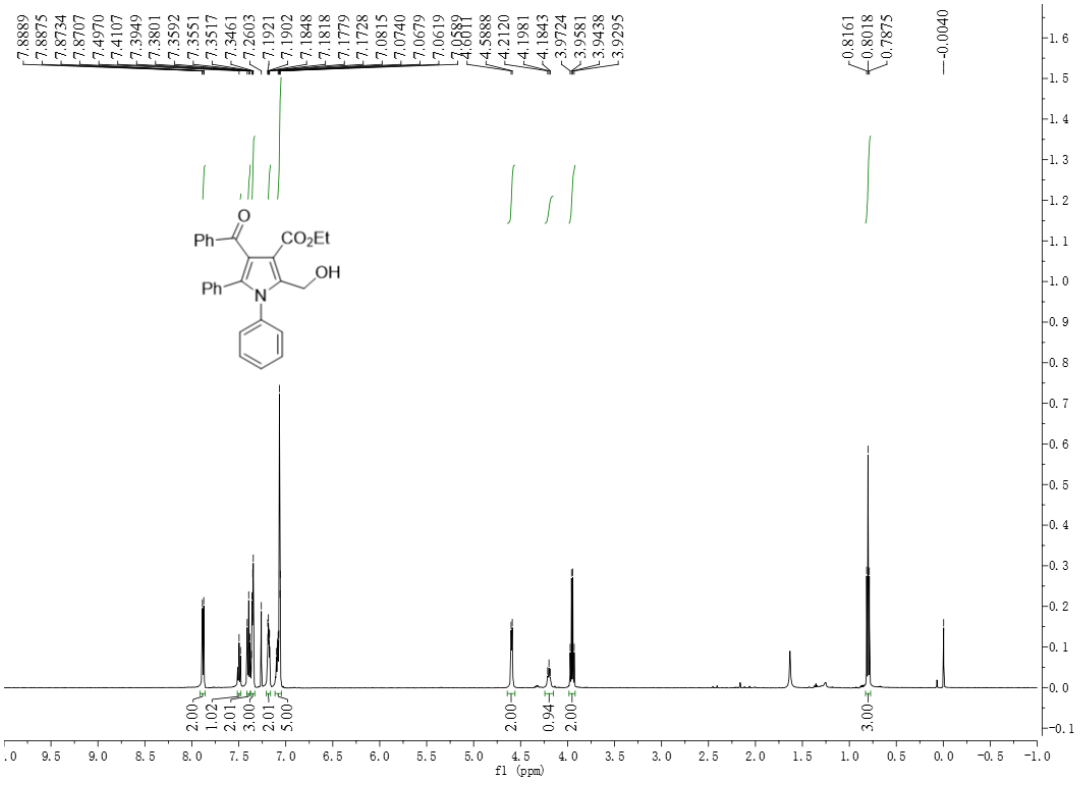


^{13}C NMR (125 MHz, $CDCl_3$)

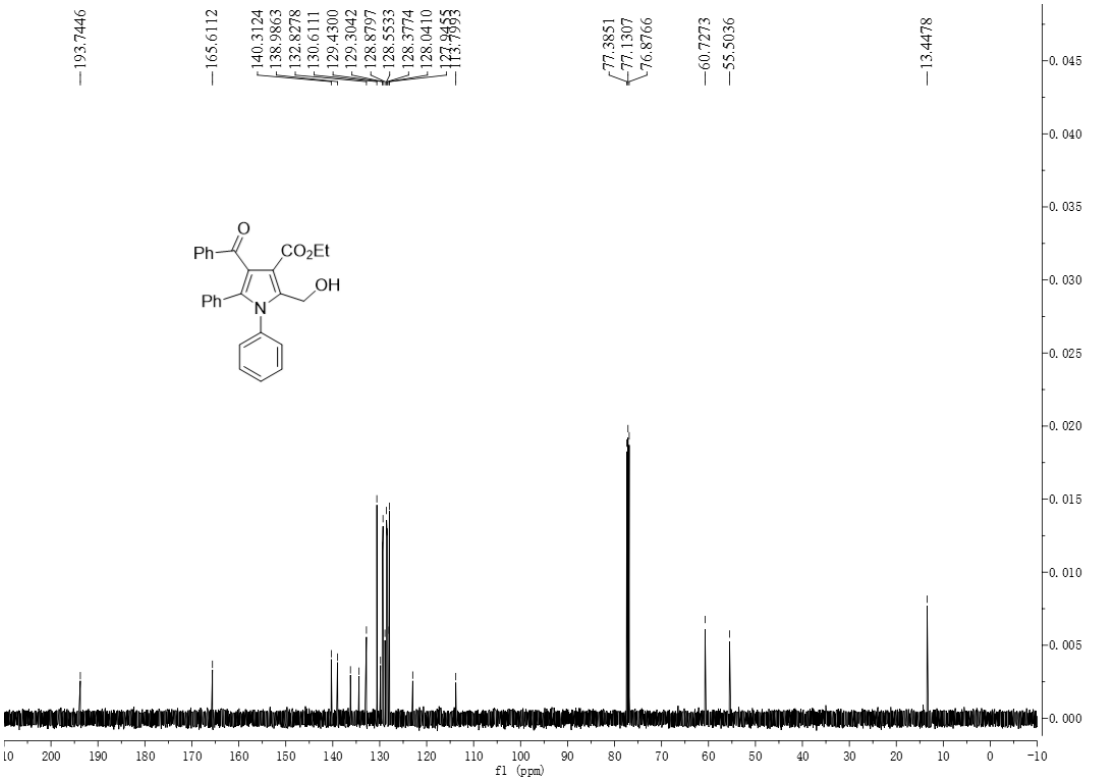


Ethyl 4-benzoyl-2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3-carboxylate (4ma)

^{1}H NMR (500 MHz, $CDCl_3$)

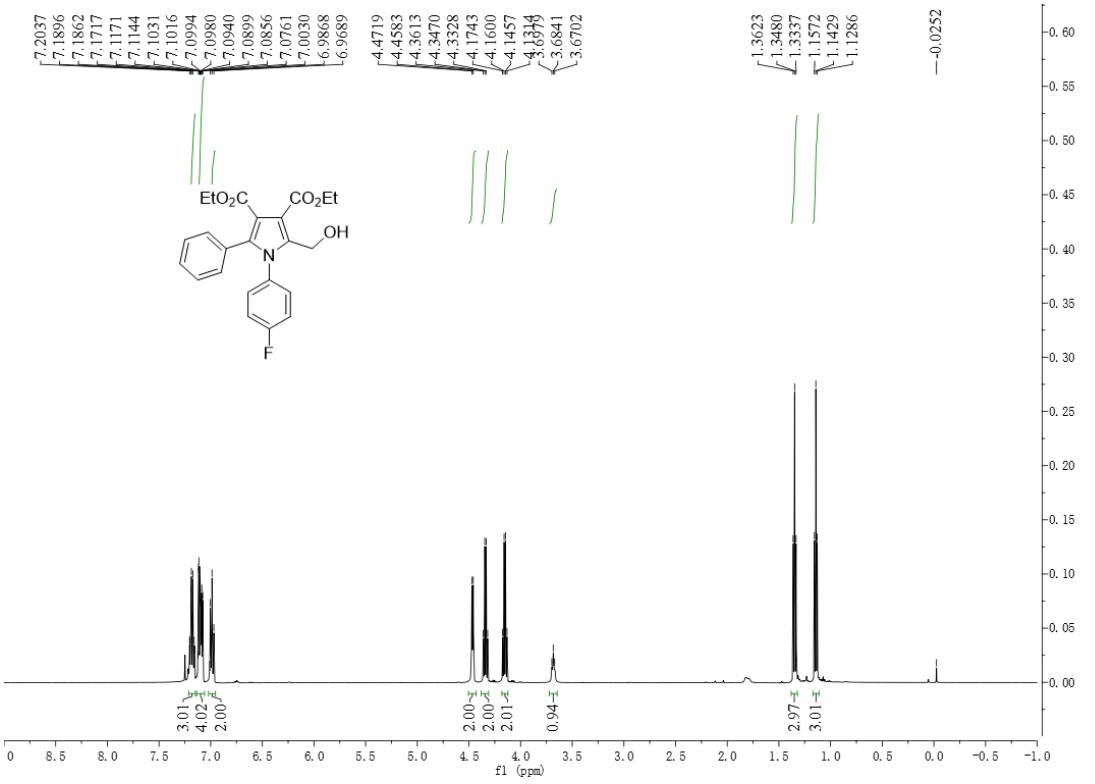


^{13}C NMR (125 MHz, $CDCl_3$)

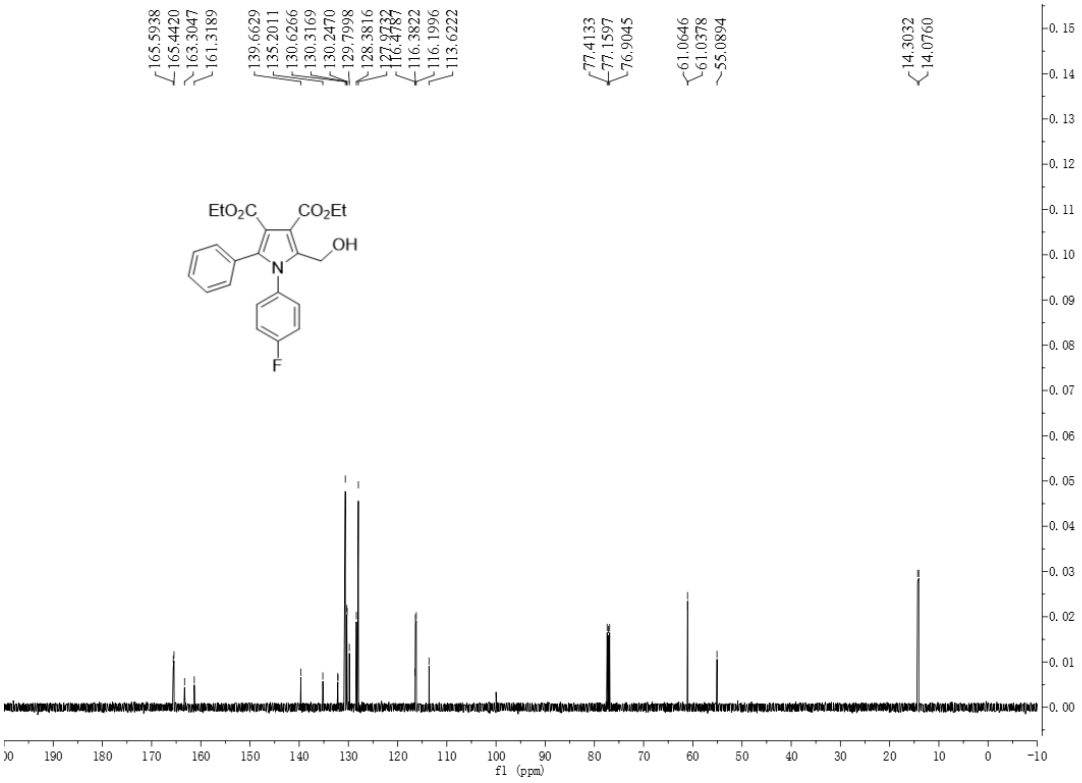


Diethyl 2-(4-fluorophenyl)-5-(hydroxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ab)

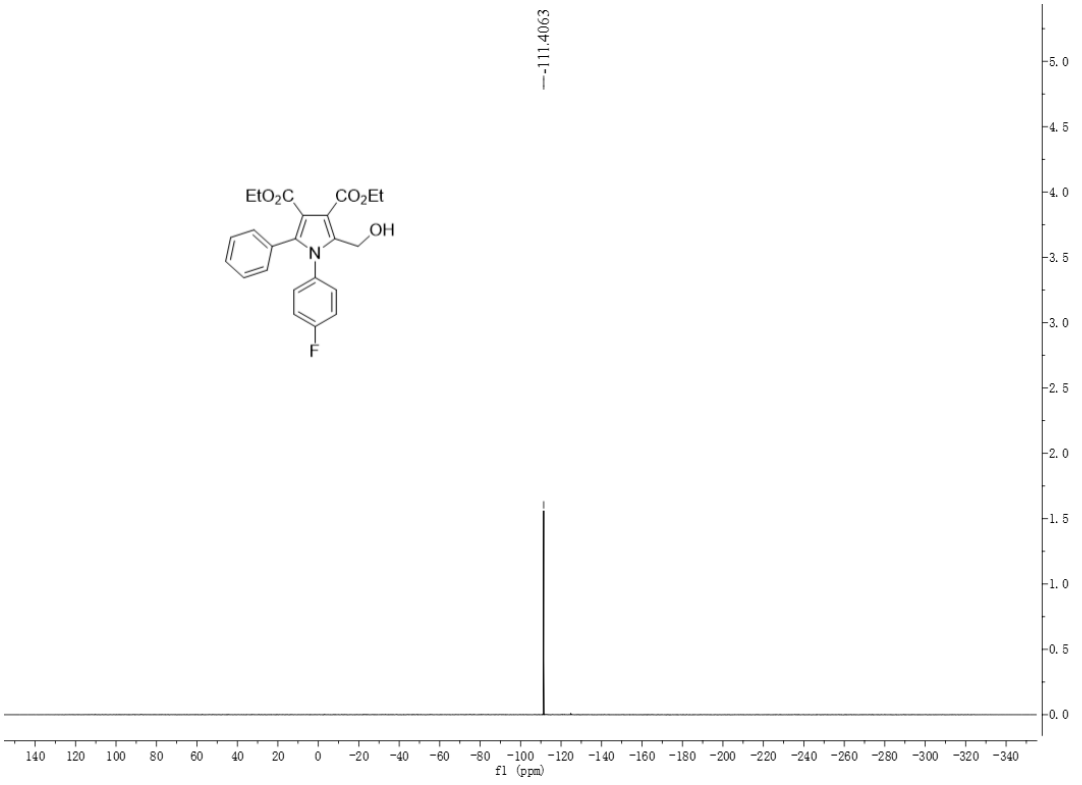
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)

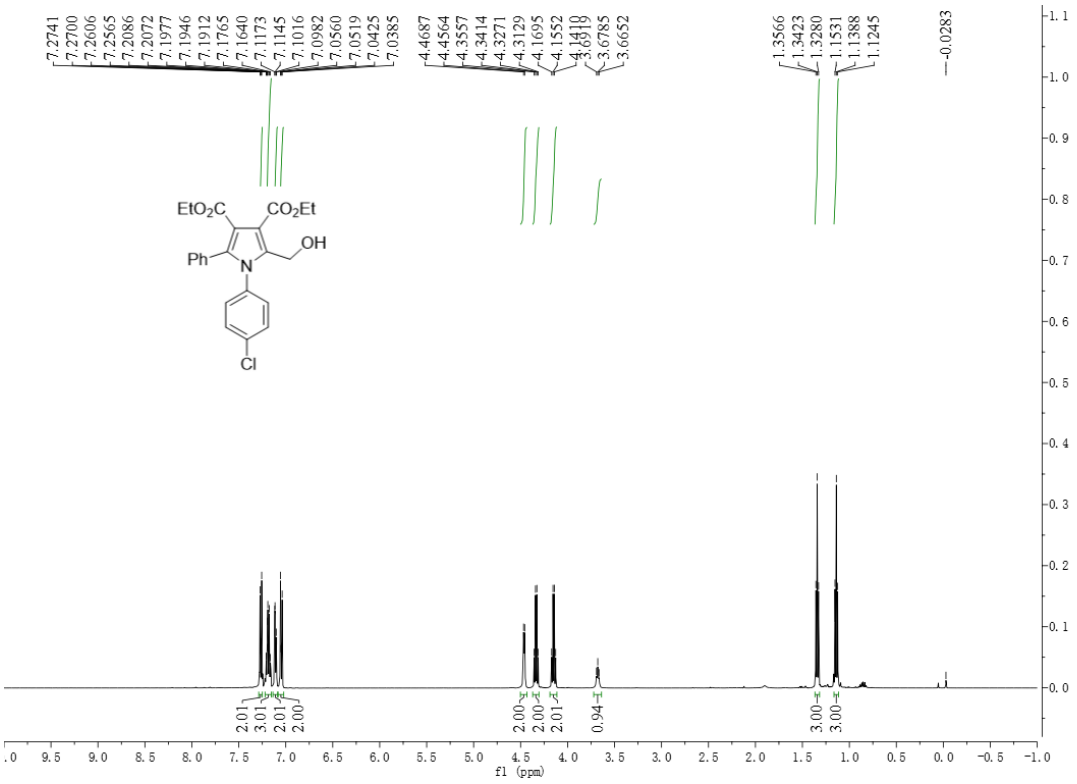


^{19}F NMR (470 MHz, $CDCl_3$)

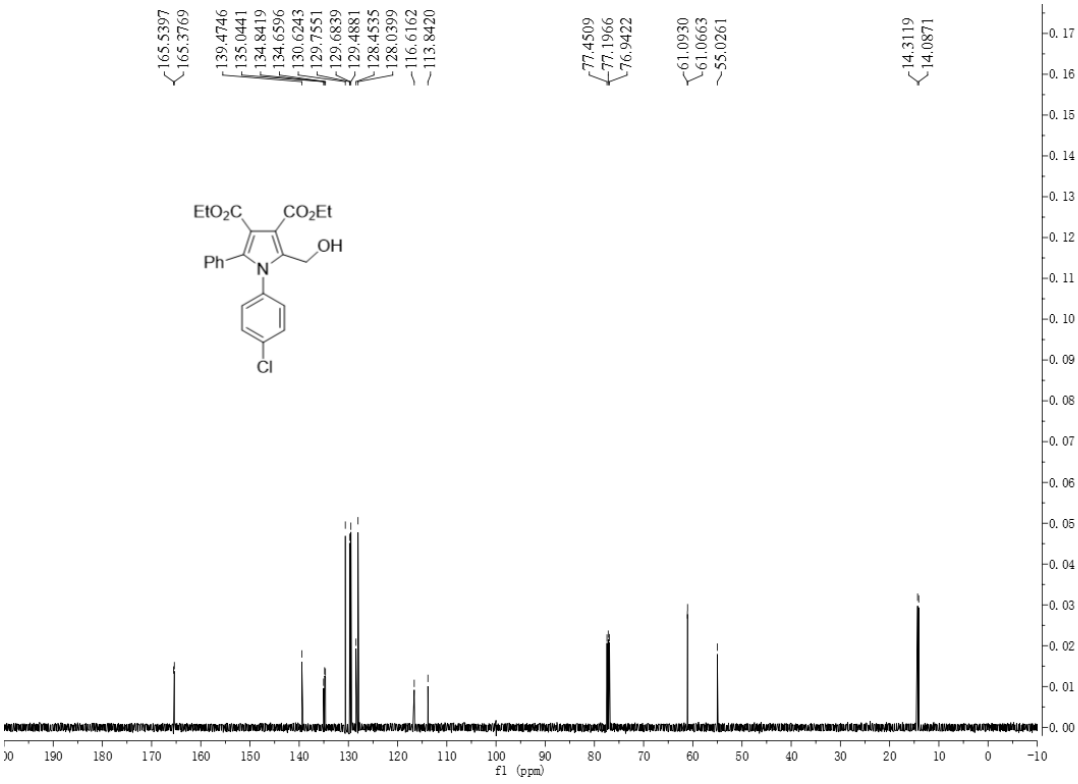


Diethyl 1-(4-chlorophenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ac)

^{1}H NMR (500 MHz, $CDCl_3$)

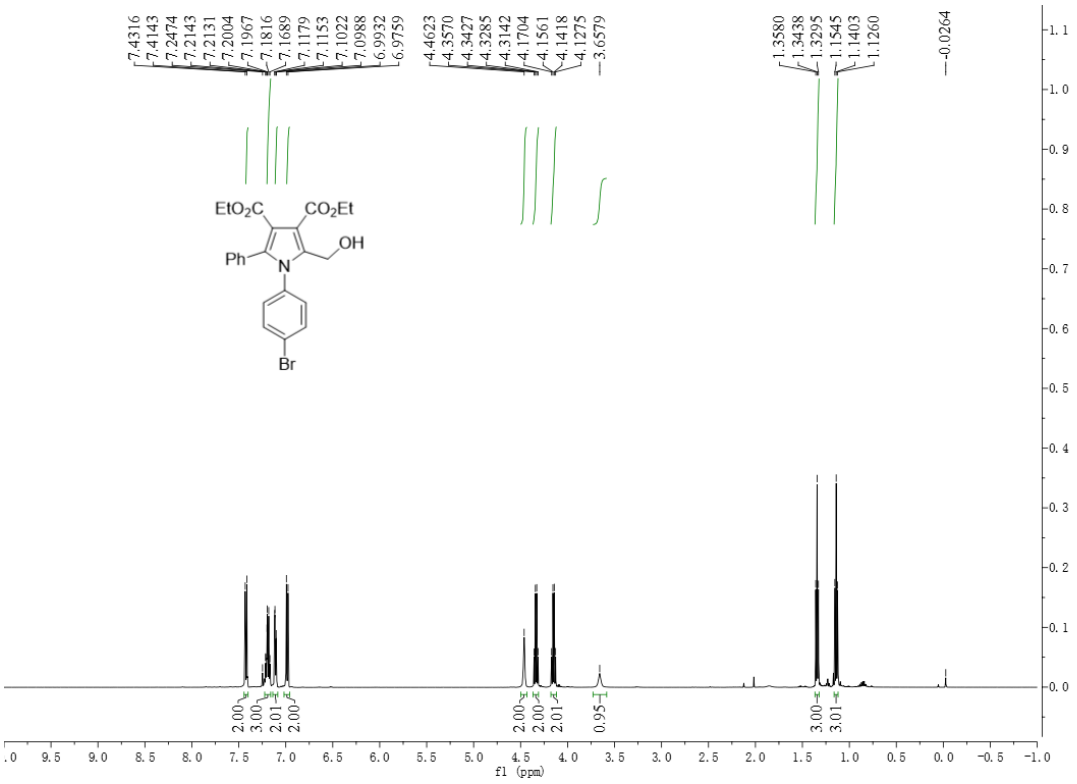


^{13}C NMR (125 MHz, $CDCl_3$)

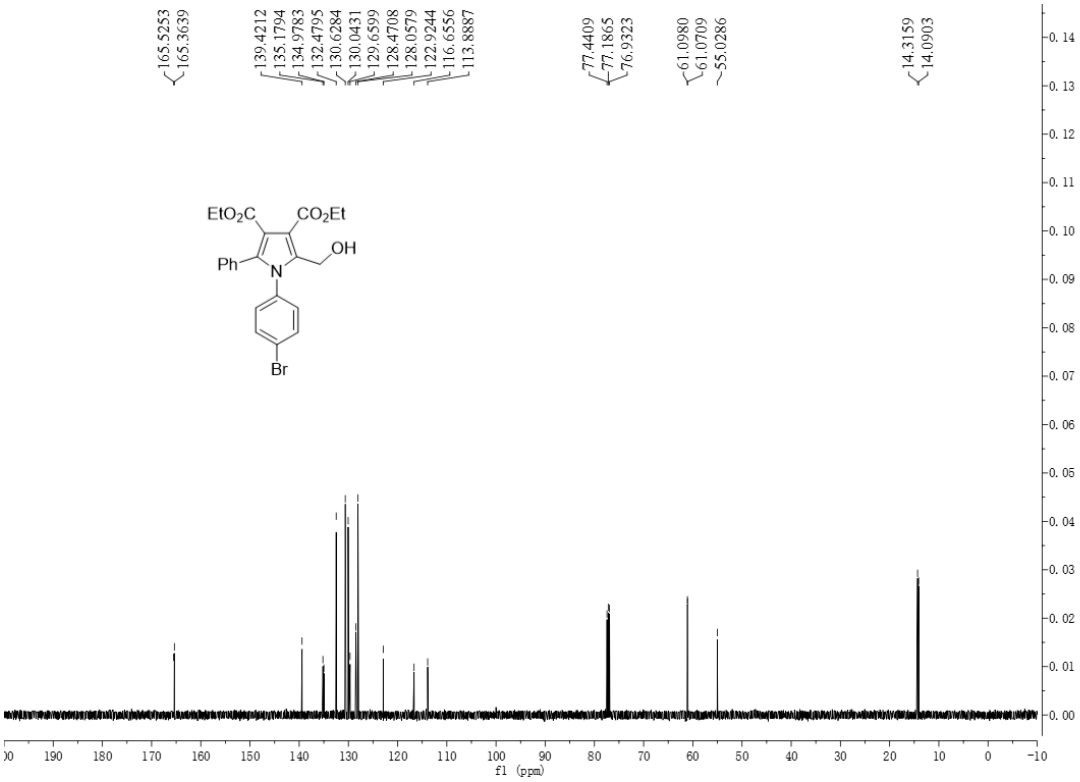


Diethyl 1-(4-bromophenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ad)

^{1}H NMR (500 MHz, $CDCl_3$)

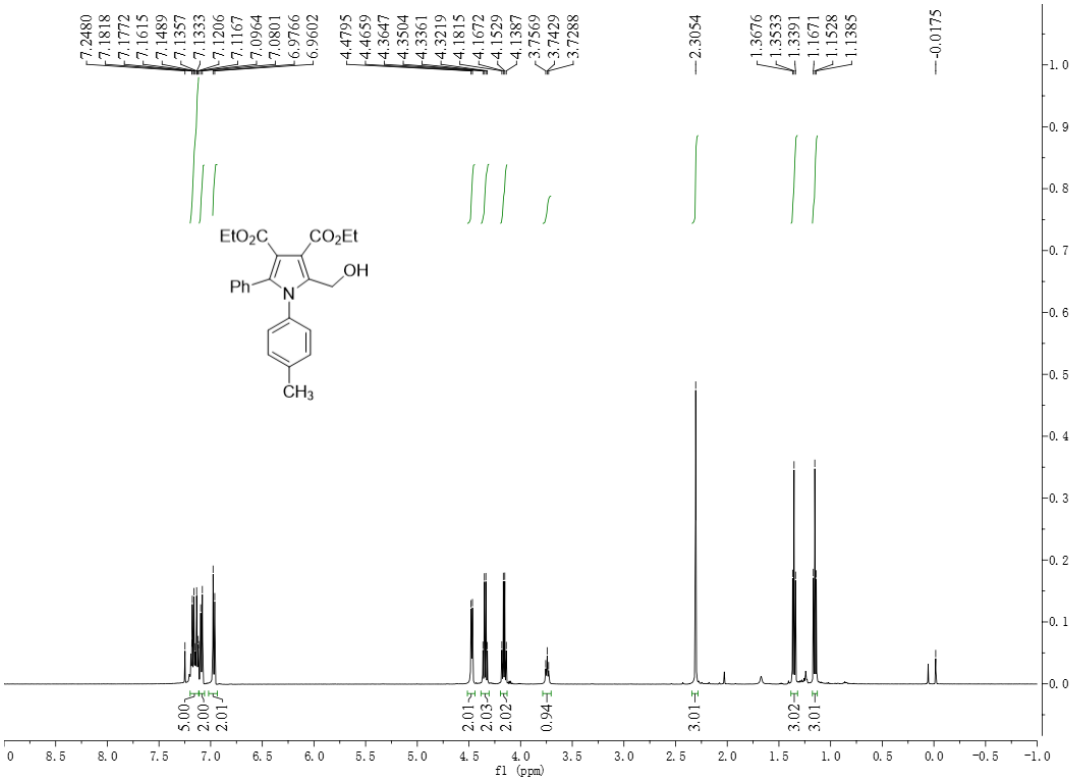


^{13}C NMR (125 MHz, $CDCl_3$)

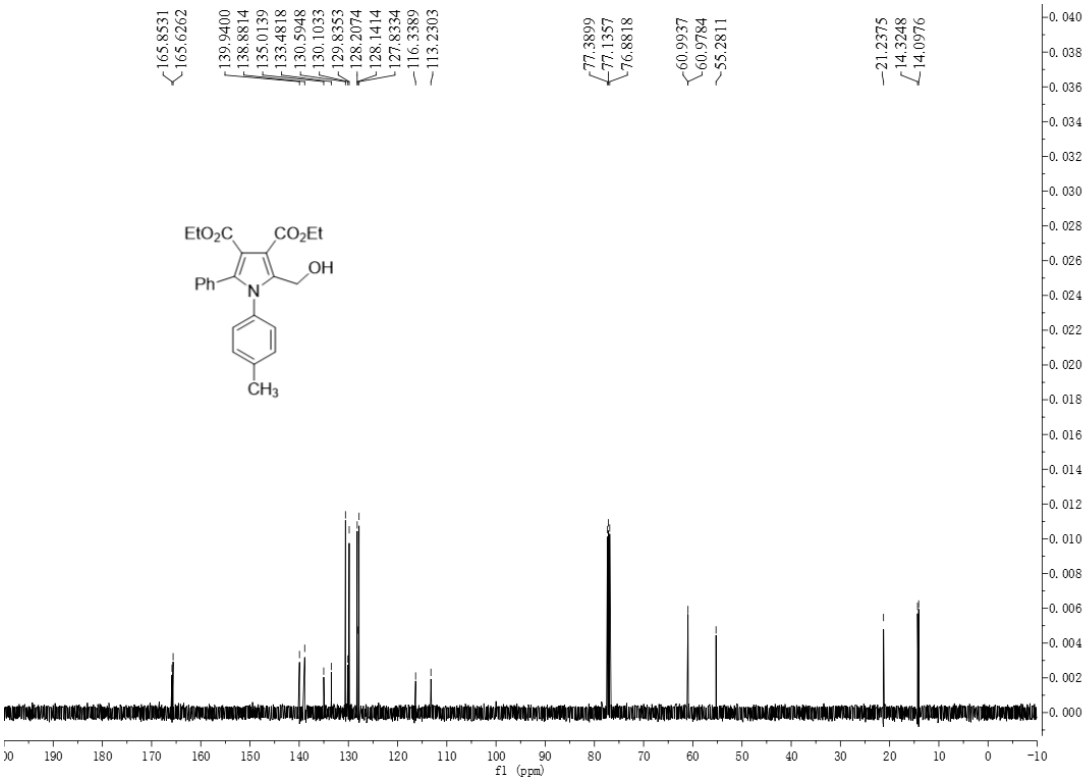


Diethyl 2-(hydroxymethyl)-5-phenyl-1-(*p*-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ae)

^{1}H NMR (500 MHz, $CDCl_3$)

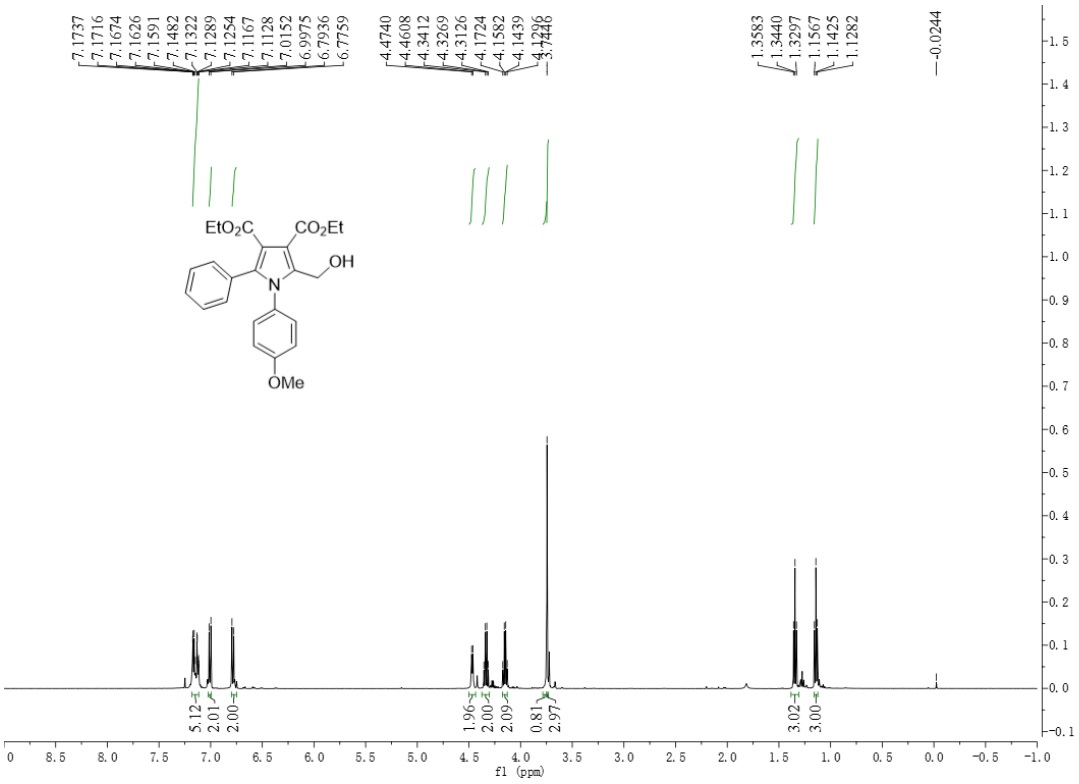


^{13}C NMR (125 MHz, $CDCl_3$)

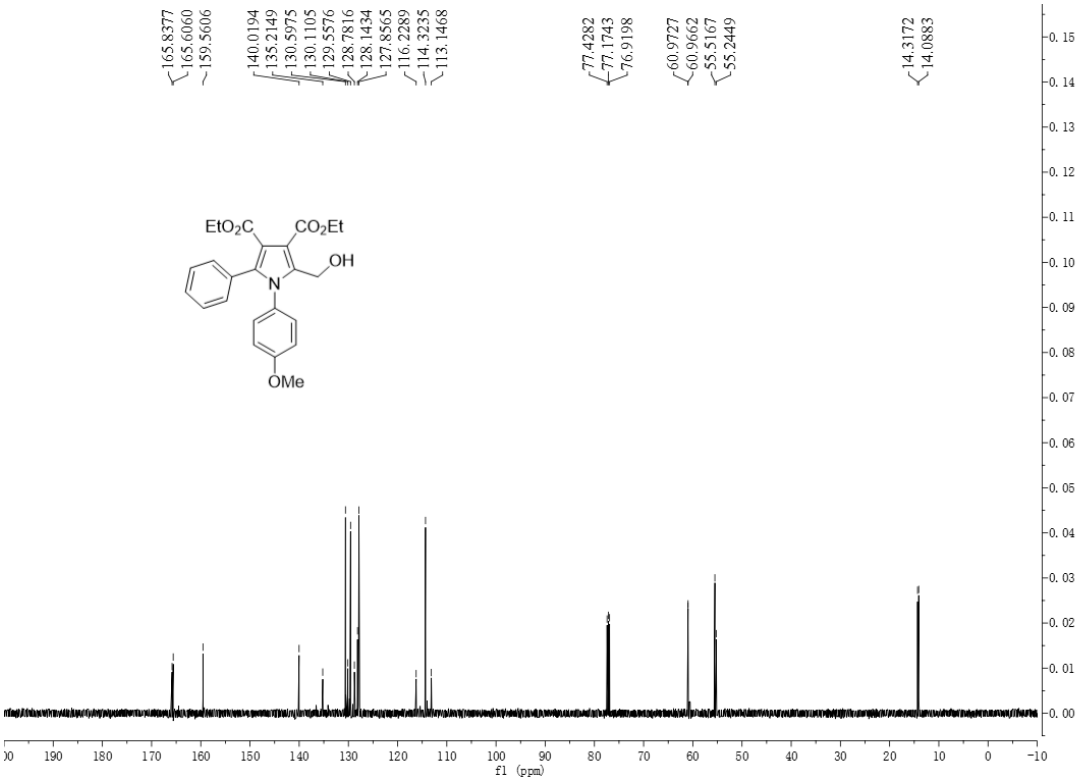


Diethyl 2-(hydroxymethyl)-1-(4-methoxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4af)

^{1}H NMR (500 MHz, $CDCl_3$)

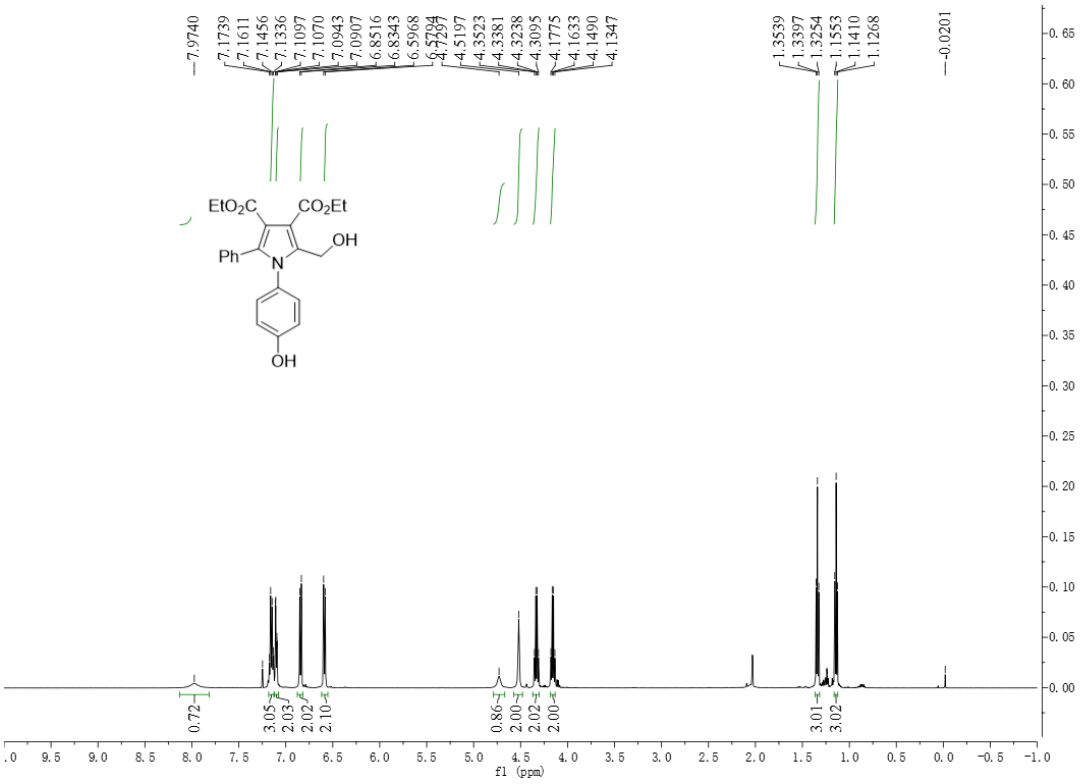


^{13}C NMR (125 MHz, $CDCl_3$)

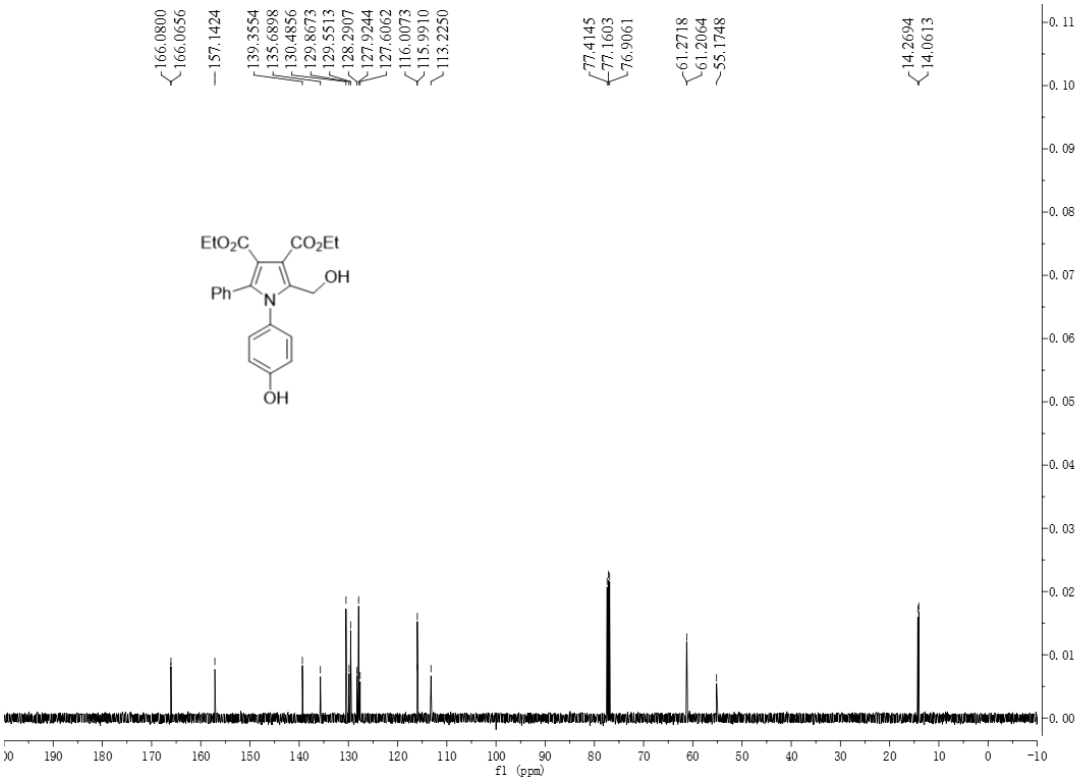


Diethyl 2-(hydroxymethyl)-1-(4-hydroxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ag)

^{1}H NMR (500 MHz, $CDCl_3$)

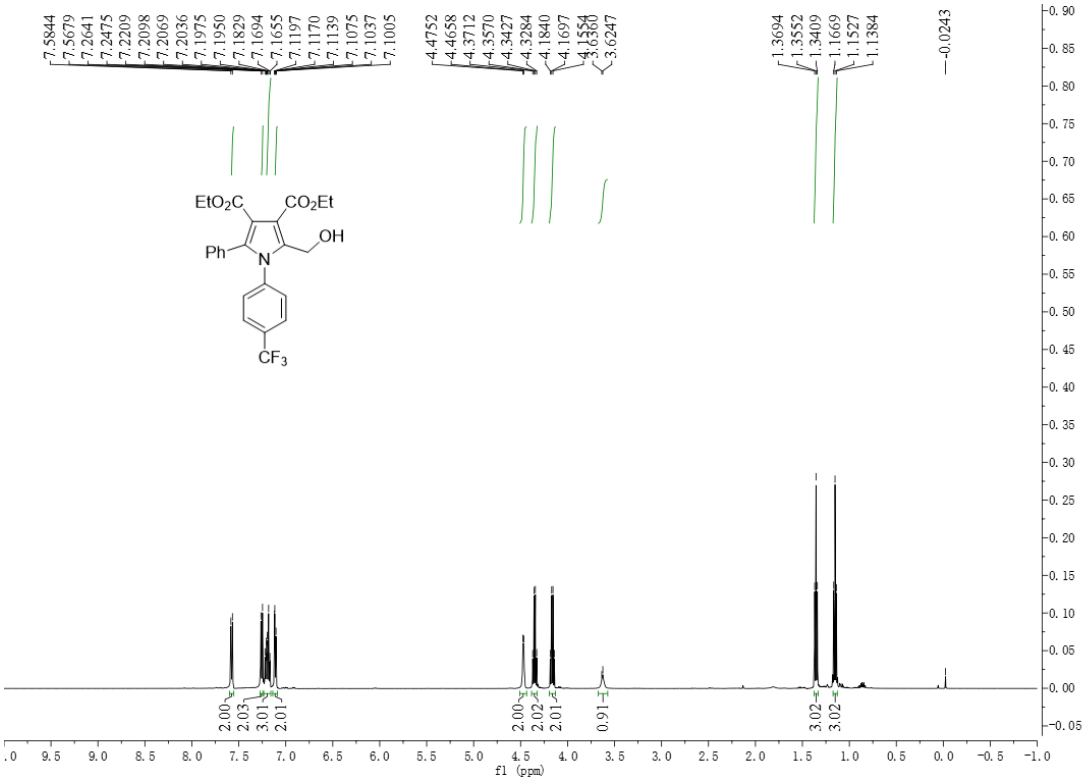


^{13}C NMR (125 MHz, $CDCl_3$)

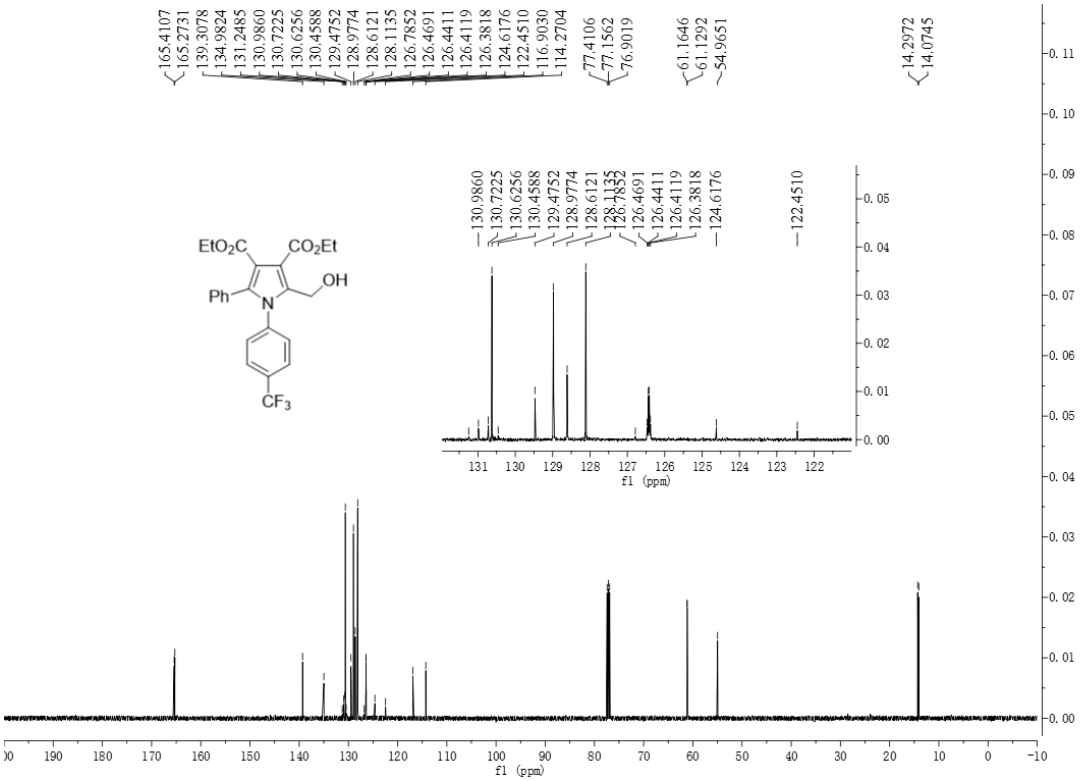


Diethyl 2-(hydroxymethyl)-5-phenyl-1-(4-(trifluoromethyl)phenyl)-1*H*-pyrrole-3,4-dicarboxylate (4ah)

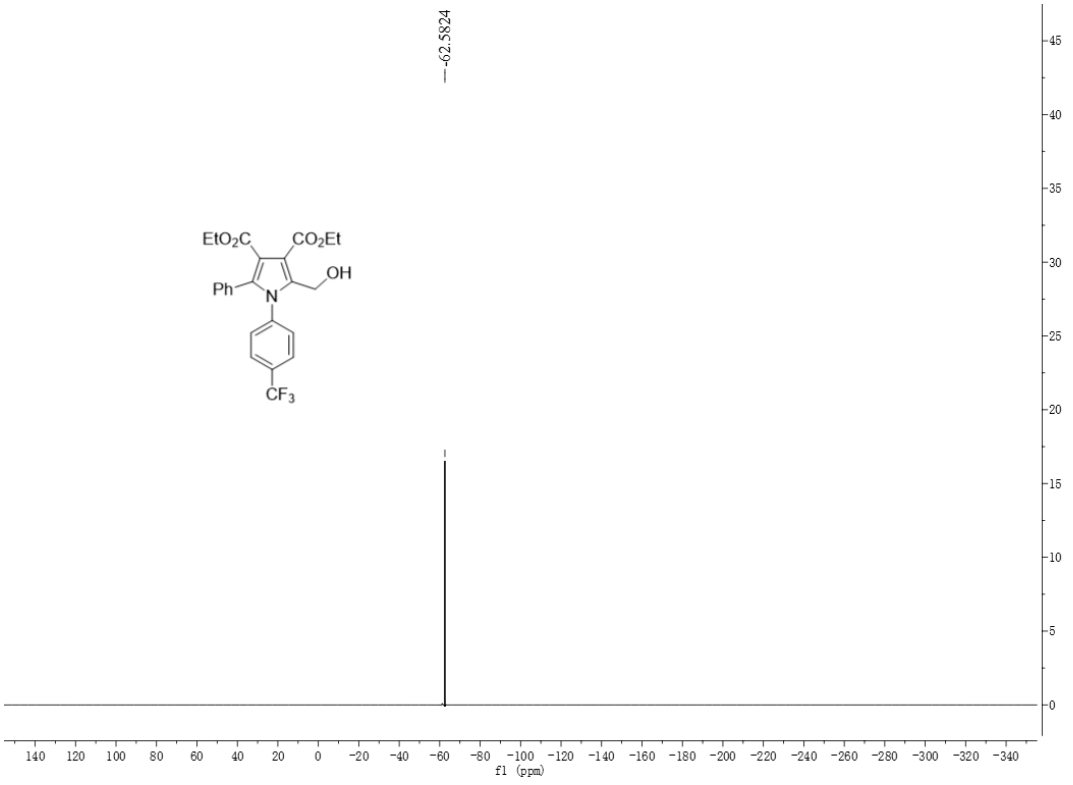
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)

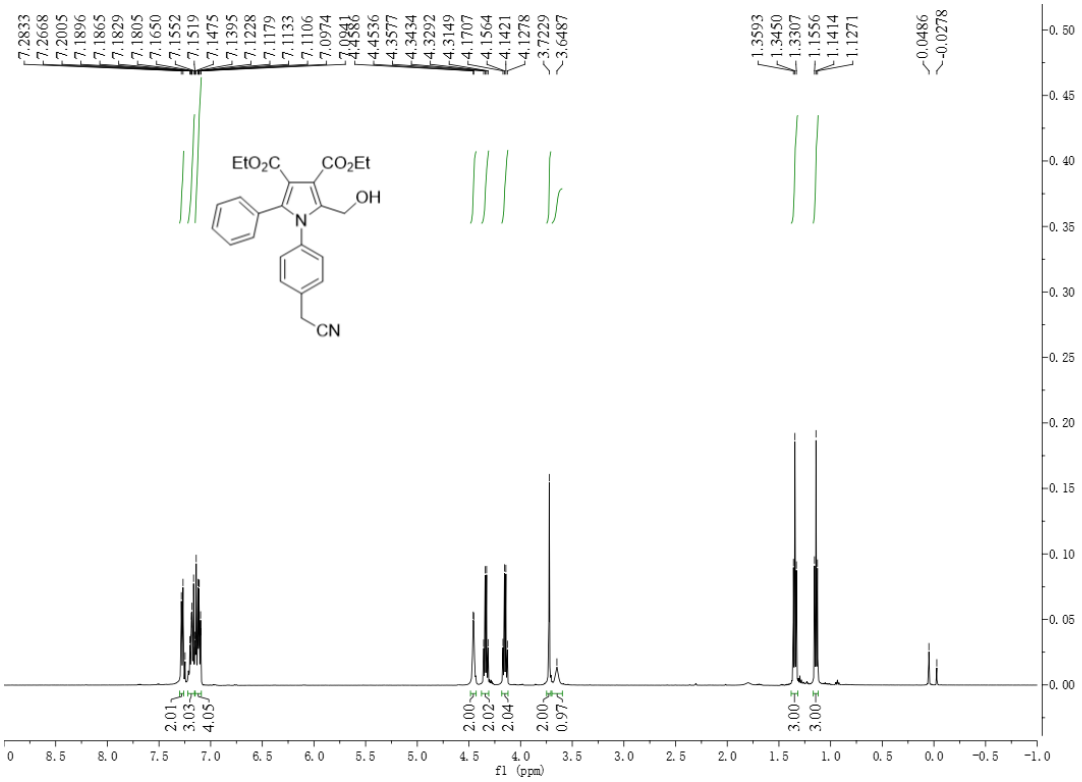


^{19}F NMR (470 MHz, $CDCl_3$)

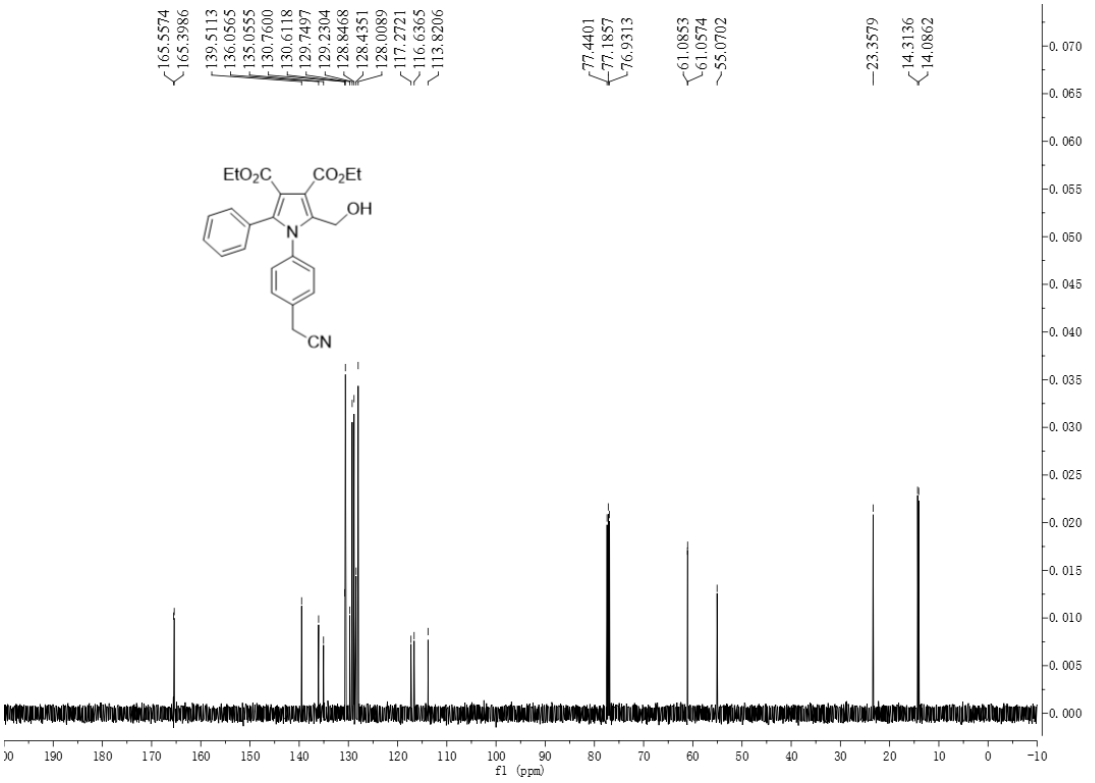


Diethyl 1-(4-(cyanomethyl)phenyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ai)

^{1}H NMR (500 MHz, $CDCl_3$)

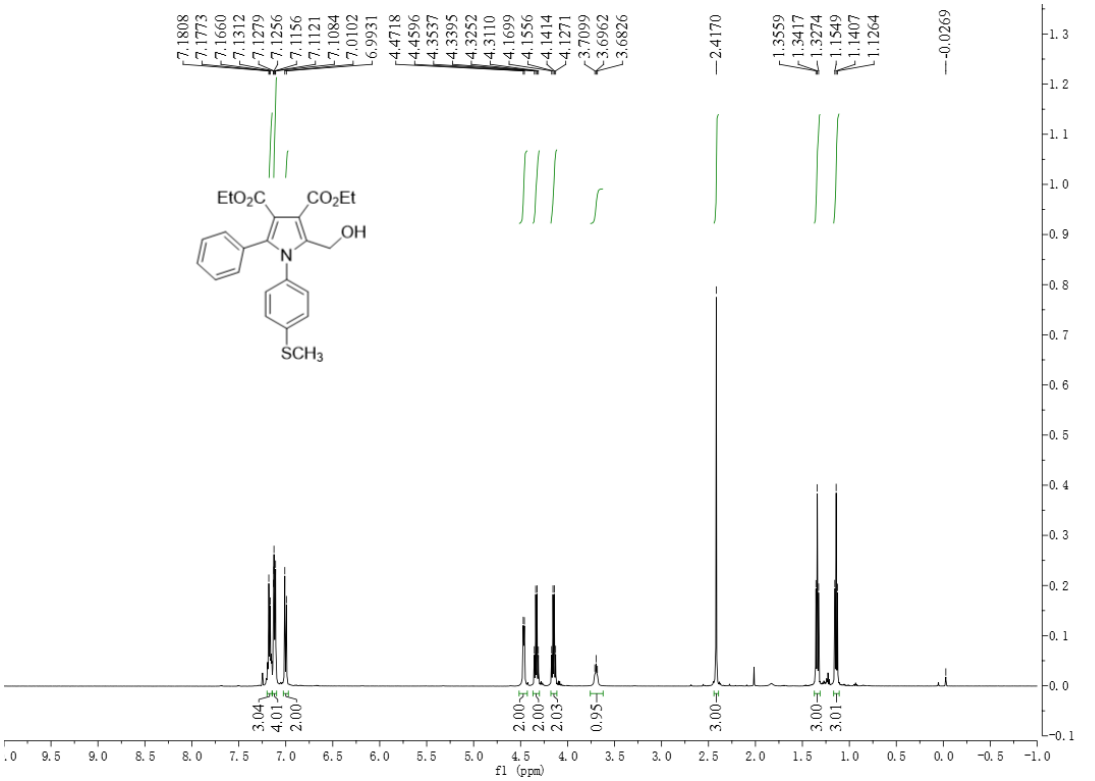


^{13}C NMR (125 MHz, $CDCl_3$)

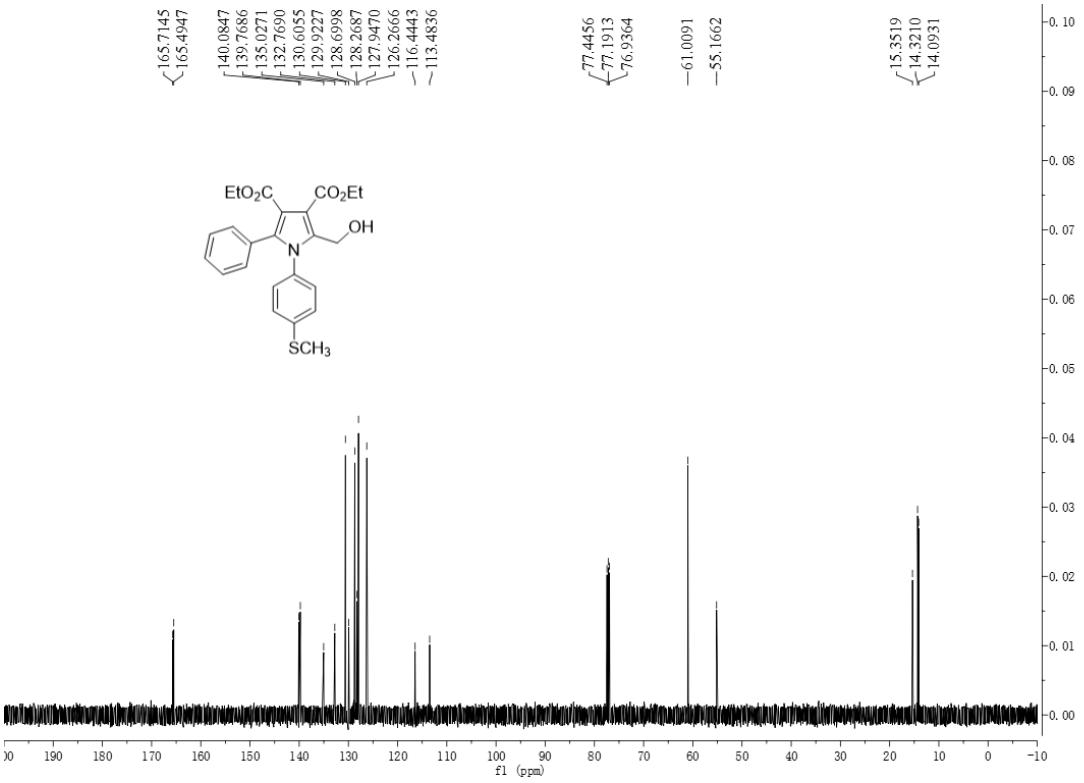


Diethyl 2-(hydroxymethyl)-1-(4-(methylthio)phenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4aj)

^{1}H NMR (500 MHz, $CDCl_3$)

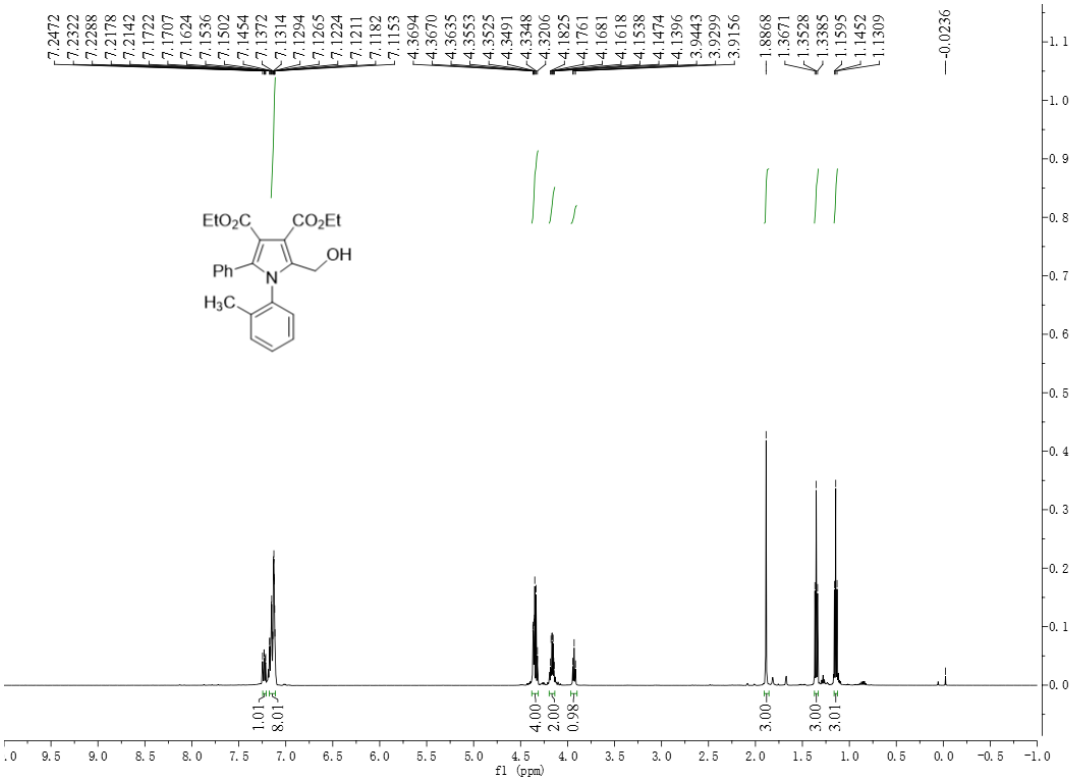


^{13}C NMR (125 MHz, $CDCl_3$)

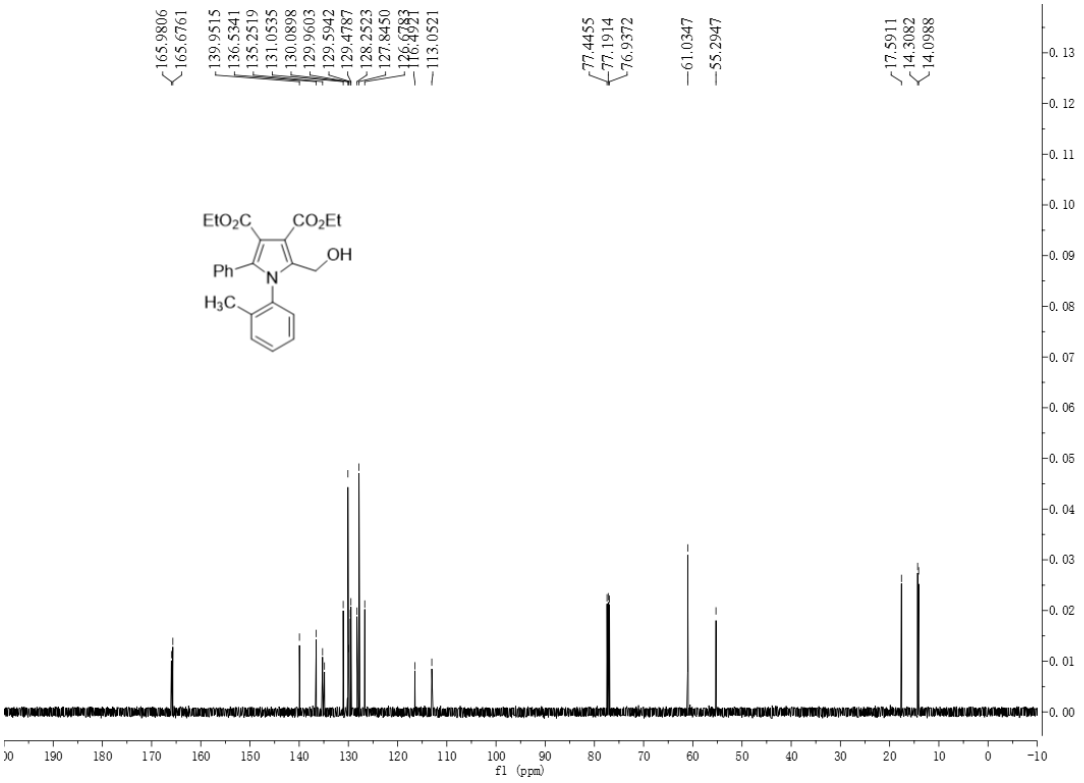


Diethyl 2-(hydroxymethyl)-5-phenyl-1-(o-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (4ak)

^{1}H NMR (500 MHz, $CDCl_3$)

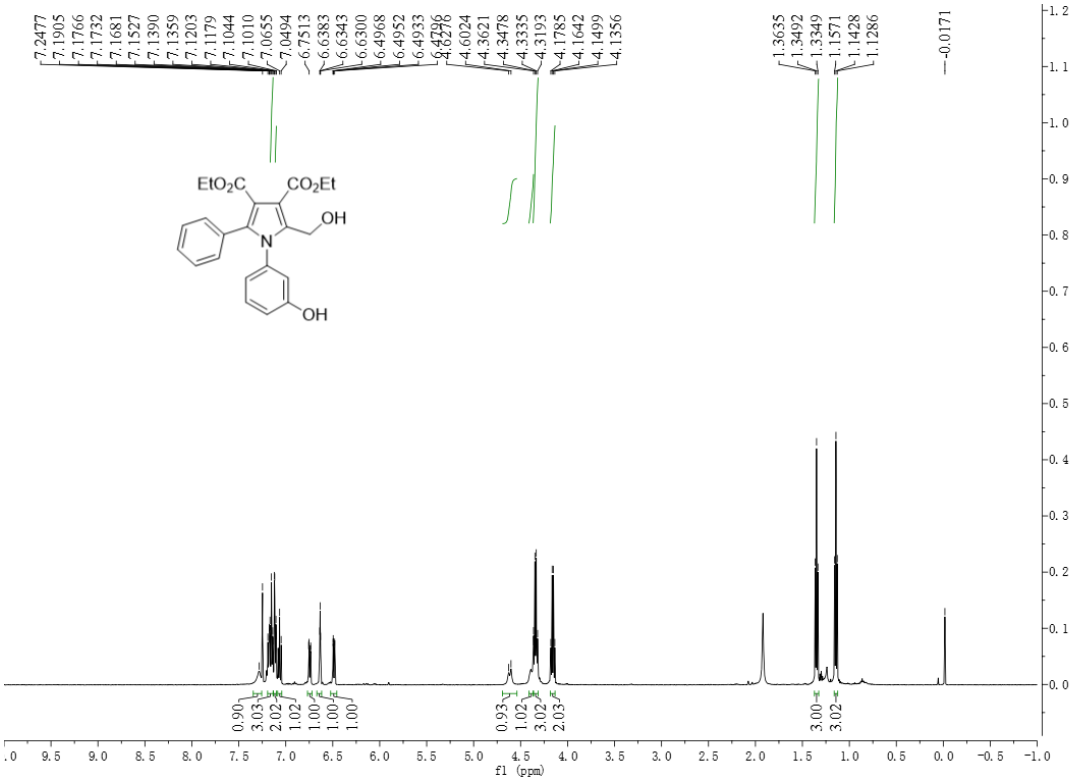


^{13}C NMR (125 MHz, $CDCl_3$)

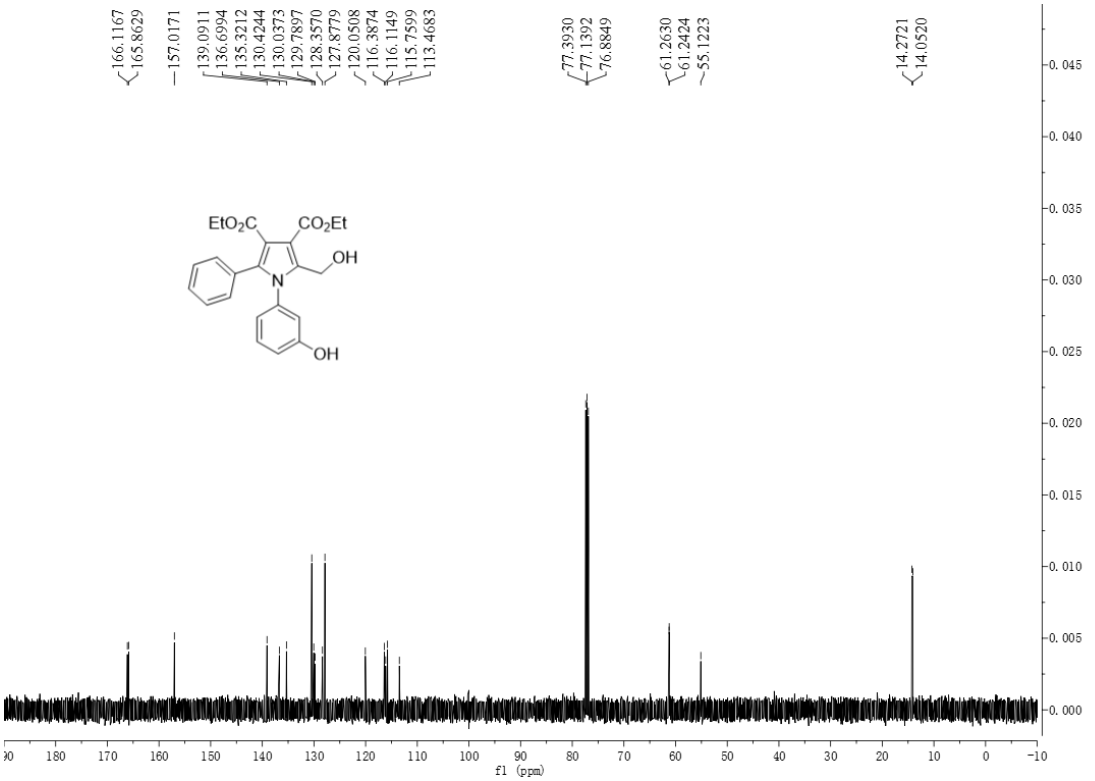


Diethyl 2-(hydroxymethyl)-1-(3-hydroxyphenyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4al)

^{1}H NMR (500 MHz, $CDCl_3$)

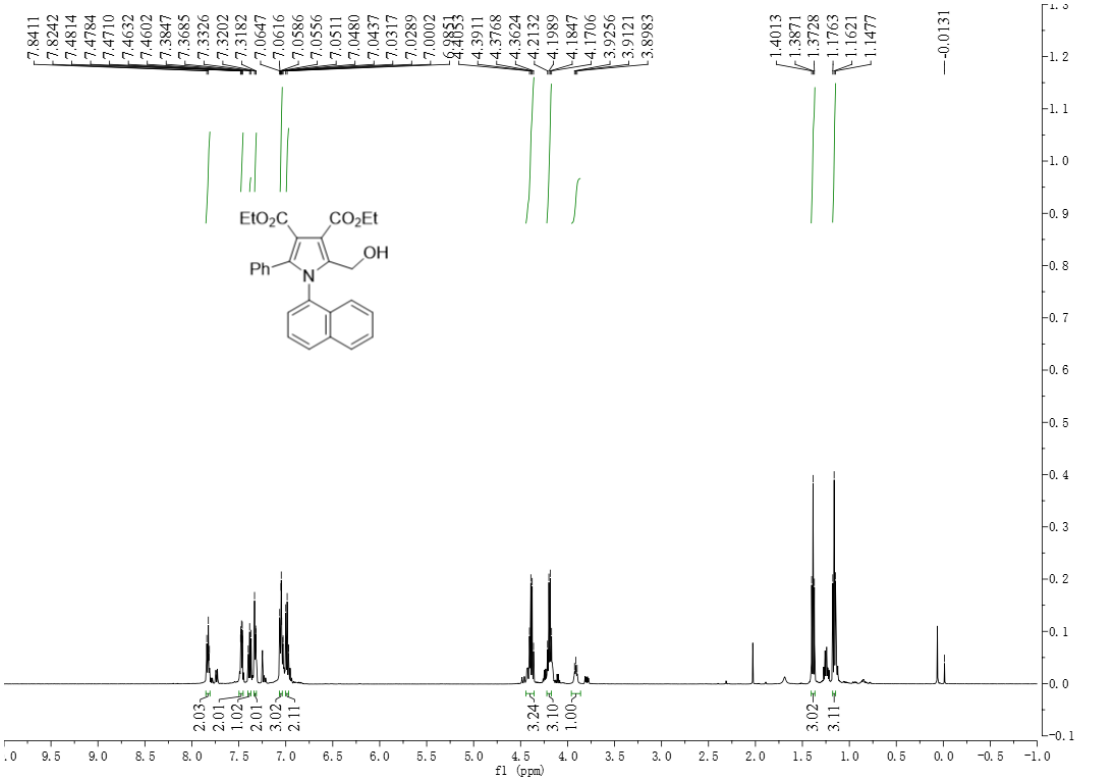


^{13}C NMR (125 MHz, $CDCl_3$)

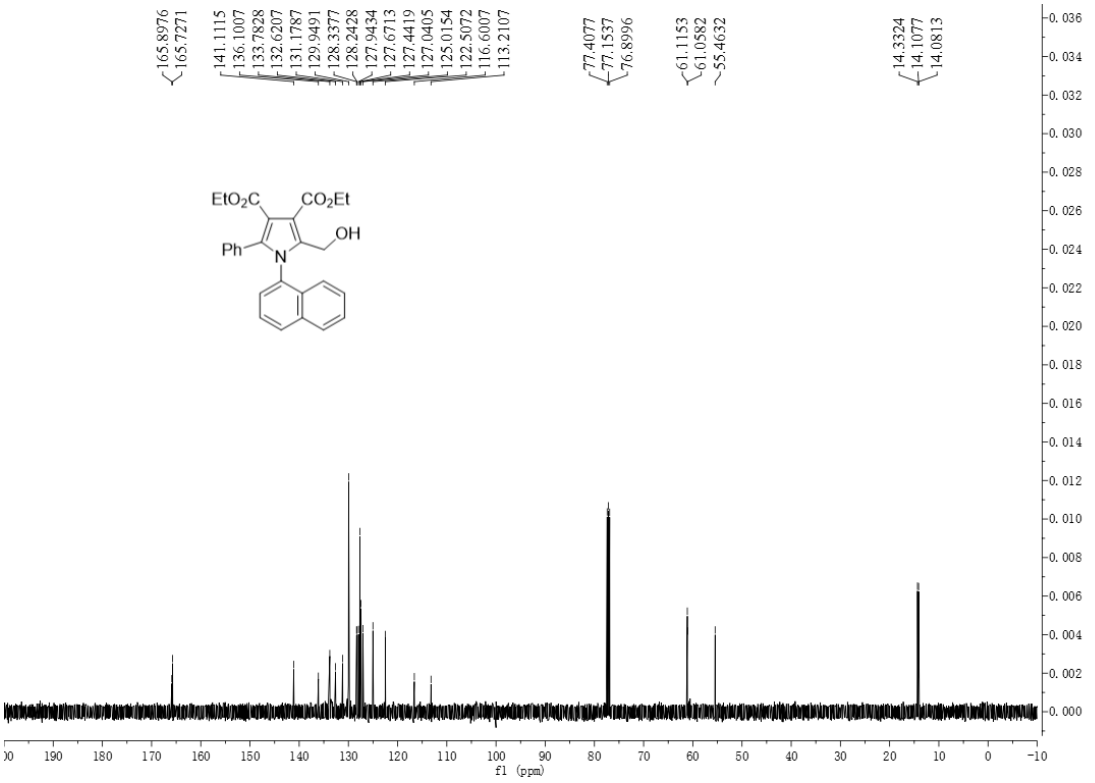


Diethyl 2-(hydroxymethyl)-1-(naphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4am)

^{1}H NMR (500 MHz, $CDCl_3$)

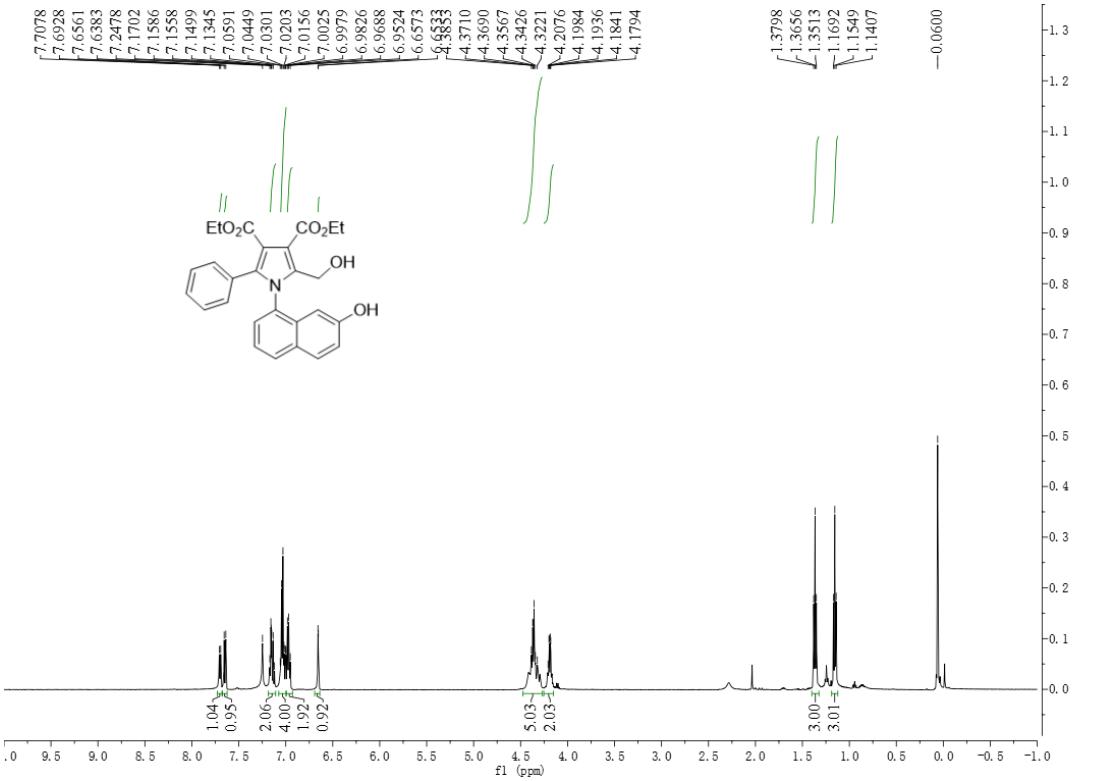


^{13}C NMR (125 MHz, $CDCl_3$)

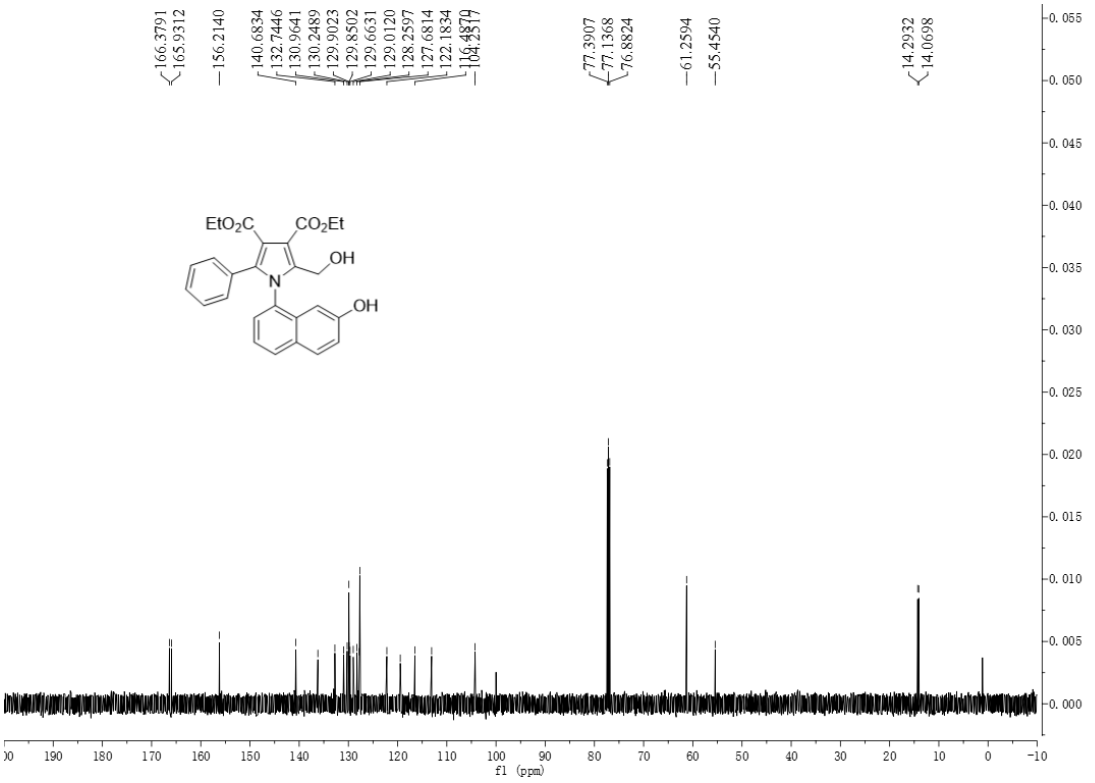


Diethyl 2-(hydroxymethyl)-1-(7-hydroxynaphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4an)

^{1}H NMR (500 MHz, $CDCl_3$)

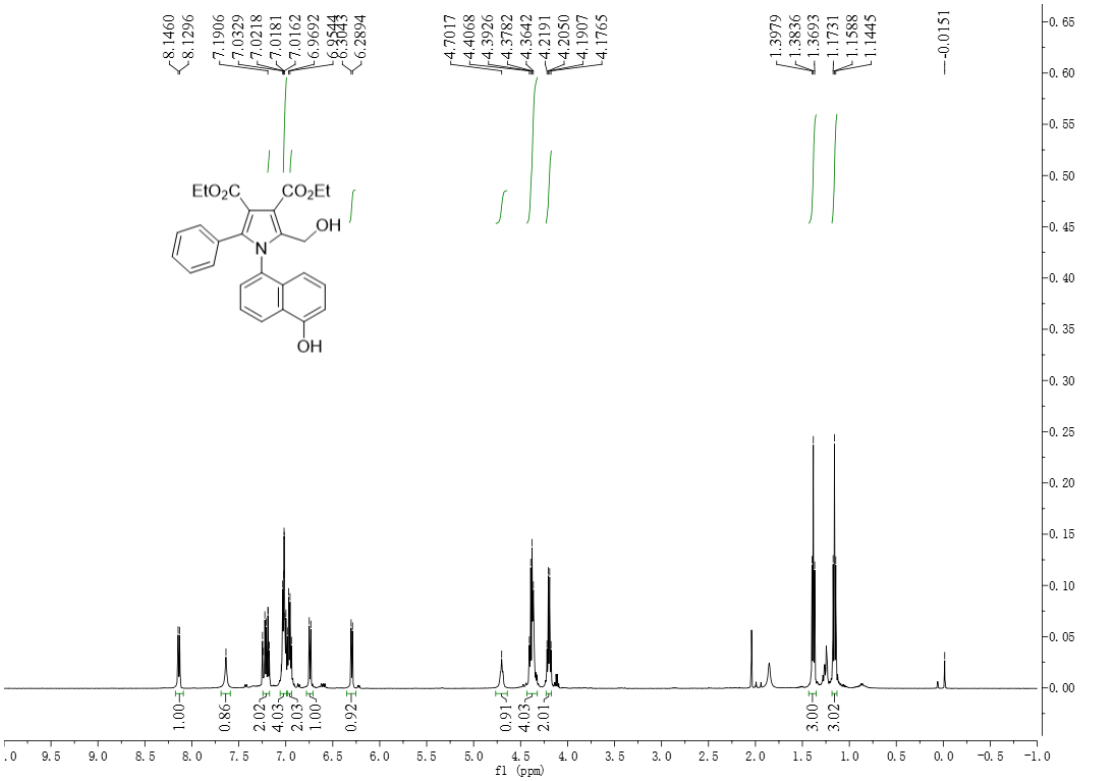


^{13}C NMR (125 MHz, $CDCl_3$)

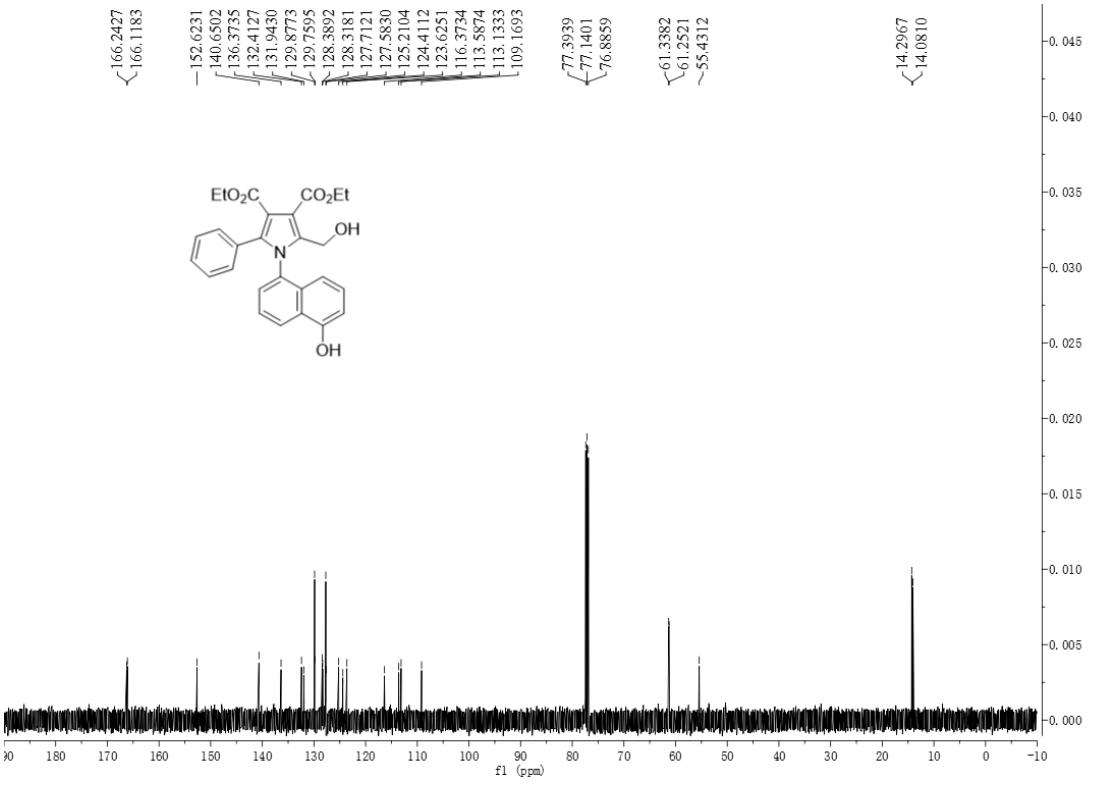


Diethyl 2-(hydroxymethyl)-1-(5-hydroxynaphthalen-1-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ao)

^{1}H NMR (500 MHz, $CDCl_3$)

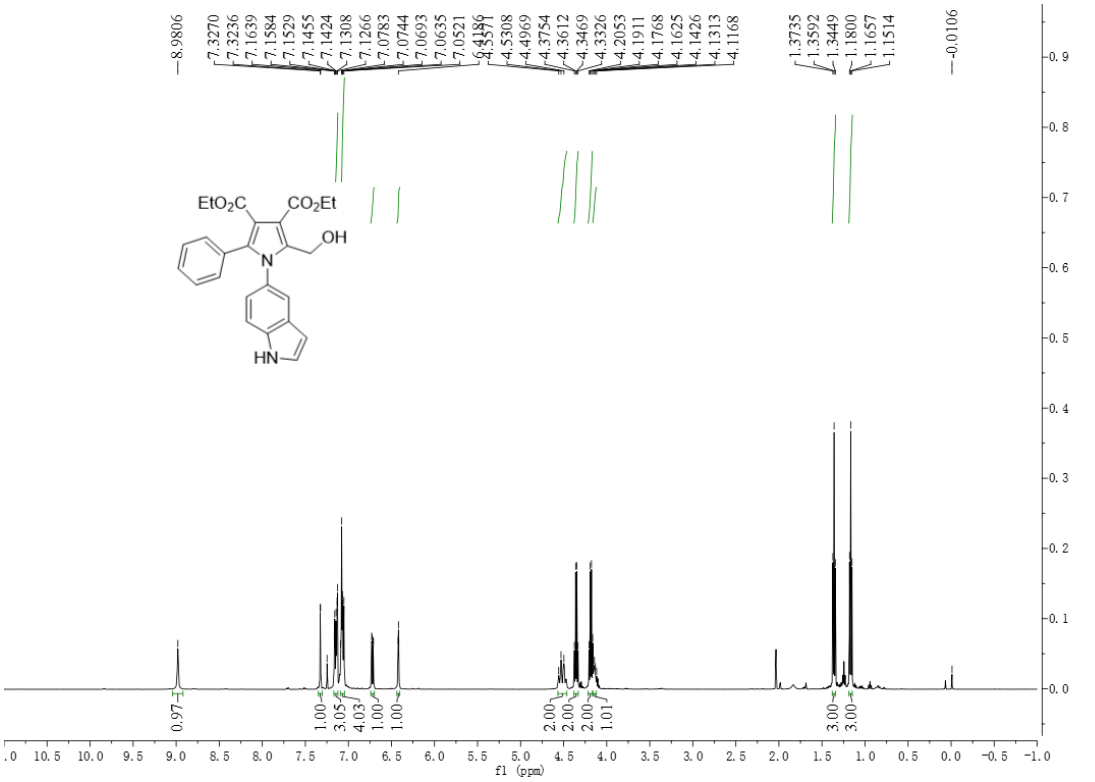


^{13}C NMR (125 MHz, $CDCl_3$)

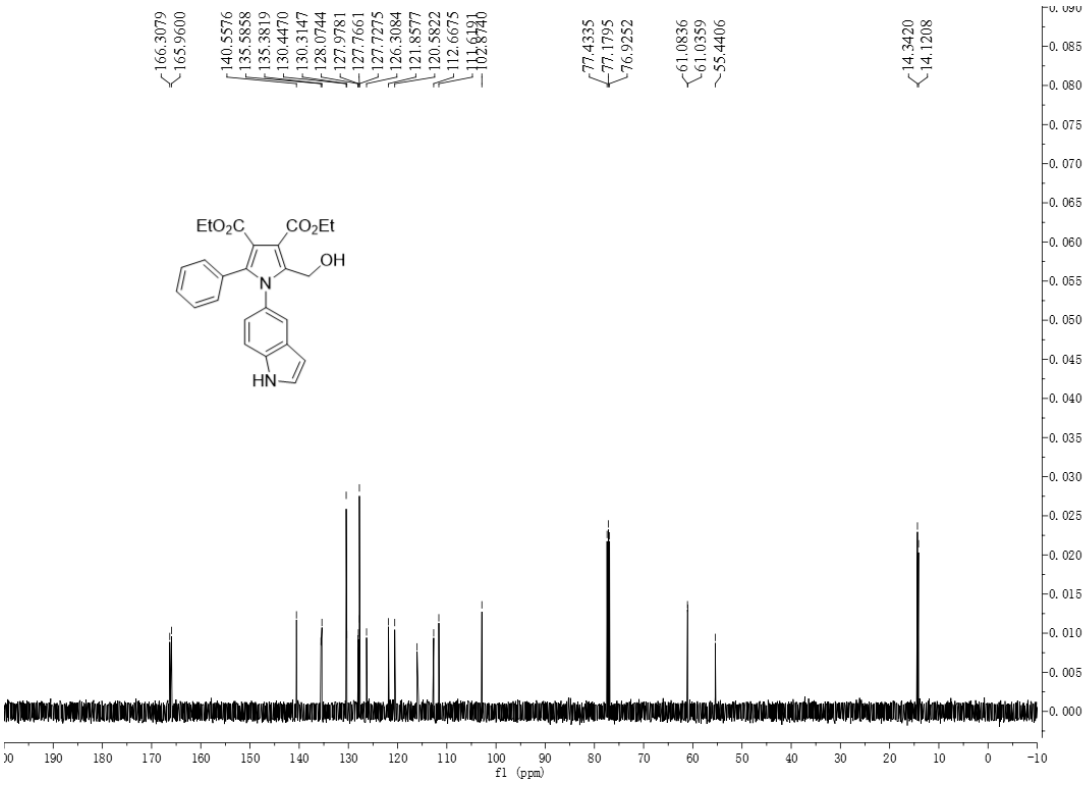


Diethyl 2-(hydroxymethyl)-1-(1*H*-indol-5-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ap)

^{1}H NMR (500 MHz, $CDCl_3$)

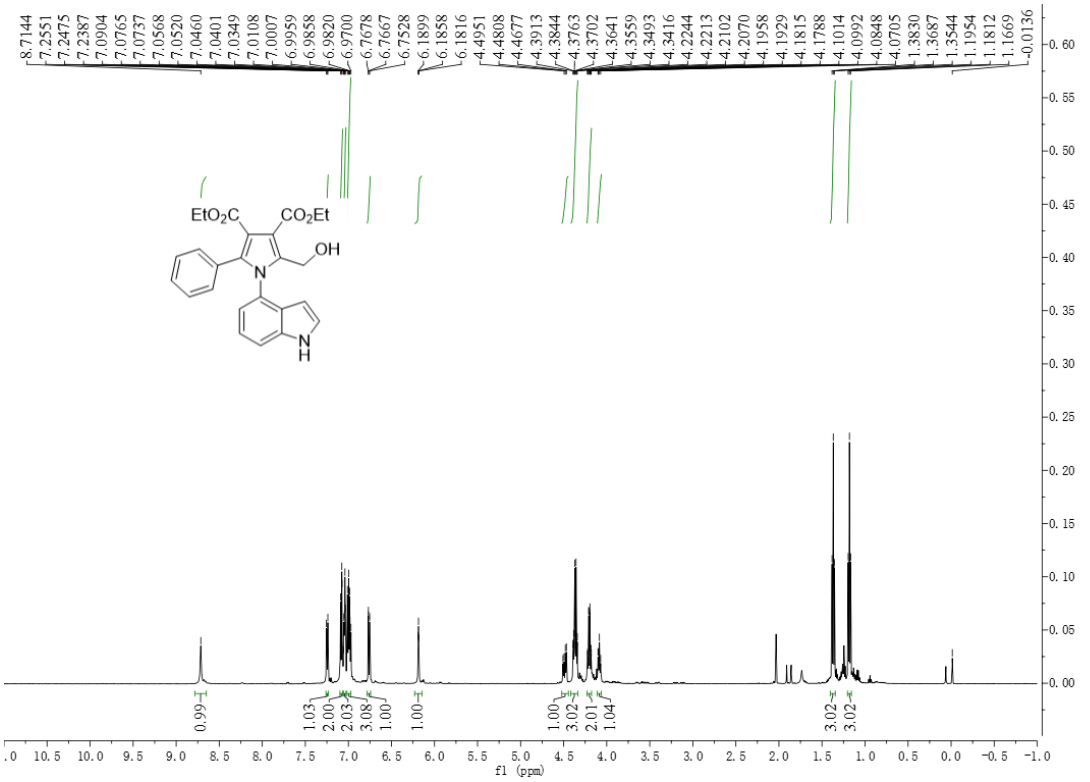


^{13}C NMR (125 MHz, $CDCl_3$)

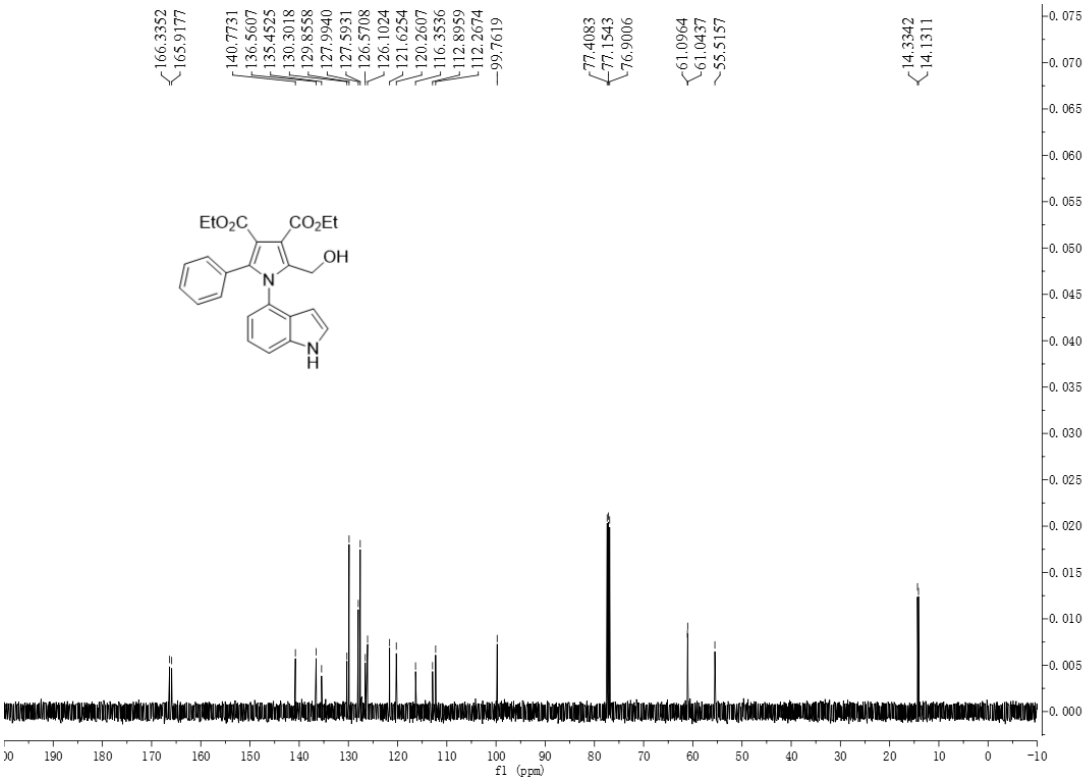


Diethyl 2-(hydroxymethyl)-1-(1*H*-indol-4-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4aq)

^{1}H NMR (500 MHz, $CDCl_3$)

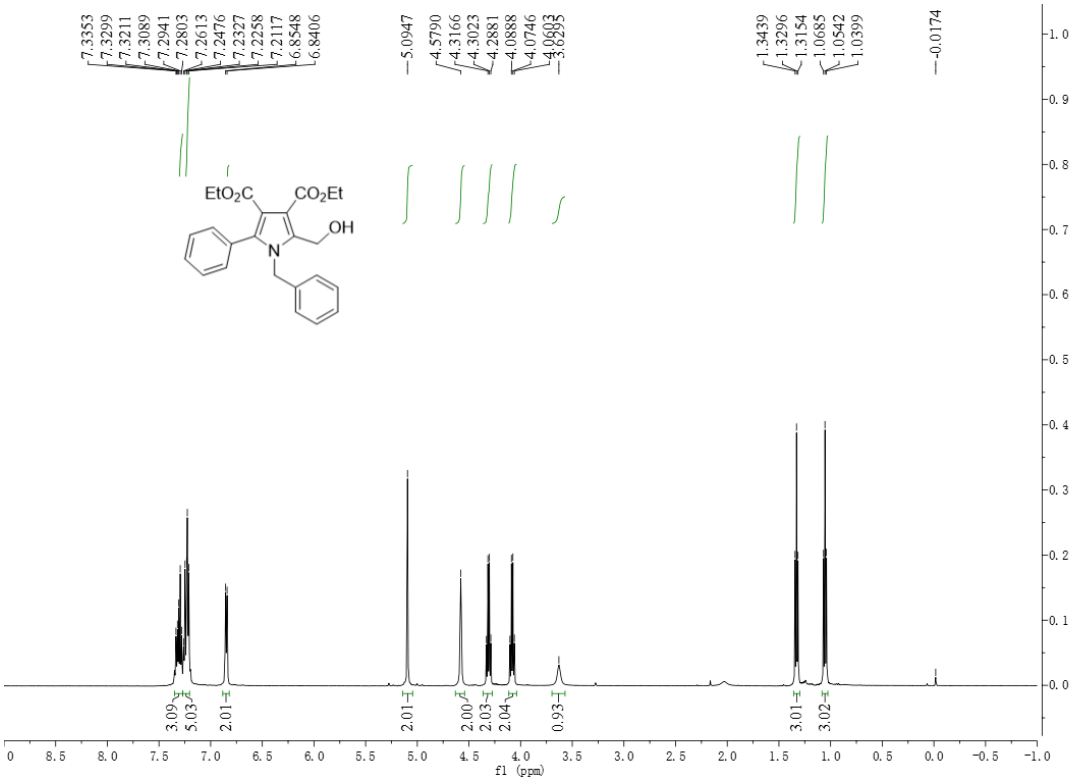


^{13}C NMR (125 MHz, $CDCl_3$)

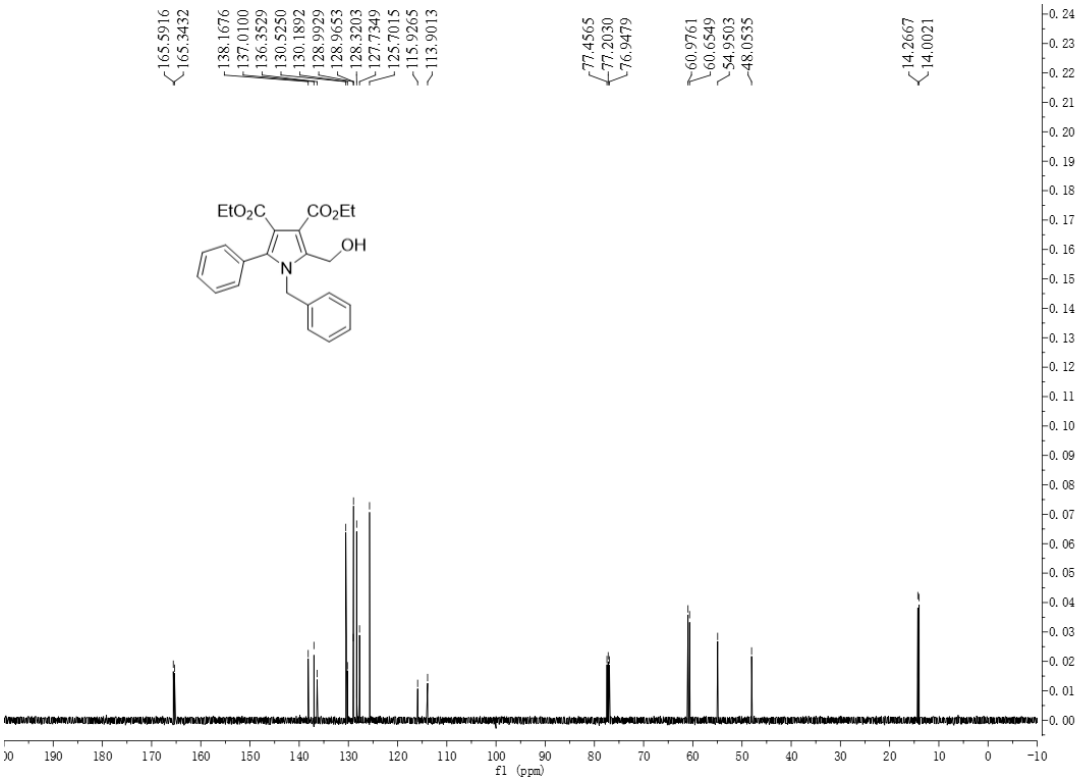


Diethyl 1-benzyl-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4ar)

^{1}H NMR (500 MHz, $CDCl_3$)

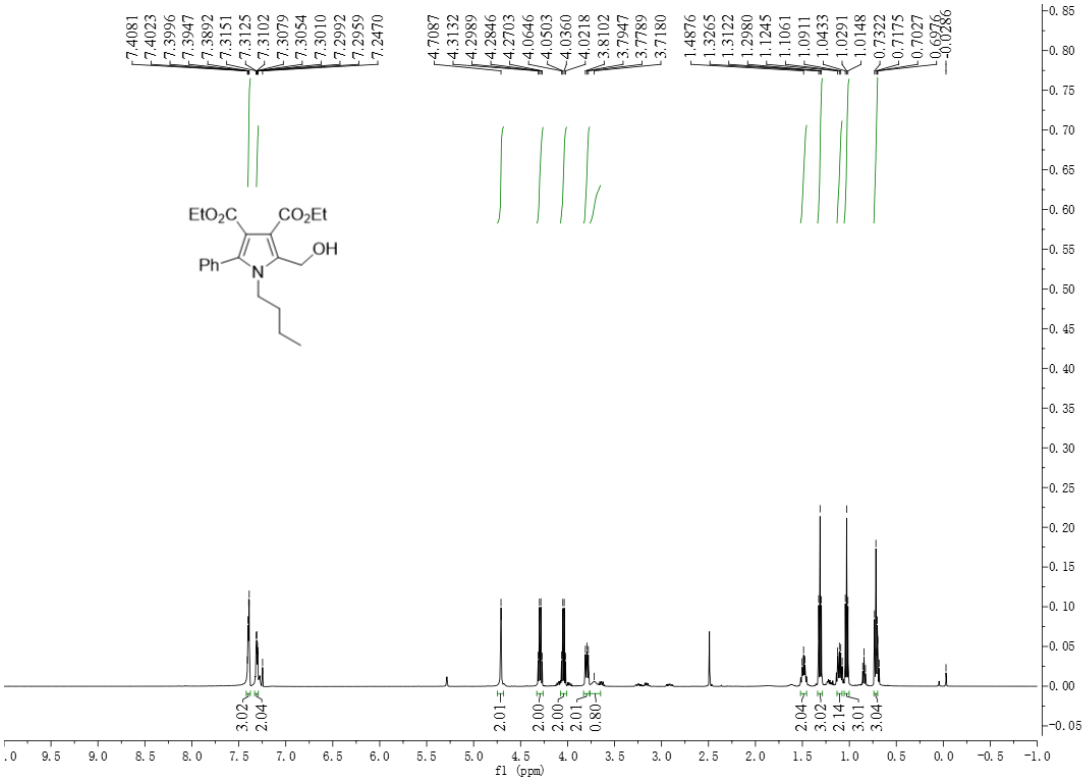


^{13}C NMR (125 MHz, $CDCl_3$)

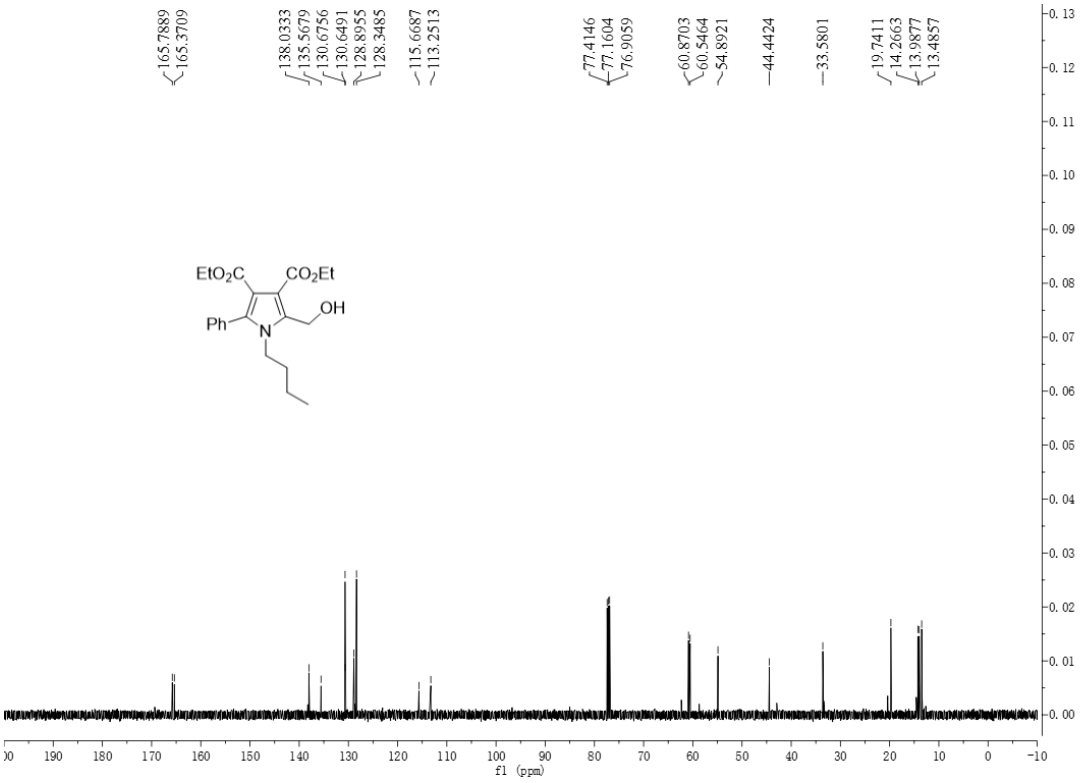


Diethyl 1-butyl-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (4as)

^{1}H NMR (500 MHz, $CDCl_3$)

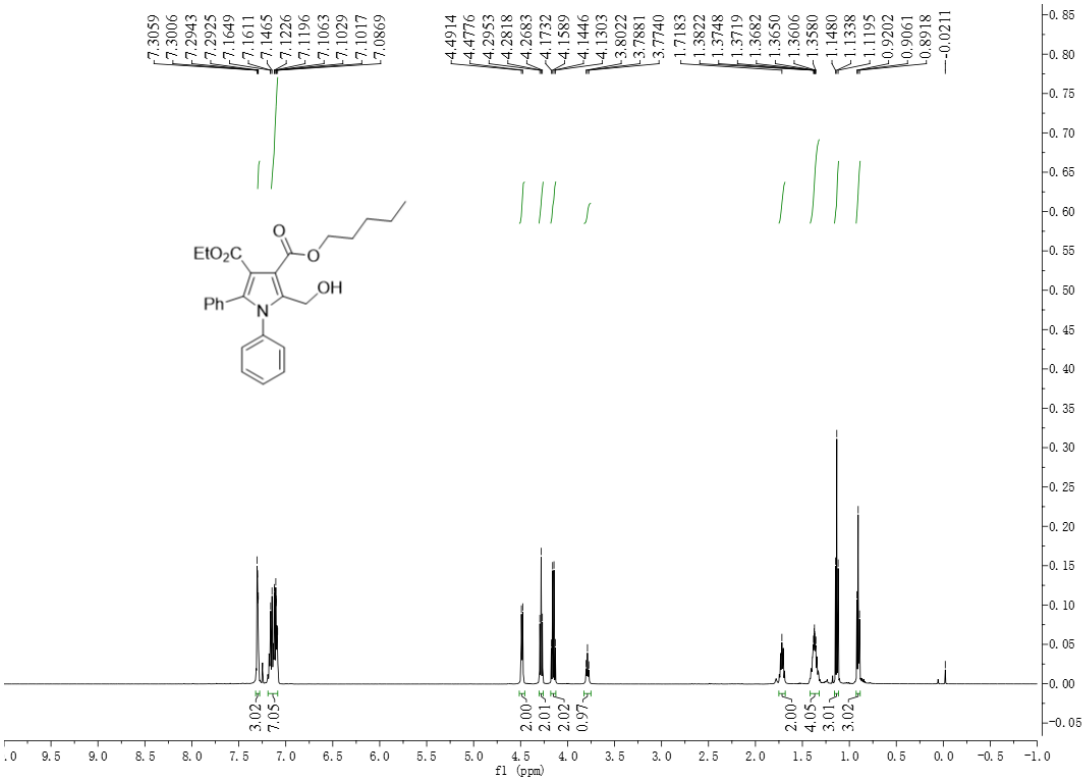


^{13}C NMR (125 MHz, $CDCl_3$)

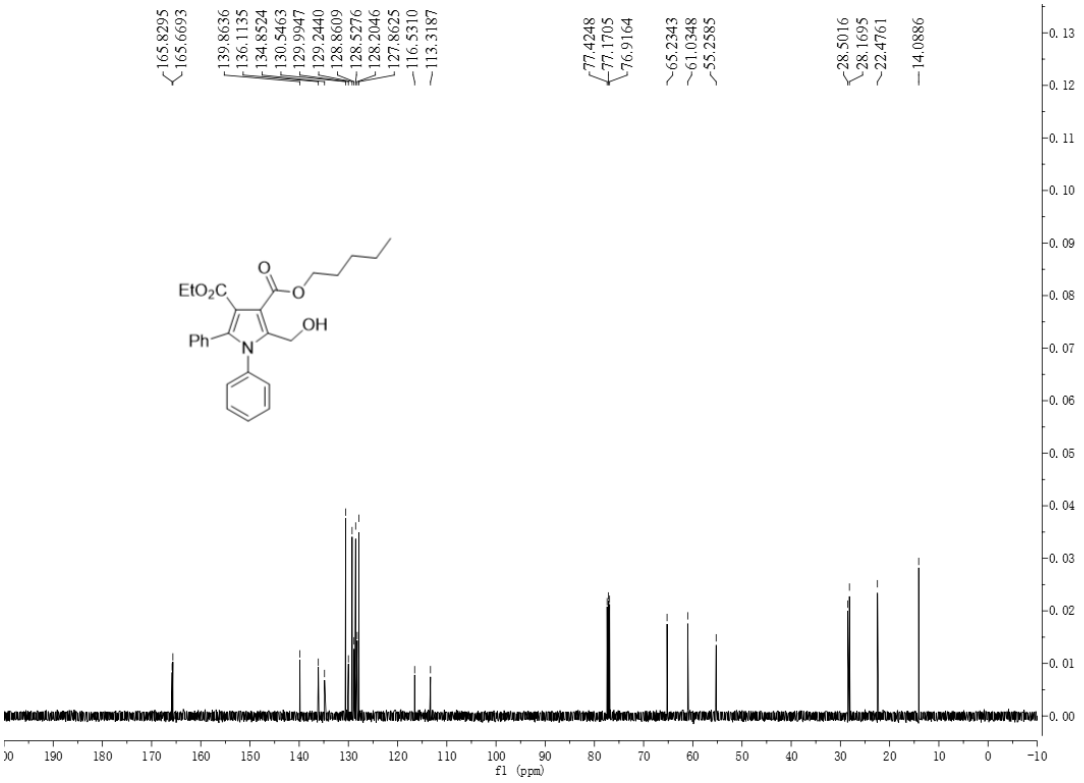


3-Ethyl 4-pentyl 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4at)

^{1}H NMR (500 MHz, $CDCl_3$)

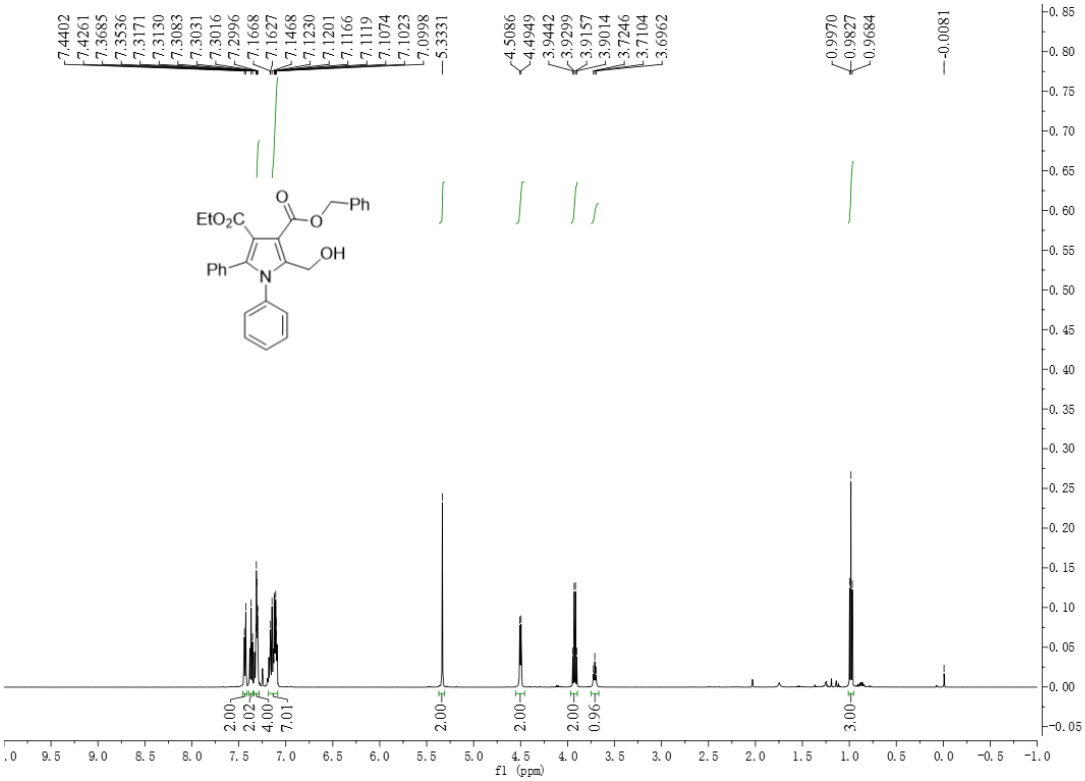


^{13}C NMR (125 MHz, $CDCl_3$)

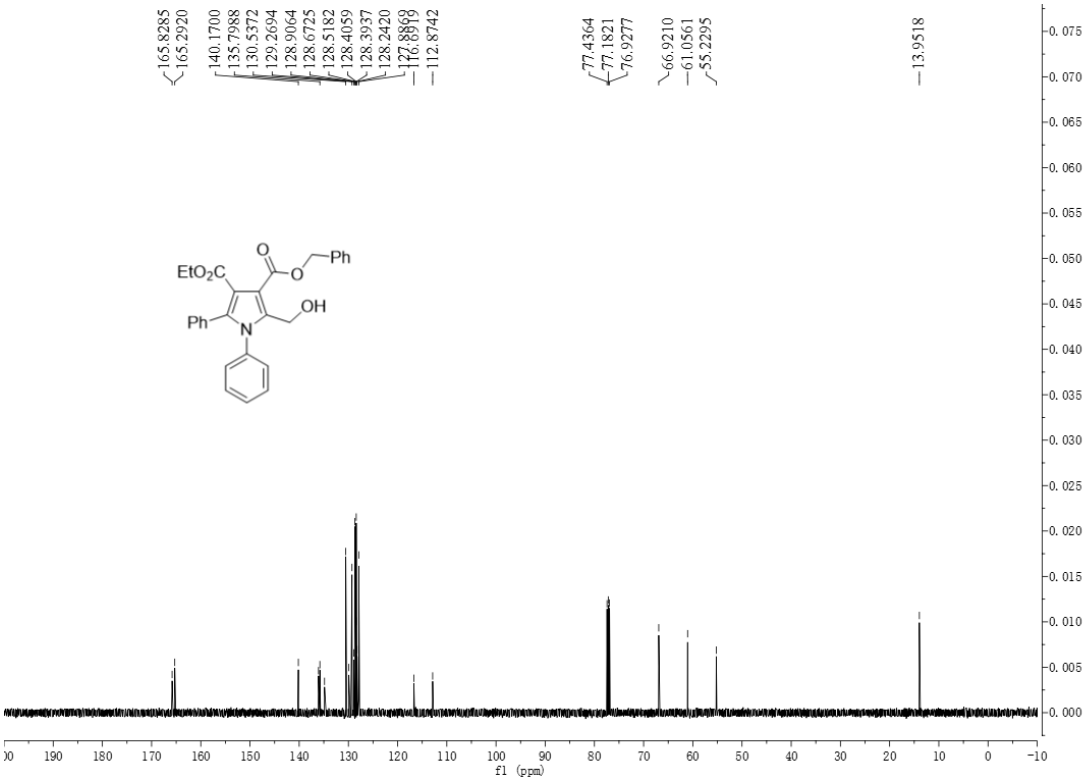


3-Benzyl 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4au)

^{1}H NMR (500 MHz, $CDCl_3$)

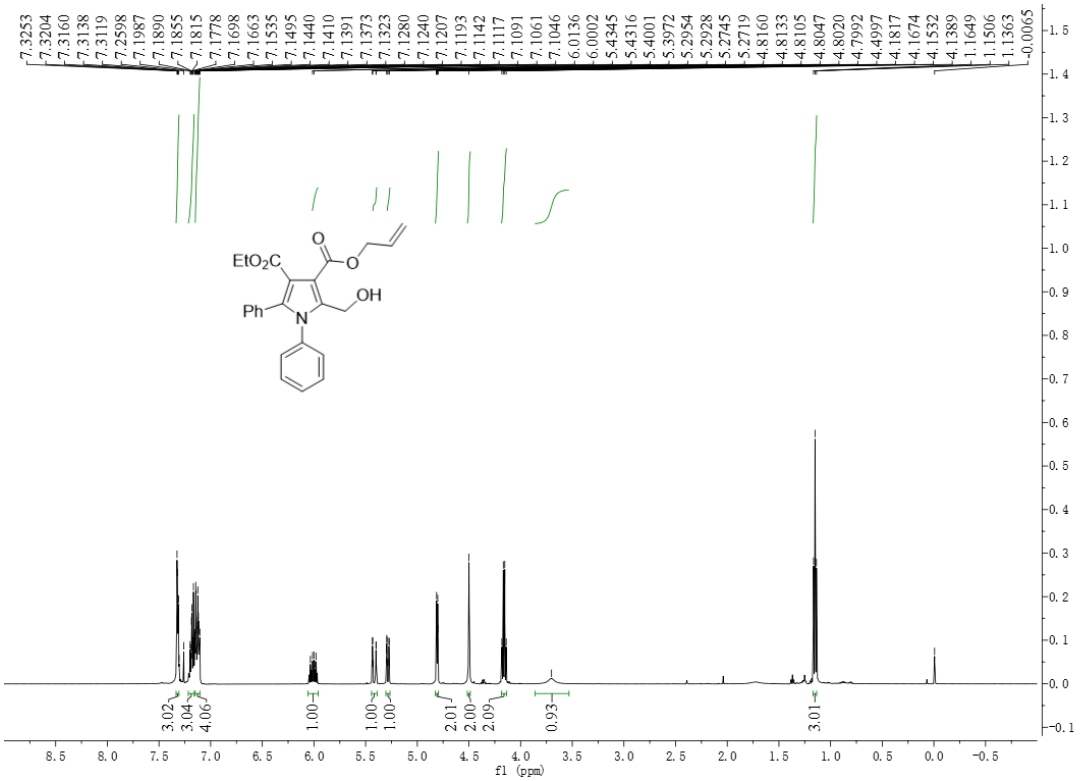


^{13}C NMR (125 MHz, $CDCl_3$)

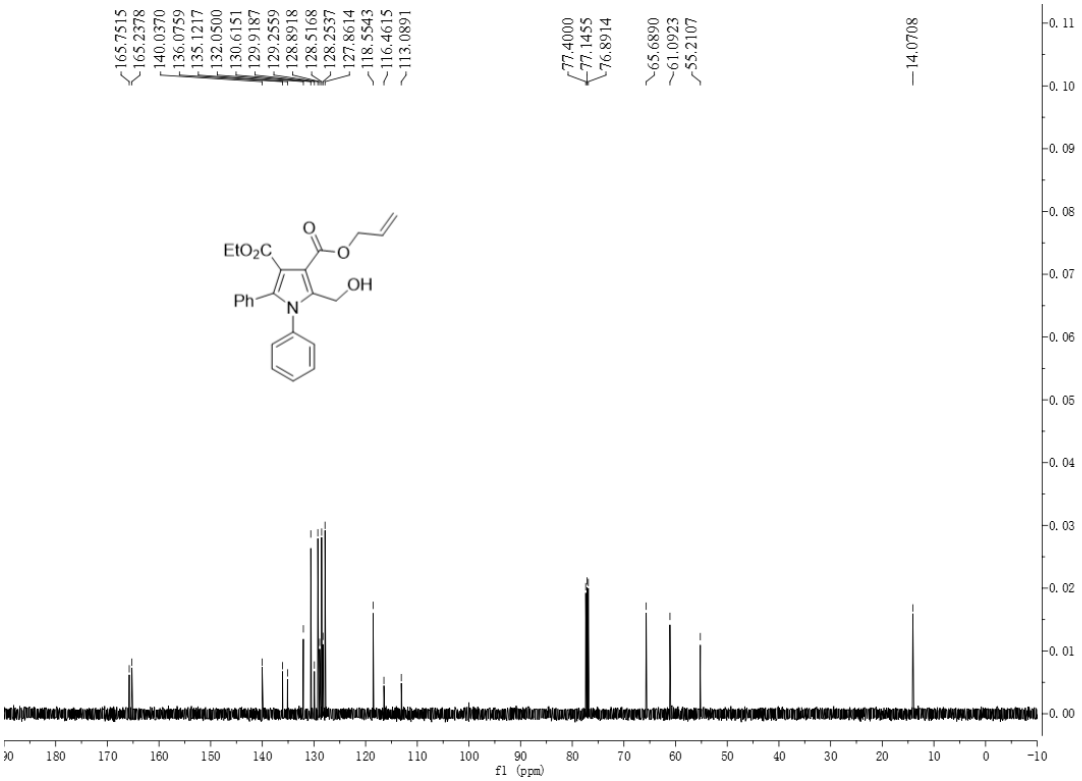


3-Allyl 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4av)

^{1}H NMR (500 MHz, $CDCl_3$)

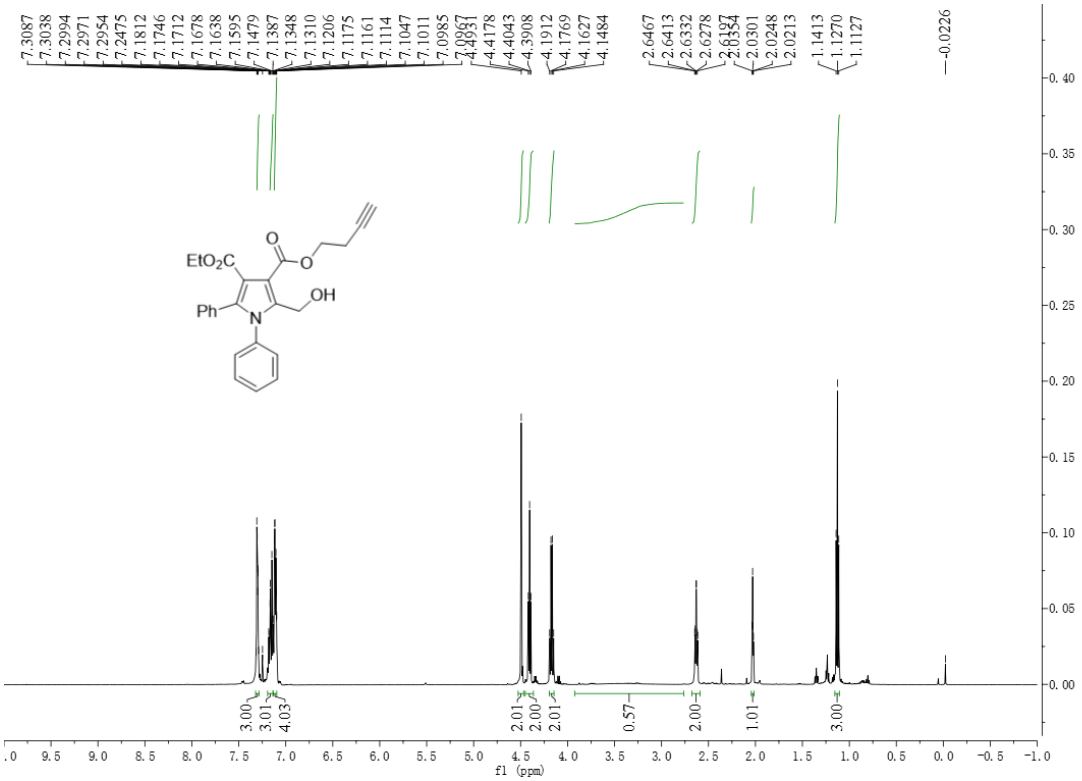


^{13}C NMR (125 MHz, $CDCl_3$)

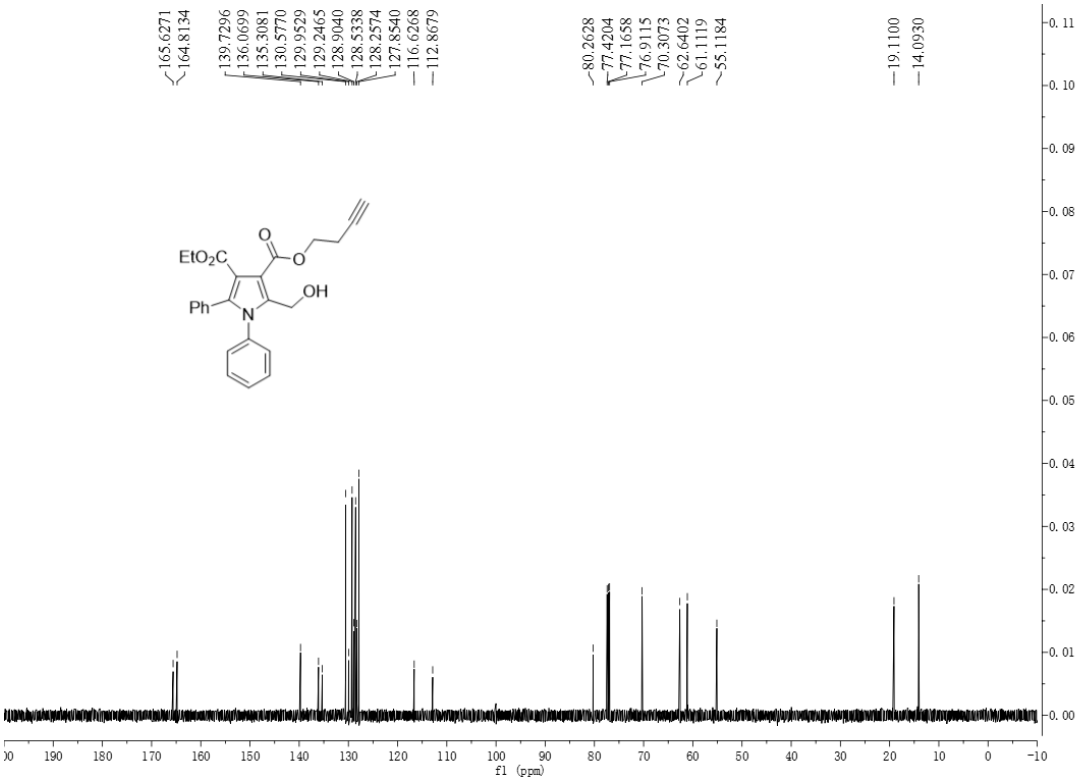


3-(But-3-yn-1-yl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4aw)

^{1}H NMR (500 MHz, $CDCl_3$)

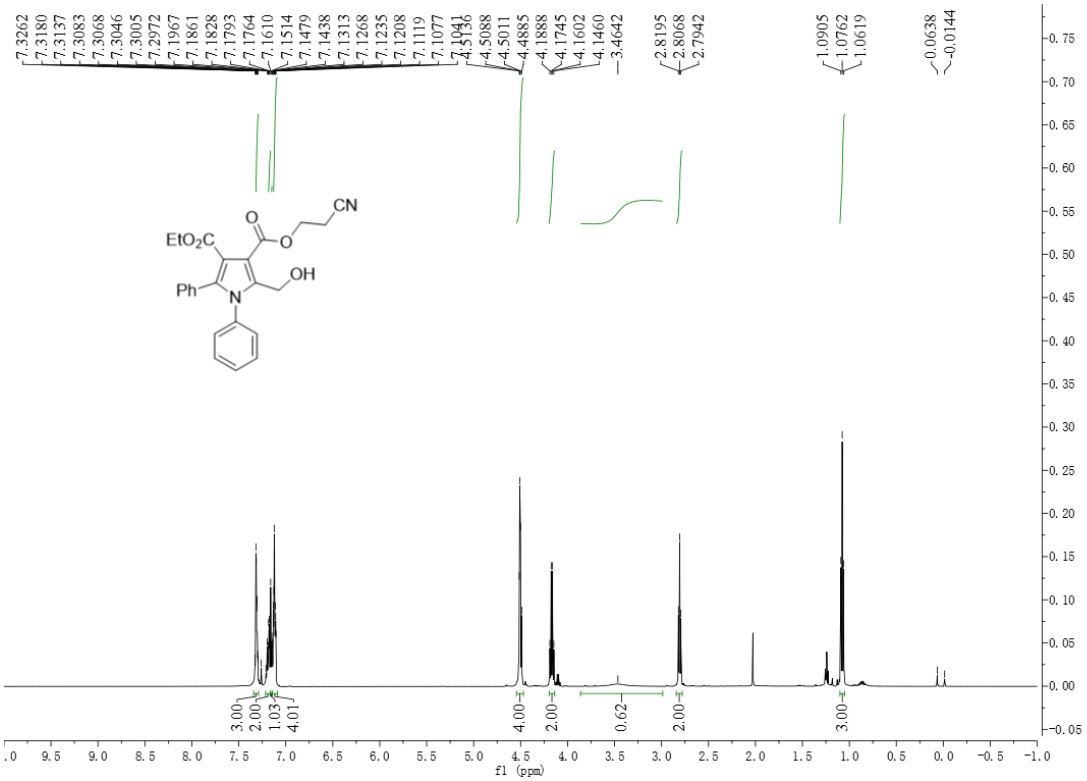


^{13}C NMR (125 MHz, $CDCl_3$)

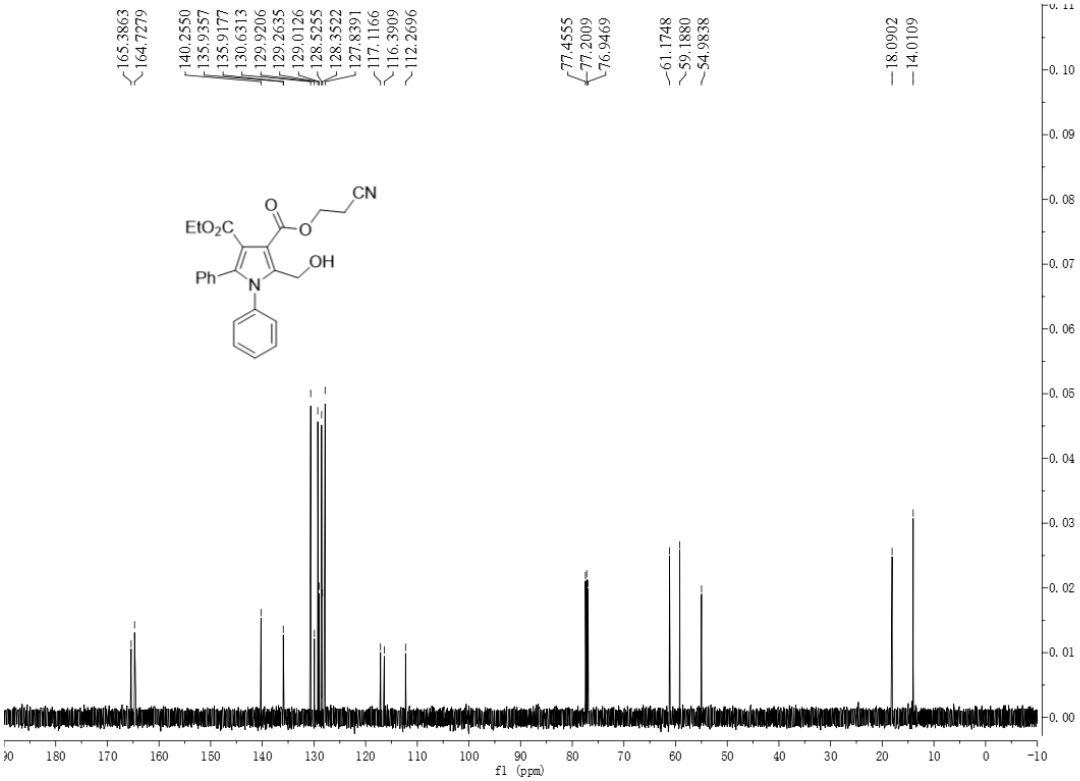


3-(2-Cyanoethyl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4ax)

^{1}H NMR (500 MHz, $CDCl_3$)

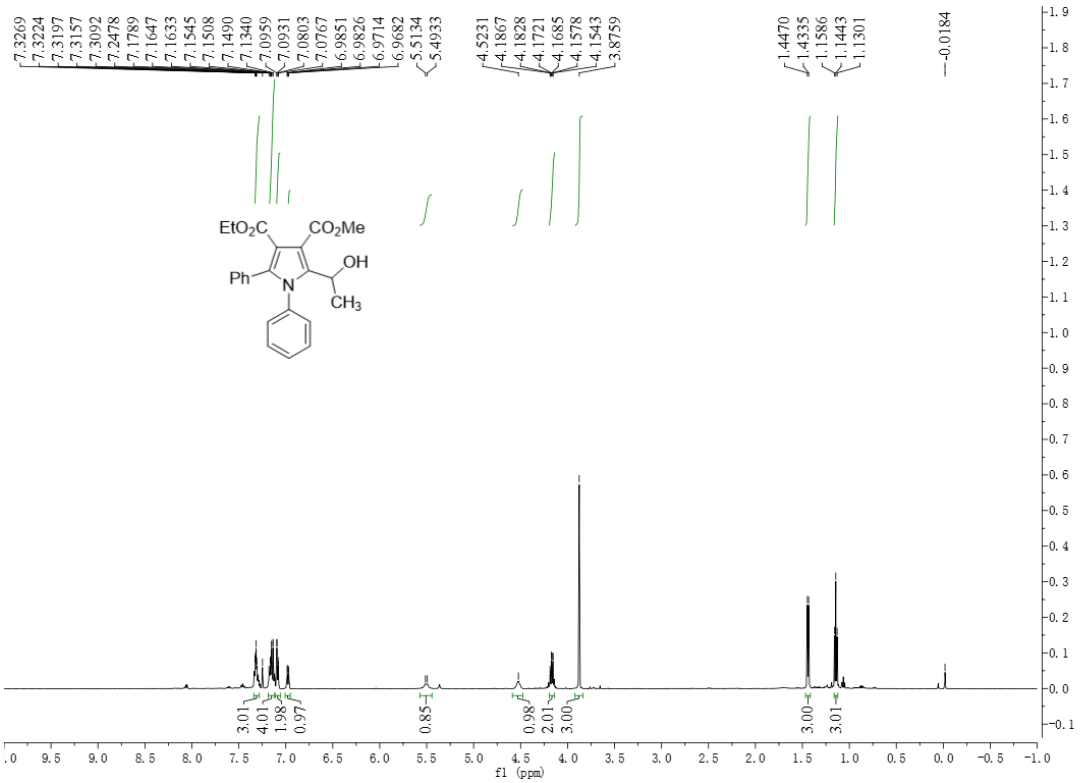


^{13}C NMR (125 MHz, $CDCl_3$)

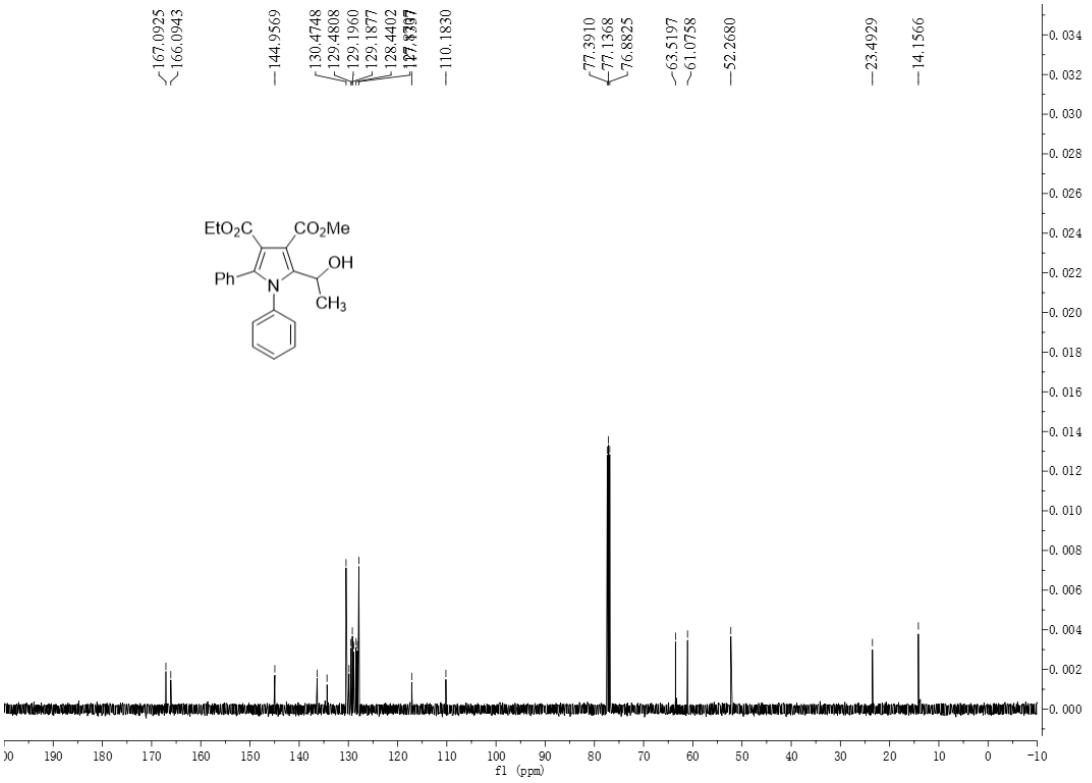


3-Ethyl 4-methyl 5-(1-hydroxyethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4ay)

^{1}H NMR (500 MHz, $CDCl_3$)

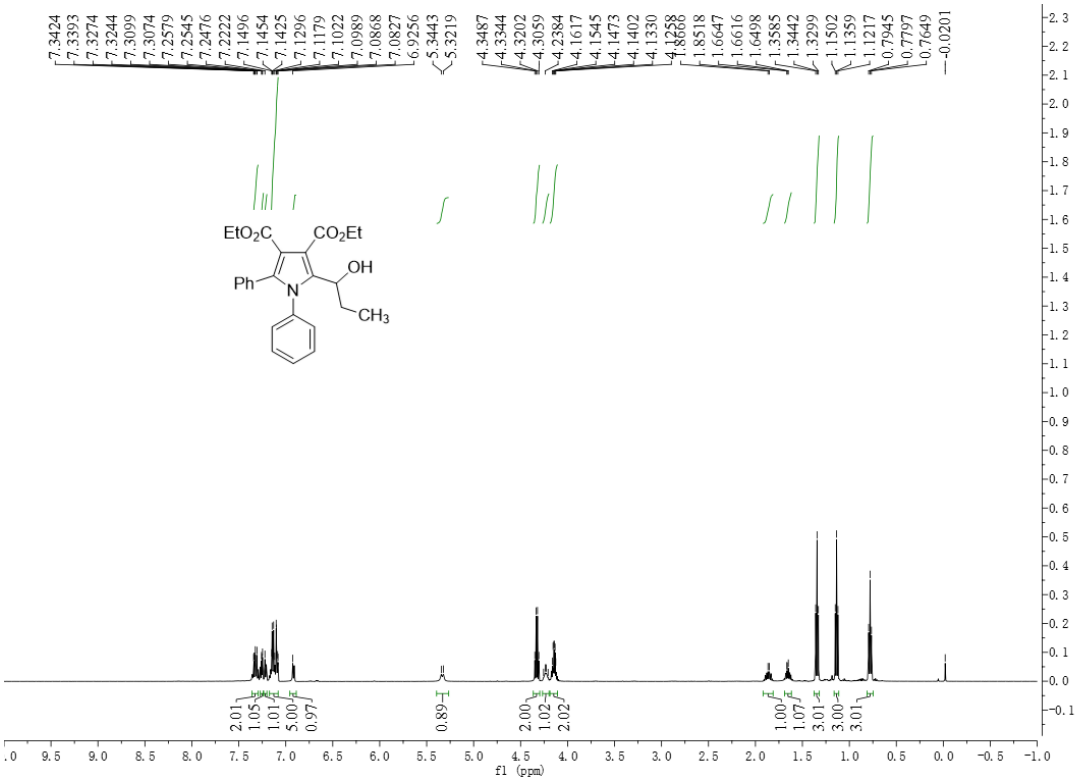


^{13}C NMR (125 MHz, $CDCl_3$)

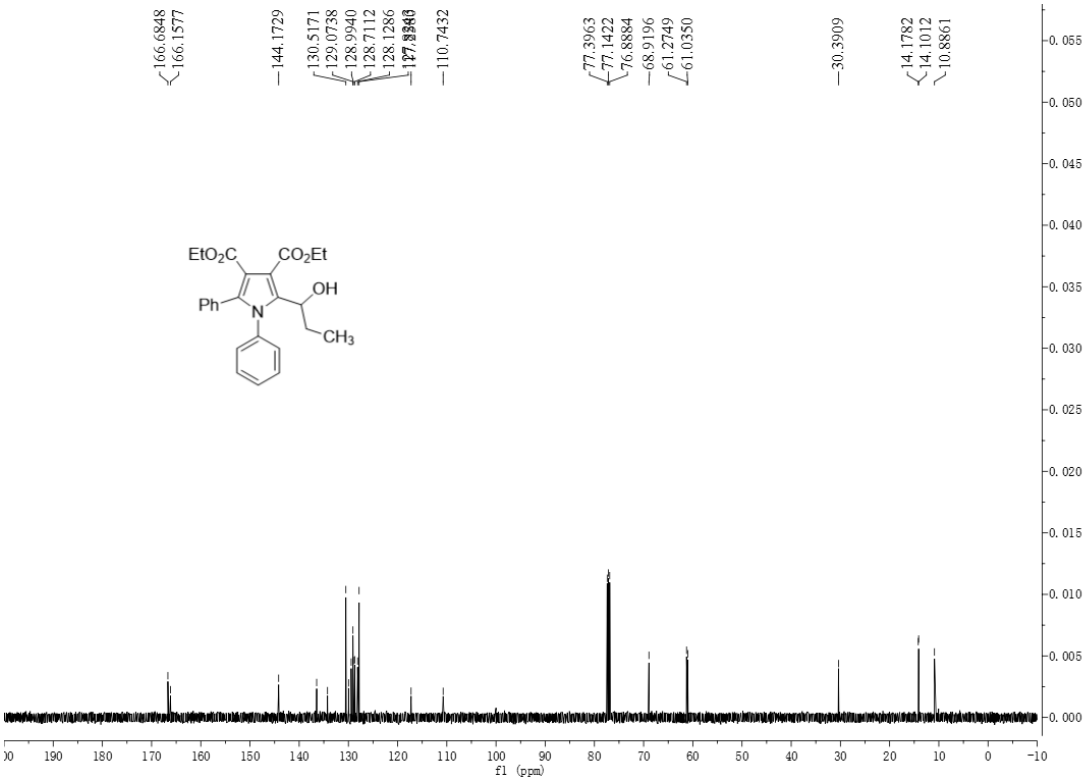


Diethyl 2-(1-hydroxypropyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (4az)

^{1}H NMR (500 MHz, $CDCl_3$)

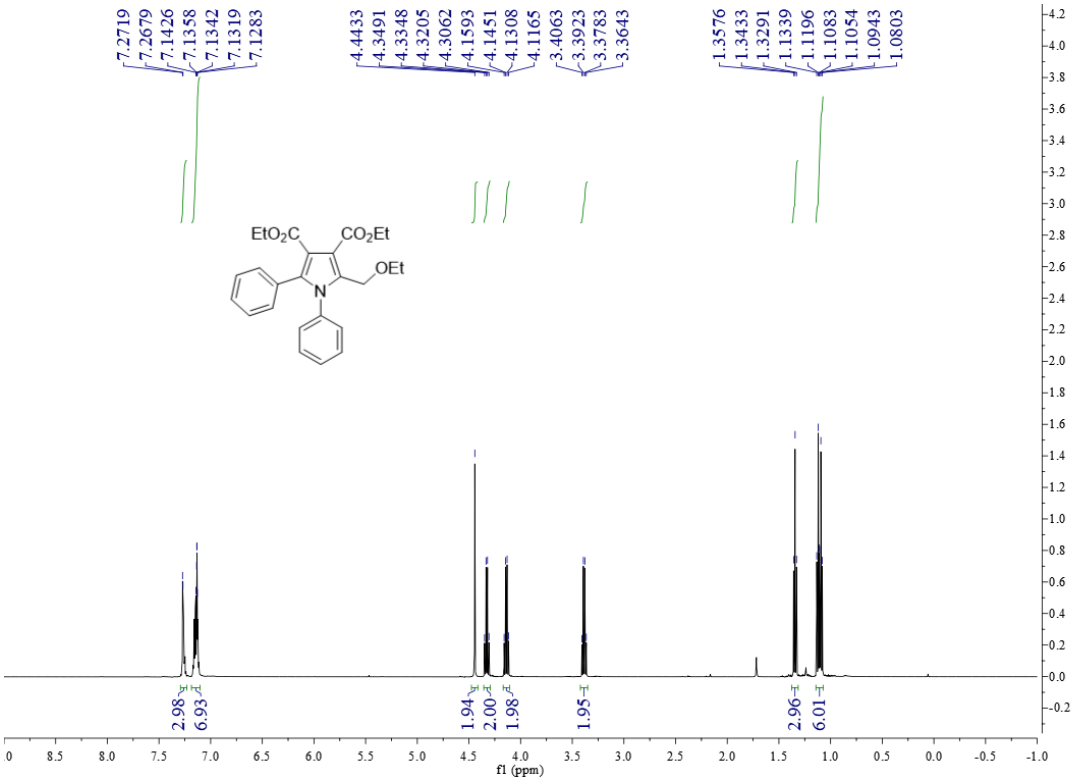


^{13}C NMR (125 MHz, $CDCl_3$)

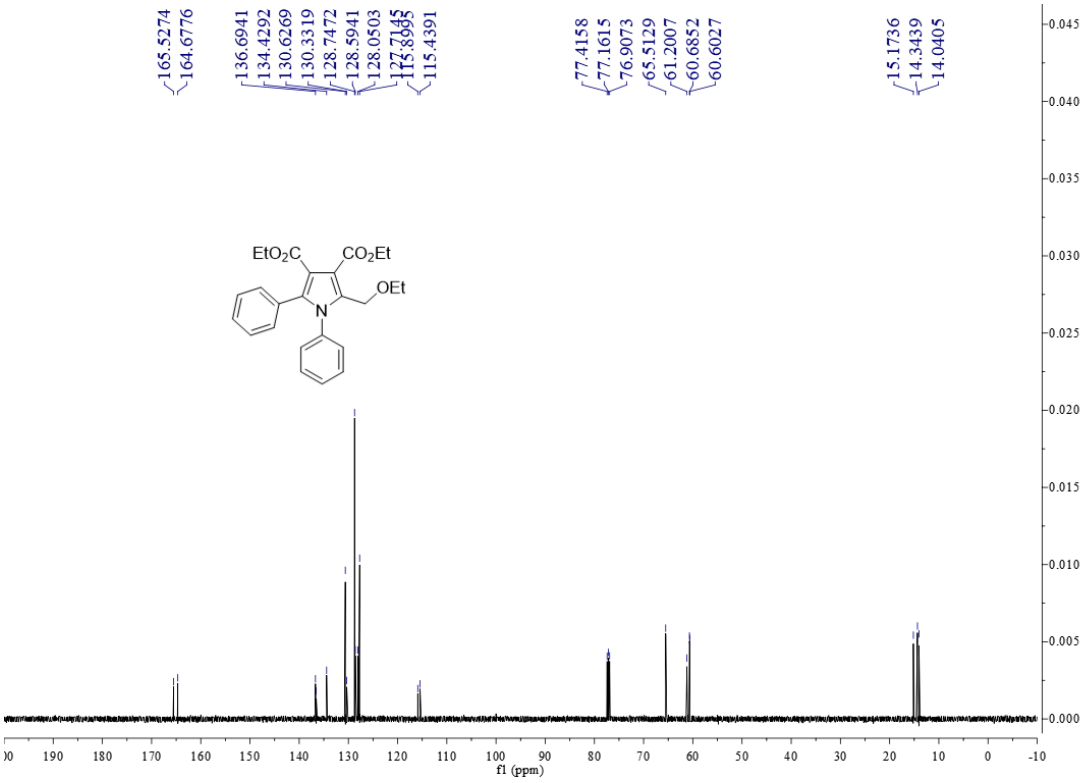


Diethyl 2-(ethoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5aa)

^{1}H NMR (500 MHz, $CDCl_3$)

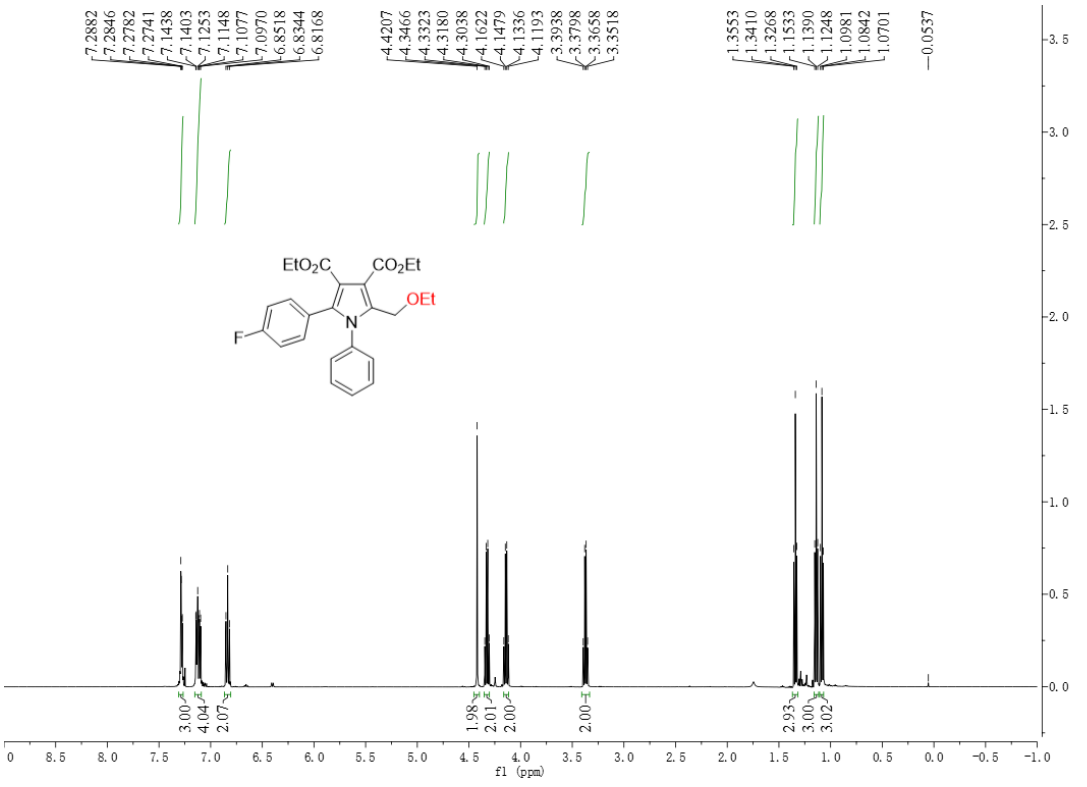


^{13}C NMR (125 MHz, $CDCl_3$)

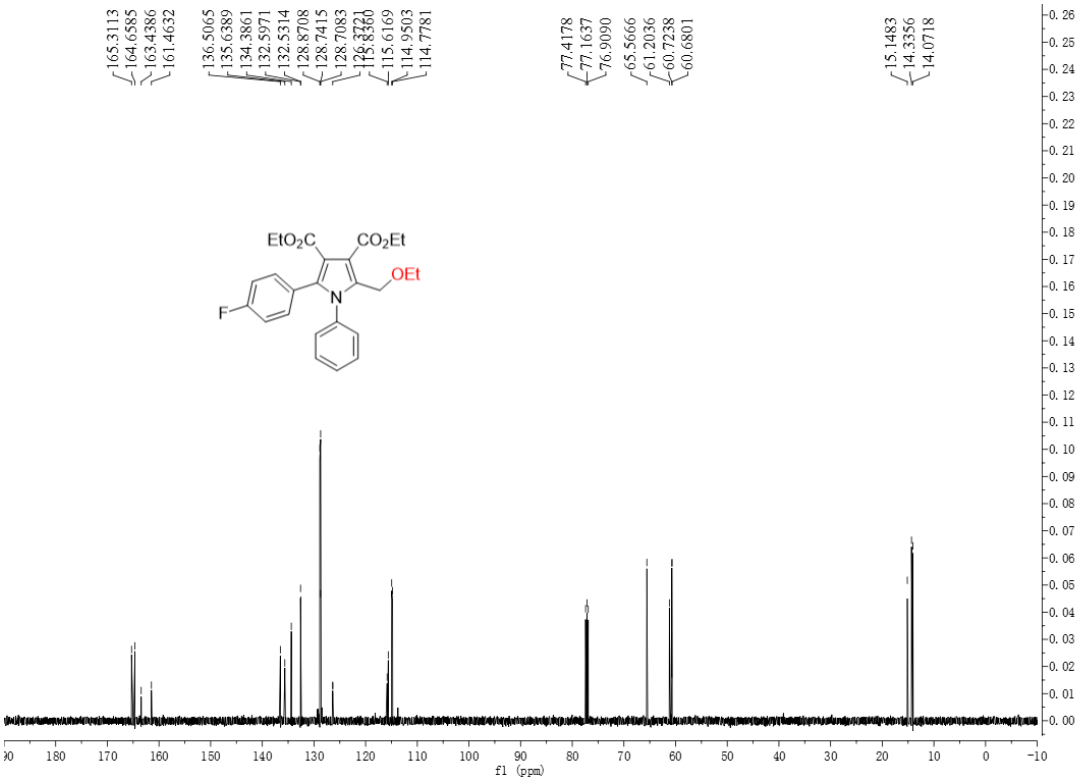


Diethyl 2-(ethoxymethyl)-5-(4-fluorophenyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ba)

^{1}H NMR (500 MHz, $CDCl_3$)

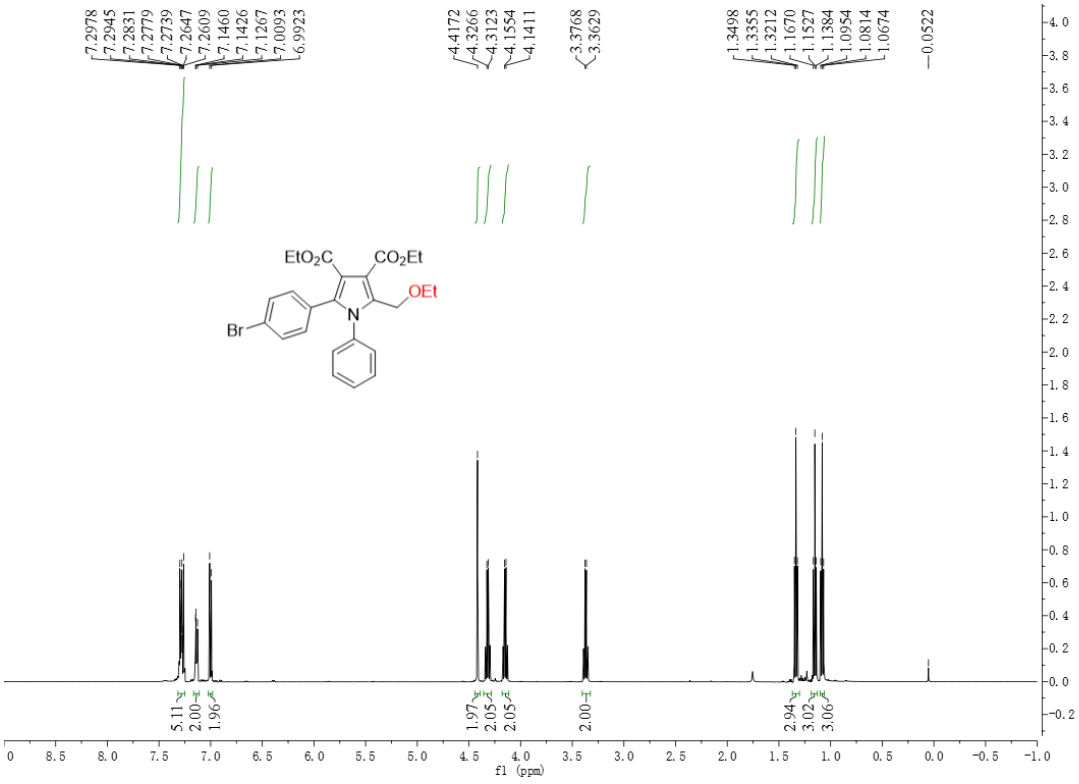


^{13}C NMR (125 MHz, $CDCl_3$)

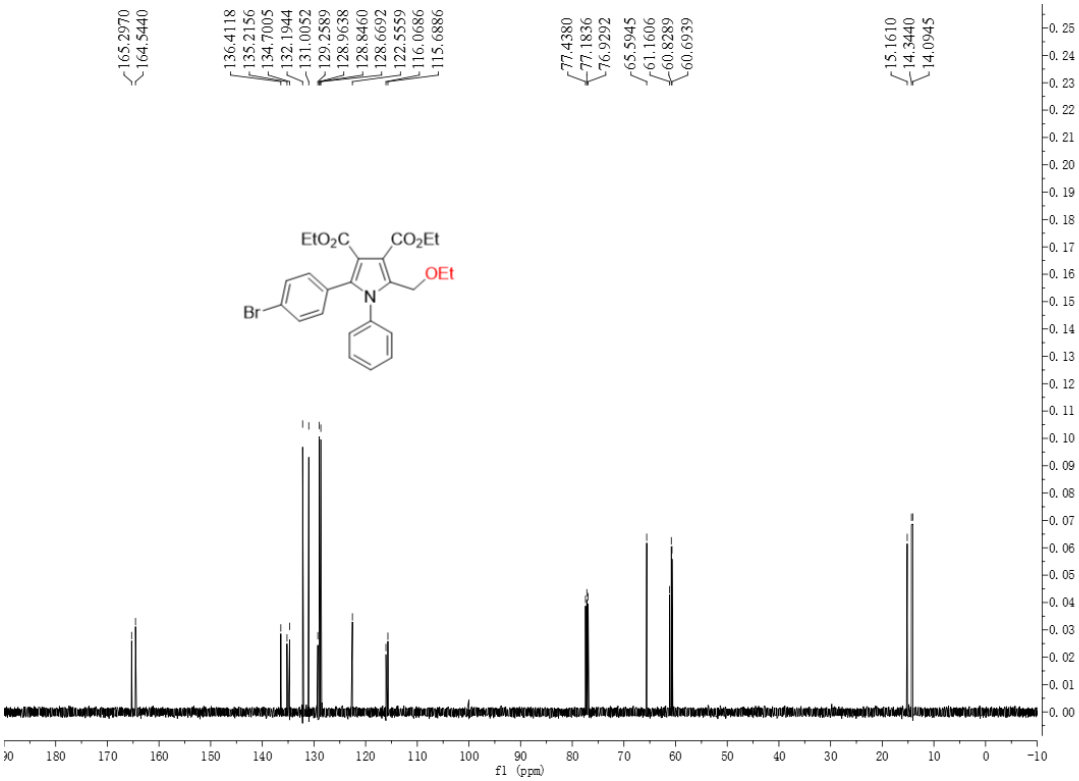


Diethyl 2-(4-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ca)

^{1}H NMR (500 MHz, $CDCl_3$)

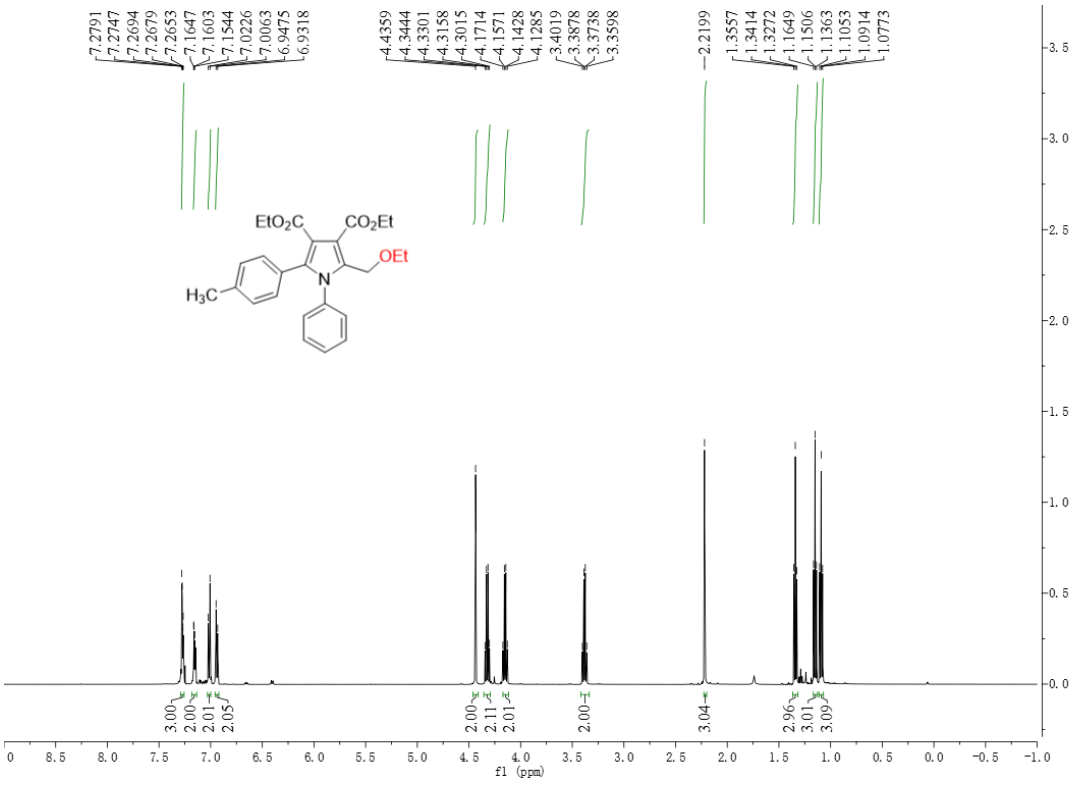


^{13}C NMR (125 MHz, $CDCl_3$)

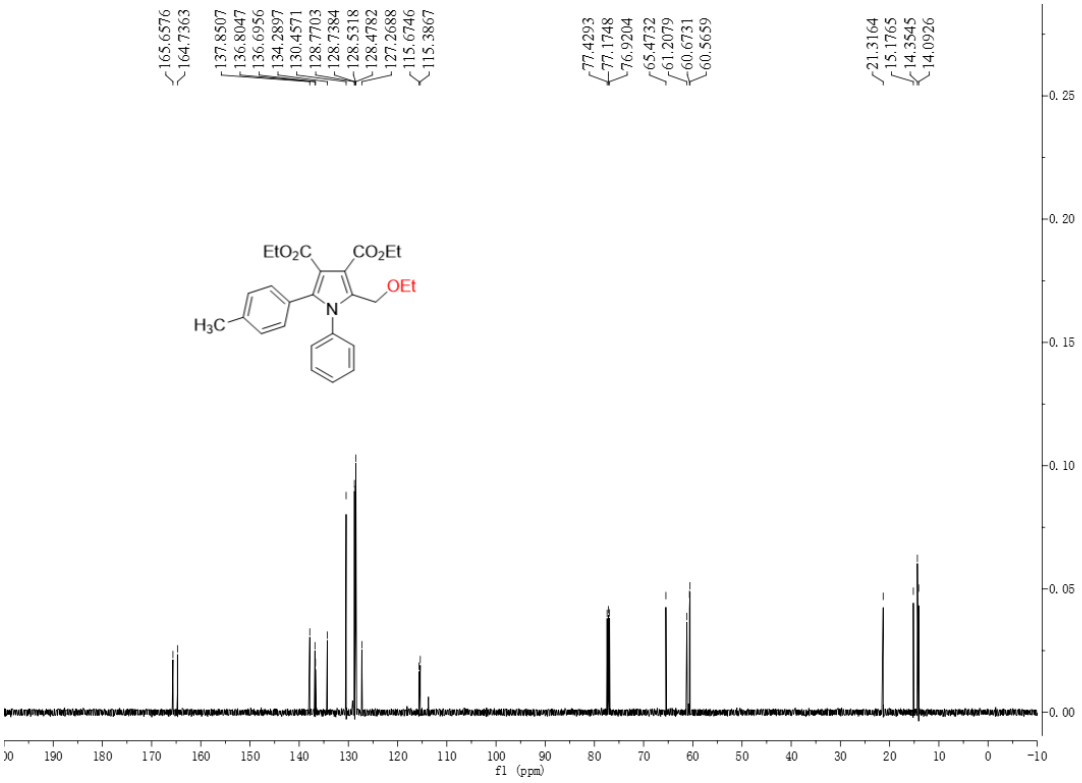


Diethyl 2-(ethoxymethyl)-1-phenyl-5-(*p*-tolyl)-1*H*-pyrrole-3,4-dicarboxylate (5da)

^{1}H NMR (500 MHz, $CDCl_3$)

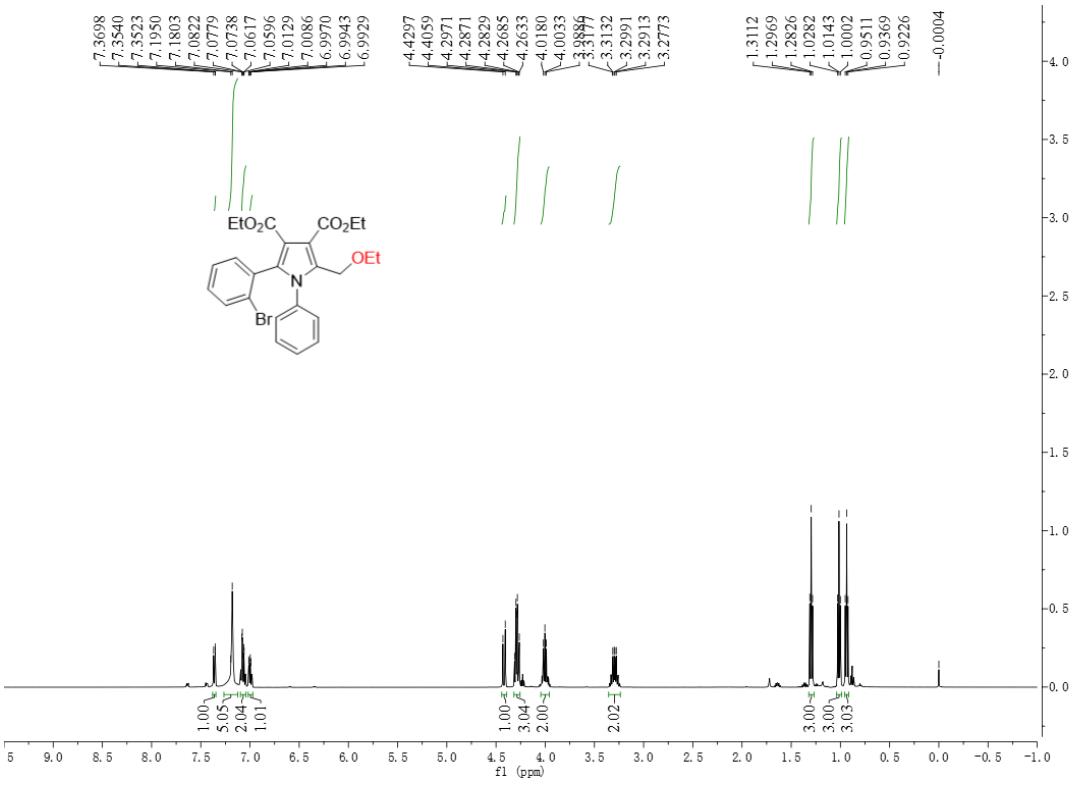


^{13}C NMR (125 MHz, $CDCl_3$)

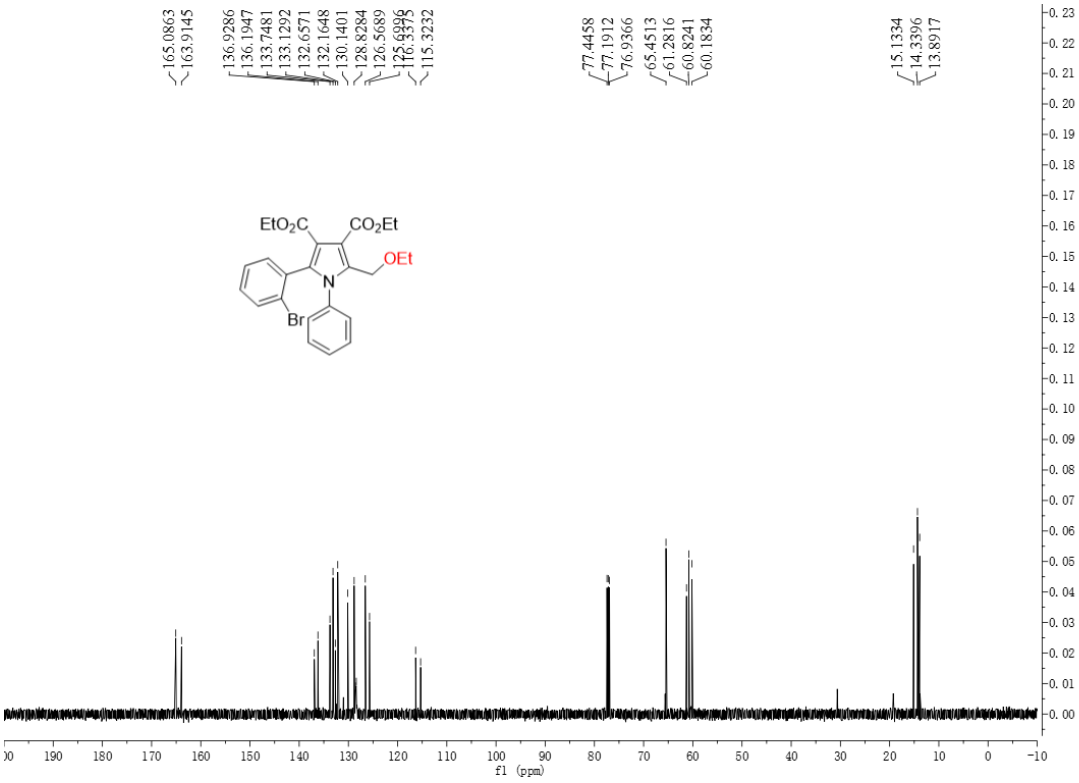


Diethyl 2-(2-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ea)

^{1}H NMR (500 MHz, $CDCl_3$)

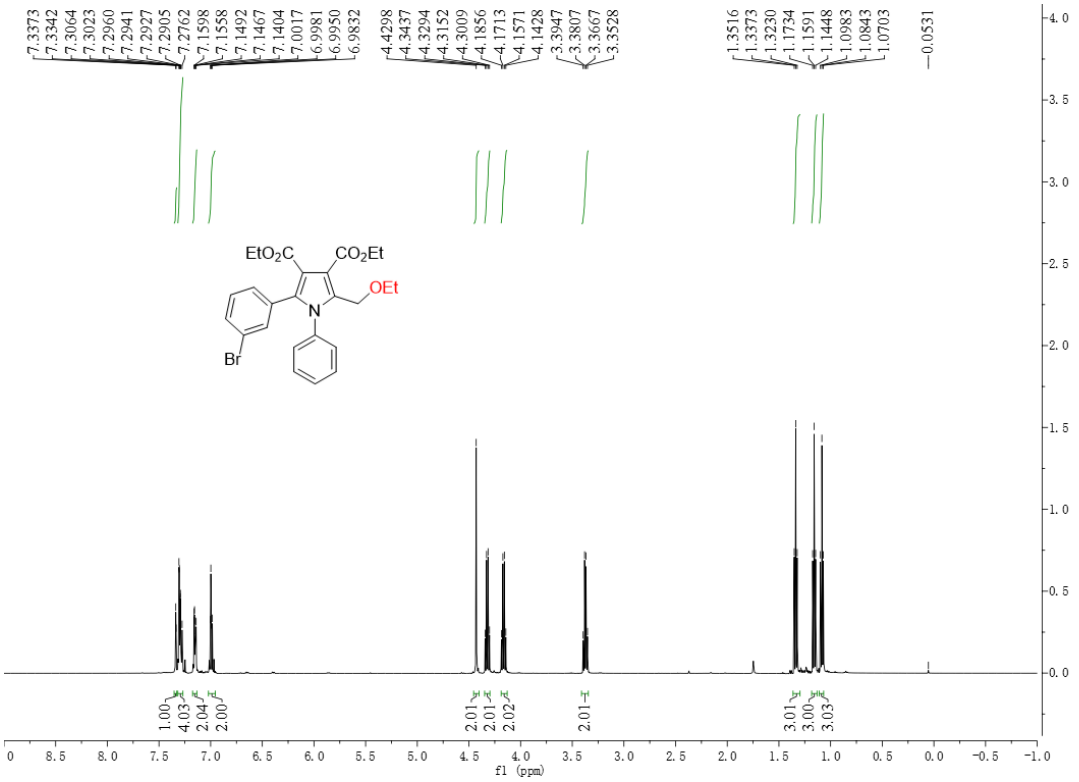


^{13}C NMR (125 MHz, $CDCl_3$)

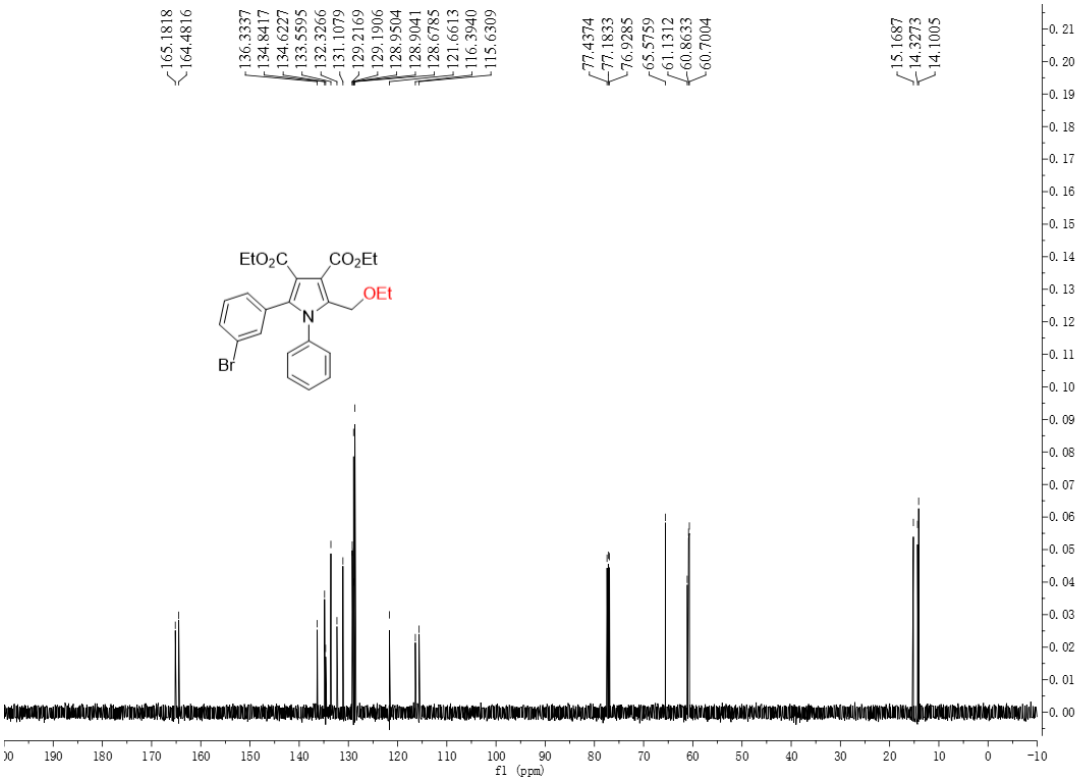


Diethyl 2-(3-bromophenyl)-5-(ethoxymethyl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5fa)

^{1}H NMR (500 MHz, $CDCl_3$)

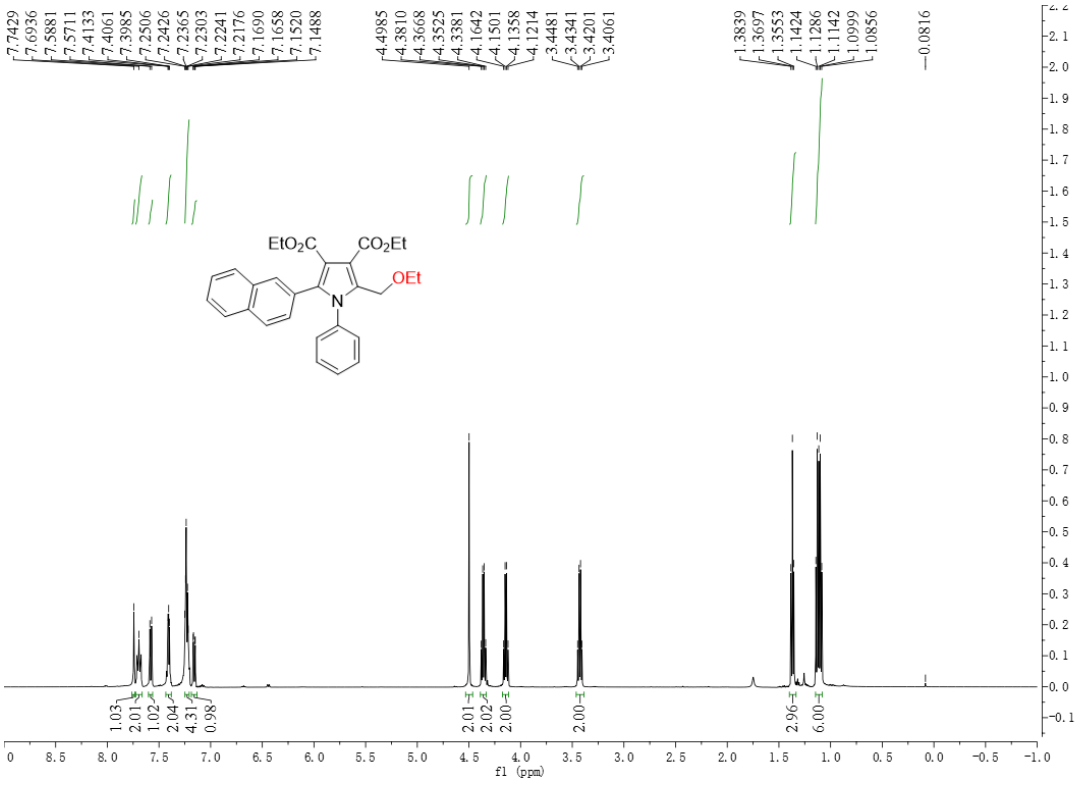


^{13}C NMR (125 MHz, $CDCl_3$)

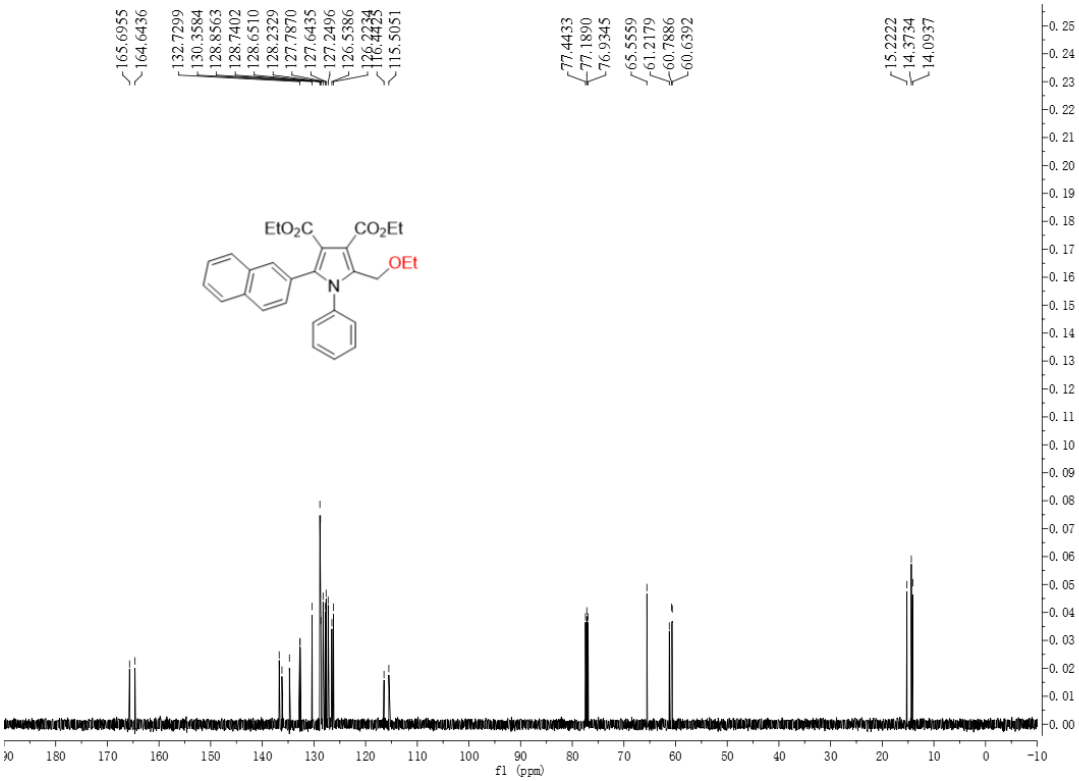


Diethyl 2-(ethoxymethyl)-5-(naphthalen-2-yl)-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ga)

^{1}H NMR (500 MHz, $CDCl_3$)

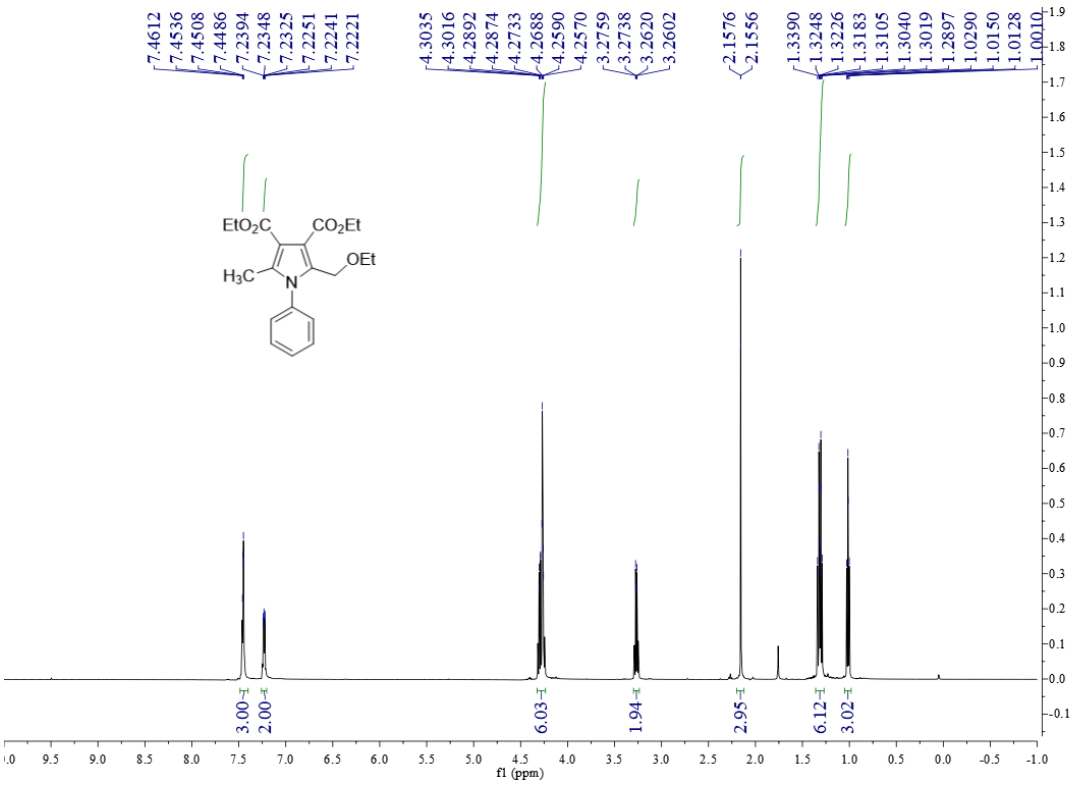


^{13}C NMR (125 MHz, $CDCl_3$)

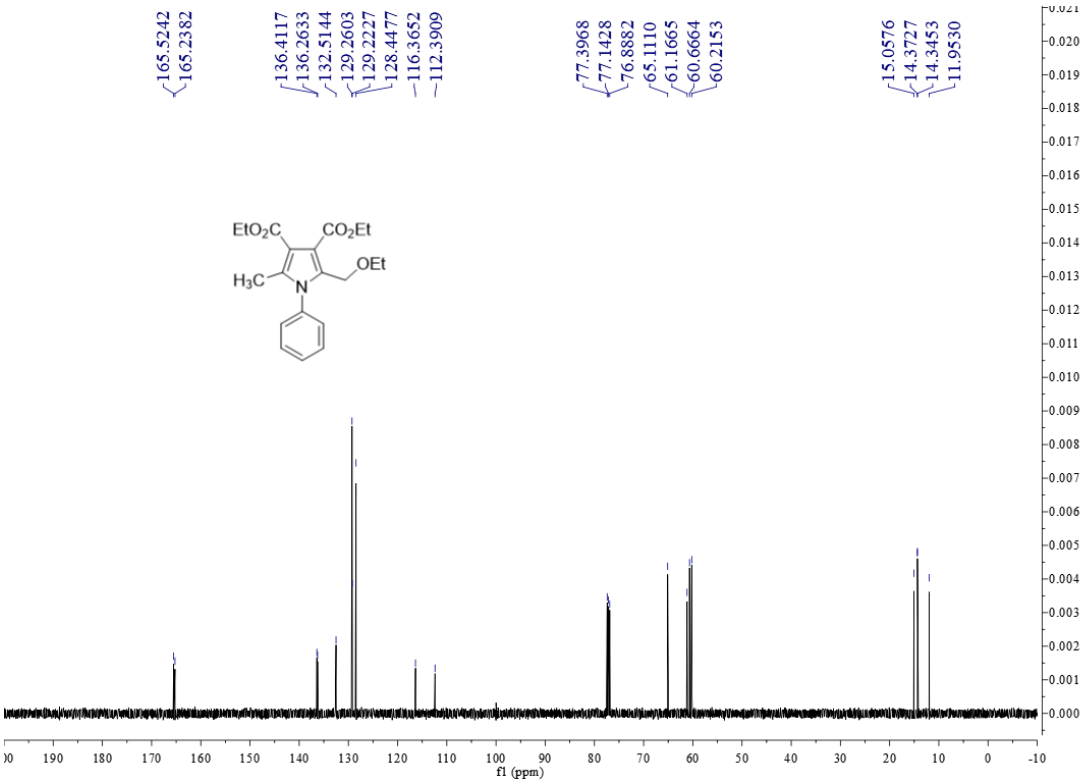


Diethyl 2-(ethoxymethyl)-5-methyl-1-phenyl-1*H*-pyrrole-3,4-dicarboxylate (5ha)

^{1}H NMR (500 MHz, $CDCl_3$)

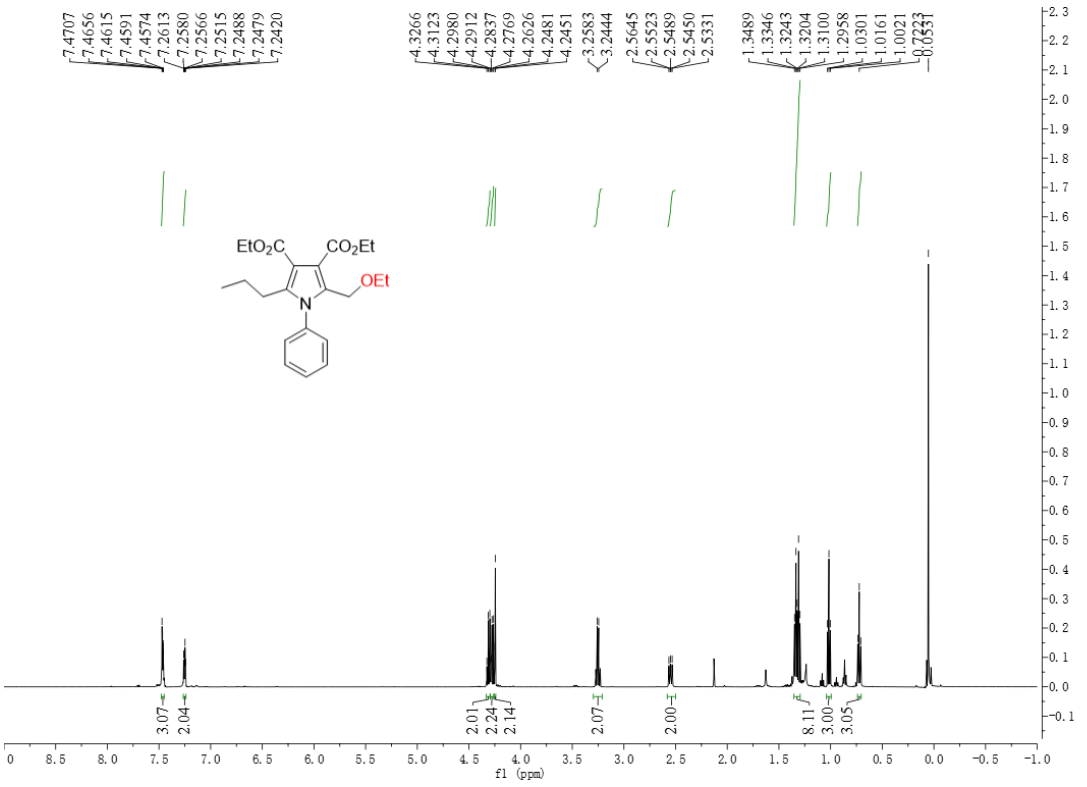


^{13}C NMR (125 MHz, $CDCl_3$)

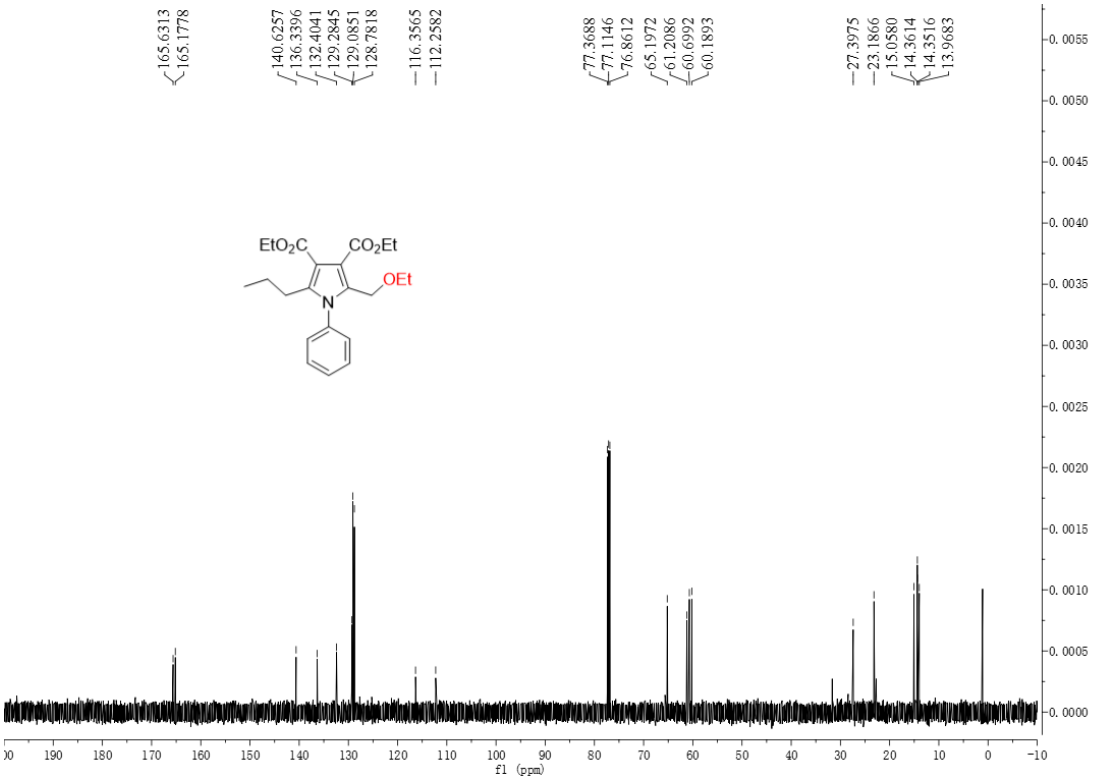


Diethyl 2-(ethoxymethyl)-1-phenyl-5-propyl-1*H*-pyrrole-3,4-dicarboxylate (5ia)

^{1}H NMR (500 MHz, $CDCl_3$)

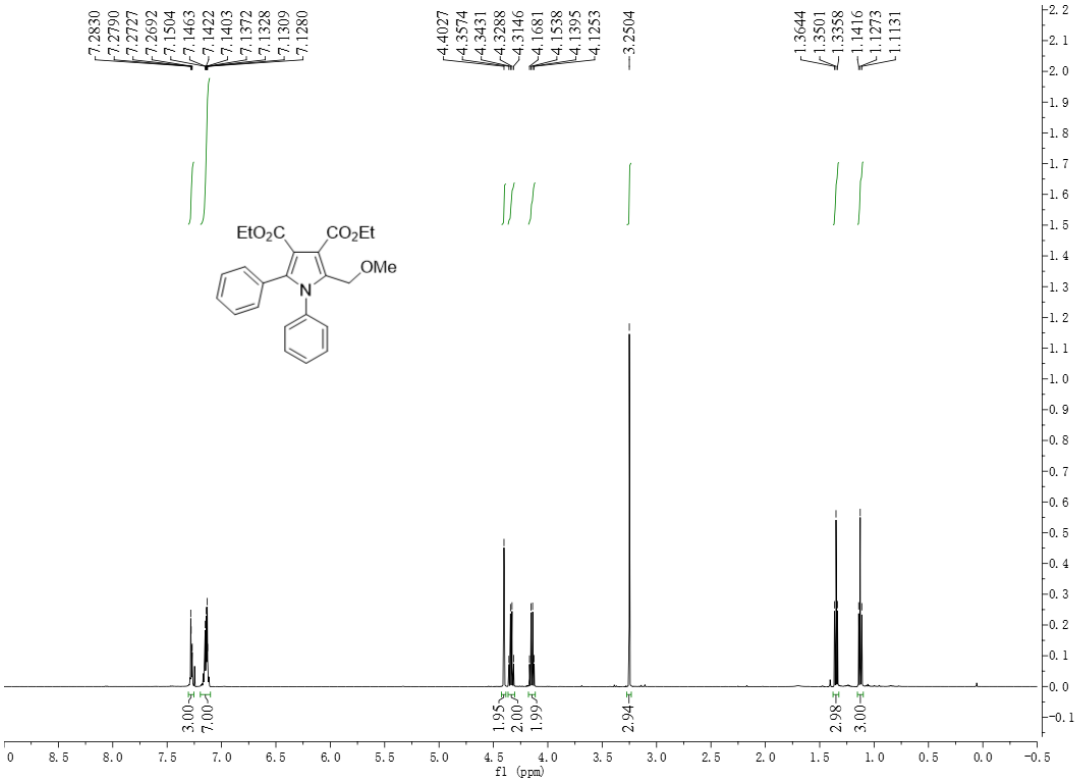


^{13}C NMR (125 MHz, $CDCl_3$)

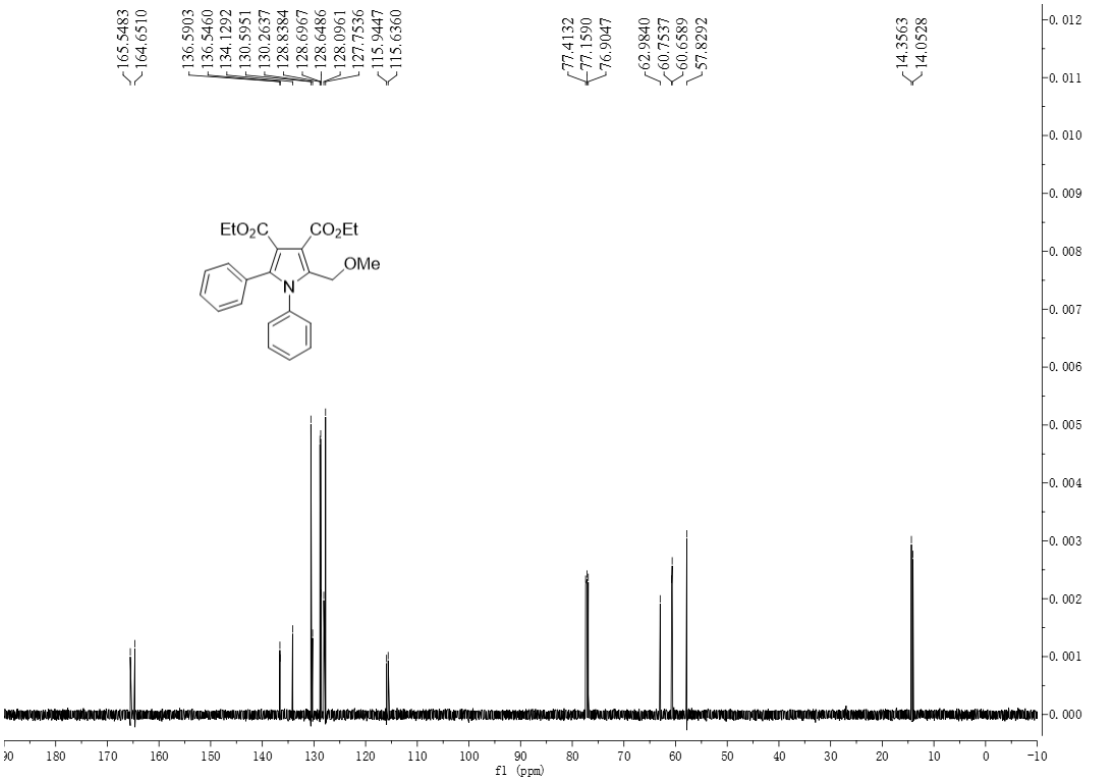


Diethyl 2-(methoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5ab)

^{1}H NMR (500 MHz, $CDCl_3$)

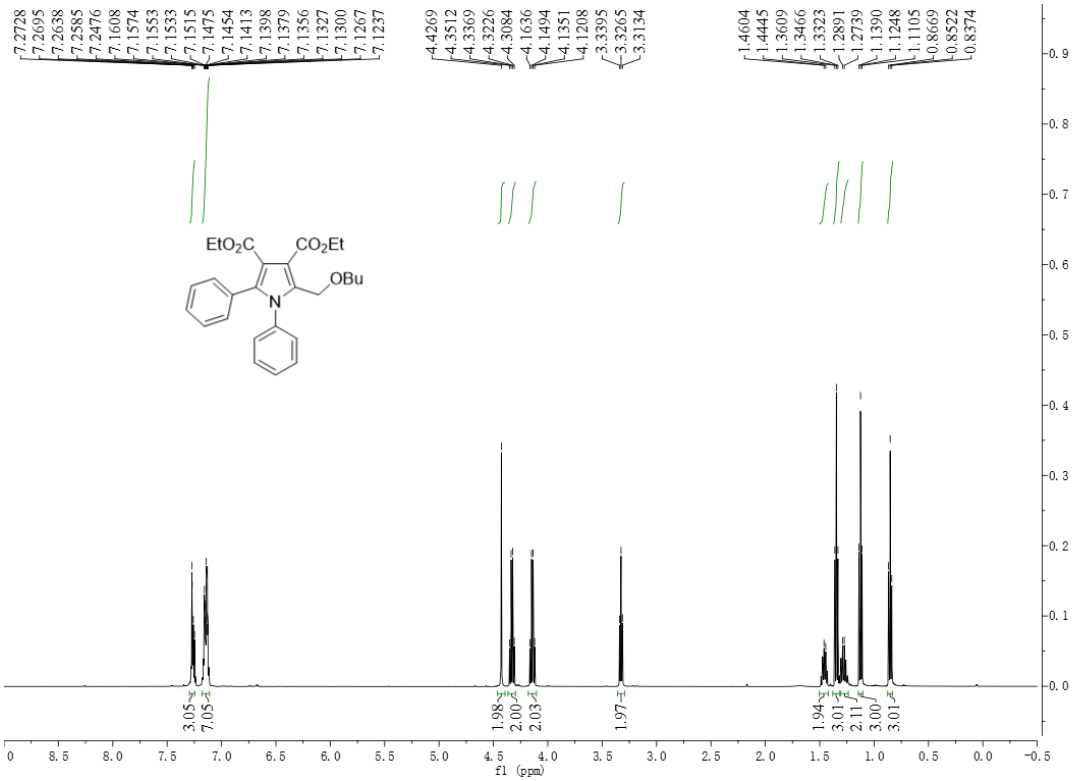


^{13}C NMR (125 MHz, $CDCl_3$)

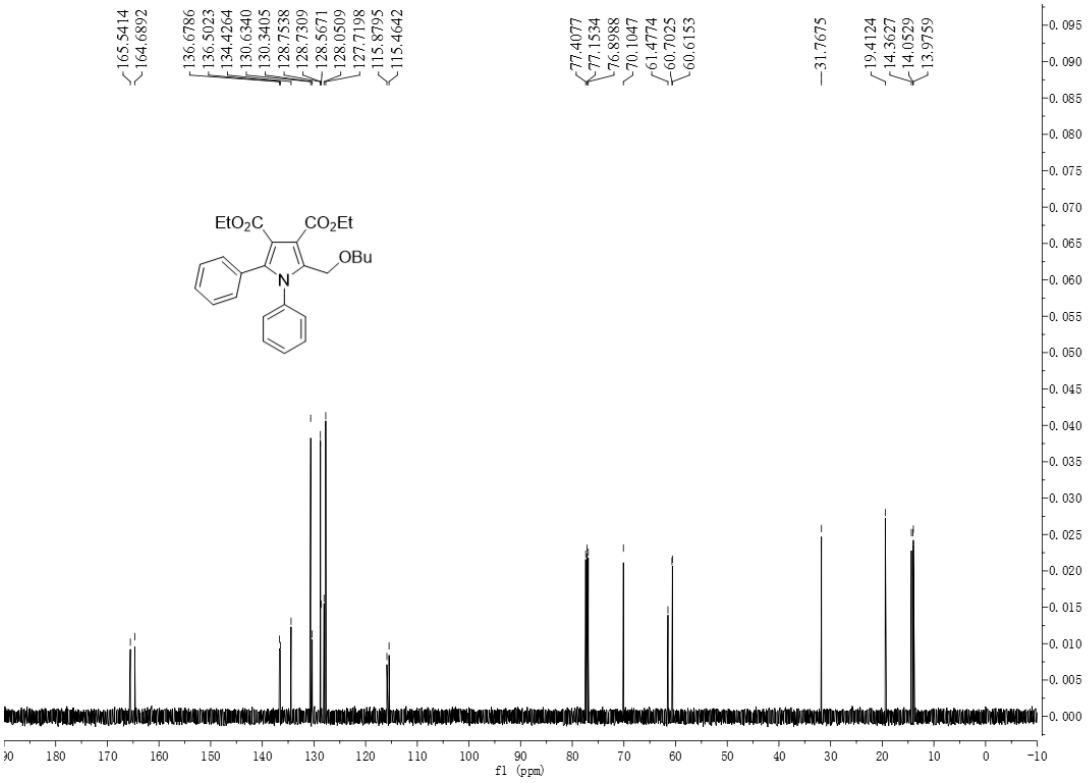


Diethyl 2-(butoxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (5ac)

^{1}H NMR (500 MHz, $CDCl_3$)

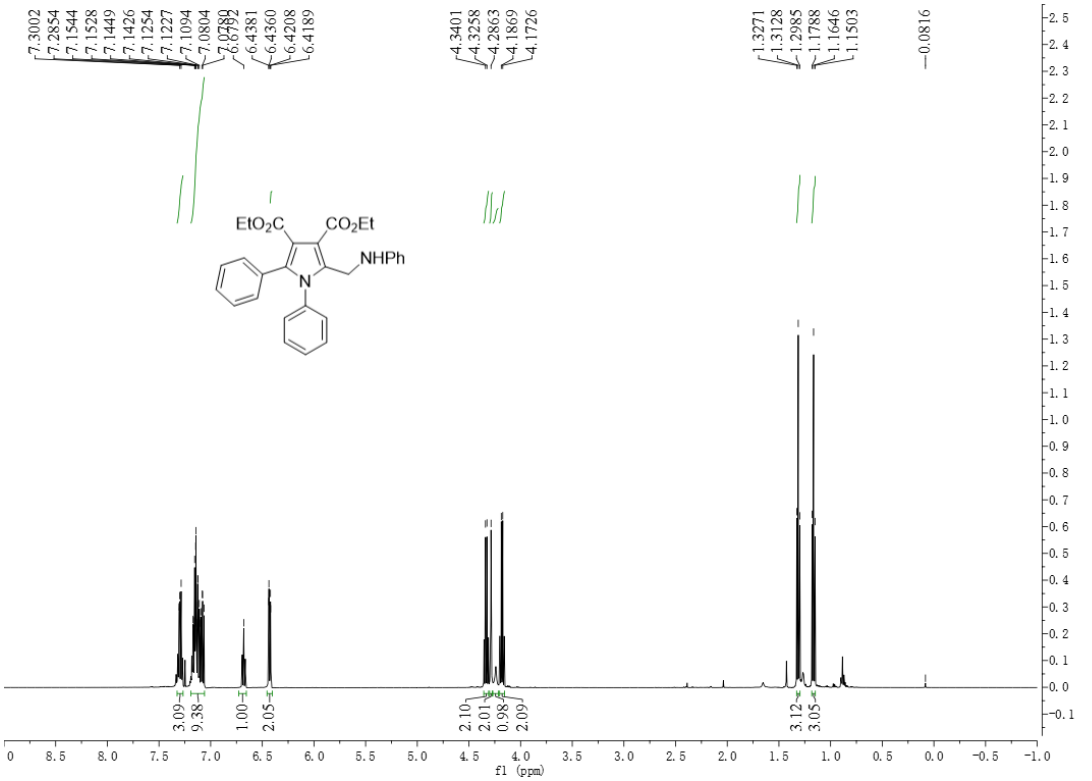


^{13}C NMR (125 MHz, $CDCl_3$)

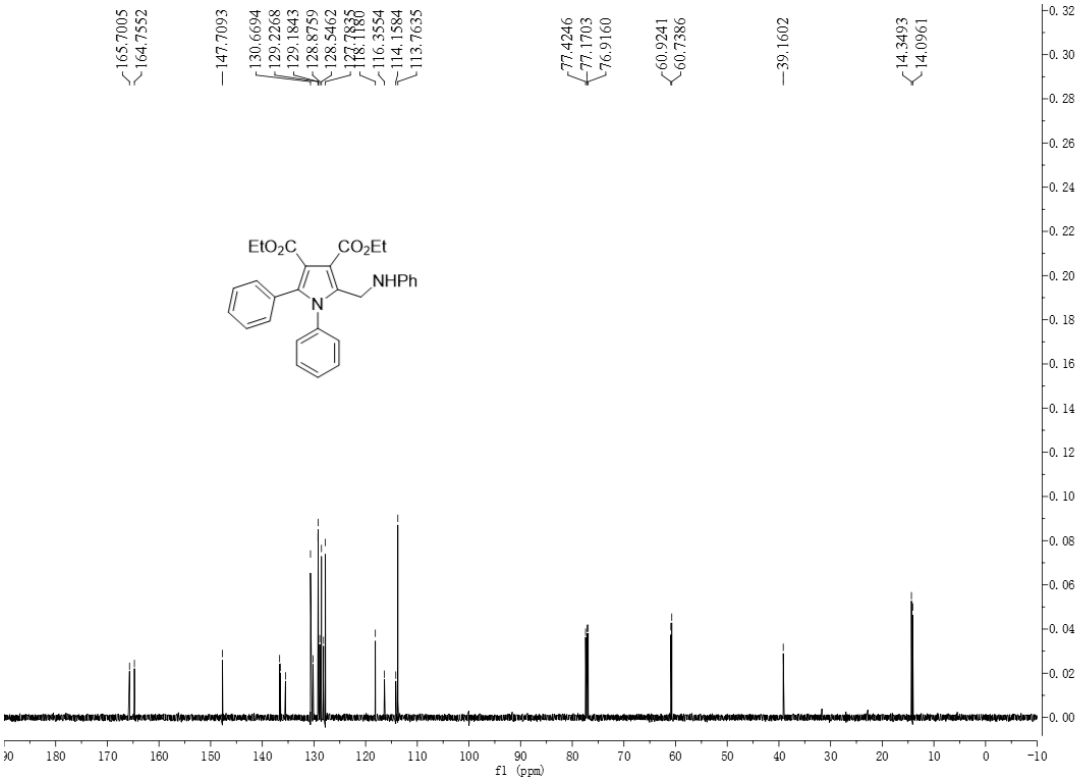


Diethyl 1,2-diphenyl-5-((phenylamino)methyl)-1*H*-pyrrole-3,4-dicarboxylate (6aa)

^{1}H NMR (500 MHz, $CDCl_3$)

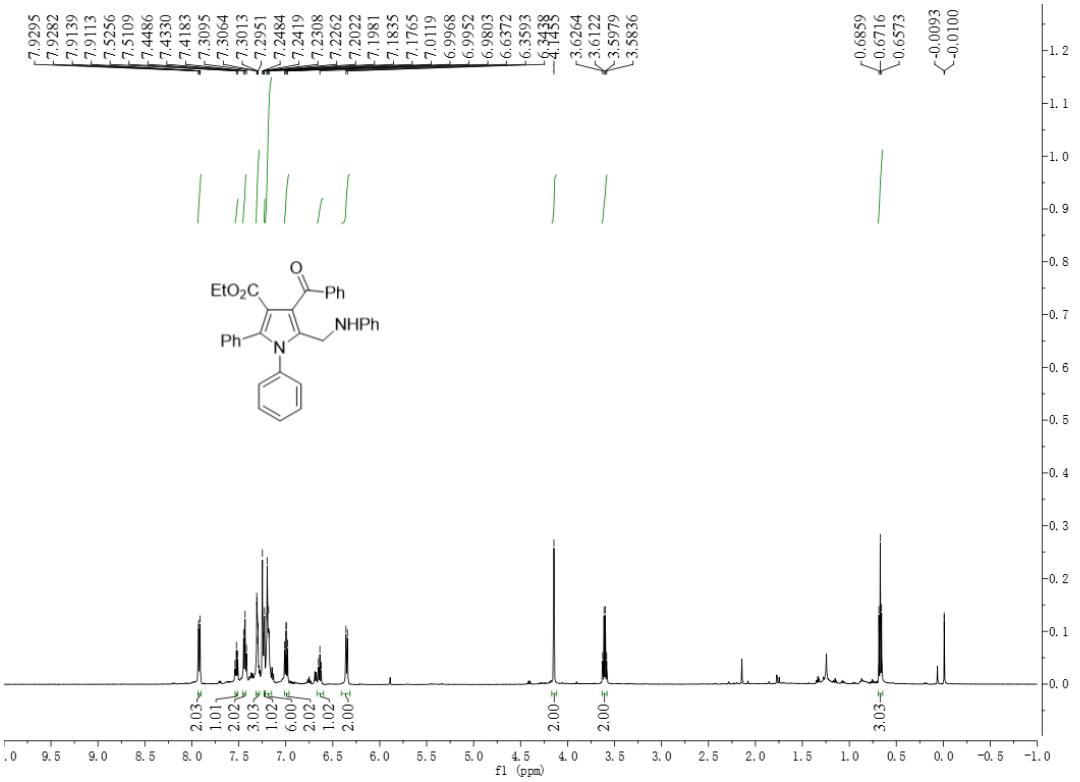


^{13}C NMR (125 MHz, $CDCl_3$)

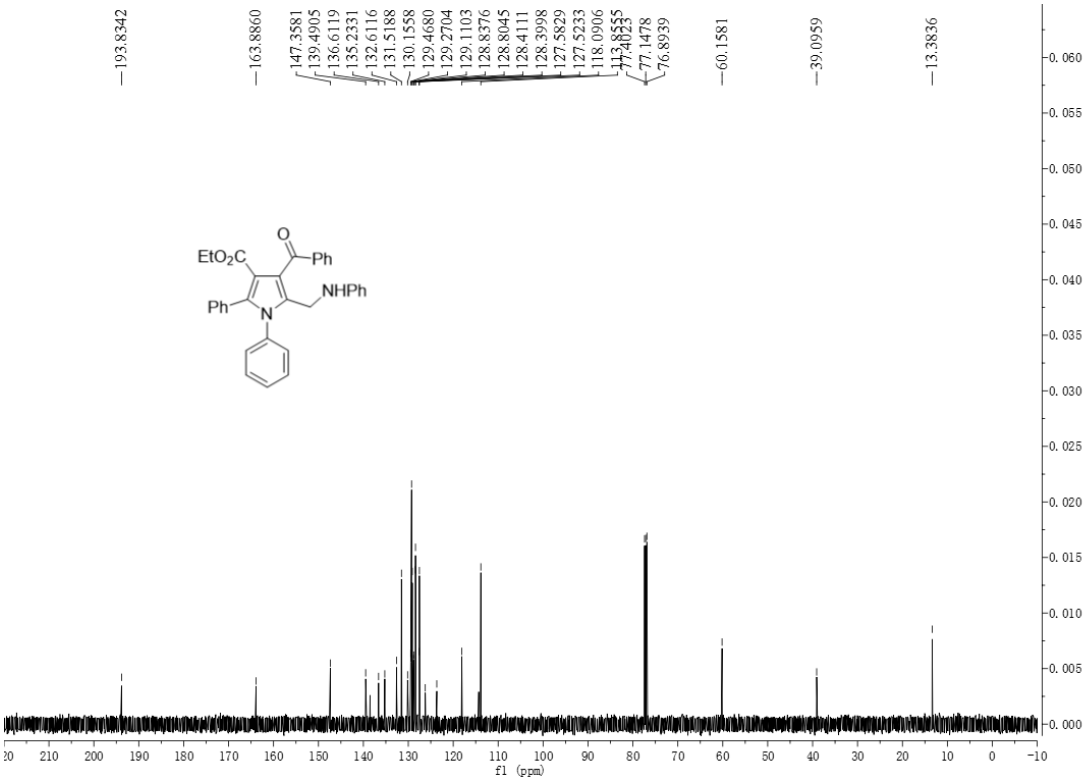


Ethyl 4-benzoyl-1,2-diphenyl-5-((phenylamino)methyl)-1H-pyrrole-3-carboxylate (6ab)

^{1}H NMR (500 MHz, $CDCl_3$)

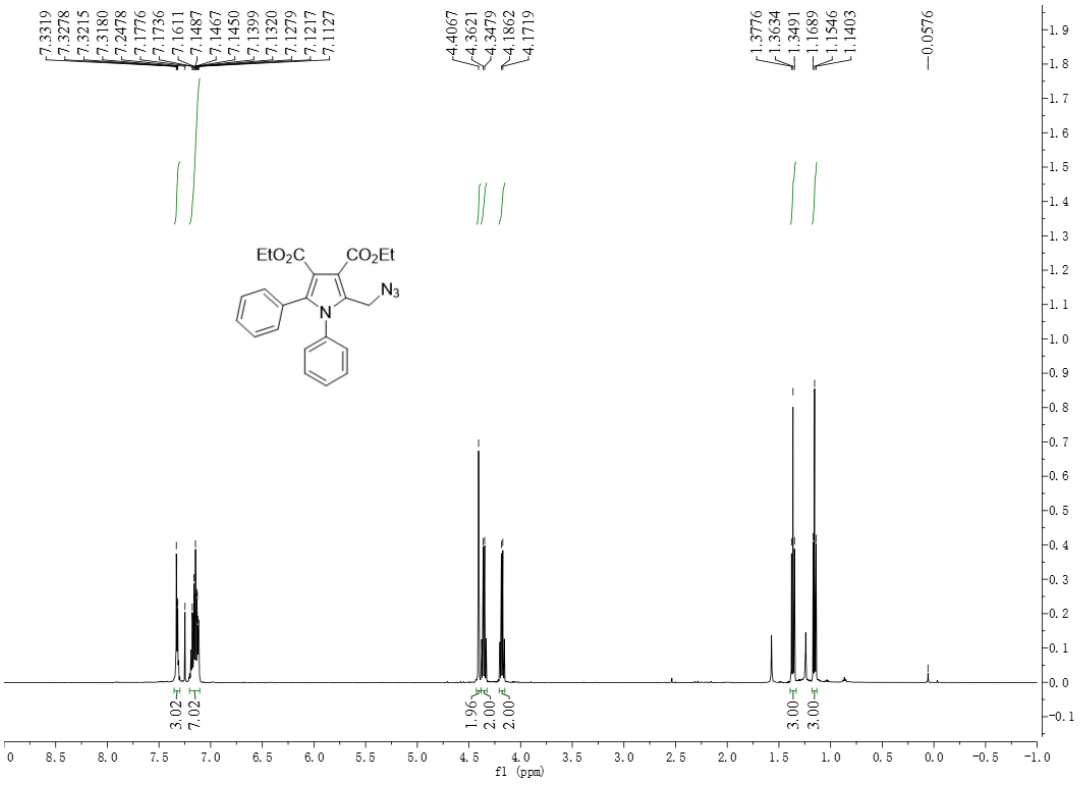


^{13}C NMR (125 MHz, $CDCl_3$)

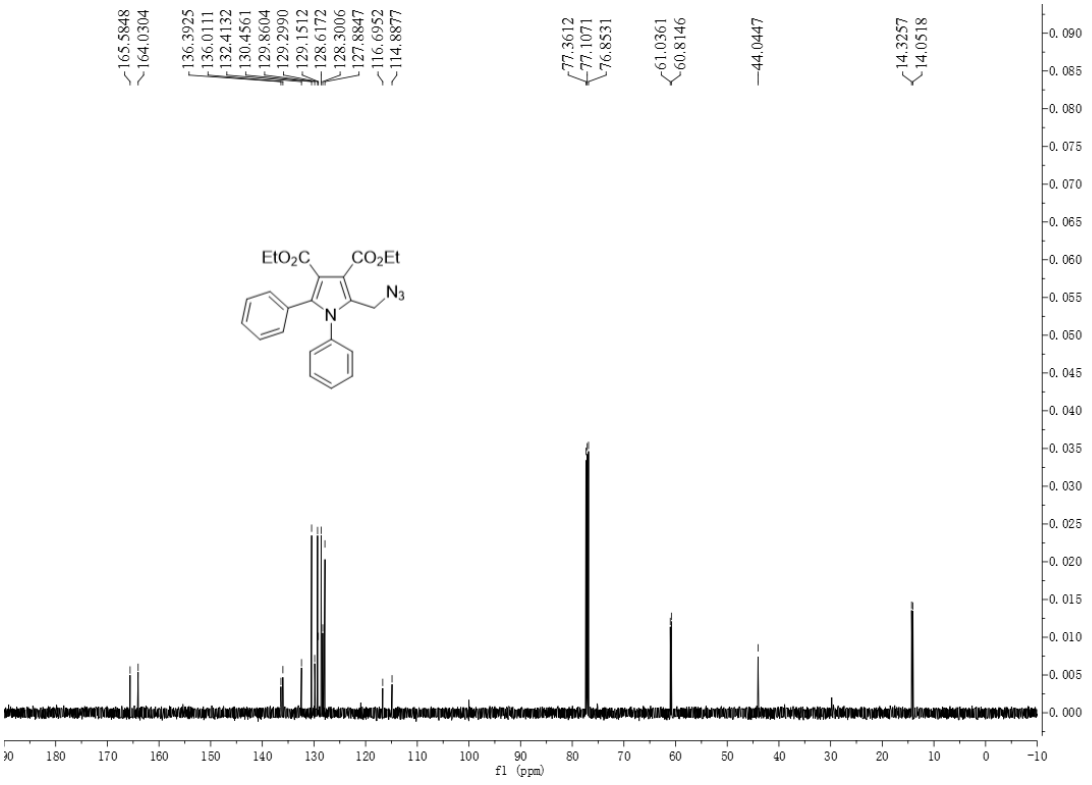


Diethyl 2-(azidomethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (7aa)

^{1}H NMR (500 MHz, $CDCl_3$)

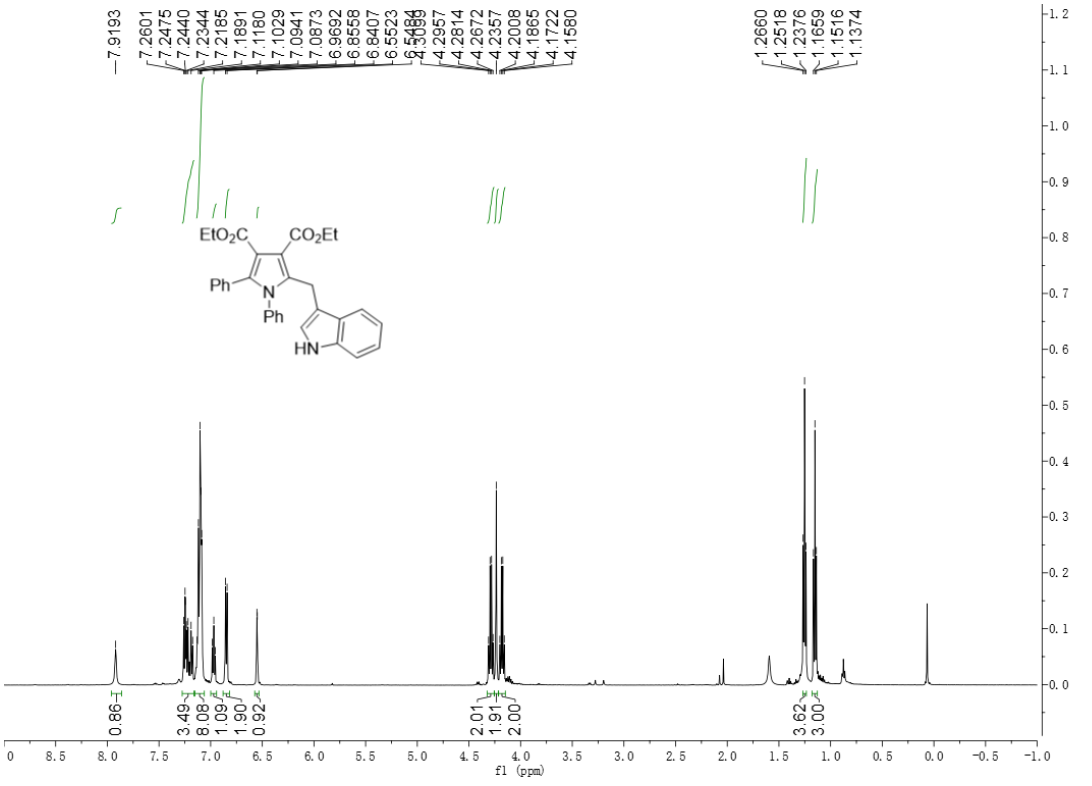


^{13}C NMR (125 MHz, $CDCl_3$)

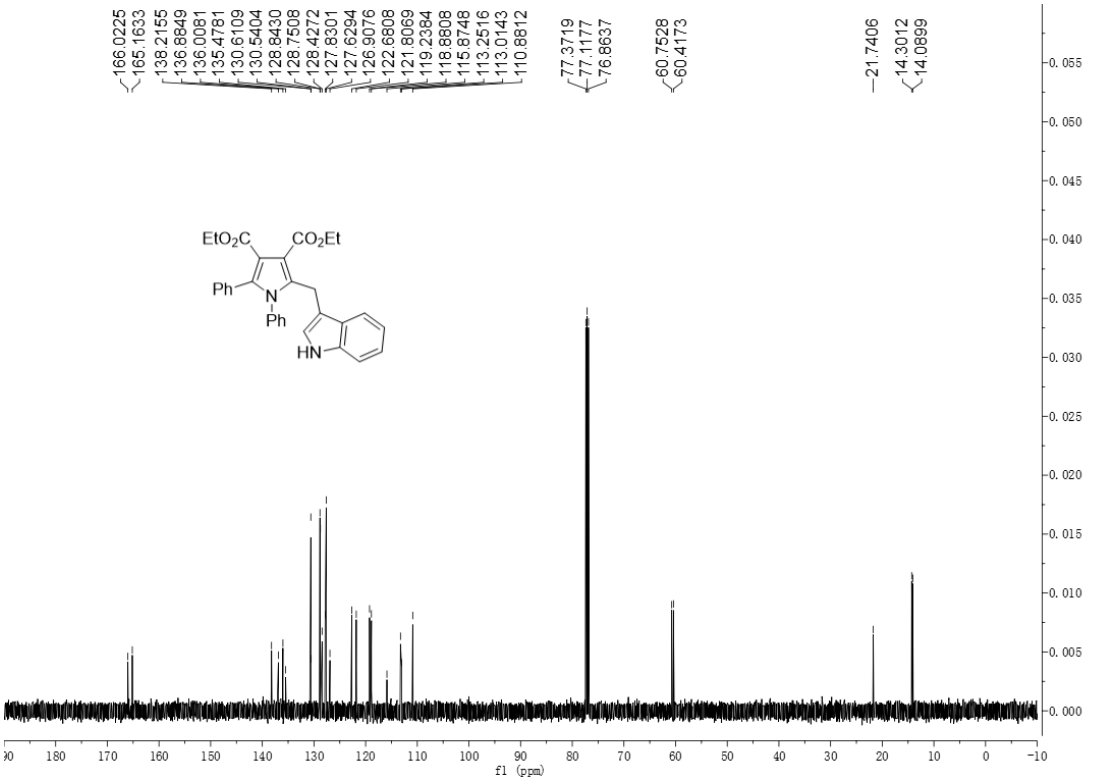


Diethyl 2-((1*H*-indol-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (8aa)

^{1}H NMR (500 MHz, $CDCl_3$)

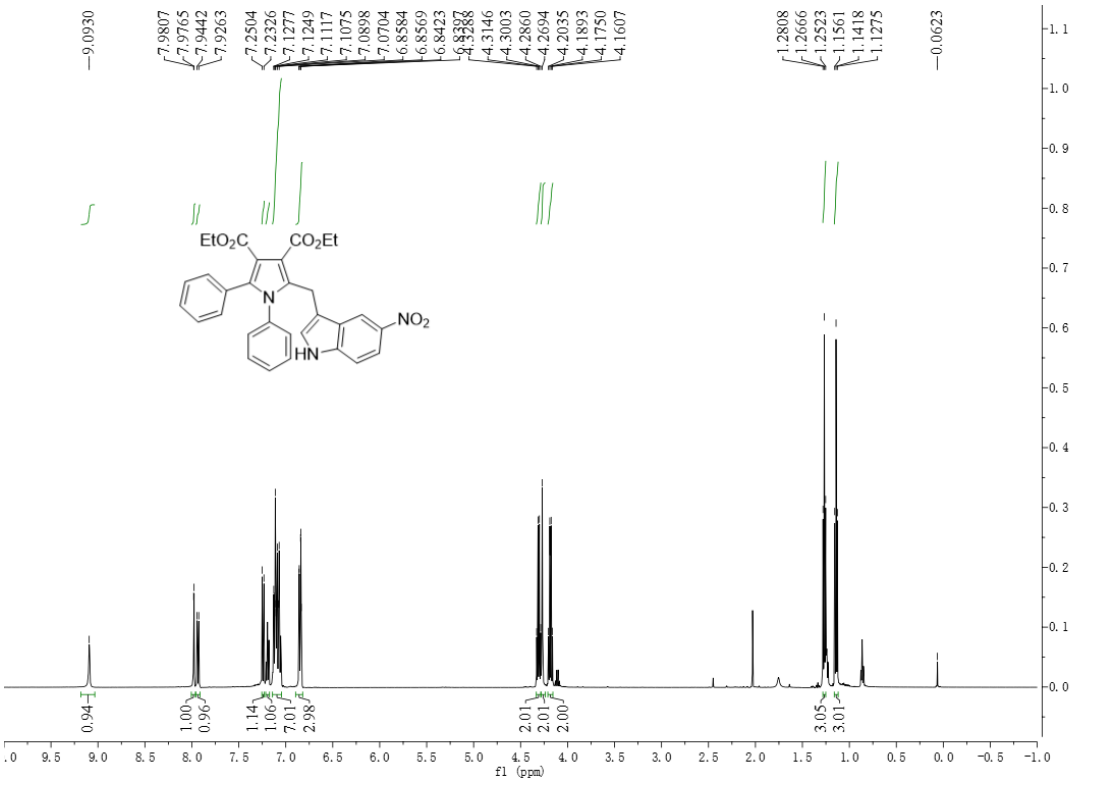


^{13}C NMR (125 MHz, $CDCl_3$)

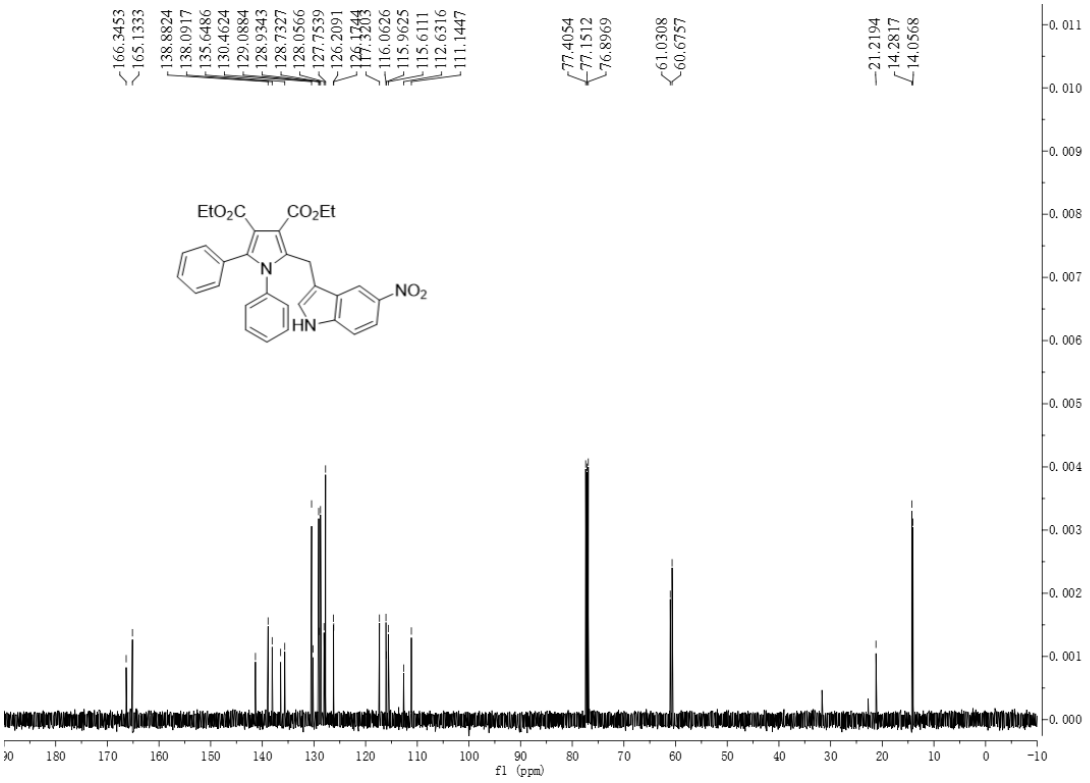


Diethyl 2-((5-nitro-1*H*-indol-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (8ab)

^{1}H NMR (500 MHz, $CDCl_3$)

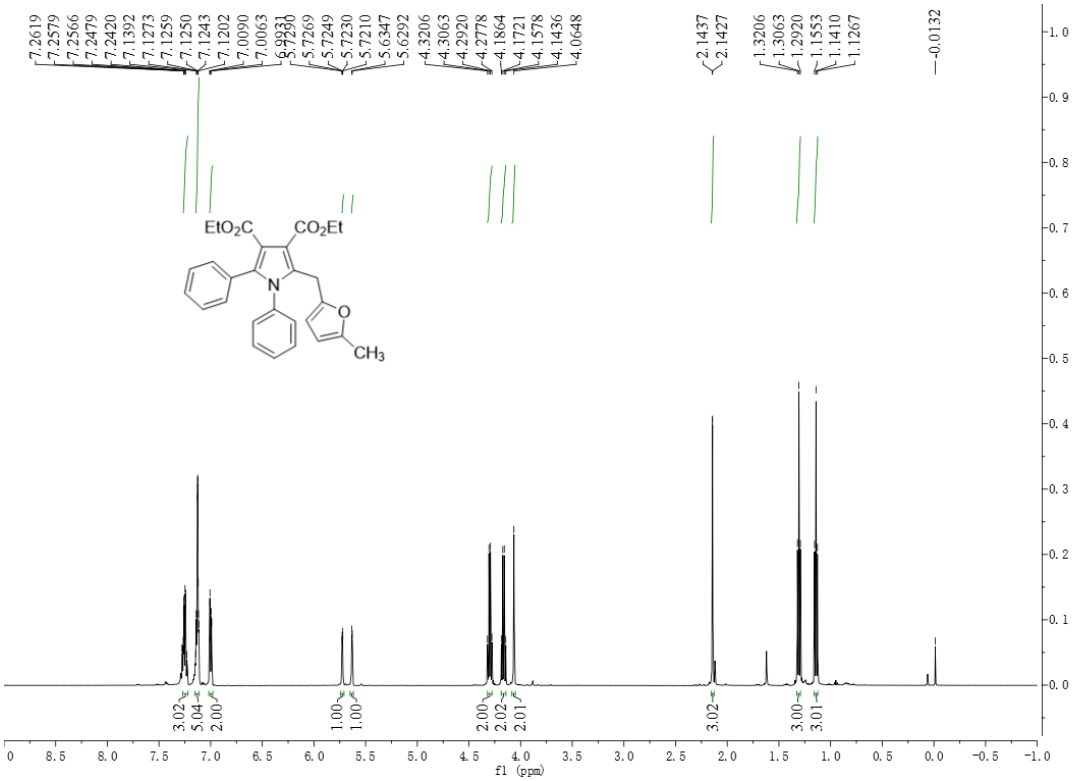


^{13}C NMR (125 MHz, $CDCl_3$)

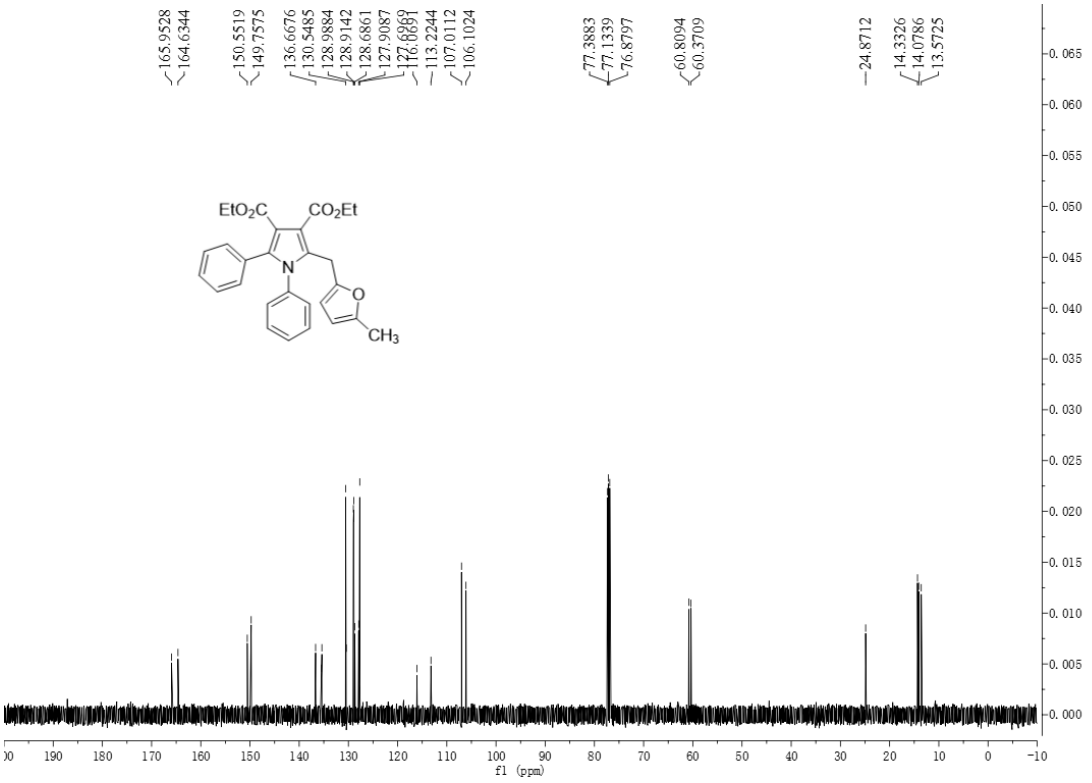


Diethyl 2-((5-methylfuran-2-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (9aa)

^{1}H NMR (500 MHz, $CDCl_3$)

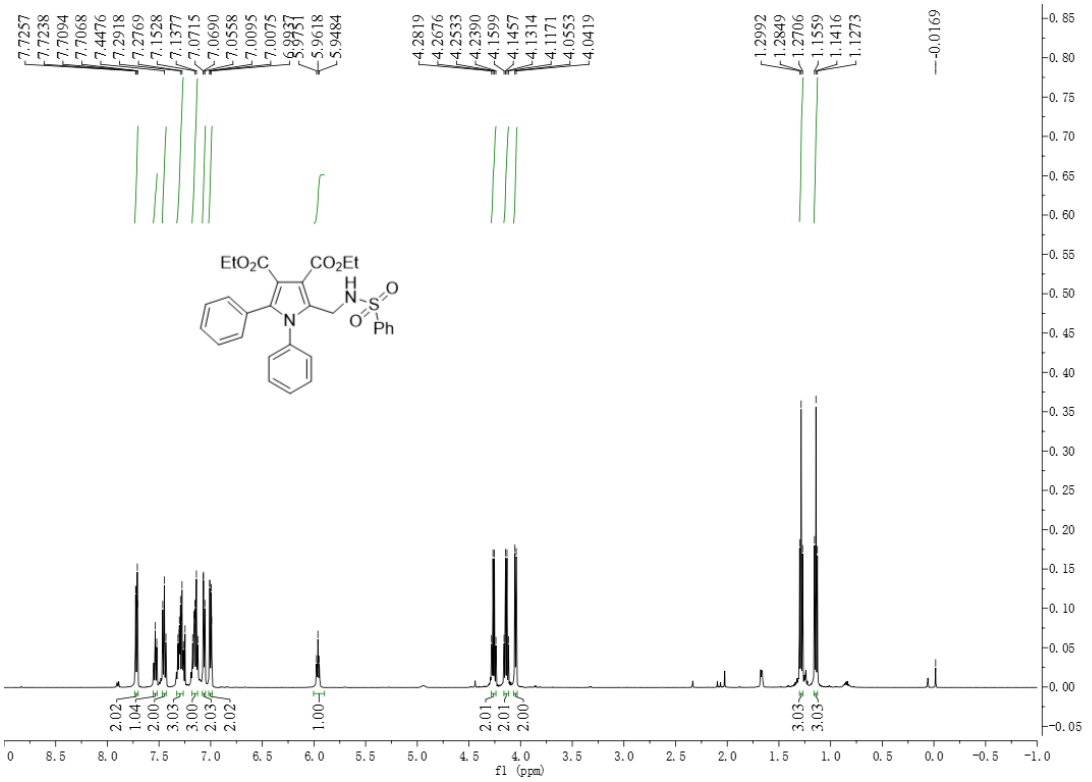


^{13}C NMR (125 MHz, $CDCl_3$)

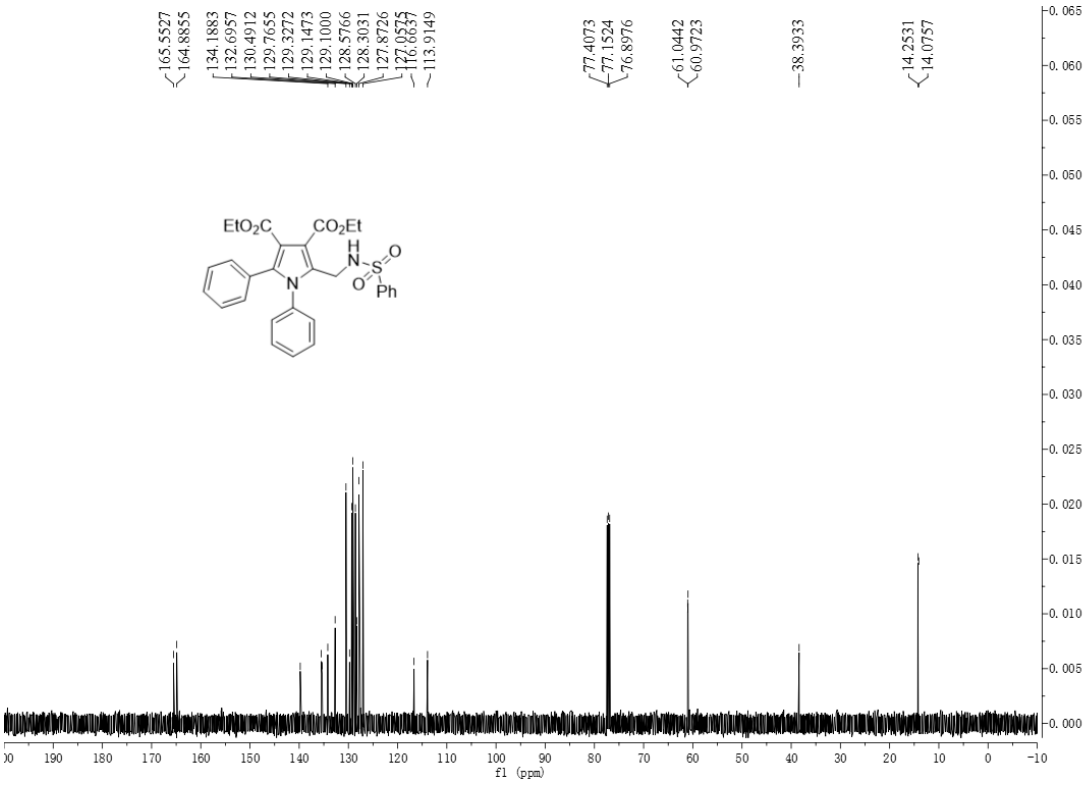


Diethyl 1,2-diphenyl-5-(phenylsulfonamidomethyl)-1*H*-pyrrole-3,4-dicarboxylate (10aa)

^{1}H NMR (500 MHz, $CDCl_3$)

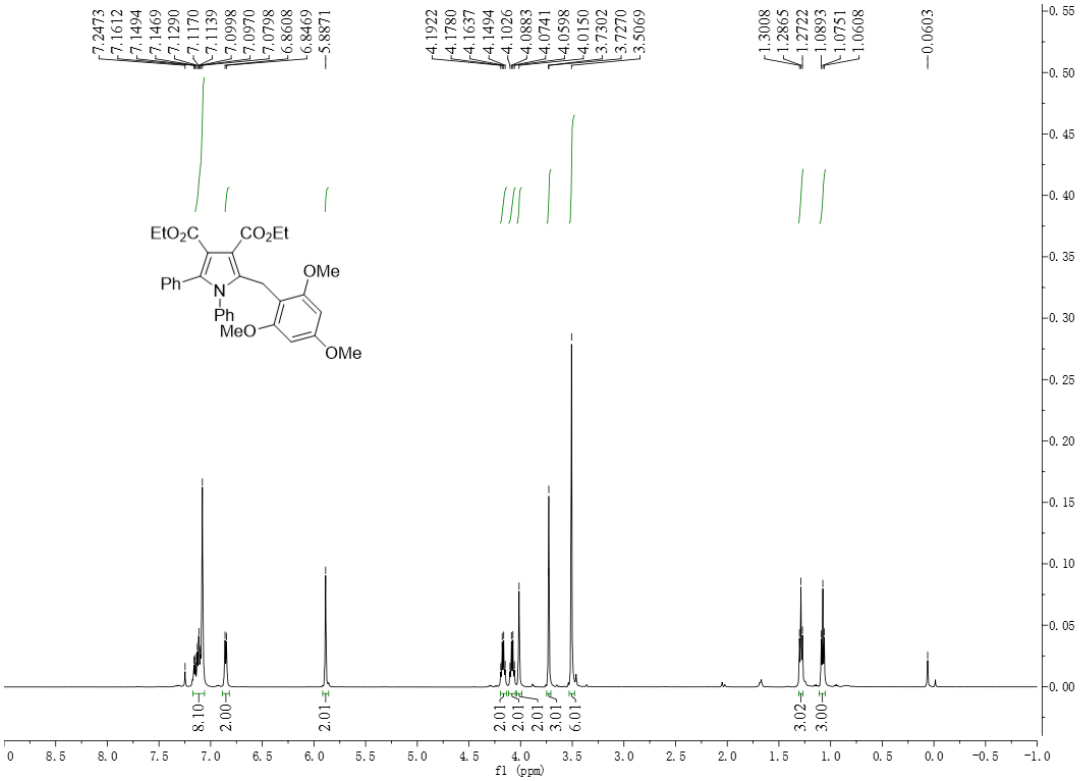


^{13}C NMR (125 MHz, $CDCl_3$)

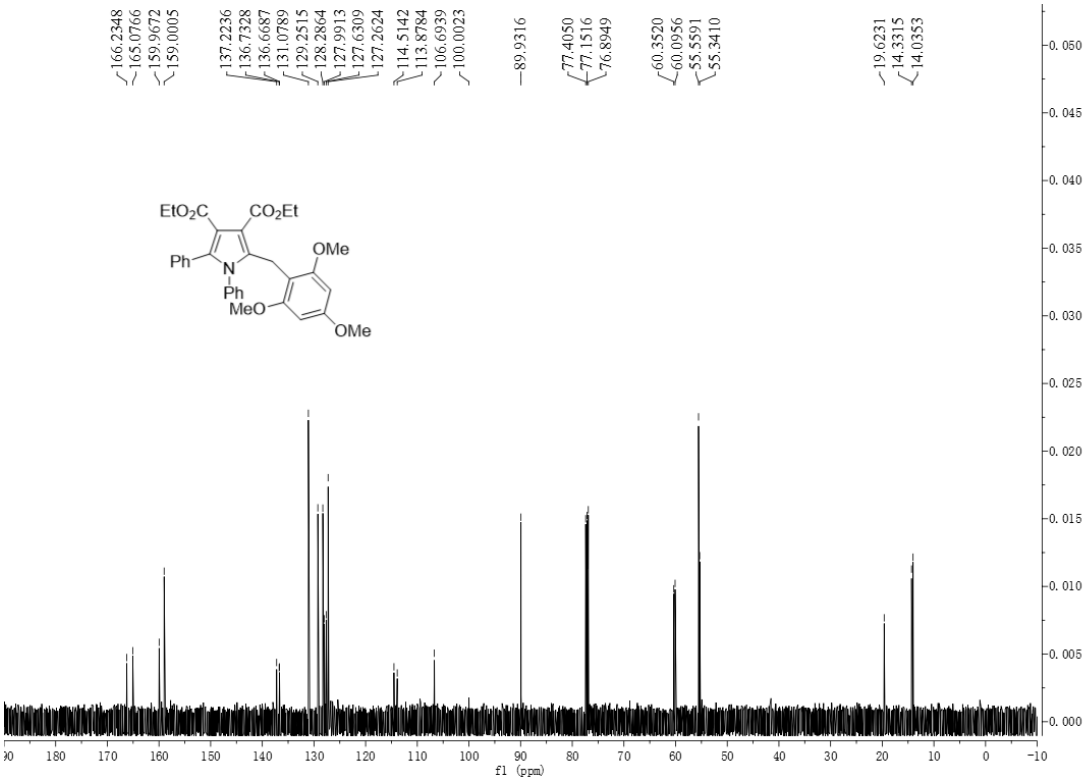


Diethyl 1,2-diphenyl-5-(2,4,6-trimethoxybenzyl)-1*H*-pyrrole-3,4-dicarboxylate (11aa)

^{1}H NMR (500 MHz, $CDCl_3$)

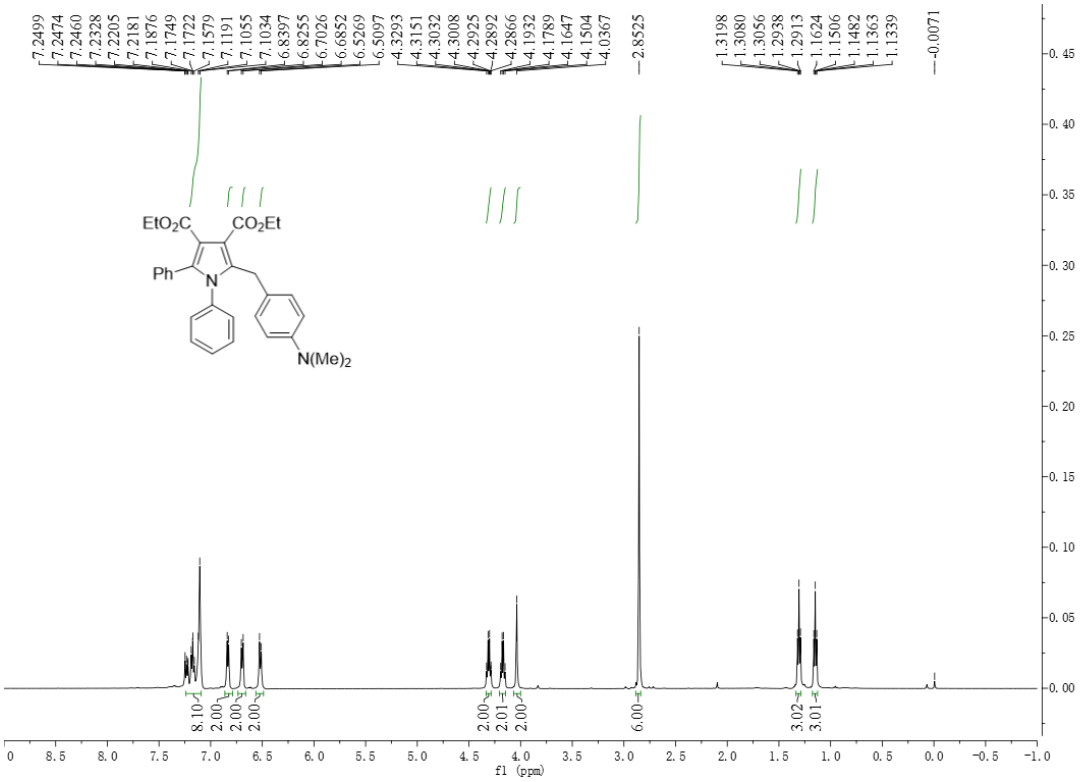


^{13}C NMR (125 MHz, $CDCl_3$)

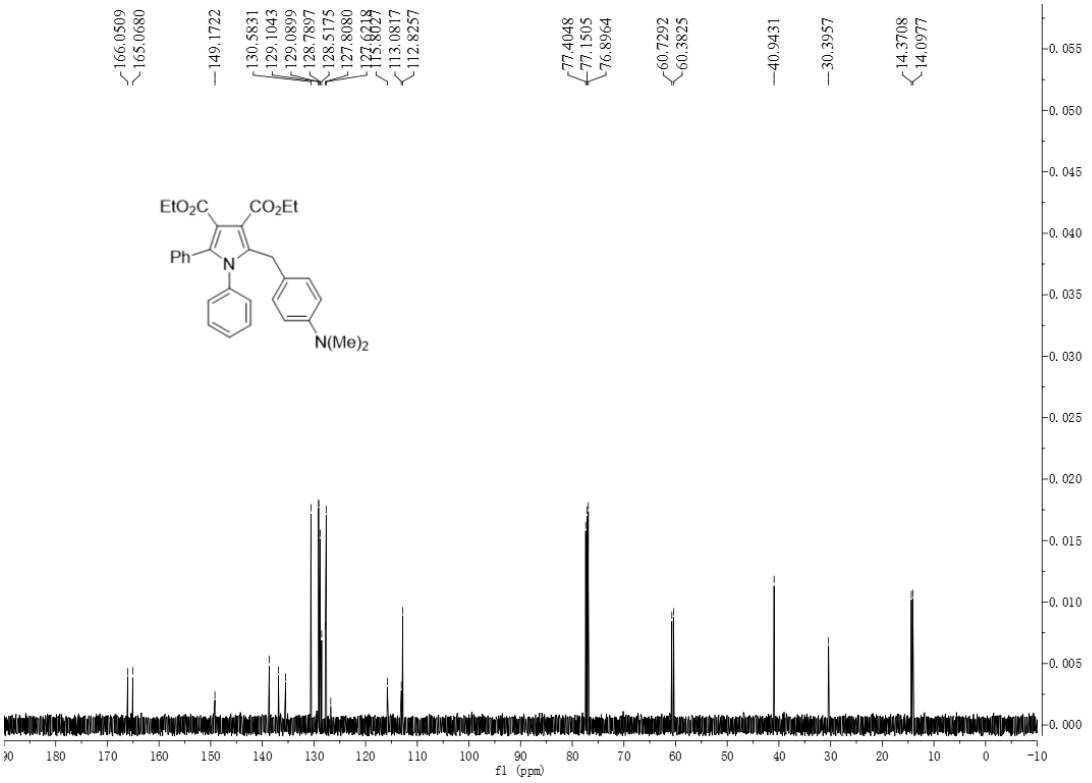


Diethyl 2-(4-(dimethylamino)benzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (12aa)

^{1}H NMR (500 MHz, $CDCl_3$)

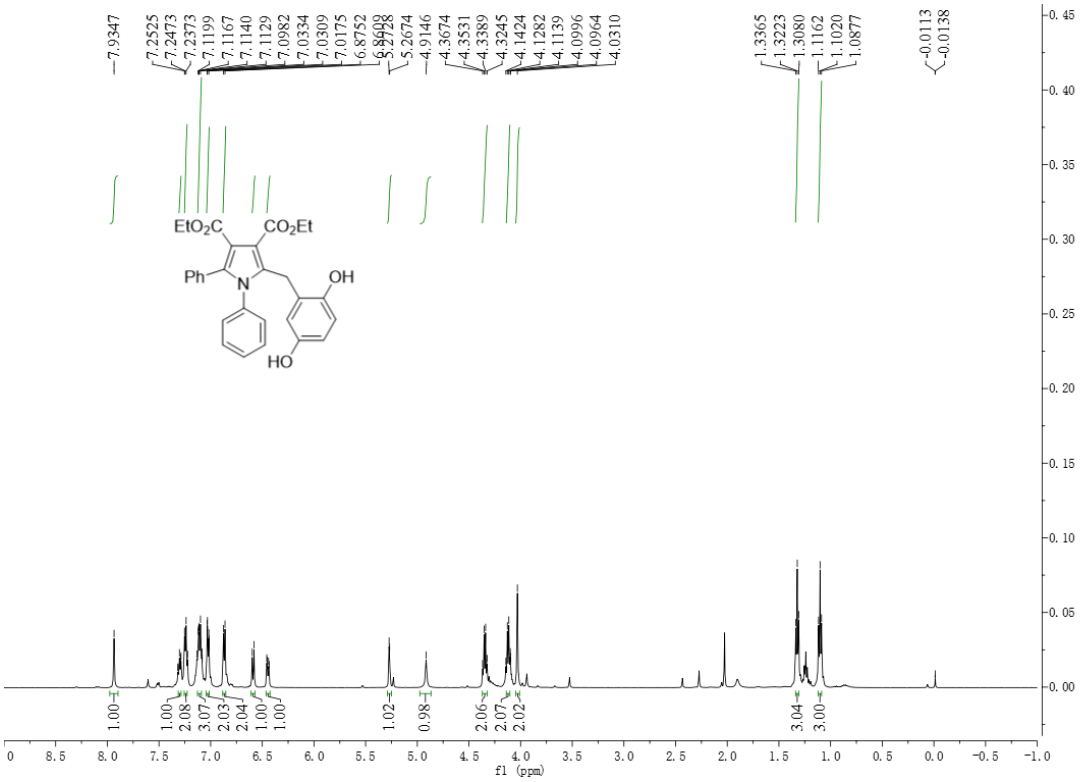


^{13}C NMR (125 MHz, $CDCl_3$)

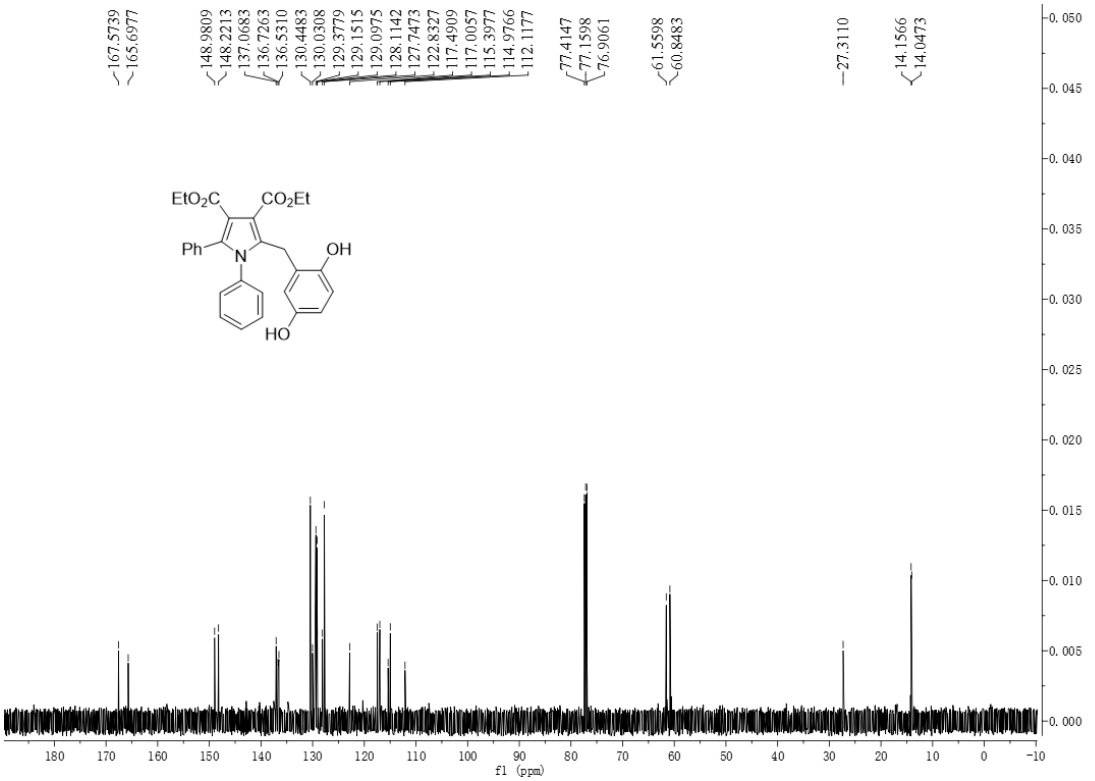


Diethyl 2-(2,5-dihydroxybenzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (13aa)

^{1}H NMR (500 MHz, $CDCl_3$)

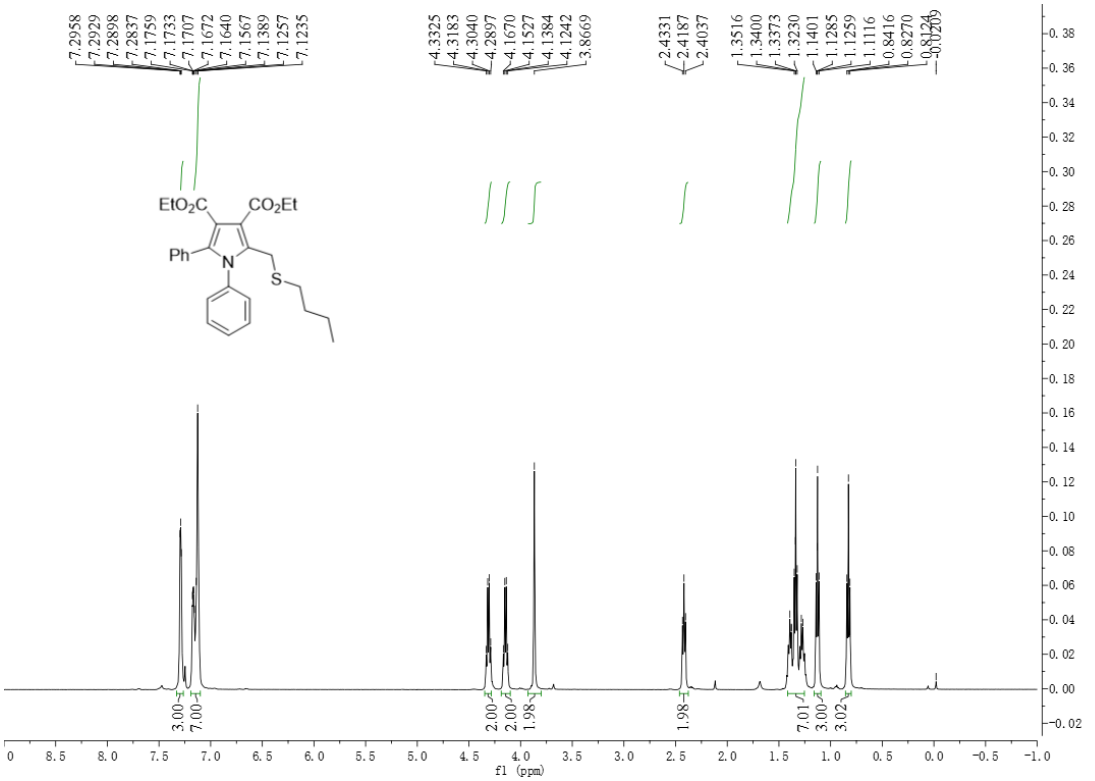


^{13}C NMR (125 MHz, $CDCl_3$)

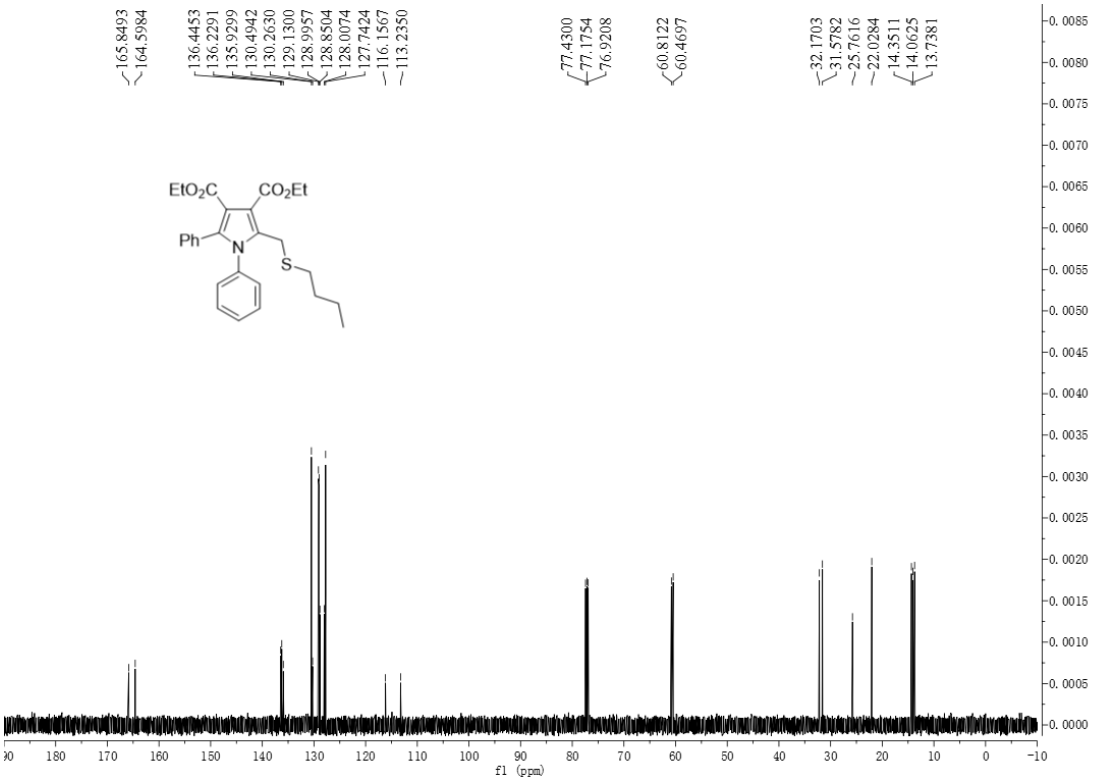


Diethyl 2-((butylthio)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (14aa)

^{1}H NMR (500 MHz, $CDCl_3$)

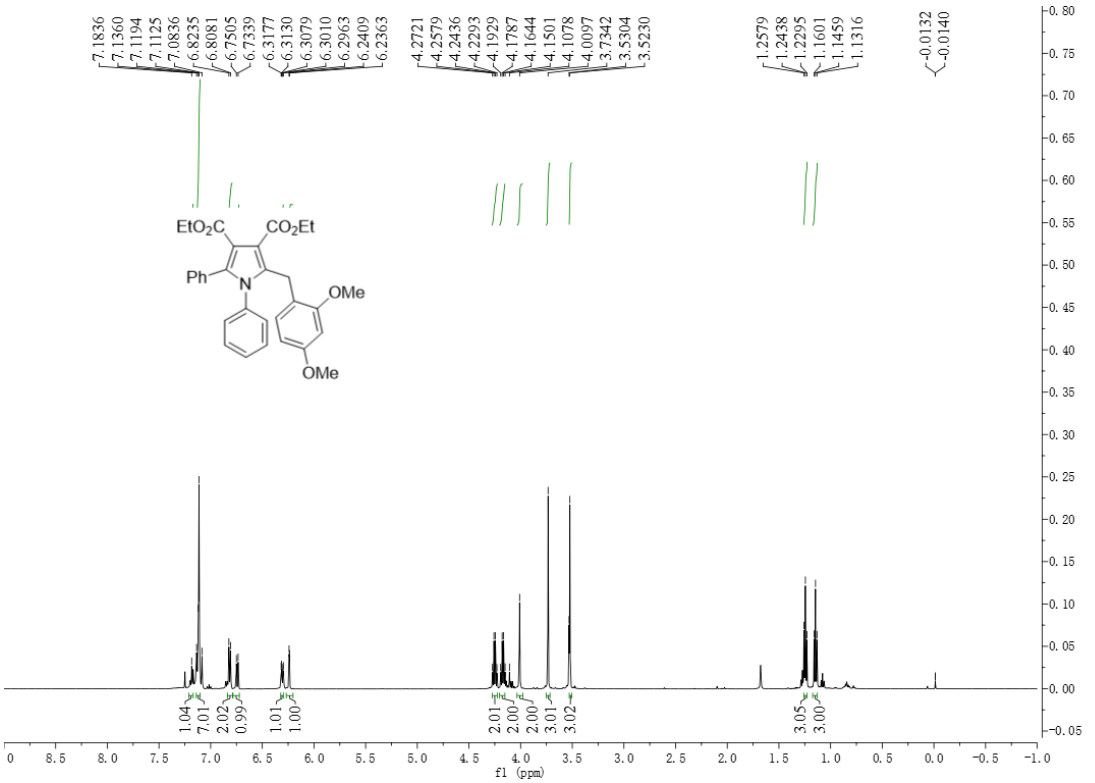


^{13}C NMR (125 MHz, $CDCl_3$)

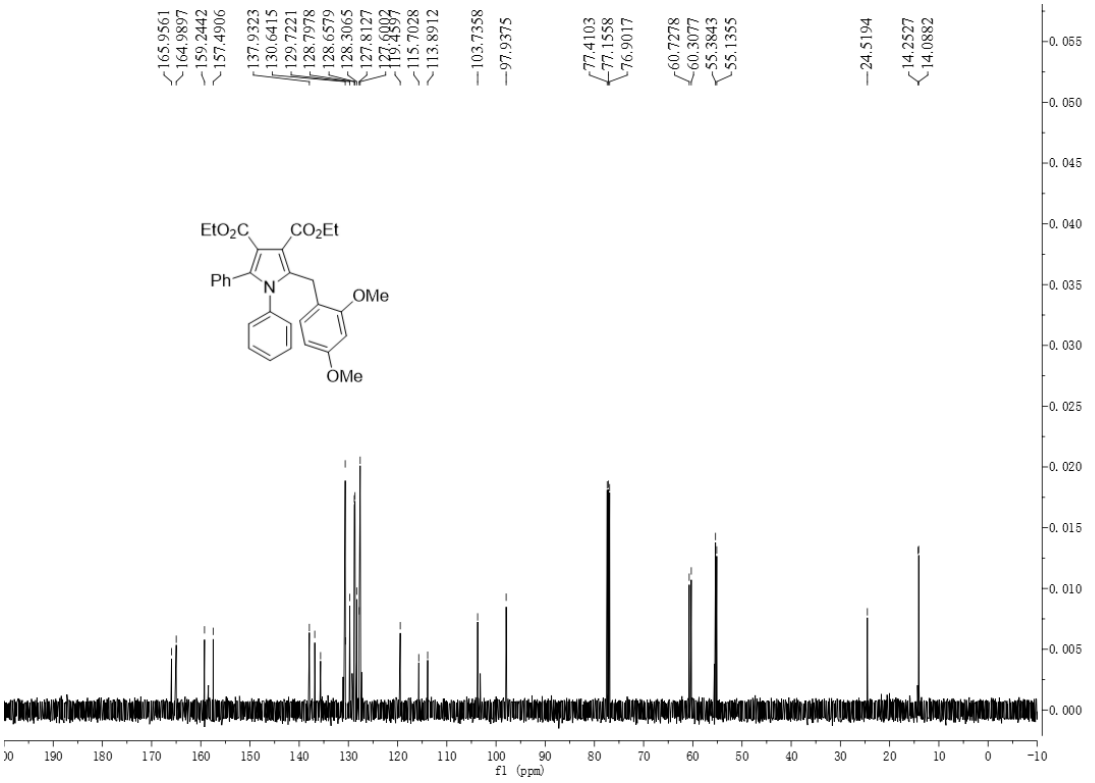


Diethyl 2-(2,4-dimethoxybenzyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (15aa)

^{1}H NMR (500 MHz, $CDCl_3$)

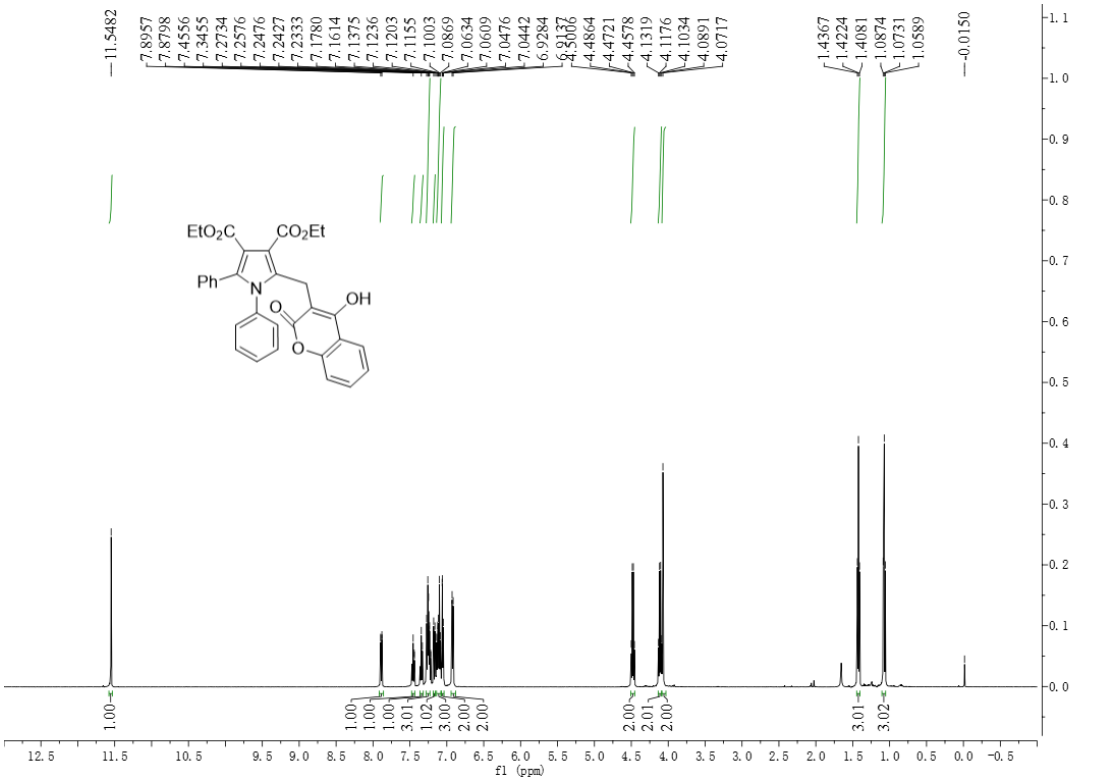


^{13}C NMR (125 MHz, $CDCl_3$)

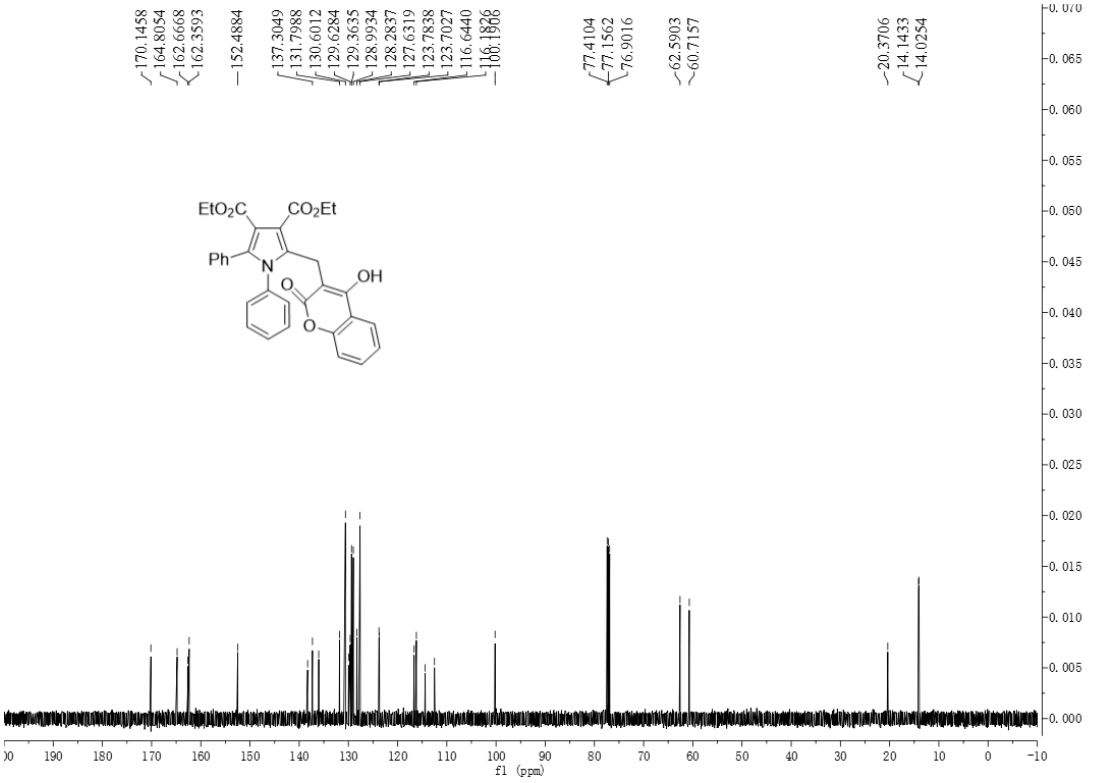


Diethyl 2-((4-hydroxy-2-oxo-2*H*-chromen-3-yl)methyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (16aa)

^{1}H NMR (500 MHz, $CDCl_3$)

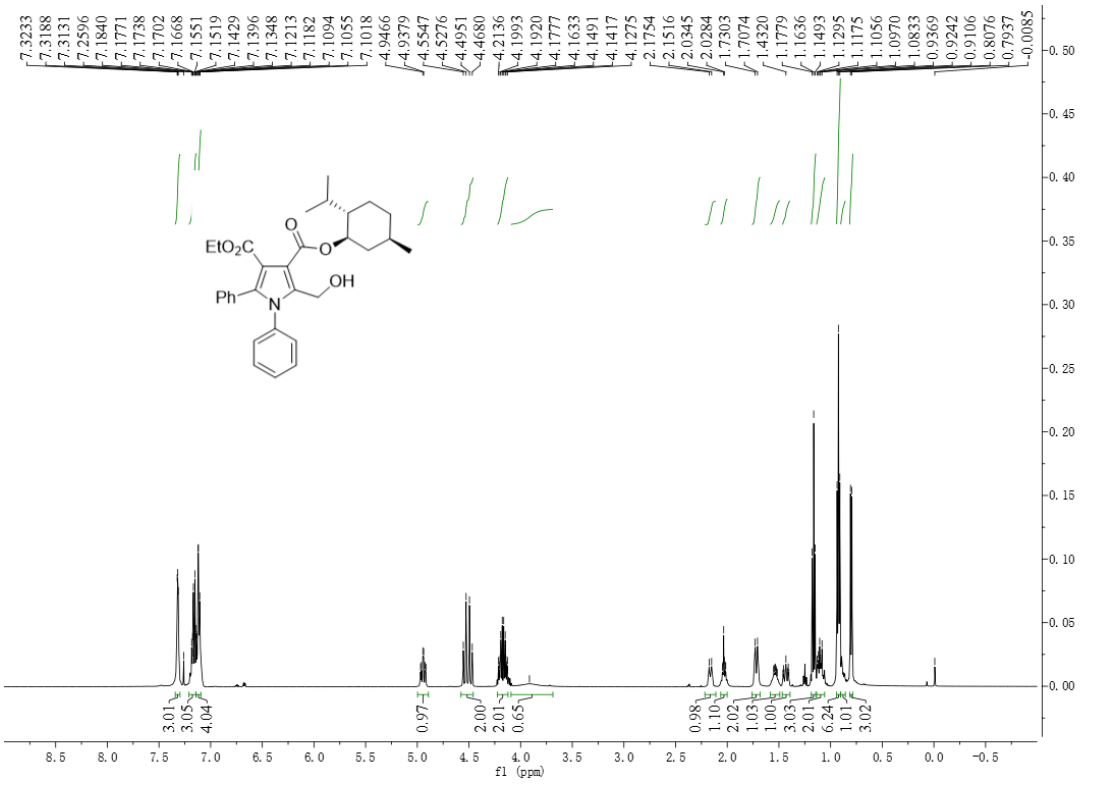


^{13}C NMR (125 MHz, $CDCl_3$)

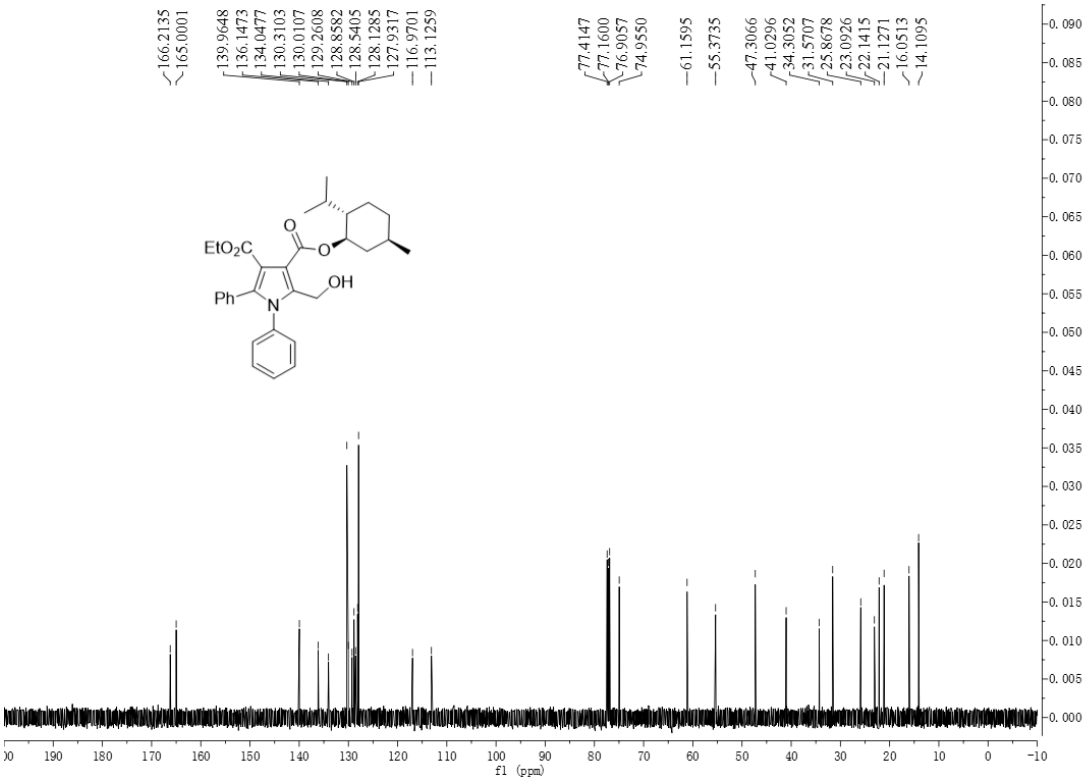


3-Ethyl 4-((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17aa)

^{1}H NMR (500 MHz, $CDCl_3$)

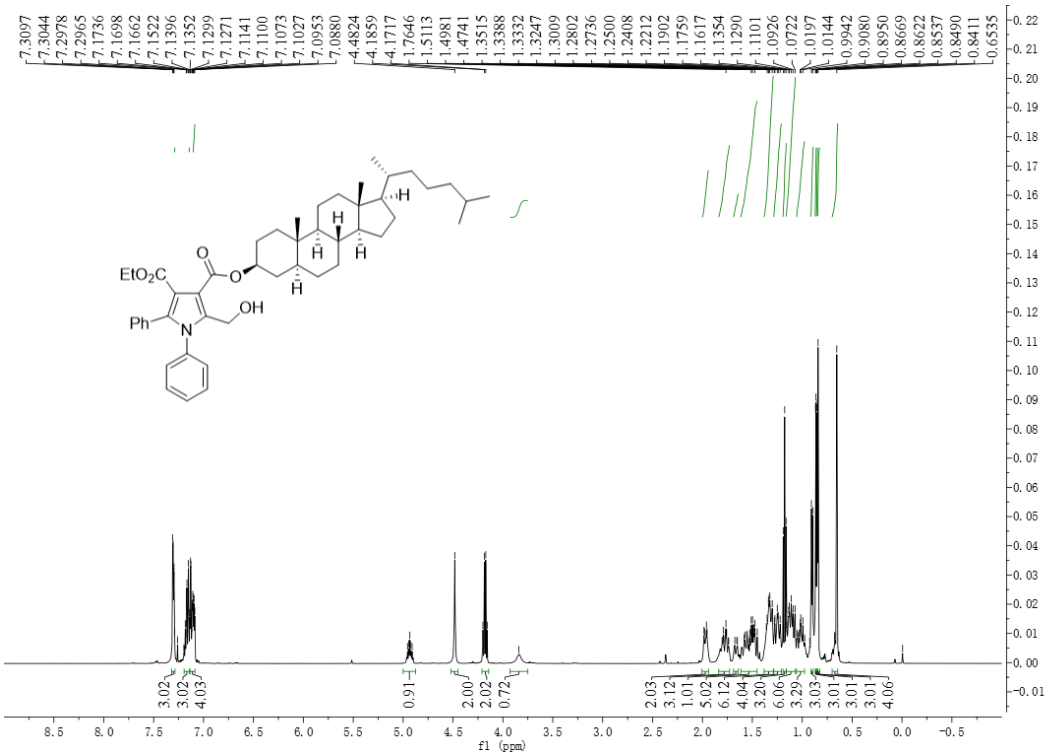


^{13}C NMR (125 MHz, $CDCl_3$)

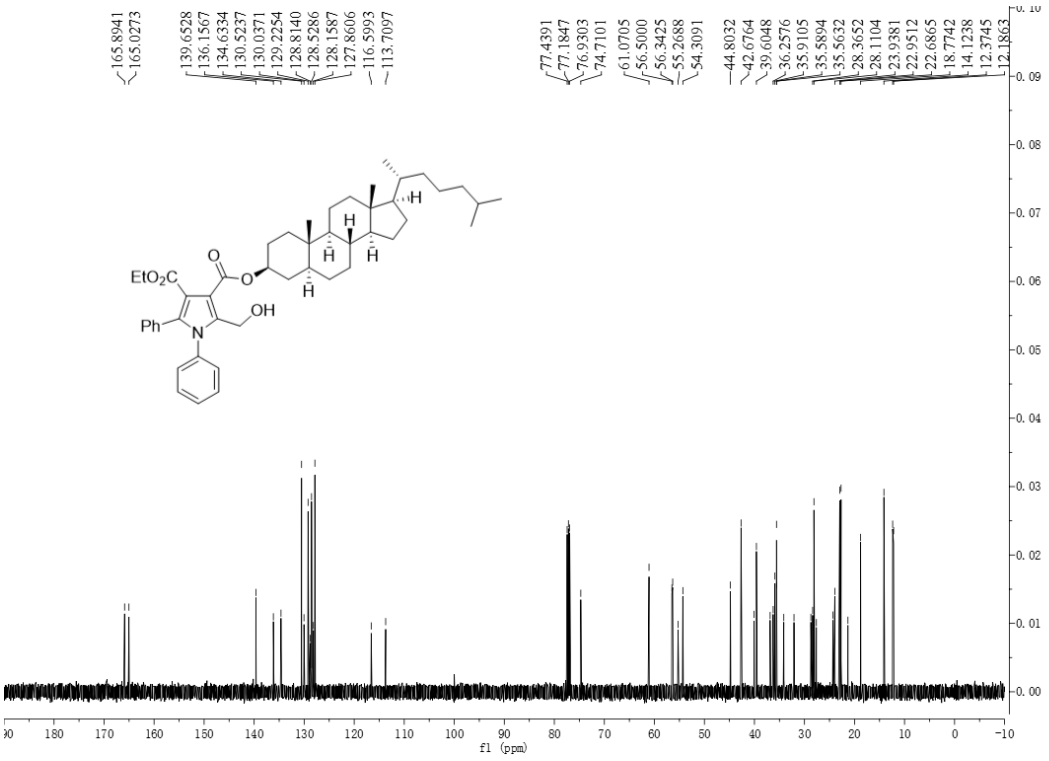


3-((3*S*,5*S*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl) 4-ethyl 2-(hydroxymethyl)-1,5-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ab)

^{1}H NMR (500 MHz, $CDCl_3$)

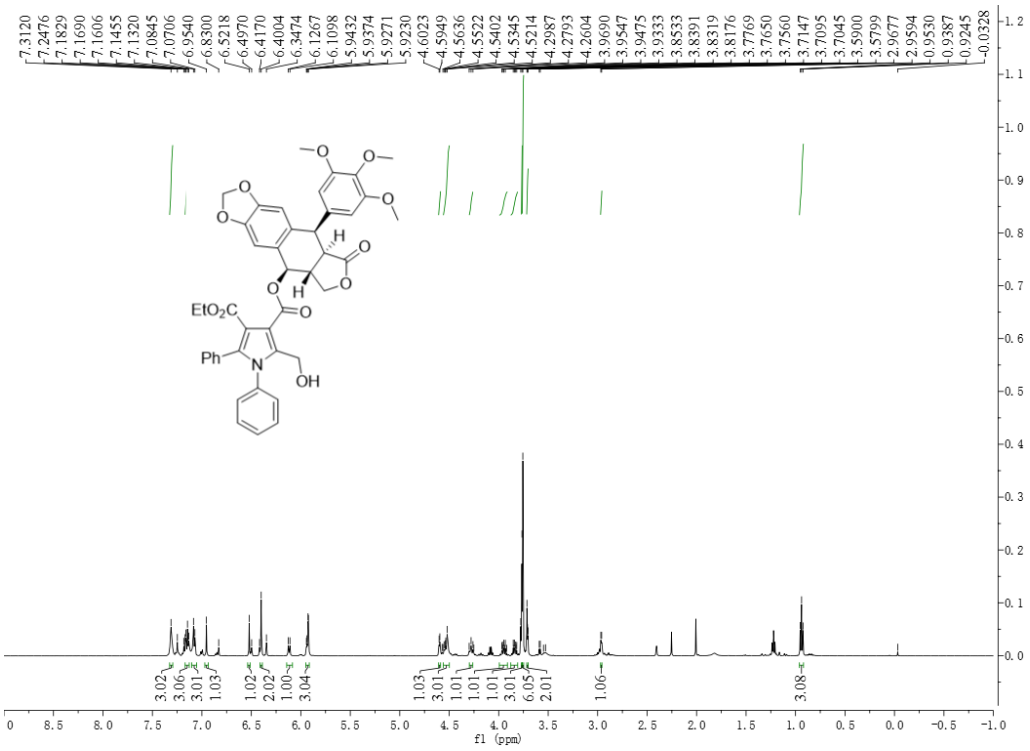


^{13}C NMR (125 MHz, $CDCl_3$)

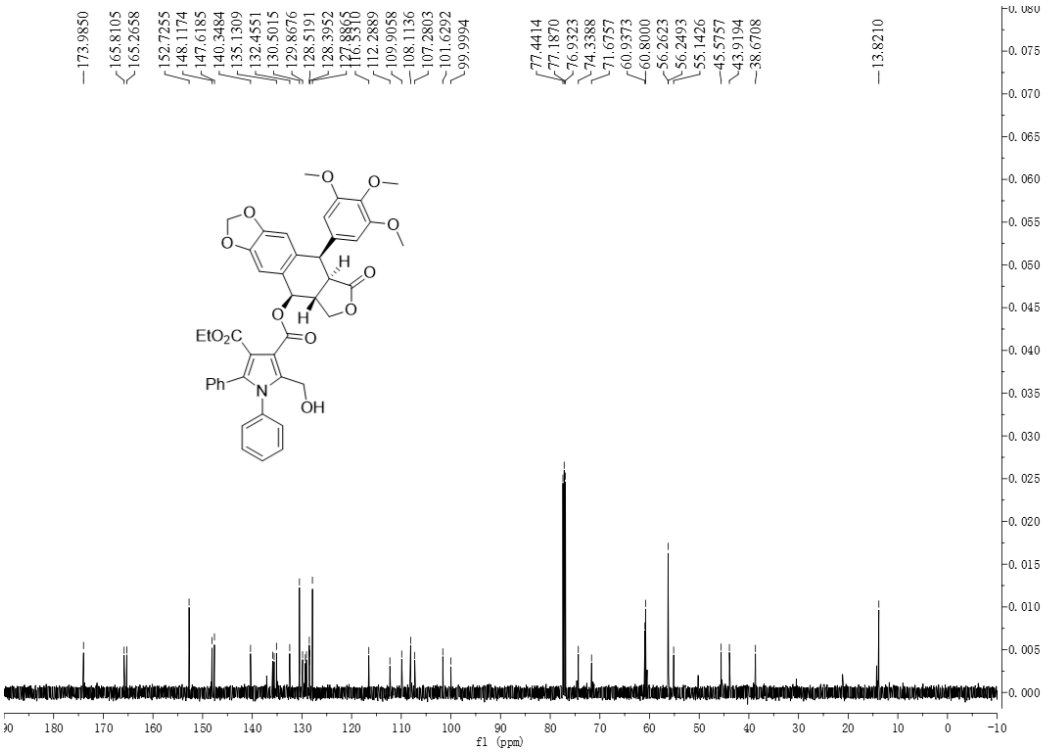


3-Ethyl 4-((5*R*,5a*R*,8a*R*,9*R*)-8-oxo-9-(3,4,5-trimethoxyphenyl)-5,5a,6,8,8a,9-hexahydrofuro [3',4':6,7]naphtho[2,3-*d*][1,3]dioxol-5-yl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ac)

^{1}H NMR (500 MHz, $CDCl_3$)

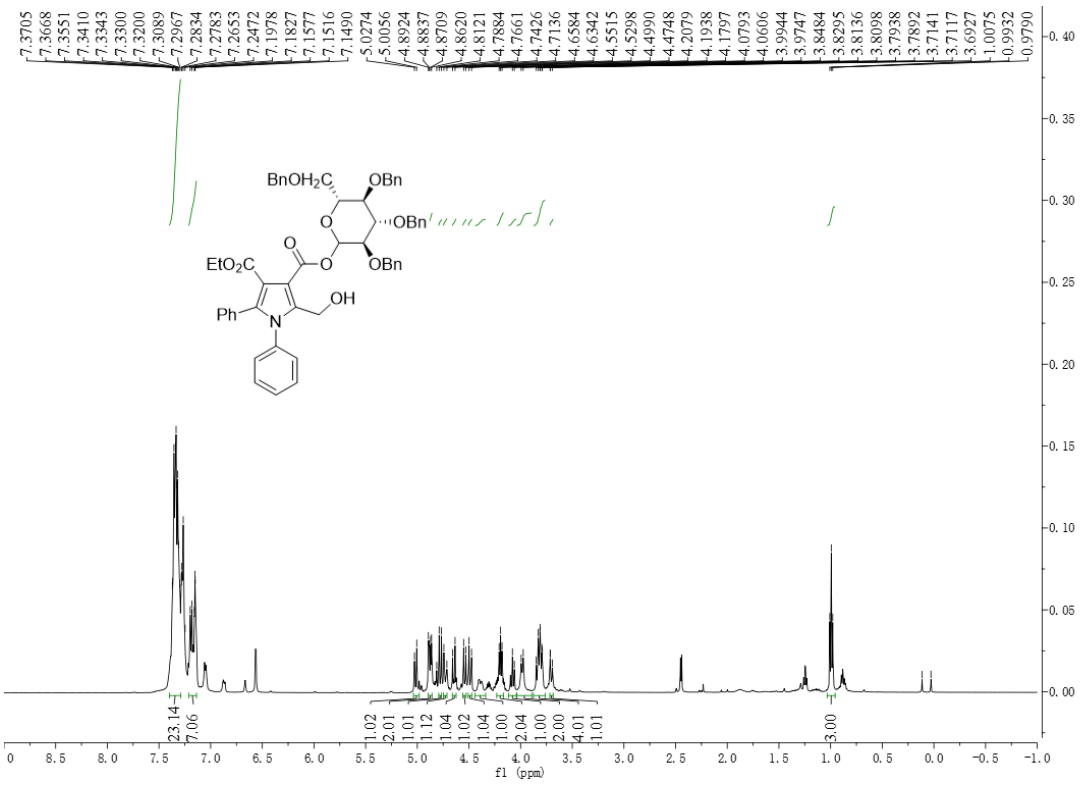


^{13}C NMR (125 MHz, $CDCl_3$)

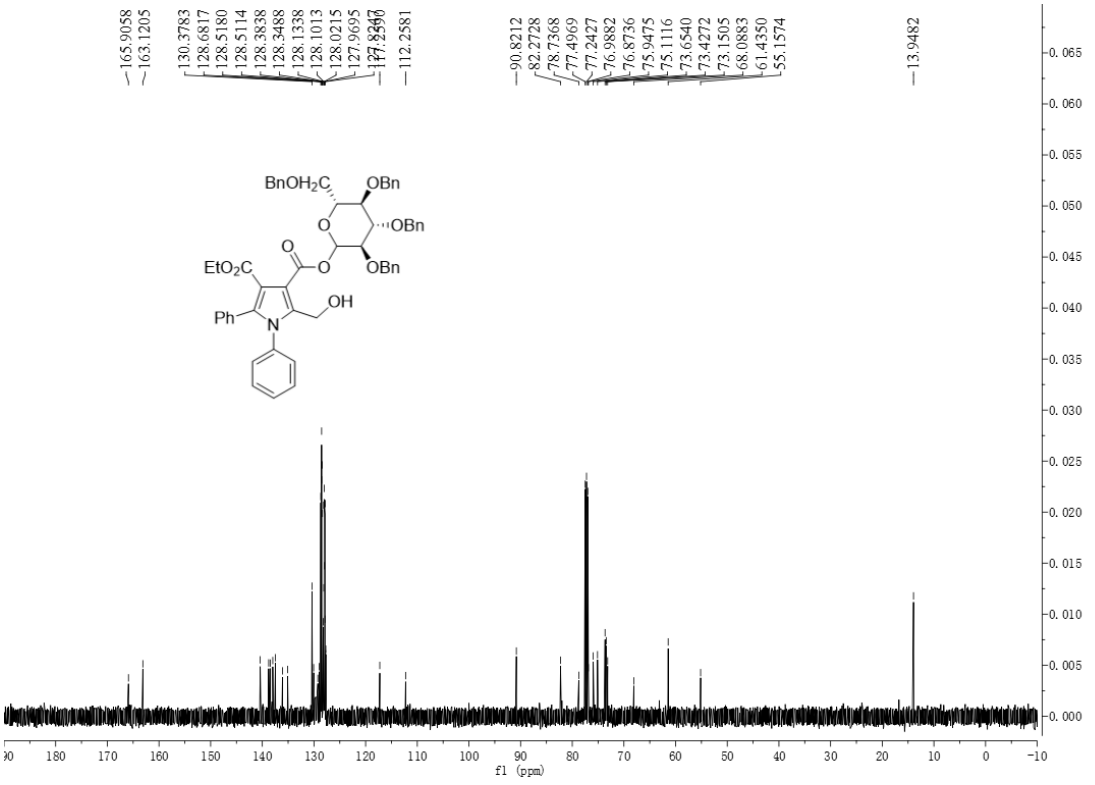


3-Ethyl 4-((3*R*,4*S*,5*R*,6*R*)-3,4,5-tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ad)

^{1}H NMR (500 MHz, $CDCl_3$)

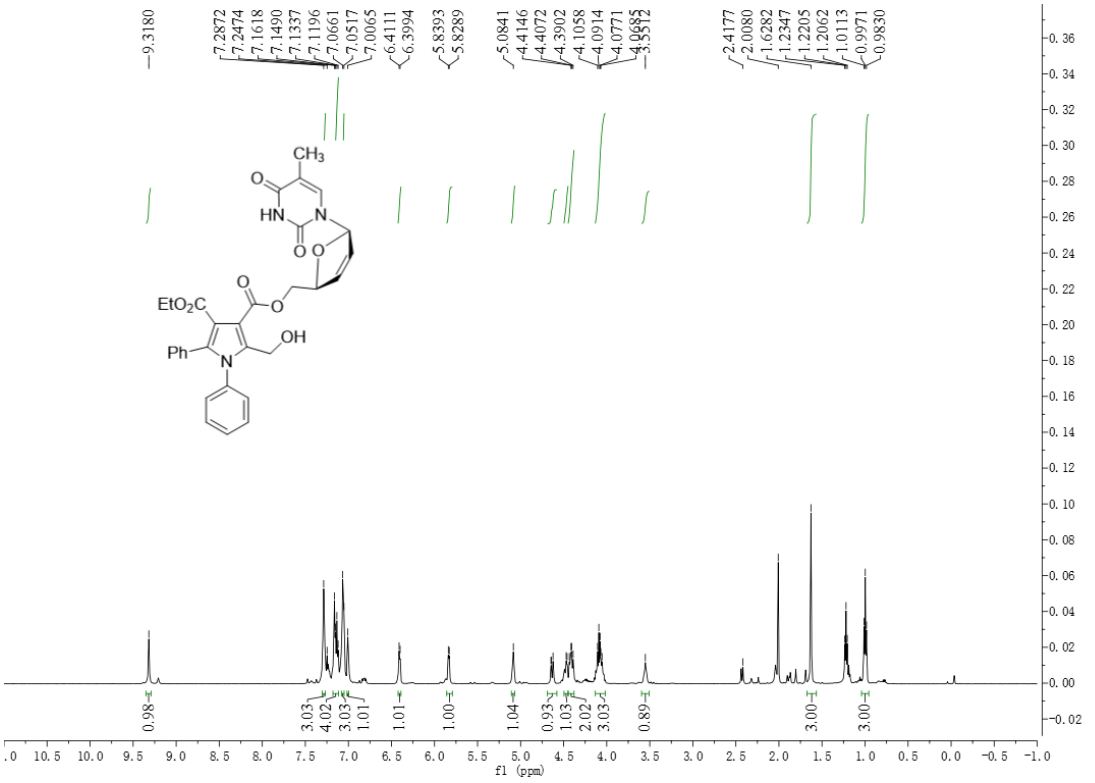


^{13}C NMR (125 MHz, $CDCl_3$)

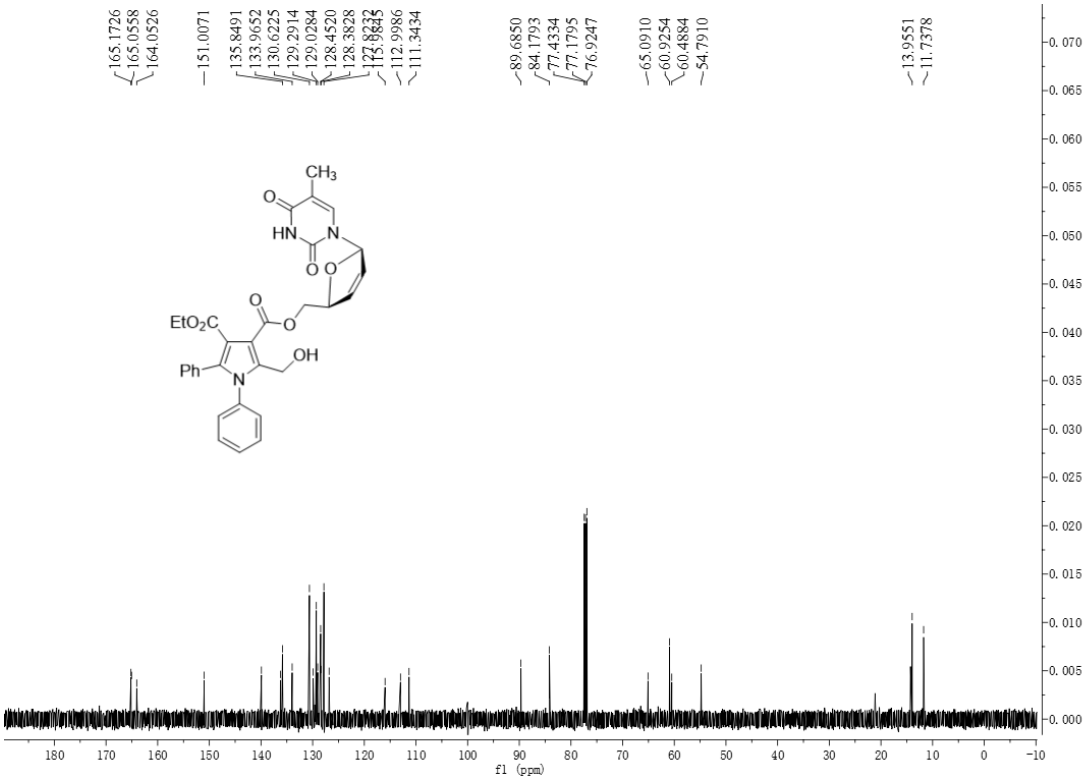


3-Ethyl 4-(((2*S*,5*R*)-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2*H*)-yl)-2,5-dihydrofuran-2-yl)methyl) 5-(hydroxymethyl)-1,2-diphenyl-1*H*-pyrrole-3,4-dicarboxylate (17ae)

^{1}H NMR (500 MHz, $CDCl_3$)

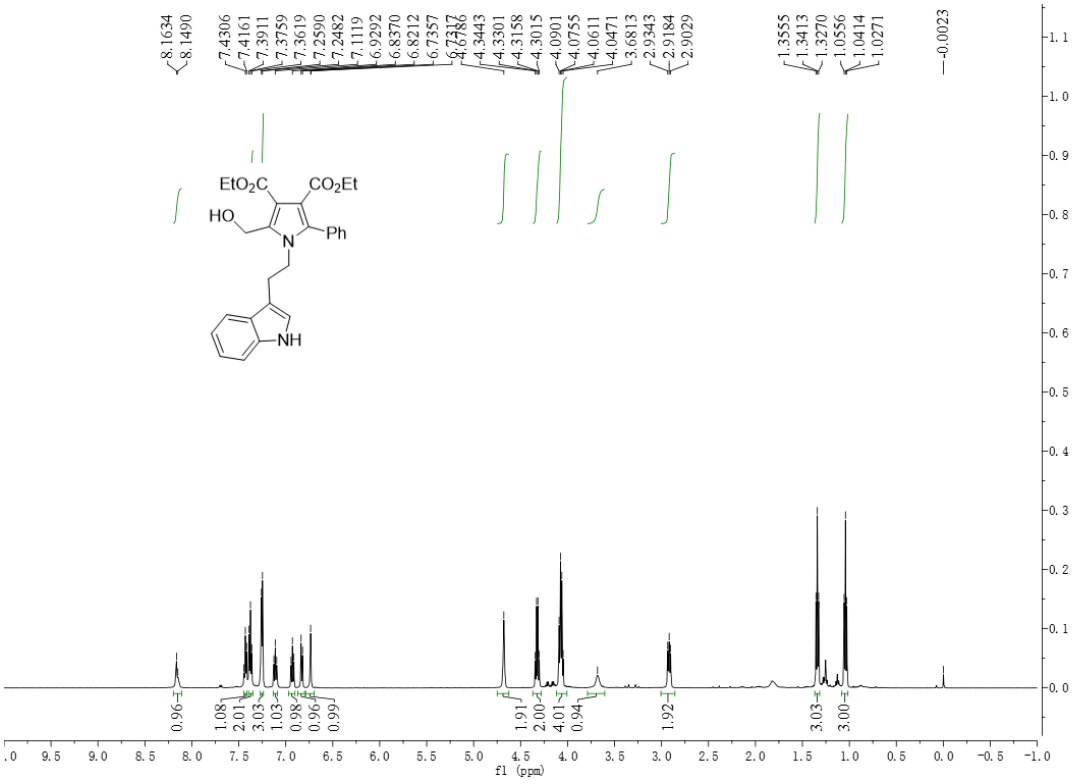


^{13}C NMR (125 MHz, $CDCl_3$)

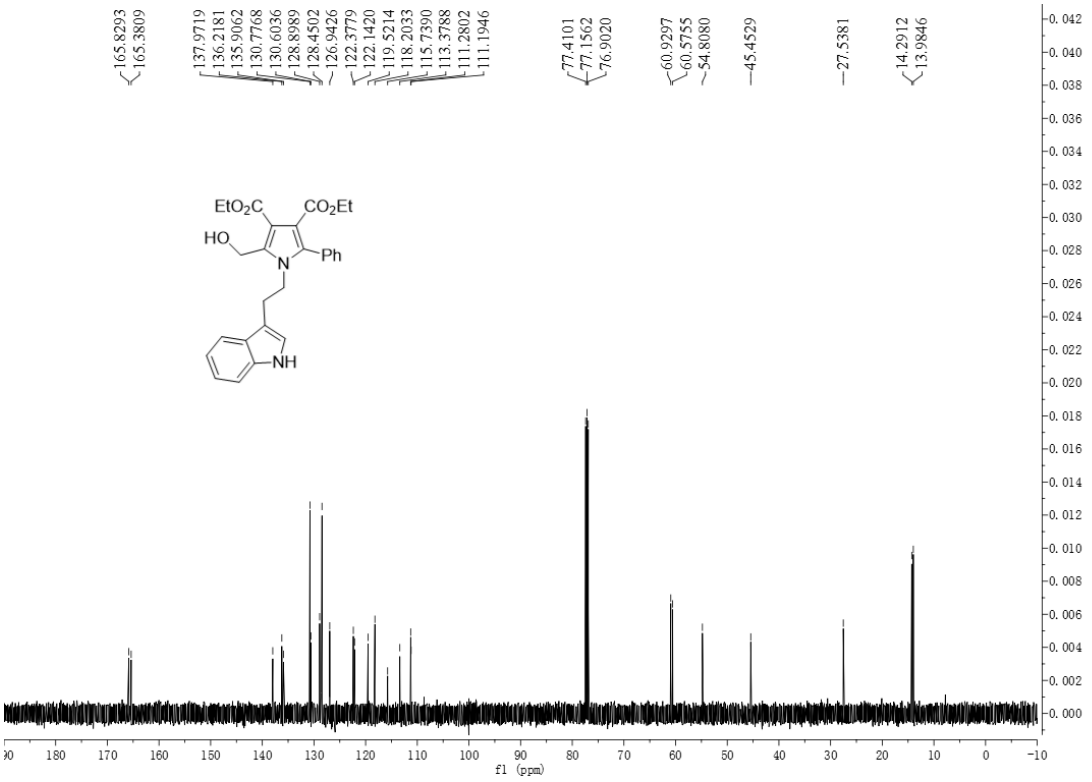


Diethyl 1-(2-(1*H*-indol-3-yl)ethyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (17af)

^{1}H NMR (500 MHz, $CDCl_3$)

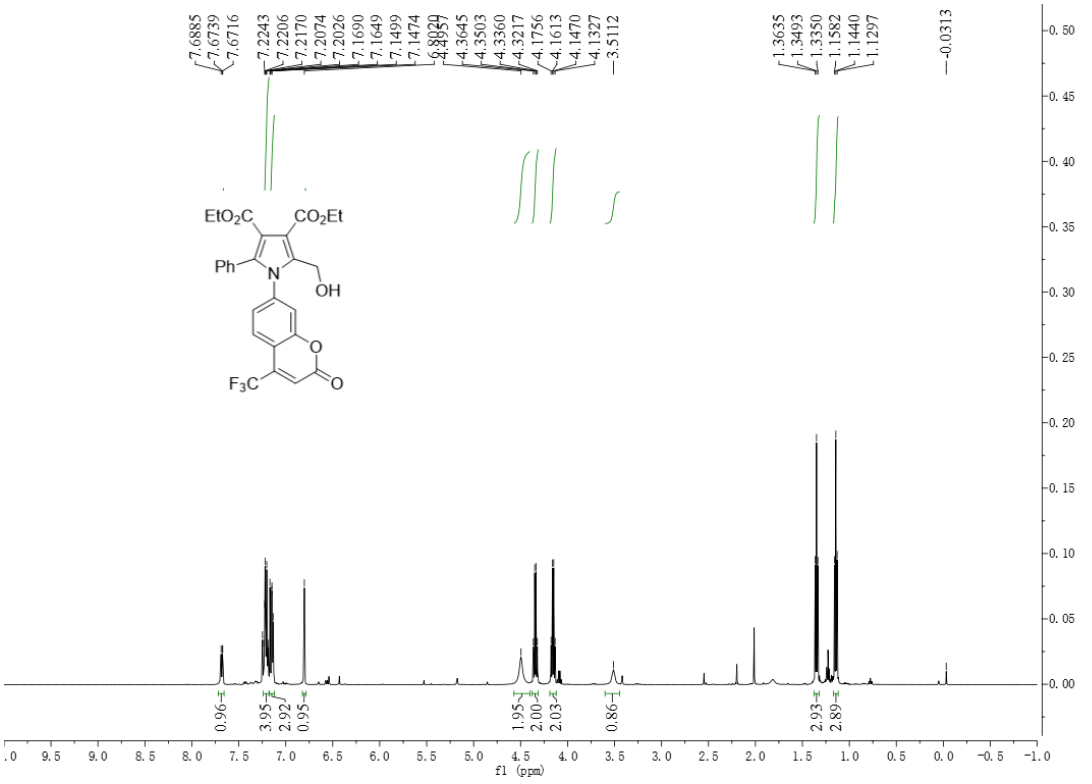


^{13}C NMR (125 MHz, $CDCl_3$)

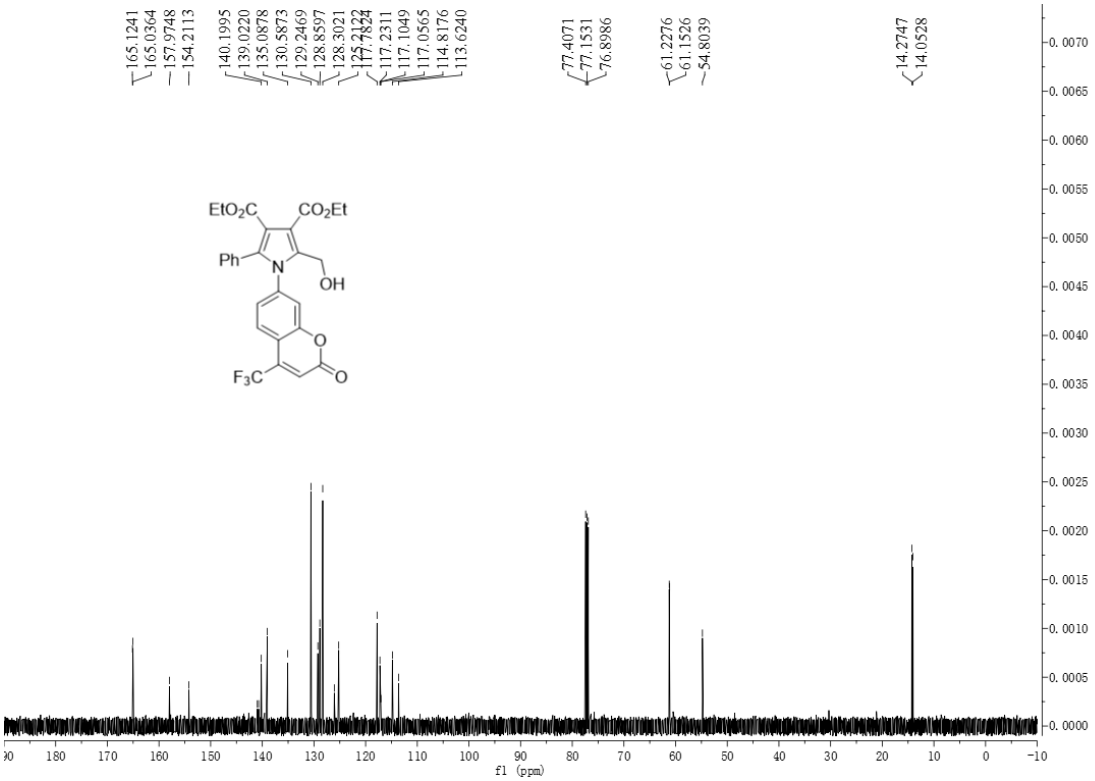


Diethyl 2-(hydroxymethyl)-1-(2-oxo-4-(trifluoromethyl)-2*H*-chromen-7-yl)-5-phenyl-1*H*-pyrrole-3,4-dicarboxylate (17ag)

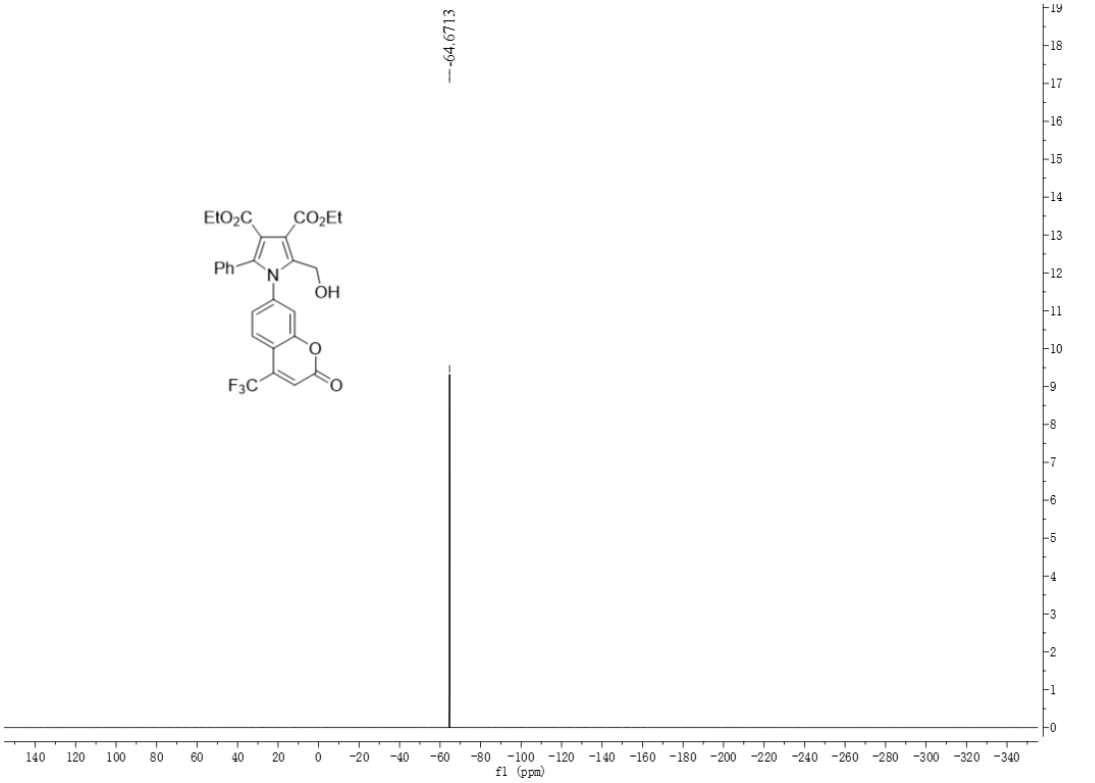
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)



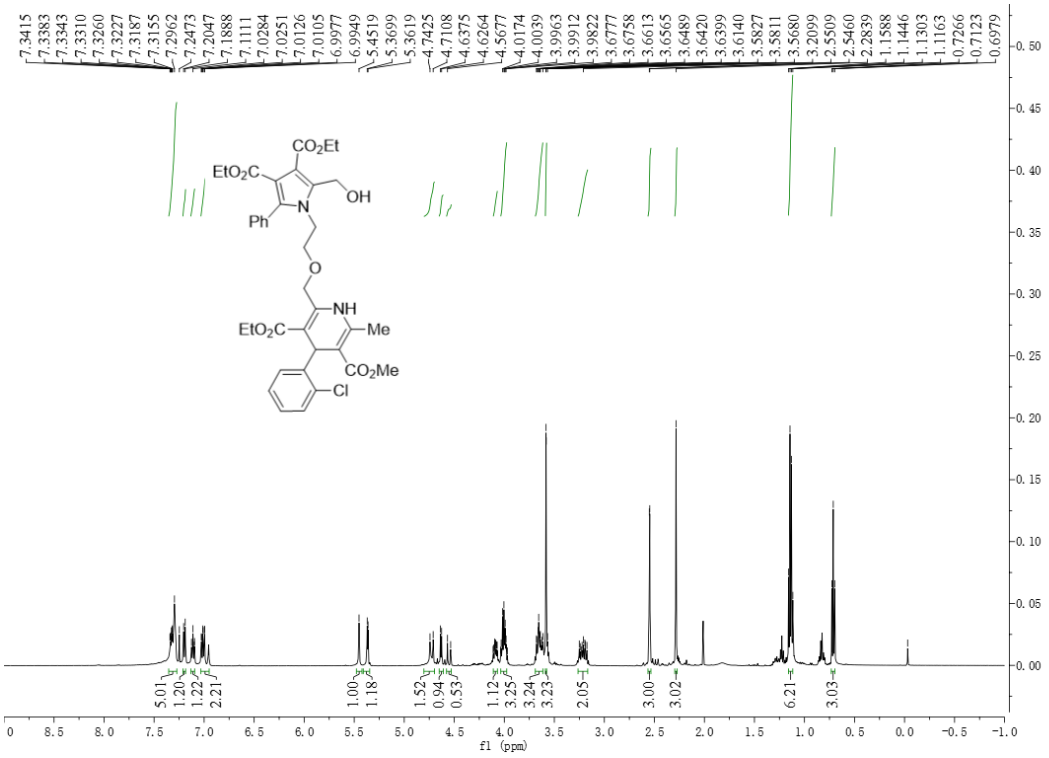
^{19}F NMR (470 MHz, $CDCl_3$)



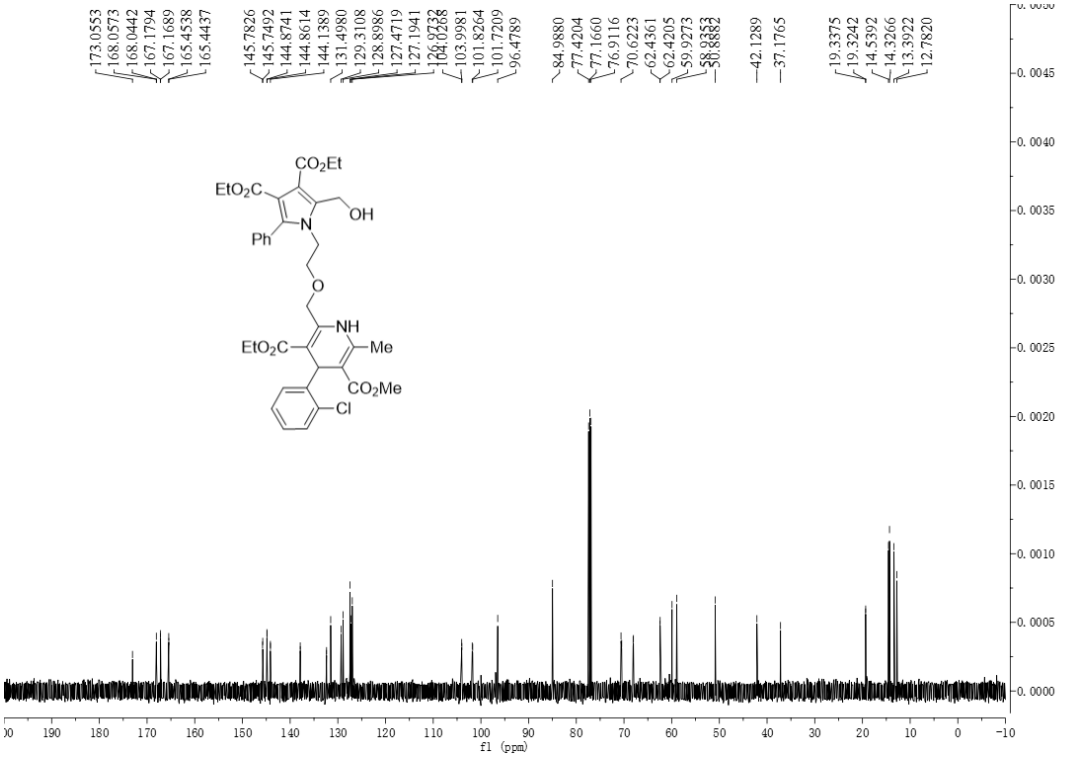
3-Ethyl 5-methyl 2-((2-(3,4-bis(ethoxycarbonyl)-2-(hydroxymethyl)-5-phenyl-1*H*-pyrrol-1-

yl)ethoxy)methyl)-4-(2-chlorophenyl)-6-methyl-1,4-dihydropyridine-3,5-dicarboxylate (17ah)

^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C NMR (125 MHz, $CDCl_3$)



Crystallographic data for compound 4ag

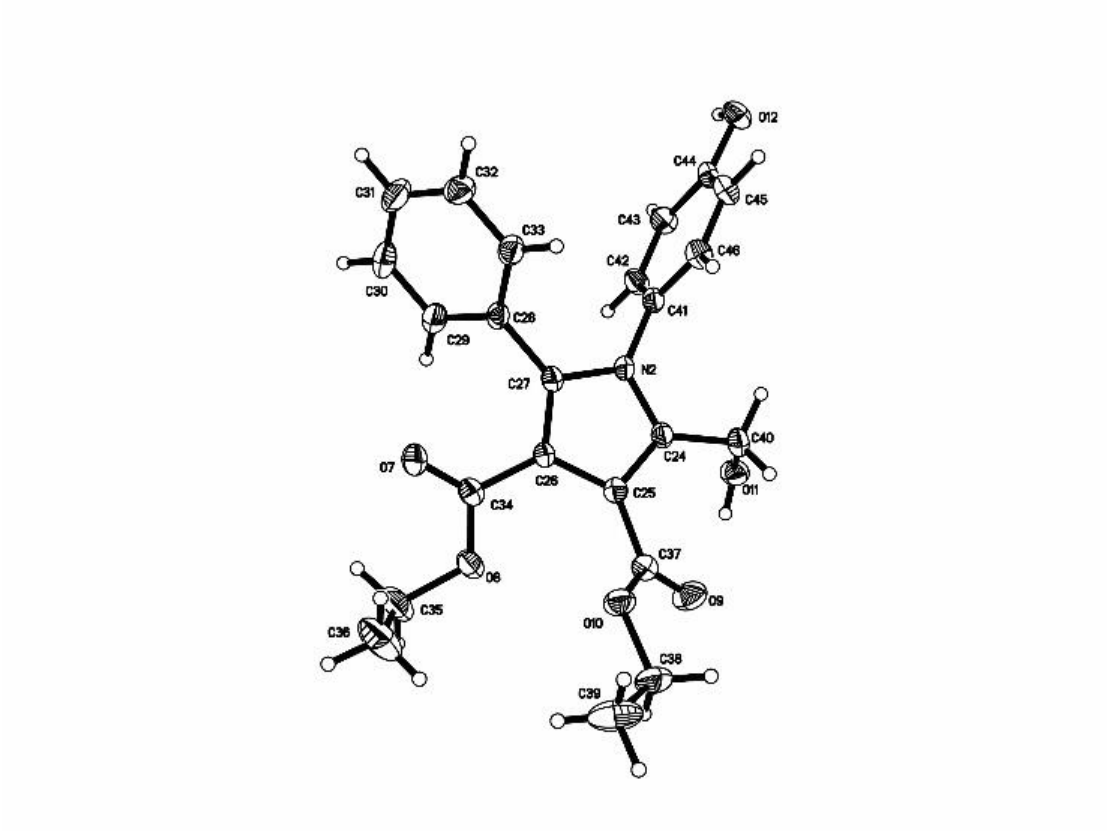


Table 1. Crystal data and structure refinement for **4ag**.

Identification code	**4ag**	
Empirical formula	C23 H23 N O6	
Formula weight	409.42	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.4110(15) Å	α= 90°.
	b = 9.4820(13) Å	β= 91.857(3)°.
	c = 36.247(4) Å	γ = 90°.
Volume	4263.4(9) $Å^3$	
Z	8	
Density (calculated)	1.276 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	1728	
Crystal size	0.120 x 0.100 x 0.030 mm^3	
Theta range for data collection	2.220 to 24.997°.	
Index ranges	-14<=h<=14, -11<=k<=11, -43<=l<=43	

Reflections collected	40423
Independent reflections	7486 [R(int) = 0.0812]
Completeness to theta = 24.997°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5882
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7486 / 58 / 573
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0793, wR2 = 0.1628
R indices (all data)	R1 = 0.1405, wR2 = 0.1858
Extinction coefficient	n/a
Largest diff. peak and hole	0.297 and -0.221 e.$Å^{-3}$

Table 2. Bond lengths [Å] and angles [°] for **4ag**.

C(1)-C(2)	1.360(5)
C(1)-N(1)	1.379(5)
C(1)-C(5)	1.480(5)
C(2)-C(3)	1.435(5)
C(2)-C(11)	1.471(6)
C(3)-C(4)	1.379(5)
C(3)-C(14)	1.463(6)
C(4)-N(1)	1.368(5)
C(4)-C(17)	1.482(5)
C(5)-C(6)	1.373(6)
C(5)-C(10)	1.379(5)
C(6)-C(7)	1.387(6)
C(6)-H(6)	0.9300
C(7)-C(8)	1.359(7)
C(7)-H(7)	0.9300
C(8)-C(9)	1.367(7)
C(8)-H(8)	0.9300
C(9)-C(10)	1.386(6)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-O(1)	1.193(5)
C(11)-O(2)	1.333(5)
C(12)-C(13B)	1.27(3)
C(12)-O(2)	1.445(5)
C(12)-C(13A)	1.456(16)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-H(12C)	0.9700
C(12)-H(12D)	0.9700
C(13A)-H(13A)	0.9600
C(13A)-H(13B)	0.9600
C(13A)-H(13C)	0.9600
C(13B)-H(13D)	0.9600
C(13B)-H(13E)	0.9600
C(13B)-H(13F)	0.9600
C(14)-O(3)	1.205(5)

C(14)-O(4)	1.317(5)
C(15)-C(16A)	1.361(18)
C(15)-O(4)	1.459(6)
C(15)-C(16B)	1.482(17)
C(15)-H(15A)	0.9700
C(15)-H(15B)	0.9700
C(15)-H(15C)	0.9700
C(15)-H(15D)	0.9700
C(16A)-H(16A)	0.9600
C(16A)-H(16B)	0.9600
C(16A)-H(16C)	0.9600
C(16B)-H(16D)	0.9600
C(16B)-H(16E)	0.9600
C(16B)-H(16F)	0.9600
C(17)-O(5)	1.416(5)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.371(5)
C(18)-C(23)	1.374(5)
C(18)-N(1)	1.442(5)
C(19)-C(20)	1.367(6)
C(19)-H(19)	0.9300
C(20)-C(21)	1.380(6)
C(20)-H(20)	0.9300
C(21)-O(6)	1.361(5)
C(21)-C(22)	1.373(6)
C(22)-C(23)	1.376(6)
C(22)-H(22)	0.9300
C(23)-H(23)	0.9300
C(24)-C(25)	1.371(5)
C(24)-N(2)	1.375(5)
C(24)-C(40)	1.492(5)
C(25)-C(26)	1.434(5)
C(25)-C(37)	1.464(5)
C(26)-C(27)	1.372(5)
C(26)-C(34)	1.462(5)
C(27)-N(2)	1.382(5)
C(27)-C(28)	1.472(5)

C(28)-C(29)	1.378(6)
C(28)-C(33)	1.388(5)
C(29)-C(30)	1.376(6)
C(29)-H(29)	0.9300
C(30)-C(31)	1.368(7)
C(30)-H(30)	0.9300
C(31)-C(32)	1.367(7)
C(31)-H(31)	0.9300
C(32)-C(33)	1.364(6)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-O(7)	1.208(5)
C(34)-O(8)	1.333(5)
C(35)-O(8)	1.452(5)
C(35)-C(36)	1.453(7)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-O(9)	1.211(5)
C(37)-O(10)	1.323(5)
C(38)-O(10)	1.453(5)
C(38)-C(39)	1.464(7)
C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-H(39A)	0.9600
C(39)-H(39B)	0.9600
C(39)-H(39C)	0.9600
C(40)-O(11)	1.424(5)
C(40)-H(40A)	0.9700
C(40)-H(40B)	0.9700
C(41)-C(42)	1.357(5)
C(41)-C(46)	1.373(5)
C(41)-N(2)	1.436(5)
C(42)-C(43)	1.388(5)
C(42)-H(42)	0.9300
C(43)-C(44)	1.367(5)

C(43)-H(43)	0.9300
C(44)-O(12)	1.369(5)
C(44)-C(45)	1.371(5)
C(45)-C(46)	1.373(5)
C(45)-H(45)	0.9300
C(46)-H(46)	0.9300
O(5)-H(5)	1.0362
O(6)-H(6A)	0.8200
O(11)-H(11)	0.79(5)
O(12)-H(12)	0.95(5)

C(2)-C(1)-N(1)	107.7(3)
C(2)-C(1)-C(5)	130.8(3)
N(1)-C(1)-C(5)	121.5(3)
C(1)-C(2)-C(3)	107.7(3)
C(1)-C(2)-C(11)	125.4(4)
C(3)-C(2)-C(11)	126.7(4)
C(4)-C(3)-C(2)	106.9(4)
C(4)-C(3)-C(14)	122.0(4)
C(2)-C(3)-C(14)	130.9(4)
N(1)-C(4)-C(3)	107.7(3)
N(1)-C(4)-C(17)	123.2(4)
C(3)-C(4)-C(17)	129.1(4)
C(6)-C(5)-C(10)	118.9(4)
C(6)-C(5)-C(1)	120.6(4)
C(10)-C(5)-C(1)	120.5(4)
C(5)-C(6)-C(7)	120.7(5)
C(5)-C(6)-H(6)	119.7
C(7)-C(6)-H(6)	119.7
C(8)-C(7)-C(6)	119.7(5)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(7)-C(8)-C(9)	120.5(5)
C(7)-C(8)-H(8)	119.7
C(9)-C(8)-H(8)	119.7
C(8)-C(9)-C(10)	119.8(5)
C(8)-C(9)-H(9)	120.1
C(10)-C(9)-H(9)	120.1

C(5)-C(10)-C(9)	120.3(4)
C(5)-C(10)-H(10)	119.9
C(9)-C(10)-H(10)	119.9
O(1)-C(11)-O(2)	123.2(4)
O(1)-C(11)-C(2)	125.8(4)
O(2)-C(11)-C(2)	111.0(4)
C(13B)-C(12)-O(2)	118.4(18)
O(2)-C(12)-C(13A)	107.0(9)
O(2)-C(12)-H(12A)	110.3
C(13A)-C(12)-H(12A)	110.3
O(2)-C(12)-H(12B)	110.3
C(13A)-C(12)-H(12B)	110.3
H(12A)-C(12)-H(12B)	108.6
C(13B)-C(12)-H(12C)	107.7
O(2)-C(12)-H(12C)	107.7
C(13B)-C(12)-H(12D)	107.7
O(2)-C(12)-H(12D)	107.7
H(12C)-C(12)-H(12D)	107.1
C(12)-C(13A)-H(13A)	109.5
C(12)-C(13A)-H(13B)	109.5
H(13A)-C(13A)-H(13B)	109.5
C(12)-C(13A)-H(13C)	109.5
H(13A)-C(13A)-H(13C)	109.5
H(13B)-C(13A)-H(13C)	109.5
C(12)-C(13B)-H(13D)	109.5
C(12)-C(13B)-H(13E)	109.5
H(13D)-C(13B)-H(13E)	109.5
C(12)-C(13B)-H(13F)	109.5
H(13D)-C(13B)-H(13F)	109.5
H(13E)-C(13B)-H(13F)	109.5
O(3)-C(14)-O(4)	124.1(4)
O(3)-C(14)-C(3)	123.6(4)
O(4)-C(14)-C(3)	112.2(4)
C(16A)-C(15)-O(4)	113.6(9)
O(4)-C(15)-C(16B)	106.1(8)
C(16A)-C(15)-H(15A)	108.8
O(4)-C(15)-H(15A)	108.8
C(16A)-C(15)-H(15B)	108.8

O(4)-C(15)-H(15B)	108.8
H(15A)-C(15)-H(15B)	107.7
O(4)-C(15)-H(15C)	110.5
C(16B)-C(15)-H(15C)	110.5
O(4)-C(15)-H(15D)	110.5
C(16B)-C(15)-H(15D)	110.5
H(15C)-C(15)-H(15D)	108.7
C(15)-C(16A)-H(16A)	109.5
C(15)-C(16A)-H(16B)	109.5
H(16A)-C(16A)-H(16B)	109.5
C(15)-C(16A)-H(16C)	109.5
H(16A)-C(16A)-H(16C)	109.5
H(16B)-C(16A)-H(16C)	109.5
C(15)-C(16B)-H(16D)	109.5
C(15)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(15)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5
H(16E)-C(16B)-H(16F)	109.5
O(5)-C(17)-C(4)	113.9(4)
O(5)-C(17)-H(17A)	108.8
C(4)-C(17)-H(17A)	108.8
O(5)-C(17)-H(17B)	108.8
C(4)-C(17)-H(17B)	108.8
H(17A)-C(17)-H(17B)	107.7
C(19)-C(18)-C(23)	120.1(4)
C(19)-C(18)-N(1)	120.0(4)
C(23)-C(18)-N(1)	119.9(3)
C(20)-C(19)-C(18)	120.4(4)
C(20)-C(19)-H(19)	119.8
C(18)-C(19)-H(19)	119.8
C(19)-C(20)-C(21)	120.0(4)
C(19)-C(20)-H(20)	120.0
C(21)-C(20)-H(20)	120.0
O(6)-C(21)-C(22)	123.4(4)
O(6)-C(21)-C(20)	117.1(4)
C(22)-C(21)-C(20)	119.5(4)
C(21)-C(22)-C(23)	120.6(4)

C(21)-C(22)-H(22)	119.7
C(23)-C(22)-H(22)	119.7
C(18)-C(23)-C(22)	119.5(4)
C(18)-C(23)-H(23)	120.3
C(22)-C(23)-H(23)	120.3
C(25)-C(24)-N(2)	107.8(3)
C(25)-C(24)-C(40)	129.2(4)
N(2)-C(24)-C(40)	123.0(3)
C(24)-C(25)-C(26)	107.5(3)
C(24)-C(25)-C(37)	120.0(4)
C(26)-C(25)-C(37)	132.0(4)
C(27)-C(26)-C(25)	107.3(3)
C(27)-C(26)-C(34)	124.1(4)
C(25)-C(26)-C(34)	128.1(3)
C(26)-C(27)-N(2)	107.6(3)
C(26)-C(27)-C(28)	131.3(3)
N(2)-C(27)-C(28)	121.0(3)
C(29)-C(28)-C(33)	118.5(4)
C(29)-C(28)-C(27)	120.8(4)
C(33)-C(28)-C(27)	120.8(4)
C(30)-C(29)-C(28)	120.8(4)
C(30)-C(29)-H(29)	119.6
C(28)-C(29)-H(29)	119.6
C(31)-C(30)-C(29)	119.9(5)
C(31)-C(30)-H(30)	120.1
C(29)-C(30)-H(30)	120.1
C(32)-C(31)-C(30)	119.9(5)
C(32)-C(31)-H(31)	120.1
C(30)-C(31)-H(31)	120.1
C(33)-C(32)-C(31)	120.7(5)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(32)-C(33)-C(28)	120.3(4)
C(32)-C(33)-H(33)	119.8
C(28)-C(33)-H(33)	119.8
O(7)-C(34)-O(8)	122.9(4)
O(7)-C(34)-C(26)	125.1(4)
O(8)-C(34)-C(26)	111.8(4)

O(8)-C(35)-C(36)	111.2(5)
O(8)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35A)	109.4
O(8)-C(35)-H(35B)	109.4
C(36)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(9)-C(37)-O(10)	123.4(4)
O(9)-C(37)-C(25)	123.4(4)
O(10)-C(37)-C(25)	113.1(4)
O(10)-C(38)-C(39)	107.7(4)
O(10)-C(38)-H(38A)	110.2
C(39)-C(38)-H(38A)	110.2
O(10)-C(38)-H(38B)	110.2
C(39)-C(38)-H(38B)	110.2
H(38A)-C(38)-H(38B)	108.5
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
O(11)-C(40)-C(24)	111.5(3)
O(11)-C(40)-H(40A)	109.3
C(24)-C(40)-H(40A)	109.3
O(11)-C(40)-H(40B)	109.3
C(24)-C(40)-H(40B)	109.3
H(40A)-C(40)-H(40B)	108.0
C(42)-C(41)-C(46)	120.1(4)
C(42)-C(41)-N(2)	119.9(3)
C(46)-C(41)-N(2)	120.0(3)
C(41)-C(42)-C(43)	120.5(4)
C(41)-C(42)-H(42)	119.7

C(43)-C(42)-H(42)	119.7
C(44)-C(43)-C(42)	119.4(4)
C(44)-C(43)-H(43)	120.3
C(42)-C(43)-H(43)	120.3
C(43)-C(44)-O(12)	122.0(4)
C(43)-C(44)-C(45)	119.9(4)
O(12)-C(44)-C(45)	118.1(3)
C(44)-C(45)-C(46)	120.5(4)
C(44)-C(45)-H(45)	119.7
C(46)-C(45)-H(45)	119.7
C(41)-C(46)-C(45)	119.6(4)
C(41)-C(46)-H(46)	120.2
C(45)-C(46)-H(46)	120.2
C(4)-N(1)-C(1)	110.0(3)
C(4)-N(1)-C(18)	124.6(3)
C(1)-N(1)-C(18)	125.2(3)
C(24)-N(2)-C(27)	109.7(3)
C(24)-N(2)-C(41)	124.3(3)
C(27)-N(2)-C(41)	125.8(3)
C(11)-O(2)-C(12)	115.6(4)
C(14)-O(4)-C(15)	116.7(4)
C(17)-O(5)-H(5)	111.0
C(21)-O(6)-H(6A)	109.5
C(34)-O(8)-C(35)	116.6(4)
C(37)-O(10)-C(38)	115.8(4)
C(40)-O(11)-H(11)	109(4)
C(44)-O(12)-H(12)	107(3)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for **4ag**.

N(1)-C(1)-C(2)-C(3)	0.8(4)
C(5)-C(1)-C(2)-C(3)	178.8(4)
N(1)-C(1)-C(2)-C(11)	-174.2(4)
C(5)-C(1)-C(2)-C(11)	3.8(7)
C(1)-C(2)-C(3)-C(4)	-0.4(4)
C(11)-C(2)-C(3)-C(4)	174.5(4)
C(1)-C(2)-C(3)-C(14)	174.3(4)
C(11)-C(2)-C(3)-C(14)	-10.8(7)
C(2)-C(3)-C(4)-N(1)	-0.2(4)
C(14)-C(3)-C(4)-N(1)	-175.4(3)
C(2)-C(3)-C(4)-C(17)	178.7(4)
C(14)-C(3)-C(4)-C(17)	3.4(7)
C(2)-C(1)-C(5)-C(6)	128.3(5)
N(1)-C(1)-C(5)-C(6)	-53.9(5)
C(2)-C(1)-C(5)-C(10)	-50.0(6)
N(1)-C(1)-C(5)-C(10)	127.8(4)
C(10)-C(5)-C(6)-C(7)	-1.2(7)
C(1)-C(5)-C(6)-C(7)	-179.5(4)
C(5)-C(6)-C(7)-C(8)	0.7(8)
C(6)-C(7)-C(8)-C(9)	0.7(8)
C(7)-C(8)-C(9)-C(10)	-1.6(8)
C(6)-C(5)-C(10)-C(9)	0.3(7)
C(1)-C(5)-C(10)-C(9)	178.6(4)
C(8)-C(9)-C(10)-C(5)	1.1(7)
C(1)-C(2)-C(11)-O(1)	131.7(5)
C(3)-C(2)-C(11)-O(1)	-42.3(7)
C(1)-C(2)-C(11)-O(2)	-47.9(5)
C(3)-C(2)-C(11)-O(2)	138.1(4)
C(4)-C(3)-C(14)-O(3)	-21.9(6)
C(2)-C(3)-C(14)-O(3)	164.1(4)
C(4)-C(3)-C(14)-O(4)	156.3(4)
C(2)-C(3)-C(14)-O(4)	-17.7(6)
N(1)-C(4)-C(17)-O(5)	-108.0(4)
C(3)-C(4)-C(17)-O(5)	73.3(6)
C(23)-C(18)-C(19)-C(20)	-1.0(6)
N(1)-C(18)-C(19)-C(20)	177.5(4)

C(18)-C(19)-C(20)-C(21)	0.5(7)
C(19)-C(20)-C(21)-O(6)	-179.4(4)
C(19)-C(20)-C(21)-C(22)	0.6(6)
O(6)-C(21)-C(22)-C(23)	178.7(4)
C(20)-C(21)-C(22)-C(23)	-1.3(6)
C(19)-C(18)-C(23)-C(22)	0.4(6)
N(1)-C(18)-C(23)-C(22)	-178.1(3)
C(21)-C(22)-C(23)-C(18)	0.8(6)
N(2)-C(24)-C(25)-C(26)	1.5(4)
C(40)-C(24)-C(25)-C(26)	-177.4(4)
N(2)-C(24)-C(25)-C(37)	-171.3(3)
C(40)-C(24)-C(25)-C(37)	9.8(6)
C(24)-C(25)-C(26)-C(27)	-1.5(4)
C(37)-C(25)-C(26)-C(27)	170.1(4)
C(24)-C(25)-C(26)-C(34)	171.1(4)
C(37)-C(25)-C(26)-C(34)	-17.3(7)
C(25)-C(26)-C(27)-N(2)	0.9(4)
C(34)-C(26)-C(27)-N(2)	-172.1(3)
C(25)-C(26)-C(27)-C(28)	178.7(4)
C(34)-C(26)-C(27)-C(28)	5.7(7)
C(26)-C(27)-C(28)-C(29)	-60.0(6)
N(2)-C(27)-C(28)-C(29)	117.6(4)
C(26)-C(27)-C(28)-C(33)	120.5(5)
N(2)-C(27)-C(28)-C(33)	-61.9(5)
C(33)-C(28)-C(29)-C(30)	-0.3(6)
C(27)-C(28)-C(29)-C(30)	-179.9(4)
C(28)-C(29)-C(30)-C(31)	0.6(7)
C(29)-C(30)-C(31)-C(32)	-0.4(8)
C(30)-C(31)-C(32)-C(33)	0.1(8)
C(31)-C(32)-C(33)-C(28)	0.1(7)
C(29)-C(28)-C(33)-C(32)	0.0(6)
C(27)-C(28)-C(33)-C(32)	179.5(4)
C(27)-C(26)-C(34)-O(7)	-23.4(6)
C(25)-C(26)-C(34)-O(7)	165.1(4)
C(27)-C(26)-C(34)-O(8)	151.6(4)
C(25)-C(26)-C(34)-O(8)	-20.0(6)
C(24)-C(25)-C(37)-O(9)	-37.8(6)
C(26)-C(25)-C(37)-O(9)	151.5(4)

C(24)-C(25)-C(37)-O(10)	138.3(4)
C(26)-C(25)-C(37)-O(10)	-32.4(6)
C(25)-C(24)-C(40)-O(11)	75.2(5)
N(2)-C(24)-C(40)-O(11)	-103.6(4)
C(46)-C(41)-C(42)-C(43)	0.4(6)
N(2)-C(41)-C(42)-C(43)	-179.3(4)
C(41)-C(42)-C(43)-C(44)	-0.2(6)
C(42)-C(43)-C(44)-O(12)	178.2(4)
C(42)-C(43)-C(44)-C(45)	-0.4(6)
C(43)-C(44)-C(45)-C(46)	0.8(6)
O(12)-C(44)-C(45)-C(46)	-177.9(4)
C(42)-C(41)-C(46)-C(45)	0.0(6)
N(2)-C(41)-C(46)-C(45)	179.7(4)
C(44)-C(45)-C(46)-C(41)	-0.5(6)
C(3)-C(4)-N(1)-C(1)	0.7(4)
C(17)-C(4)-N(1)-C(1)	-178.3(4)
C(3)-C(4)-N(1)-C(18)	-174.0(3)
C(17)-C(4)-N(1)-C(18)	7.0(6)
C(2)-C(1)-N(1)-C(4)	-0.9(4)
C(5)-C(1)-N(1)-C(4)	-179.1(3)
C(2)-C(1)-N(1)-C(18)	173.7(3)
C(5)-C(1)-N(1)-C(18)	-4.5(5)
C(19)-C(18)-N(1)-C(4)	-76.5(5)
C(23)-C(18)-N(1)-C(4)	102.0(4)
C(19)-C(18)-N(1)-C(1)	109.6(4)
C(23)-C(18)-N(1)-C(1)	-71.9(5)
C(25)-C(24)-N(2)-C(27)	-1.0(4)
C(40)-C(24)-N(2)-C(27)	178.0(3)
C(25)-C(24)-N(2)-C(41)	-177.5(3)
C(40)-C(24)-N(2)-C(41)	1.5(6)
C(26)-C(27)-N(2)-C(24)	0.0(4)
C(28)-C(27)-N(2)-C(24)	-178.0(3)
C(26)-C(27)-N(2)-C(41)	176.5(3)
C(28)-C(27)-N(2)-C(41)	-1.6(6)
C(42)-C(41)-N(2)-C(24)	94.7(5)
C(46)-C(41)-N(2)-C(24)	-85.0(5)
C(42)-C(41)-N(2)-C(27)	-81.2(5)
C(46)-C(41)-N(2)-C(27)	99.0(5)

O(1)-C(11)-O(2)-C(12)	-5.7(7)
C(2)-C(11)-O(2)-C(12)	173.9(4)
C(13B)-C(12)-O(2)-C(11)	142(3)
C(13A)-C(12)-O(2)-C(11)	174.9(11)
O(3)-C(14)-O(4)-C(15)	-5.3(7)
C(3)-C(14)-O(4)-C(15)	176.5(4)
C(16A)-C(15)-O(4)-C(14)	167.3(18)
C(16B)-C(15)-O(4)-C(14)	-150.4(12)
O(7)-C(34)-O(8)-C(35)	3.0(6)
C(26)-C(34)-O(8)-C(35)	-172.1(4)
C(36)-C(35)-O(8)-C(34)	-83.2(6)
O(9)-C(37)-O(10)-C(38)	2.0(6)
C(25)-C(37)-O(10)-C(38)	-174.1(4)
C(39)-C(38)-O(10)-C(37)	-178.0(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Hydrogen bonds for **4ag** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(19)-H(19)...O(2)#1	0.93	2.57	3.427(5)	153.6
C(23)-H(23)...O(1)#2	0.93	2.49	3.368(5)	157.6
C(36)-H(36C)...O(7)	0.96	2.65	3.131(7)	111.6
C(43)-H(43)...O(5)	0.93	2.62	3.305(5)	130.9
C(46)-H(46)...O(7)#3	0.93	2.48	3.189(5)	133.5
O(5)-H(5)...O(3)	1.04	2.23	2.945(4)	125.0
O(5)-H(5)...O(9)#4	1.04	2.05	2.916(4)	139.0
O(6)-H(6A)...O(11)	0.82	1.90	2.688(4)	160.7
O(11)-H(11)...O(3)#5	0.79(5)	2.34(5)	2.993(4)	141(5)
O(11)-H(11)...O(9)	0.79(5)	2.40(5)	2.997(4)	134(5)
O(12)-H(12)...O(5)	0.95(5)	1.78(5)	2.731(4)	176(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+1 #2 -x,-y+1,-z+1 #3 -x+1,y+1/2,-z+3/2

#4 x-1,y,z #5 x+1,y,z