

Supporting Information

TBAI-catalyzed C-H bond activation to construct C_(sp3)-O bond in water: the synthesis of indole-3-carboxylic- α -esters under metal-free conditions

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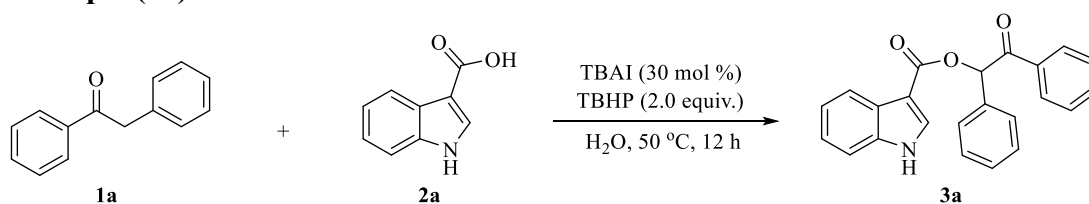
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1. General methods

All reactions were performed in flame-dried glassware in an atmosphere, unless otherwise noted. Column chromatographic purification of products was carried out by using silica gel (200~300 mesh). The commercial reagents were used without further purification. ^1H NMR spectra were recorded at 400 MHz, and ^{13}C NMR spectra were recorded at 100 MHz in $\text{CDCl}_3/\text{DMSO}-d_6$ (containing 0.03% TMS) solution. ^1H NMR spectra were recorded with tetramethylsilane ($\delta = 0.00$ ppm) as internal reference; ^{13}C NMR spectra were recorded with CDCl_3 ($\delta = 77.00$ ppm) as internal reference. ^1H NMR spectra were recorded with $\text{DMSO}-d_6$ ($\delta = 2.50$ ppm) as internal reference; ^{13}C NMR spectra were recorded with $\text{DMSO}-d_6$ ($\delta = 39.52$ ppm) as internal reference. High-resolution mass spectra (HRMS) were performed on an electrospray ionization (ESI) Fourier transform mass spectrometer (FTMS, Thermo Q-Exactive Focus). Single crystal X-ray diffraction data were collected in a Rigaku XtaLAB Synergy.

2. Synthesis of products 3-17

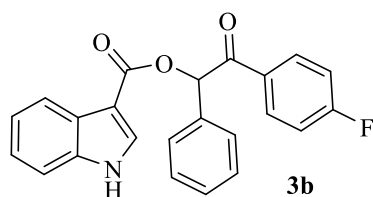
Example (3a):



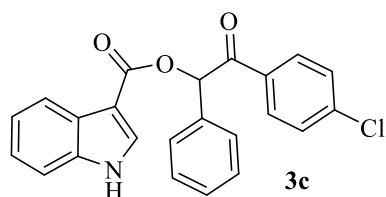
Benzyl phenyl ketone **1a** (39.2 mg, 0.2 mmol), indole-3-carboxylic acid **2a** (48.3 mg, 0.3 mmol), TBAI (22.2 mg, 0.06 mmol), and H_2O (2 mL) were placed in a Schlenk tube, then TBHP (70% in water, 55.0 μL , 0.4 mmol) was added into the above mixture under air condition. After the completion of the addition, the reaction mixture was allowed to react at $50\text{ }^\circ\text{C}$ (oil bath) for 12 h. Subsequently, the reaction mixture was cooled to room temperature, and then extracted with ethyl acetate. The organic layer was dried with anhydrous Na_2SO_4 . After removal of the ethyl acetate under reduced pressure, the residue was purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1-3:1) to afford 2-oxo-1,2-diphenylethyl-1H-indole-3-carboxylate **3a** (white solid, 58.8 mg, 83% yield).

2-Oxo-1,2-diphenylethyl-1H-indole-3-carboxylate (3a). Following the general procedure, the crude product was purified using silica gel column chromatography

(petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3a** (white solid, 58.8 mg, 83% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.96 (s, 1H), 8.17-8.12 (m, 1H), 8.08-8.02 (m, 2H), 7.93-7.89 (m, 1H), 7.63-7.57 (m, 2H), 7.56-7.50 (m, 1H), 7.45-7.33 (m, 6H), 7.25-7.16 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.9, 164.3, 136.1, 134.8, 134.2, 133.5, 132.0, 129.1, 129.1, 128.9, 128.7, 125.8, 123.2, 122.2, 121.5, 111.6, 107.6, 76.8. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{17}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 378.1101; found: 378.1103.

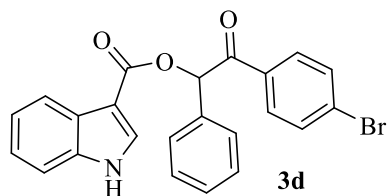


2-(4-Fluorophenyl)-2-oxo-1-phenylethyl-1H-indole-3-carboxylate (3b). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3b** (brown solid, 108.0 mg, 72% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.04 (s, 1H), 8.15-8.10 (m, 1H), 8.09-8.04 (m, 2H), 7.88 (d, $J = 3.2$ Hz, 1H), 7.59-7.55 (m, 2H), 7.43-7.31 (m, 4H), 7.23-7.17 (m, 2H), 7.12-7.05 (m, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.4, 165.9 ($J_{\text{C-F}} = 254.0$ Hz), 164.3, 136.1, 134.0, 132.1, 131.6 ($J_{\text{C-F}} = 10.0$ Hz), 131.1 ($J_{\text{C-F}} = 3.0$ Hz), 129.3, 129.2, 128.6, 125.8, 123.2, 122.2, 121.4, 115.9 ($J_{\text{C-F}} = 22.0$ Hz), 111.7, 107.3, 76.7. ^{19}F NMR (376 MHz, CDCl_3) δ -103.7. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{FNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 396.1006; found: 396.1003.

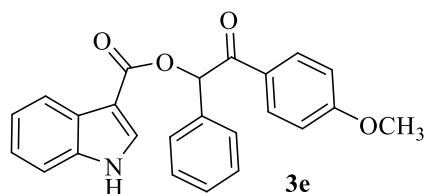


2-(4-Chlorophenyl)-2-oxo-1-phenylethyl-1H-indole-3-carboxylate (3c). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3c** (yellow solid, 62.6 mg, 40% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.91 (s, 1H), 8.14 (dd, $J_1 = 6.0$ Hz, $J_2 = 3.2$ Hz, 1H), 7.99-7.95 (m, 2H), 7.92 (d, $J = 3.2$ Hz, 1H), 7.59-7.56 (m, 2H), 7.41-7.35 (m, 6H), 7.24-7.21 (m, 2H), 7.09 (s, 1H). ^{13}C NMR

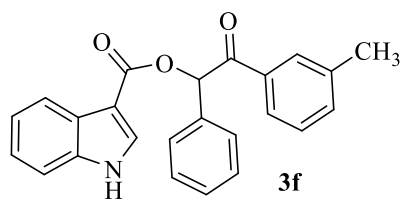
(100 MHz, CDCl₃) δ 193.7, 164.3, 139.9, 136.1, 133.9, 133.1, 132.0, 129.3, 129.2, 129.0, 128.6, 125.8, 123.3, 122.2, 121.4, 111.6, 107.5, 76.8. HRMS (ESI, m/z) calcd. for C₂₃H₁₆ClNO₃Na [M+Na]⁺ calc.: 412.0711; found: 412.0716.



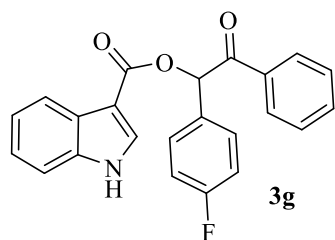
2-(4-Bromophenyl)-2-oxo-1-phenylethyl-1H-indole-3-carboxylate (3d). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3d** (brown solid, 104.1 mg, 60% yield); ¹H NMR (400 MHz, DMSO-d₆) δ 12.09 (s, 1H), 8.19 (d, *J* = 3.2 Hz, 1H), 8.08-8.04 (m, 2H), 7.94 (d, *J* = 7.2 Hz, 1H), 7.77-7.73 (m, 2H), 7.69-7.65 (m, 2H), 7.53-7.49 (m, 1H), 7.47-7.36 (m, 3H), 7.32 (s, 1H), 7.24-7.14 (m, 2H). ¹³C NMR (100 MHz, DMSO-d₆) δ 193.8, 163.7, 136.5, 133.8, 133.5, 133.2, 132.1, 130.7, 129.2, 129.1, 128.7, 128.1, 125.6, 122.6, 121.1, 120.3, 112.6, 105.5, 76.0. HRMS (ESI, m/z) calcd. for C₂₃H₁₆BrNO₃Na [M+Na]⁺ calc.: 456.0206; found: 456.0209.



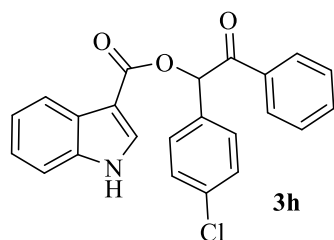
2-(4-Methoxyphenyl)-2-oxo-1-phenylethyl-1H-indole-3-carboxylate (3e). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3e** (brown solid, 55.8 mg, 36% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.88 (s, 1H), 8.19-8.16 (m, 1H), 8.07-8.02 (m, 2H), 7.95 (d, *J* = 2.8 Hz, 1H), 7.62-7.58 (m, 2H), 7.42-7.34 (m, 4H), 7.25-7.20 (m, 2H), 7.15 (s, 1H), 6.92-6.88 (m, 2H), 3.83 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 193.1, 164.2, 163.8, 136.1, 134.8, 131.9, 131.3, 129.0, 129.0, 128.6, 127.7, 125.9, 123.2, 122.2, 121.6, 113.9, 111.5, 107.8, 76.5. HRMS (ESI, m/z) calcd. for C₂₄H₁₉NO₄Na [M+Na]⁺ calc.: 408.1206; found: 408.1210.



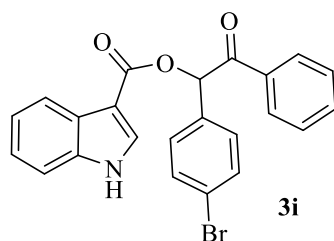
2-Oxo-1-phenyl-2-(*m*-tolyl)ethyl-1*H*-indole-3-carboxylate (3f). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3f** (brown solid, 85.8, 58% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.20 (s, 1H), 8.14-8.11 (m, 1H), 7.87-7.83 (m, 3H), 7.60-7.56 (m, 2H), 7.39- 7.30 (m, 6H), 7.20-7.16 (m, 3H), 2.35 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.3, 164.4, 138.6, 136.1, 134.8, 134.4, 134.2, 132.2, 129.4, 129.1, 129.1, 128.6, 128.5, 126.1, 125.8, 123.1, 122.1, 121.3, 111.7, 107.3, 76.7, 21.3. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 392.1257; found: 392.1260.



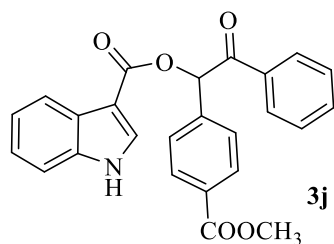
1-(4-Fluorophenyl)-2-oxo-2-phenylethyl-1*H*-indole-3-carboxylate (3g). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3g** (white solid, 118.6 mg, 79% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.09 (s, 1H), 8.14-8.10 (m, 1H), 8.04-8.01 (m, 2H), 7.87 (d, $J = 2.8$ Hz, 1H), 7.59-7.52 (m, 3H), 7.46-7.41 (m, 2H), 7.36-7.33 (m, 1H), 7.24-7.19 (m, 2H), 7.16 (s, 1H), 7.10-7.05 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.8, 164.2, 163.1 ($J_{\text{C-F}} = 247.0$ Hz), 136.1, 134.6, 133.7, 132.1, 130.6 ($J_{\text{C-F}} = 9.0$ Hz), 130.1 ($J_{\text{C-F}} = 3.0$ Hz), 128.9, 128.8, 125.8, 123.2, 122.2, 121.3, 116.2 ($J_{\text{C-F}} = 22.0$ Hz), 111.7, 107.3, 75.9. ^{19}F NMR (376 MHz, CDCl_3) δ -111.8. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{FNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 396.1006; found: 396.1009.



1-(4-Chlorophenyl)-2-oxo-2-phenylethyl-1H-indole-3-carboxylate (3h). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3h** (white solid, 57.9 mg, 37% yield); ^1H NMR (400 MHz, DMSO- d_6) δ 12.10 (s, 1H), 8.20 (d, J = 3.2 Hz, 1H), 8.15-8.12 (m, 2H), 7.93 (d, J = 7.2 Hz, 1H), 7.74-7.69 (m, 2H), 7.68-7.62 (m, 1H), 7.60-7.50 (m, 5H), 7.39 (s, 1H), 7.24-7.15 (m, 2H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 194.2, 163.5, 136.5, 134.1, 134.0, 133.9, 133.4, 133.2, 130.5, 129.1, 129.0, 128.7, 125.6, 122.6, 121.5, 120.3, 112.5, 105.4, 75.2. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{ClNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 412.0711; found: 412.0716.

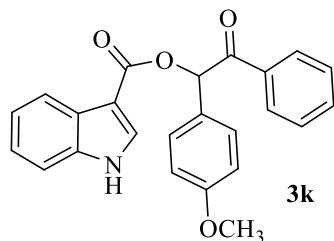


1-(4-Bromophenyl)-2-oxo-2-phenylethyl-1H-indole-3-carboxylate (3i). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3i** (brown solid, 57.2 mg, 33% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.95 (s, 1H), 8.15-8.11 (m, 1H), 8.04-8.00 (m, 2H), 7.91 (d, J = 3.2 Hz, 1H), 7.56-7.50 (m, 3H), 7.48-7.41 (m, 4H), 7.39-7.35 (m, 1H), 7.25-7.22 (m, 2H), 7.13 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.4, 164.1, 136.1, 134.6, 133.7, 133.3, 132.3, 132.1, 130.2, 128.9, 128.8, 125.8, 123.5, 123.3, 122.3, 121.4, 111.6, 107.4, 75.9. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{BrNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 456.0206; found: 456.0208.



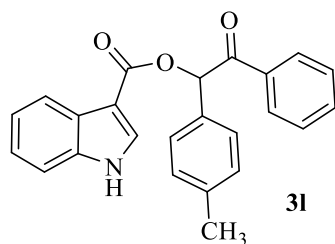
1-(4-(Methoxycarbonyl)phenyl)-2-oxo-2-phenylethyl-1*H*-indole-3-carboxylate

(3j). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3j** (brown solid, 78.9 mg, 48% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.82 (s, 1H), 8.17-8.13 (m, 1H), 8.07 -8.00 (m, 4H), 7.97 (d, J = 2.8 Hz, 1H), 7.69-7.66 (m, 2H), 7.57-7.52 (m, 1H), 7.46-7.38 (m, 3H), 7.25-7.23 (m, 2H), 7.20 (s, 1H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.3, 166.5, 164.0, 139.1, 136.1, 134.7, 133.7, 132.0, 130.7, 130.3, 128.9, 128.8, 128.5, 125.8, 123.4, 122.3, 121.4, 111.6, 107.5, 76.2, 52.3. HRMS (ESI, m/z) calcd. for $\text{C}_{25}\text{H}_{19}\text{NO}_5\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 436.1155; found: 436.1160.

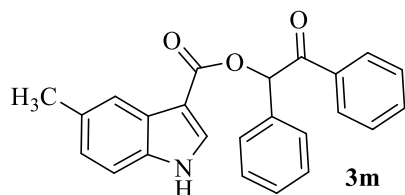


1-(4-Methoxyphenyl)-2-oxo-2-phenylethyl-1*H*-indole-3-carboxylate **(3k).**

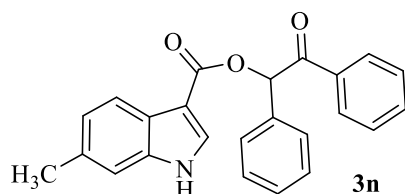
Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3k** (brown solid, 81.2 mg, 53% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.13 (s, 1H), 8.14-8.11 (m, 1H), 8.05-8.01 (m, 2H), 7.85 (d, J = 2.8 Hz, 1H), 7.54-7.48 (m, 3H), 7.44-7.39 (m, 2H), 7.35-7.32 (m, 1H), 7.22-7.17 (m, 2H), 7.13 (s, 1H), 6.93-6.88 (m, 2H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.0, 164.5, 160.2, 136.1, 134.8, 133.5, 132.1, 130.2, 128.9, 128.7, 126.1, 125.8, 123.1, 122.1, 121.4, 114.5, 111.7, 107.5, 76.4, 55.3. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 408.1206; found: 408.1209.



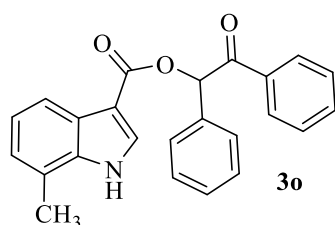
2-Oxo-2-phenyl-1-(*p*-tolyl)ethyl-1*H*-indole-3-carboxylate (3l). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3l** (brown solid, 99.0 mg, 67% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.15 (s, 1H), 8.14-8.11 (m, 1H), 8.06-8.02 (m, 2H), 7.84 (d, $J = 3.2$ Hz, 1H), 7.54-7.46 (m, 3H), 7.44-7.39 (m, 2H), 7.34-7.31 (m, 1H), 7.21-7.17 (m, 4H), 7.14 (s, 1H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.1, 164.4, 139.2, 136.1, 134.8, 133.5, 132.1, 131.1, 129.8, 128.9, 128.7, 125.8, 123.1, 122.1, 121.4, 111.7, 107.4, 76.7, 21.2. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 392.1257; found: 392.1263.



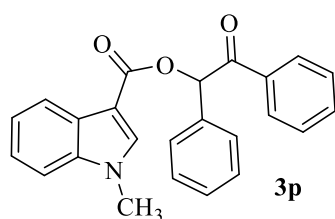
2-Oxo-1,2-diphenylethyl-5-methyl-1*H*-indole-3-carboxylate (3m). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3m** (brown solid, 104.8 mg, 71% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.77 (s, 1H), 8.07-8.03 (m, 2H), 7.96 (s, 1H), 7.90 (d, $J = 3.2$ Hz, 1H), 7.62-7.58 (m, 2H), 7.56-7.51 (m, 1H), 7.46-7.35 (m, 5H), 7.26-7.25 (m, 1H), 7.15 (s, 1H), 7.05 (dd, $J_1 = 8.6$ Hz, $J_2 = 1.6$ Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.8, 164.3, 134.9, 134.4, 134.3, 133.5, 131.8, 131.7, 129.1, 129.0, 128.9, 128.7, 128.7, 126.2, 124.8, 121.2, 111.2, 107.0, 76.7, 21.5. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 392.1257; found: 392.1256.



2-Oxo-1,2-diphenylethyl-6-methyl-1*H*-indole-3-carboxylate (3n). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3n** (brown solid, 88.1 mg, 60% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.74 (s, 1H), 8.06-8.00 (m, 3H), 7.86 (d, *J* = 3.2 Hz, 1H), 7.61-7.57 (m, 2H), 7.55-7.50 (m, 1H), 7.45-7.35 (m, 5H), 7.16-7.15 (m, 2H), 7.06 (dd, *J*₁ = 8.0 Hz, *J*₂ = 1.2 Hz, 1H), 2.43 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 194.7, 164.3, 136.5, 134.9, 133.4, 133.2, 131.4, 129.1, 129.1, 128.9, 128.7, 128.7, 124.0, 123.7, 121.1, 111.4, 107.6, 76.7, 21.6. HRMS (ESI, *m/z*) calcd. for C₂₄H₁₉NO₃Na [M+Na]⁺ calc.: 392.1257; found: 392.1255.

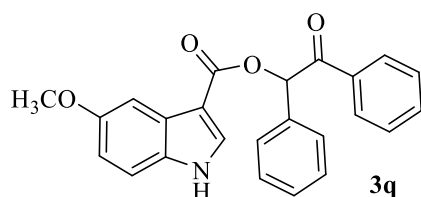


2-Oxo-1,2-diphenylethyl-7-methyl-1*H*-indole-3-carboxylate (3o). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3o** (white solid, 84.8 mg, 57% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.99 (s, 1H), 8.06-8.02 (m, 2H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.91 (d, *J* = 2.8 Hz, 1H), 7.61-7.57 (m, 2H), 7.55-7.49 (m, 1H), 7.44-7.34 (m, 5H), 7.17 (s, 1H), 7.12-7.07 (m, 1H), 6.97 (d, *J* = 7.2 Hz, 1H), 2.43 (s, 3H). ¹³C NMR (100 MHz, CDCl₃) δ 195.1, 164.4, 135.7, 134.9, 134.2, 133.5, 131.7, 129.1, 129.1, 128.9, 128.7, 125.4, 123.7, 122.3, 120.8, 119.0, 107.8, 76.8, 16.4. HRMS (ESI, *m/z*) calcd. for C₂₄H₁₉NO₃Na [M+Na]⁺ calc.: 392.1257; found: 392.1259.

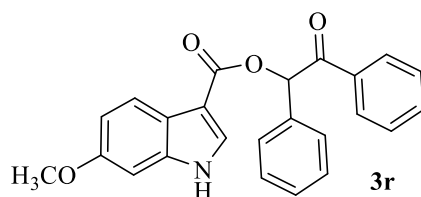


2-Oxo-1,2-diphenylethyl-1-methyl-1*H*-indole-3-carboxylate (3p). Following the general procedure, the crude product was purified using silica gel column

chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3p** (brown solid, 101.1 mg, 68% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.20-8.17 (m, 1H), 8.05-8.01(m, 2H), 7.87 (s, 1H), 7.62-7.59 (m, 2H), 7.54-7.48 (m, 1H), 7.43-7.37 (m, 4H), 7.37-7.31 (m, 2H), 7.35-7.23 (m, 2H) 7.16 (s, 1H), 3.80 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.5, 164.0, 137.2, 135.9, 135.0, 134.4, 133.3, 129.0, 128.9, 128.7, 128.6, 126.8, 122.9, 122.1, 121.7, 109.8, 105.9, 76.7, 33.4. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 392.1257; found: 392.1262.

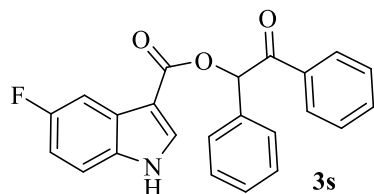


2-Oxo-1,2-diphenylethyl-5-methoxy-1H-indole-3-carboxylate (3q). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3q** (brown solid, 86.7 mg, 56% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.99 (s, 1H), 8.06-8.03 (m, 2H), 7.84 (d, $J = 3.2$ Hz, 1H), 7.61-7.58 (m, 3H), 7.56-7.50 (m, 1H), 7.45-7.34 (m, 5H), 7.22 (d, $J = 8.8$ Hz, 1H), 7.14 (s, 1H), 6.83 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.4$ Hz, 1H), 3.78 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.9, 164.3, 155.8, 134.8, 134.2, 133.6, 132.1, 130.9, 129.2, 129.1, 128.9, 128.7, 128.7, 126.7, 113.9, 112.4, 107.2, 102.4, 76.7, 55.5. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 408.1206; found: 408.1209.

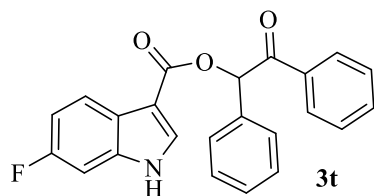


2-Oxo-1,2-diphenylethyl-6-methoxy-1H-indole-3-carboxylate (3r). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3r** (brown solid, 84.5 mg, 55% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.06 (s, 1H), 8.05-8.01 (m, 2H), 7.95 (d, $J = 8.8$ Hz, 1H), 7.71 (d, $J = 2.8$ Hz, 1H), 7.59-7.56 (m, 2H), 7.53-7.48 (m, 1H), 7.43-7.33 (m, 5H), 7.14 (s, 1H), 6.83 (dd, $J_1 = 8.8$ Hz, $J_2 =$

2.0 Hz, 1H), 6.77 (d, $J = 2.4$ Hz, 1H), 3.73 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.1, 164.4, 156.9, 137.0, 134.8, 134.2, 133.6, 131.1, 129.1, 129.1, 128.9, 128.7, 128.6, 121.9, 119.9, 111.9, 107.3, 95.0, 76.7, 55.5. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 408.1206; found: 468.1209.

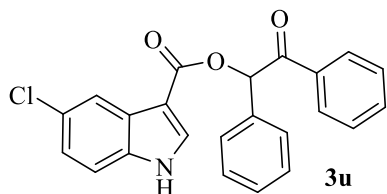


2-Oxo-1,2-diphenylethyl-5-fluoro-1H-indole-3-carboxylate (3s). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3s** (white solid, 99.2 mg, 66% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.21 (s, 1H), 8.06-8.02 (m, 2H), 7.86 (d, $J = 3.2$ Hz, 1H), 7.69 (dd, $J_1 = 9.6$ Hz, $J_2 = 2.4$ Hz, 1H), 7.59-7.51 (m, 3H), 7.46-7.36 (m, 5H), 7.26-7.22 (m, 1H), 7.15 (s, 1H), 6.94-6.88 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.2, 164.0, 159.2 ($J_{\text{C-F}} = 236.0$ Hz), 134.7, 134.0, 133.7, 133.2, 132.5, 129.3, 129.2, 128.9, 128.8, 128.7, 126.5 ($J_{\text{C-F}} = 11.0$ Hz), 112.5 ($J_{\text{C-F}} = 10.0$ Hz), 111.7 ($J_{\text{C-F}} = 26.0$ Hz), 107.6 ($J_{\text{C-F}} = 4.0$ Hz), 106.7 ($J_{\text{C-F}} = 25.0$ Hz), 76.9. ^{19}F NMR (376 MHz, CDCl_3) δ -121.1. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{FNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 396.1006; found: 396.1011.

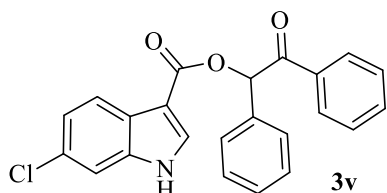


2-Oxo-1,2-diphenylethyl-6-fluoro-1H-indole-3-carboxylate (3t). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3t** (brown solid, 123.9 mg, 83% yield); ^1H NMR (400 MHz, CDCl_3) δ 9.30 (s, 1H), 8.06-8.03 (m, 2H), 7.96 (dd, $J_1 = 8.8$ Hz, $J_2 = 5.6$ Hz, 1H), 7.79 (d, $J = 3.2$ Hz, 1H), 7.59-7.56 (m, 2H), 7.55-7.52 (m, 1H), 7.46-7.36 (m, 5H), 7.16 (s, 1H), 7.00 (dd, $J_1 = 9.2$ Hz, $J_2 = 2.0$ Hz, 1H), 6.94-6.87 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 195.3, 164.1, 160.2 ($J_{\text{C-F}} = 238.0$ Hz), 136.2 ($J_{\text{C-F}} = 12.0$ Hz), 134.7, 133.9, 133.7, 132.4 ($J_{\text{C-F}}$

= 3.0 Hz), 129.3, 129.2, 128.9, 128.8, 128.7, 122.2 ($J_{\text{C-F}} = 9.0$ Hz), 122.1 ($J_{\text{C-F}} = 1.0$ Hz), 110.7 ($J_{\text{C-F}} = 24.0$ Hz), 107.4, 98.1 ($J_{\text{C-F}} = 26.0$ Hz), 76.9. ^{19}F NMR (376 MHz, CDCl_3) δ -119.3. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{FNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 396.1006; found: 396.1011.

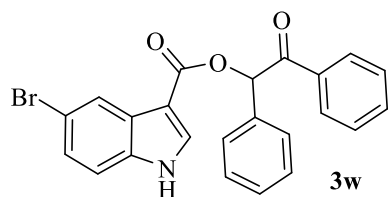


2-Oxo-1,2-diphenylethyl-5-chloro-1H-indole-3-carboxylate (3u). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3u** (white solid, 105.1 mg, 67% yield); ^1H NMR (400 MHz, DMSO-d_6) δ 12.27 (s, 1H), 8.27 (s, 1H), 8.15-8.11 (m, 2H), 7.91 (d, $J = 2.0$ Hz, 1H), 7.71-7.67 (m, 2H), 7.66-7.62 (m, 1H), 7.55 (s, 1H), 7.53-7.50 (m, 2H), 7.47-7.38 (m, 3H), 7.36 (s, 1H), 7.24 (dd, $J_1 = 8.4$ Hz, $J_2 = 2.0$ Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 194.2, 163.3, 135.0, 134.8, 134.2, 134.0, 133.9, 129.2, 129.1, 129.0, 128.8, 128.7, 126.8, 126.3, 122.7, 119.6, 114.3, 105.4, 76.3. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{16}\text{ClNO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 412.0711; found: 412.0716.

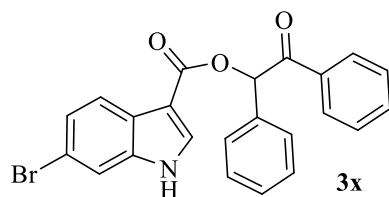


2-Oxo-1,2-diphenylethyl-6-chloro-1H-indole-3-carboxylate (3v). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3v** (brown solid, 73.2 mg, 47% yield); ^1H NMR (400 MHz, DMSO-d_6) δ 12.17 (s, 1H), 8.23 (d, $J = 2.8$ Hz, 1H), 8.14-8.10 (m, 2H), 7.92 (d, $J = 8.4$ Hz, 1H), 7.70-7.67 (m, 2H), 7.66-7.61 (m, 1H), 7.57 (d, $J = 2.0$ Hz, 1H), 7.55-7.50 (m, 2H), 7.46-7.37 (m, 3H), 7.34 (s, 1H), 7.21 (dd, $J_1 = 8.4$ Hz, $J_2 = 2.0$ Hz, 1H). ^{13}C NMR (100 MHz, DMSO-d_6) δ 194.2, 163.3, 136.9, 134.3, 134.2, 134.0, 133.8, 129.1, 129.0, 128.9, 128.7, 128.6, 127.2, 124.4, 121.9, 121.6, 112.2, 105.8, 76.3. HRMS (ESI, m/z) calcd. for

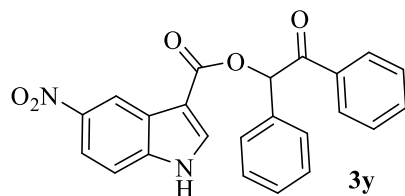
C₂₃H₁₆ClNO₃Na [M+Na]⁺ calc.: 412.0711; found: 412.0716.



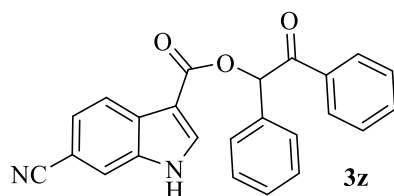
2-Oxo-1,2-diphenylethyl-5-bromo-1H-indole-3-carboxylate (3w). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3w** (white solid, 83.0 mg, 48% yield); ¹H NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), 8.21 (s, 1H), 8.06 (d, *J* = 7.6 Hz, 2H), 7.86 (d, *J* = 3.2 Hz, 1H), 7.61-7.54 (m, 3H), 7.47-7.36 (m, 5H), 7.31-7.28 (m, 1H), 7.24-7.20 (m, 1H), 7.14 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 195.3, 163.8, 134.7, 133.9, 133.7, 132.6, 129.3, 129.2, 129.0, 128.8, 128.7, 127.4, 126.2, 124.1, 115.7, 113.0, 107.0, 76.9. HRMS (ESI, *m/z*) calcd. for C₂₃H₁₆BrNO₃Na [M+Na]⁺ calc.: 456.0206; found: 456.0202.



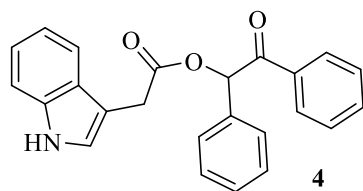
2-Oxo-1,2-diphenylethyl-6-bromo-1H-indole-3-carboxylate (3x). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3x** (brown solid, 61.2 mg, 35% yield); ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.17 (s, 1H), 8.21 (d, *J* = 2.4 Hz, 1H), 8.14-8.10 (m, 2H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.71-7.66 (m, 3H), 7.65-7.62 (m, 1H), 7.55-7.50 (m, 2H), 7.46-7.37 (m, 3H), 7.34-7.31 (m, 2H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 194.2, 163.3, 137.4, 134.2, 134.2, 134.0, 133.8, 129.0, 128.9, 128.7, 128.7, 124.7, 124.5, 122.0, 115.2, 105.8, 76.3. HRMS (ESI, *m/z*) calcd. for C₂₃H₁₆BrNO₃Na [M+Na]⁺ calc.: 456.0206; found: 456.0211.



2-Oxo-1,2-diphenylethyl-5-nitro-1*H*-indole-3-carboxylate (3y). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3y** (yellow solid, 40.8 mg, 25% yield); ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.71 (s, 1H), 8.86 (d, *J* = 2.0 Hz, 1H), 8.48 (d, *J* = 2.0 Hz, 1H), 8.16-8.10 (m, 3H), 7.74-7.69 (m, 3H), 7.68-7.63 (m, 1H), 7.57-7.51 (m, 2H), 7.48-7.40 (m, 4H). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 194.1, 162.9, 142.6, 139.7, 137.0, 134.1, 134.0, 133.8, 129.3, 129.1, 129.0, 128.8, 128.7, 125.1, 118.0, 116.9, 113.4, 107.7, 76.6. HRMS (ESI, *m/z*) calcd. for C₂₃H₁₆N₂O₅Na [M+Na]⁺ calc.: 423.0951; found: 423.0956.

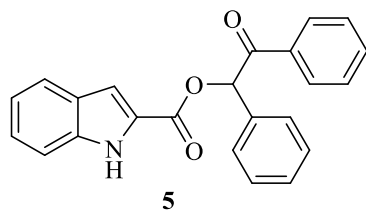


2-Oxo-1,2-diphenylethyl-6-cyano-1*H*-indole-3-carboxylate (3z). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **3z** (white solid, 55.4 mg, 36% yield); ¹H NMR (400 MHz, CDCl₃) δ 9.92 (s, 1H), 8.08-8.05 (m, 2H), 7.98-7.94 (m, 2H), 7.67-7.65 (m, 1H), 7.61-7.56 (m, 3H), 7.49-7.40 (m, 5H), 7.30 (dd, *J*₁ = 8.0 Hz *J*₂ = 1.2 Hz, 1H), 7.17 (s, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 195.7, 163.4, 135.0, 134.9, 134.5, 134.1, 133.5, 129.6, 129.4, 129.0, 128.9, 128.7, 124.8, 122.0, 119.9, 116.7, 107.9, 105.8, 77.2. HRMS (ESI, *m/z*) calcd. for C₂₄H₁₆N₂O₃Na [M+Na]⁺ calc.: 403.1053; found: 403.1059.

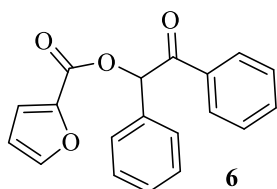


2-Oxo-1,2-diphenylethyl-2-(1*H*-indol-3-yl)acetate (4). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **4** (yellow liquid, 91.2 mg, 62% yield); ¹H NMR (400 MHz, CDCl₃) δ 8.12 (s, 1H), 7.92-7.89 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.51-7.44 (m, 3H), 7.38-7.29 (m, 6H), 7.19-7.14 (m, 2H),

7.12-7.07 (m, 1H), 6.89 (s, 1H), 4.00-3.89 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 194.0, 171.5, 136.0, 134.6, 133.5, 133.4, 129.3, 129.1, 128.8, 128.6, 128.6, 127.2, 123.3, 122.1, 119.6, 118.8, 111.1, 107.8, 77.9, 30.9. HRMS (ESI, m/z) calcd. for $\text{C}_{24}\text{H}_{19}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 392.1257; found: 392.1263.

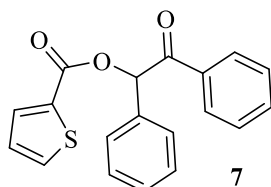


2-Oxo-1,2-diphenylethyl-1H-indole-2-carboxylate (5). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **5** (white solid, 111.4 mg, 78% yield, $dr = 2.0:1.0$); ^1H NMR (400 MHz, CDCl_3) δ ^1H NMR (400 MHz, CDCl_3 , major isomer) δ 9.14 (s, 1H), 8.01-7.97 (m, 2H), 7.66 (dd, $J_1 = 8.2$ Hz, $J_2 = 0.8$ Hz, 1H), 7.57 (d, $J = 1.6$ Hz, 1H), 7.52-7.49 (m, 1H), 7.42-7.37 (m, 7H), 7.32-7.29 (m, 2H), 7.14-7.09 (m, 2H); (minor isomer) δ 9.52 (s, 0.50H), 8.01-7.97 (m, 1.59H), 7.63 (dd, $J_1 = 7.4$ Hz, $J_2 = 2.0$ Hz, 1H), 7.59 (d, $J = 2.0$ Hz, 1H), 7.54-7.51 (m, 1H), 7.37-7.33 (m, 3.52 H), 7.28-7.25 (m, 1H), 7.21-7.17 (m, 1H). ^{13}C NMR (100 MHz, CDCl_3 , major isomer) δ 193.4, 161.1, 137.1, 134.5, 133.6, 133.5, 129.5, 129.2, 128.9, 128.8, 128.7, 127.4, 126.3, 125.7, 122.7, 120.8, 112.0, 110.2, 77.9; (minor isomer) δ 193.2, 159.9, 136.5, 134.4, 133.7, 133.2, 131.4, 129.6, 129.2, 129.1, 128.9, 128.7, 126.9, 123.5, 121.7, 112.2, 78.1. HRMS (ESI, m/z) calcd. for $\text{C}_{23}\text{H}_{17}\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 378.1101; found: 378.1098.

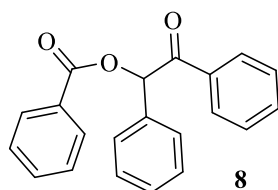


2-Oxo-1,2-diphenylethyl-furan-2-carboxylate (6). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **6** (white solid, 63.3 mg, 52% yield); ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.10-8.07 (m, 2H), 8.03-8.01 (m, 1H),

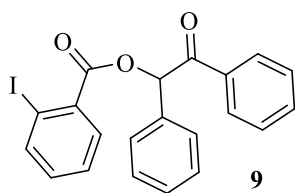
7.66-7.60 (m, 3H), 7.54-7.49 (m, 2H), 7.45-7.38 (m, 4H), 7.36 (s, 1H), 6.73 (dd, $J_1 = 3.4$ Hz, $J_2 = 2.0$ Hz, 1H). ^{13}C NMR (100 MHz, DMSO- d_6) δ 193.4, 157.2, 148.2, 143.2, 134.0, 133.8, 133.2, 129.4, 129.1, 129.0, 128.8, 128.7, 119.4, 112.6, 77.3. HRMS (ESI, m/z) calcd. for $\text{C}_{19}\text{H}_{14}\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 329.0784; found: 329.0789.



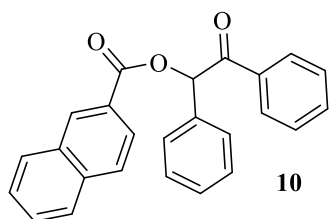
2-Oxo-1,2-diphenylethyl-thiophene-2-carboxylate (7). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **7** (white solid, 109.5 mg, 85% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.00-7.97 (m, 2H), 7.89 (dd, $J_1 = 3.6$ Hz, $J_2 = 1.2$ Hz, 1H), 7.59 (dd, $J_1 = 5.2$ Hz, $J_2 = 1.2$ Hz, 1H), 7.57-7.54 (m, 2H), 7.53-7.50 (m, 1H), 7.44-7.35 (m, 5H), 7.12-7.09 (m, 1H), 7.05 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.5, 161.6, 134.6, 134.3, 133.5, 133.2, 132.7, 129.3, 129.1, 128.9, 128.7, 128.6, 127.8, 78.0. HRMS (ESI, m/z) calcd. for $\text{C}_{19}\text{H}_{14}\text{O}_3\text{SNa}$ $[\text{M}+\text{Na}]^+$ calc.: 345.0556; found: 345.0561.



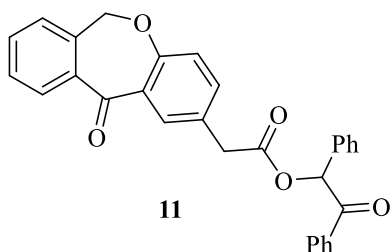
2-Oxo-1,2-diphenylethyl benzoate (8). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **8** (white solid, 67.6 mg, 53% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.14-8.11 (m, 2H), 8.02-7.99 (m, 2H), 7.60-7.54 (m, 3H), 7.53-7.50 (m, 1H), 7.46-7.41 (m, 4H), 7.40-7.35 (m, 3H), 7.10 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.7, 166.0, 134.7, 133.7, 133.5, 133.4, 130.0, 129.4, 129.3, 129.1, 128.8, 128.7, 128.4, 77.9. HRMS (ESI, m/z) calcd. for $\text{C}_{21}\text{H}_{16}\text{O}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 339.0992; found: 339.0990.



2-Oxo-1,2-diphenylethyl-2-iodobenzoate (9). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **9** (white solid, 130.3 mg, 74% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.07 (dd, $J_1 = 8.0$ Hz, $J_2 = 1.6$ Hz, 1H), 8.01-7.97 (m, 3H), 7.58-7.54 (m, 2H), 7.54-7.50 (m, 1H), 7.44-7.35 (m, 6H), 7.19-7.14 (m, 1H), 7.13 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.5, 165.7, 141.4, 134.5, 133.8, 133.6, 133.3, 133.1, 131.8, 129.5, 129.2, 128.9, 128.8, 128.7, 128.0, 94.5, 78.5. HRMS (ESI, m/z) calcd. for $\text{C}_{21}\text{H}_{15}\text{IO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 464.9958; found: 464.9966.

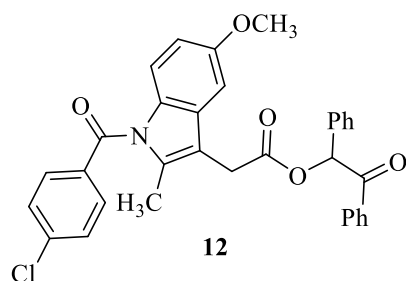


2-Oxo-1,2-diphenylethyl-2-naphthoate (10). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **10** (yellow solid, 133.1 mg, 91% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.70 (s, 1H), 8.12 (dd, $J_1 = 8.4$ Hz, $J_2 = 2.0$ Hz, 1H), 8.05-8.01 (m, 2H), 7.95 (d, $J = 8.4$ Hz, 1H), 7.89-7.85 (m, 2H), 7.64-7.61 (m, 2H), 7.60-7.56 (m, 1H), 7.55-7.51 (m, 2H), 7.45-7.42 (m, 3H), 7.41-7.38 (m, 2H), 7.16 (s, 1H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.7, 166.2, 135.7, 134.7, 133.8, 133.5, 132.4, 131.7, 129.4, 129.3, 129.2, 128.9, 128.8, 128.7, 128.4, 128.2, 127.8, 126.6, 126.5, 125.4, 78.0. HRMS (ESI, m/z) calcd. for $\text{C}_{25}\text{H}_{18}\text{O}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 389.1148; found: 389.1153.



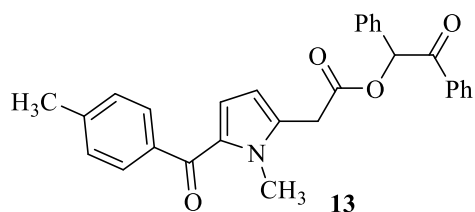
2-Oxo-1,2-diphenylethyl-2-(11-oxo-6,11-dihydrodibenzo[*b,e*]oxepin-2-yl)acetate

(11). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **11** (white solid, 126.9 mg, 69% yield); ^1H NMR (400 MHz, CDCl_3) δ 8.13 (s, 1H), 7.92-7.86 (m, 3H), 7.57-7.52 (m, 1H), 7.51-7.46 (m, 5H), 7.39-7.34 (m, 6H), 7.02 (d, $J = 8.8$ Hz, 1H), 6.87 (s, 1H), 5.17 (s, 2H), 3.88-3.77 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.6, 190.8, 171.0, 160.5, 140.4, 136.5, 135.5, 134.5, 133.5, 133.3, 132.7, 132.6, 129.5, 129.3, 129.2, 129.1, 128.8, 128.6, 127.8, 127.2, 125.0, 121.1, 78.1, 73.6, 39.6. HRMS (ESI, m/z) calcd. for $\text{C}_{30}\text{H}_{22}\text{O}_5\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 485.1359; found: 485.1362.



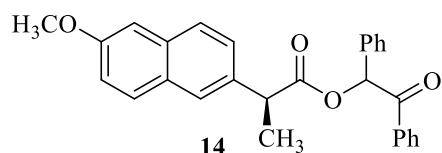
2-Oxo-1,2-diphenylethyl-2-(1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate

(12). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **12** (brown oil, 170.2 mg, 77% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.89-7.86 (m, 2H), 7.62-7.59 (m, 2H), 7.47-7.39 (m, 5H), 7.35-7.30 (m, 5H), 7.01-7.00 (m, 1H), 6.94-6.91 (m, 1H), 6.87 (s, 1H), 6.66 (dd, $J_1 = 8.8$ Hz, $J_2 = 2.4$ Hz, 1H), 3.84 (s, 2H), 3.78 (s, 3H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.5, 170.2, 168.2, 156.0, 139.0, 135.8, 134.3, 133.8, 133.4, 133.3, 131.1, 130.6, 130.4, 129.2, 129.0, 128.9, 128.6, 128.5, 128.4, 114.8, 112.1, 112.0, 100.9, 78.1, 55.5, 29.8, 13.3. HRMS (ESI, m/z) calcd. for $\text{C}_{33}\text{H}_{26}\text{ClNO}_5\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 574.1392; found: 574.1397.



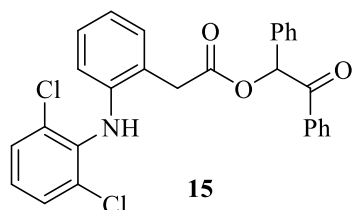
2-Oxo-1,2-diphenylethyl-2-(1-methyl-5-(4-methylbenzoyl)-1H-pyrrol-2-yl)acetate

(13). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **13** (brown oil, 103.8 mg, 57% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.92-7.89 (m, 2H), 7.70 (d, J = 8.4 Hz, 2H), 7.50-7.44 (m, 3H), 7.38-7.32 (m, 5H), 7.23-7.20 (m, 2H), 6.90 (s, 1H), 6.66 (d, J = 4.0 Hz, 1H), 6.15 (d, J = 4.4 Hz, 1H), 3.94-3.82 (m, 5H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.2, 185.7, 168.9, 141.7, 137.2, 134.3, 133.8, 133.5, 133.0, 131.3, 129.4, 129.3, 129.1, 128.7, 128.6, 128.5, 122.1, 109.6, 78.4, 33.1, 32.4, 21.4. HRMS (ESI, m/z) calcd. for $\text{C}_{29}\text{H}_{25}\text{NO}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 474.1676; found: 474.1684.



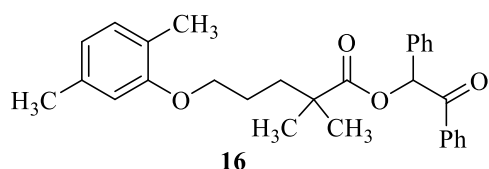
2-Oxo-1,2-diphenylethyl-(2S)-2-(6-methoxynaphthalen-2-yl)propanoate (14).

Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **14** (yellow oil, 99.0 mg, 58% yield, dr = 1.0:1.0); isomer 1 + isomer 2: ^1H NMR (400 MHz, CDCl_3) δ 7.92-7.89 (m, 2H, isomer 1), 7.84-7.81 (m, 2H, isomer 2), 7.70-7.63 (m, 3H, isomer 1 + 3H, isomer 2), 7.47-7.20 (m, 9H, isomer 1 + 9H, isomer 2), 7.14-7.07 (m, 2H, isomer 1 + 2H, isomer 2), 6.82-6.80 (m, 1H, isomer 1 + 1H, isomer 2), 4.13-3.98 (m, 1H, isomer 1 + 1H, isomer 2), 3.87(s, 1H, isomer 1), 3.85 (s, 1H, isomer 2), 1.66-1.60 (m, 3H, isomer 1 + 3H, isomer 2). ^{13}C NMR (100 MHz, CDCl_3) δ 193.9, 193.7, 174.2, 173.9, 157.5, 135.1, 134.9, 134.6, 134.5, 133.7, 133.6, 133.5, 133.4, 133.2, 129.3, 129.2, 129.0, 129.0, 128.9, 128.9, 128.8, 128.8, 128.7, 128.6, 128.5, 128.4, 128.3, 128.2, 127.0, 127.0, 126.4, 126.3, 126.1, 126.1, 118.8, 118.7, 105.5, 105.4, 77.9, 77.7, 55.2, 55.1, 45.1, 45.0, 18.7, 18.4. HRMS (ESI, m/z) calcd. for $\text{C}_{28}\text{H}_{24}\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 447.1567; found: 447.1573.



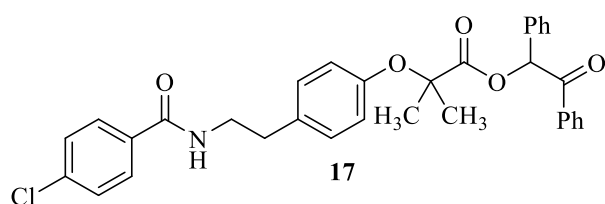
2-Oxo-1,2-diphenylethyl-2-((2,6-dichlorophenyl)amino)phenyl)acetate (15).

Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **15** (yellow oil, 136.5 mg, 70% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.89 (d, $J = 8.8$ Hz, 2H), 7.46-7.40 (m, 3H), 7.34-7.30 (m, 5H), 7.28-7.23 (m, 3H), 7.11-7.07 (m, 1H), 6.96-6.87(m, 3H), 6.64 (s, 1H), 6.54 (d, $J = 8.0$ Hz, 1H), 4.06-3.93 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.2, 171.7, 142.7, 137.9, 134.3, 133.4, 133.2, 130.9, 129.3, 129.3, 129.1, 128.7, 128.7, 128.6, 128.5, 128.0, 124.4, 123.8, 122.2, 118.7, 78.3, 38.0. HRMS (ESI, m/z) calcd. for $\text{C}_{28}\text{H}_{21}\text{Cl}_2\text{NO}_3\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 512.0791; found: 512.0798.



2-Oxo-1,2-diphenylethyl-5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate (16).

Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **16** (yellow oil, 149.0 mg, 84% yield, $dr = 2.0:1.0$); ^1H NMR (400 MHz, CDCl_3 , major isomer) δ 7.93 (d, $J = 8.4$ Hz, 2H), 7.50-7.44 (m, 3H), 7.39-7.29 (m, 5H), 6.99 (d, $J = 7.6$ Hz, 1H), 6.79 (s, 1H), 6.65 (d, $J = 7.6$ Hz, 1H), 6.61 (s, 1H), 3.91 (s, 2H), 2.29 (s, 3H), 2.14(s, 3H), 1.88-1.74 (m, 4H), 1.31 (s, 3H), 1.29 (s, 3H); (minor isomer) δ 7.97 (d, $J = 7.6$ Hz, 1H), 7.65-7.60 (m, 0.47H), 7.50-7.44 (m, 1H), 2.29 (s, 0.17H), 2.14 (s, 0.15H), 1.88-1.74 (m, 0.25H), 1.31 (s, 0.17H), 1.29 (s, 0.94H). ^{13}C NMR (100 MHz, CDCl_3 , major isomer) δ 194.2, 177.3, 156.9, 136.3, 134.8, 133.6, 133.3, 130.2, 129.8, 128.9, 128.7, 128.5, 123.5, 120.5, 111.9, 77.3, 67.9, 42.0, 37.0, 25.1, 25.0, 24.9, 21.3, 15.7; (minor isomer) δ 194.5, 134.8, 132.9, 129.0, 129.0, 128.2. HRMS (ESI, m/z) calcd. for $\text{C}_{29}\text{H}_{32}\text{O}_4\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 467.2193; found: 467.2199.



2-Oxo-1,2-diphenylethyl-2-(4-(2-(4-chlorobenzamido)ethyl)phenoxy)-2-methylpropanoate (17). Following the general procedure, the crude product was purified using silica gel column chromatography (petroleum ether / ethyl acetate = 5:1-3:1) to produce the desired product **17** (yellow oil, 150.1 mg, 67% yield); ^1H NMR (400 MHz, CDCl_3) δ 7.91 (d, J = 7.6 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.51-7.46 (m, 1H), 7.42-7.35 (m, 4H), 7.34-7.25 (m, 5H), 7.04 (d, J = 8.4 Hz, 2H), 6.89-6.86 (m, 3H), 6.56-6.46 (m, 1H), 3.58 (q, J = 6.8 Hz, 2H), 2.80 (t, J = 6.8 Hz, 2H), 1.68 (s, 3H), 1.66 (s, 3H). ^{13}C NMR (100 MHz, CDCl_3) δ 193.4, 173.6, 166.4, 153.8, 137.3, 134.4, 133.5, 133.0, 132.9, 132.5, 129.3, 129.3, 129.0, 128.7, 128.6, 128.5, 128.3, 128.2, 119.9, 79.1, 78.1, 41.2, 34.6, 25.9, 24.9. HRMS (ESI, m/z) calcd. for $\text{C}_{33}\text{H}_{30}\text{ClNO}_5\text{Na}$ $[\text{M}+\text{Na}]^+$ calc.: 578.1705; found: 578.1710.

3. Gram-scale synthesis of **3a**

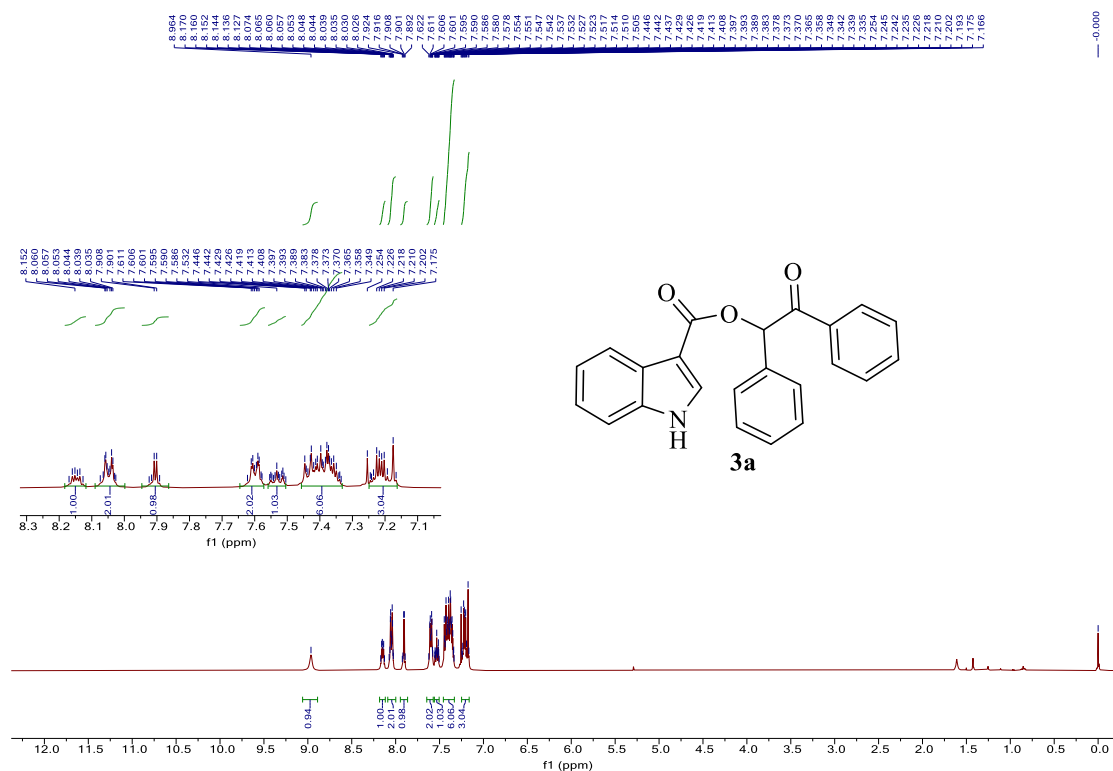
Benzyl phenyl ketone **1a** (0.785 g, 4 mmol), indole-3-carboxylic acid **2a** (0.967 g, 6 mmol), TBAI (0.443 g, 1.2 mmol) and H_2O (20 mL) were placed in an Schlenk tube, then TBHP (70% in water, 1.1 mL, 8 mmol) was added into the above mixture under air condition. After the completion of the addition, the reaction mixture was allowed to react at 50 °C (oil bath) for 12 h. Subsequently, the reaction mixture was cooled to room temperature, and then extracted with ethyl acetate. The organic layer was dried with anhydrous Na_2SO_4 . After removal of the ethyl acetate under reduced pressure, the residue was purified by column chromatography on silica gel (petroleum ether / ethyl acetate = 5:1-3:1) to afford 2-oxo-1,2-diphenylethyl-1*H*-indole-3-carboxylate **3a** (white solid, 1.13 g, 79% yield).

4. Crystal Preparation Methods of **3a**

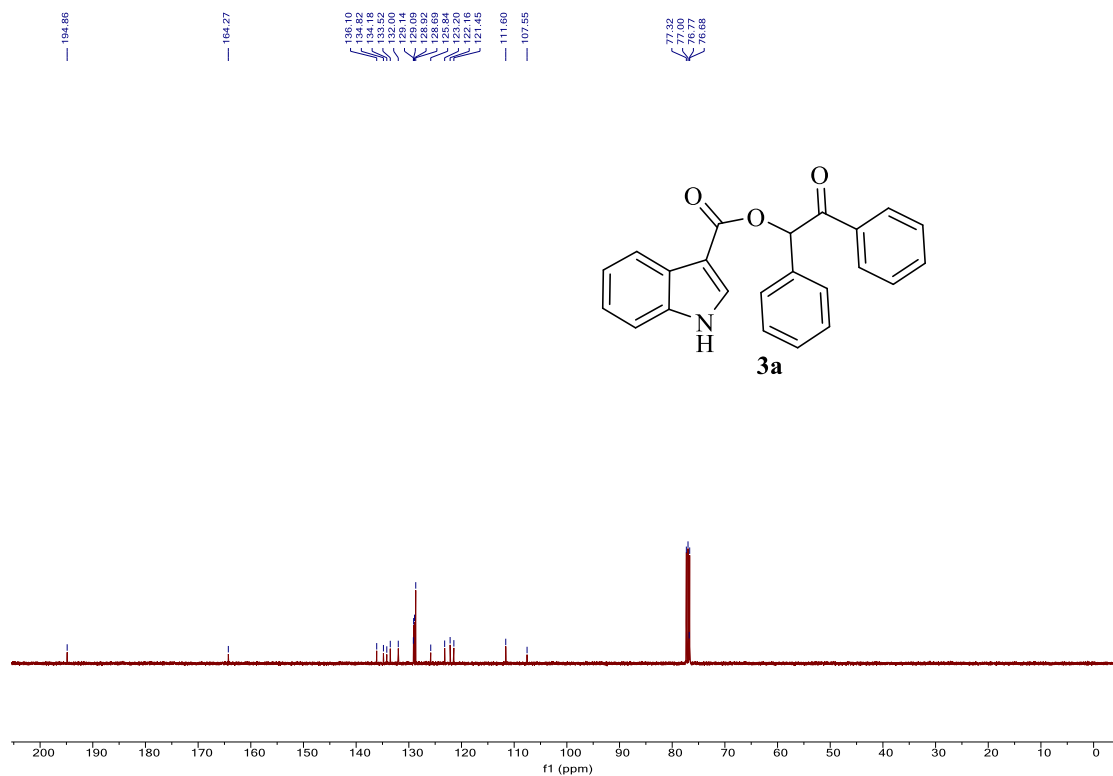
In a 50 mL round bottom flask, 50 mg of **3a** was dissolved in 3 mL DCM. Subsequently, 3 mL petroleum ether was added to the flask. The prepared solution was well shaken and kept at room temperature until crystals had precipitated out. The crystals were carefully picked out for single crystal X-ray diffraction.

5. ^1H NMR and ^{13}C NMR Spectra of Products 3-17

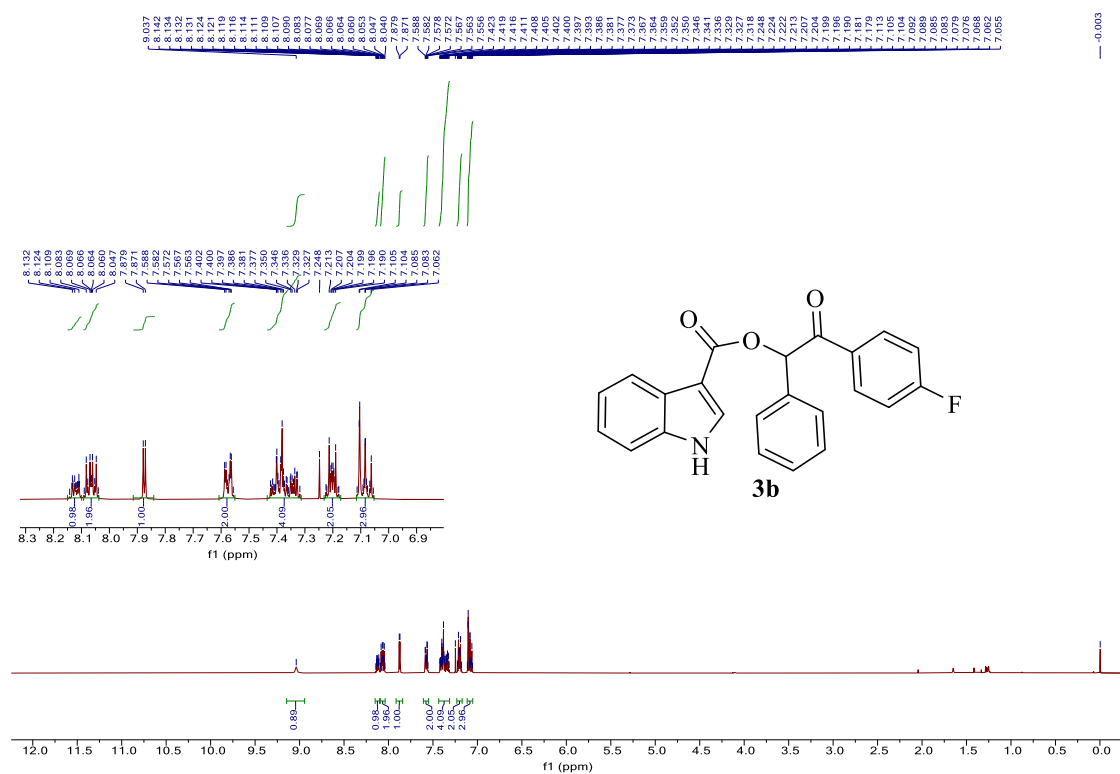
The ^1H NMR spectrum of **3a** (400 MHz, CDCl_3)



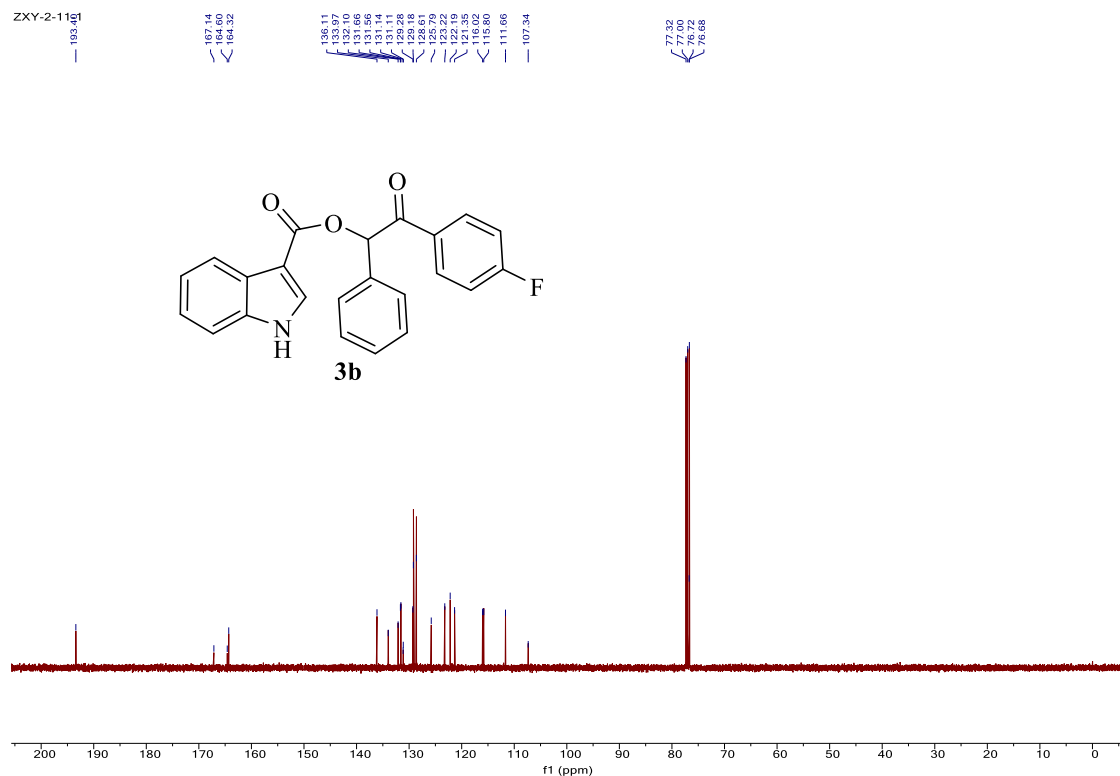
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3a** (100 MHz, CDCl_3)



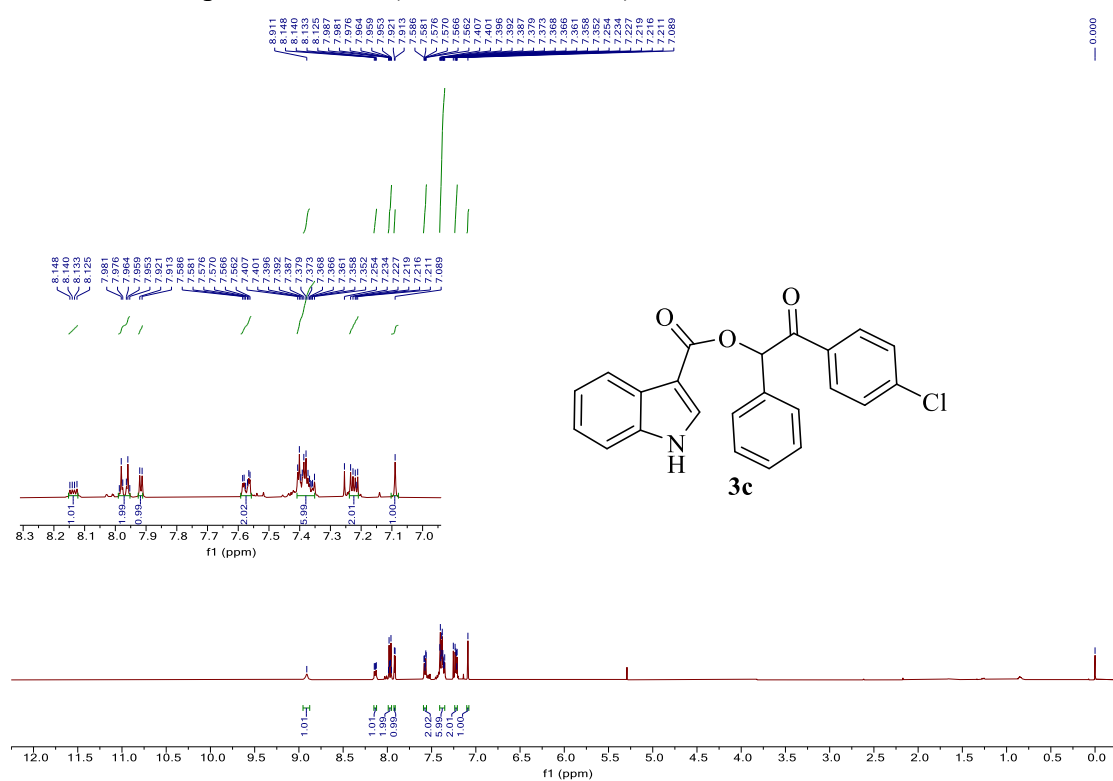
The ^1H NMR spectrum of **3b** (400 MHz, CDCl_3)



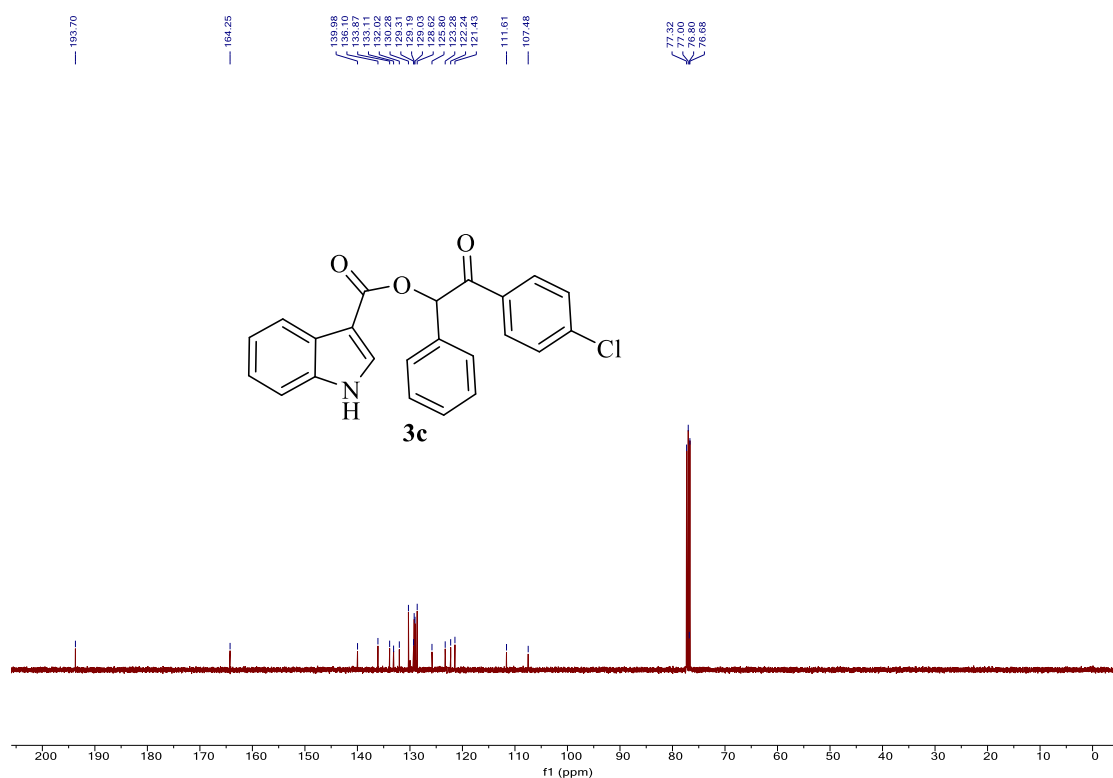
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3b** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **3c** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3c** (100 MHz, CDCl_3)



Chemical structure of 3d: O=C1C(=O)OC2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4C5=CC=C(C=C5)Br

¹H NMR spectrum (CDCl₃):

- Chemical shift range:** 7.149 – 8.194 ppm.
- Integration values:** 0.97, 2.00, 1.00, 0.95, 2.01, 1.02, 1.02, 0.98, 2.04.
- Peak list (ppm):** 8.194, 8.186, 8.172, 8.060, 8.045, 7.928, 7.909, 7.759, 7.742, 7.737, 7.684, 7.657, 7.522, 7.500, 7.502, 7.460, 7.445, 7.424, 7.438, 7.405, 7.387, 7.371, 7.218, 7.215, 7.195, 7.189, 7.169, 7.166, 3.367, 2.500, 2.500, 2.495, 2.481.

Chemical structure of **3d** is shown above the spectrum. The structure is an indole-3-carboxylate derivative: Indole-3-carboxylic acid benzyl ester with a 4-bromobenzoyl group on the benzylic carbon.

¹³C NMR spectrum (CDCl₃) of **3d**. The x-axis is labeled f1 (ppm) and ranges from 200 to 0. The spectrum shows peaks at the following chemical shifts (ppm): 193.80, 163.66, 135.50, 134.66, 133.22, 133.45, 132.55, 130.70, 129.20, 128.13, 128.11, 128.65, 127.55, 122.59, 121.56, 119.35, 112.57, 105.49, 76.01 (triplet), and a cluster of peaks between 38 and 41 ppm.

[illegible]

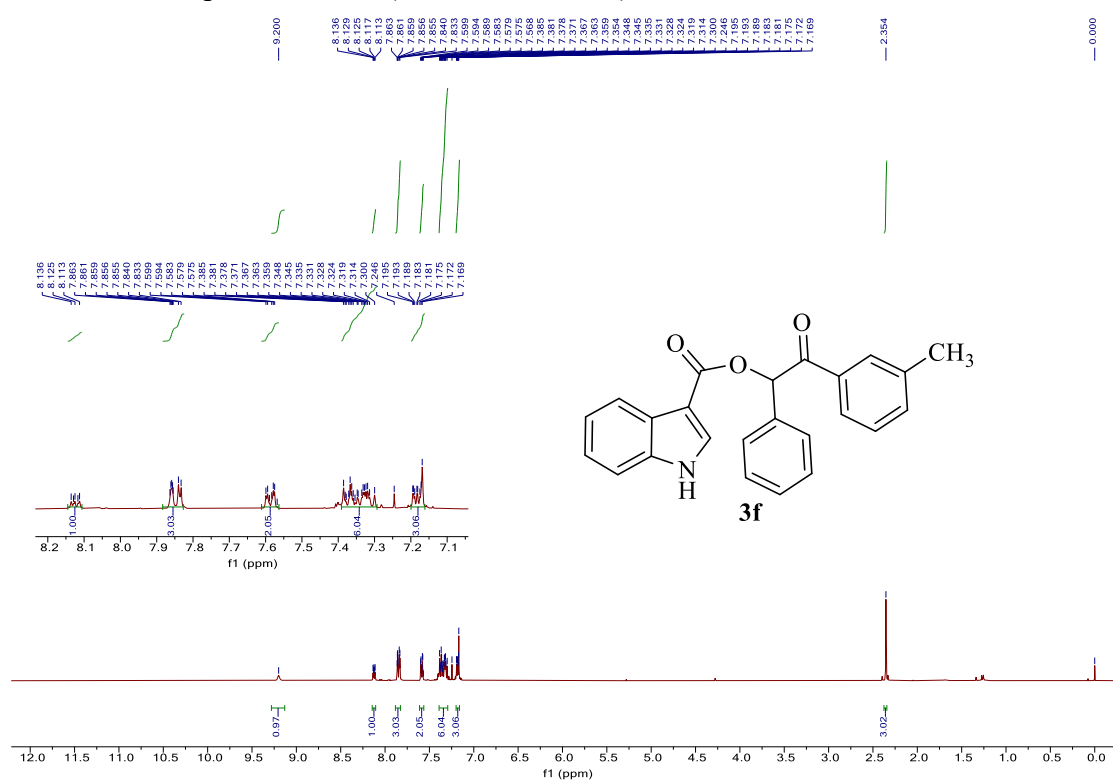
Chemical structure of **3e** is shown above the spectrum. The structure is a benzimidazole derivative with a benzimidazole core, a benzyl group, and a 4-methoxybenzoyl group.

The ¹³C NMR spectrum (CDCl₃) shows the following chemical shifts (ppm):

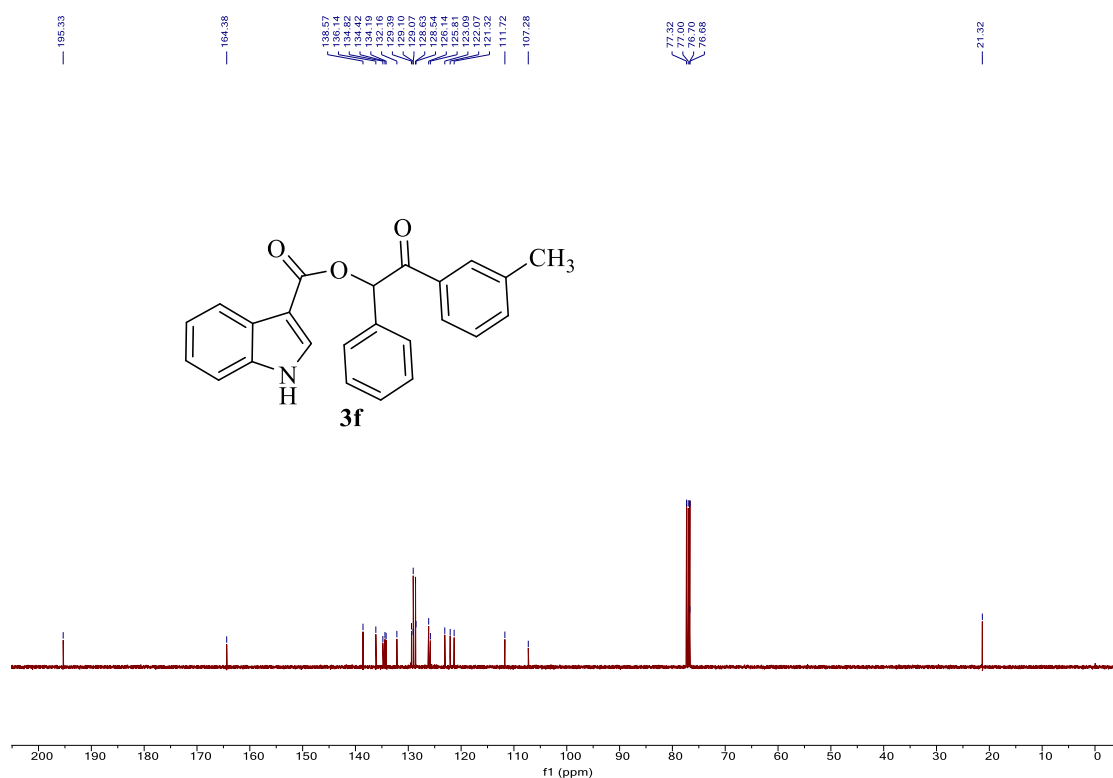
- 193.08
- 163.24
- 163.78
- 136.11
- 135.16
- 131.91
- 131.30
- 130.00
- 128.99
- 128.61
- 127.71
- 125.91
- 123.19
- 121.15
- 121.56
- 113.92
- 113.13
- 107.80
- 77.92
- 77.52
- 77.00
- 76.68
- 76.48
- 55.46

The spectrum displays a series of peaks corresponding to these chemical shifts, with a prominent solvent triplet for CDCl₃ centered around 77 ppm.

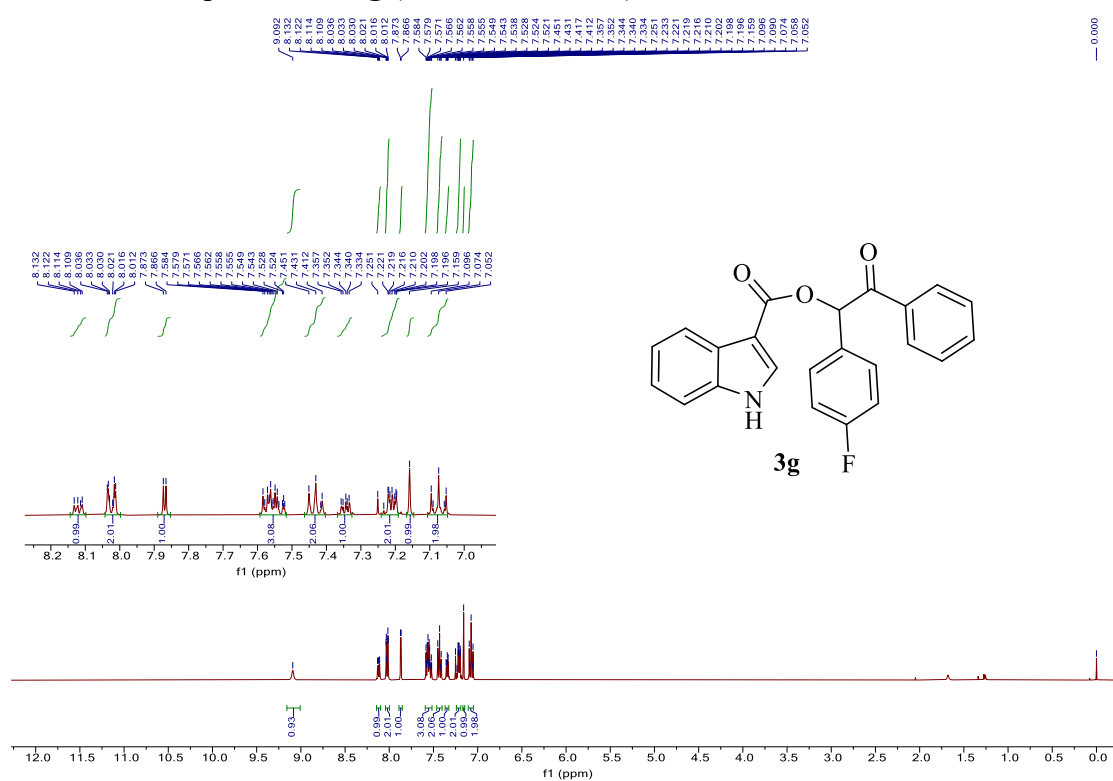
The ^1H NMR spectrum of **3f** (400 MHz, CDCl_3)



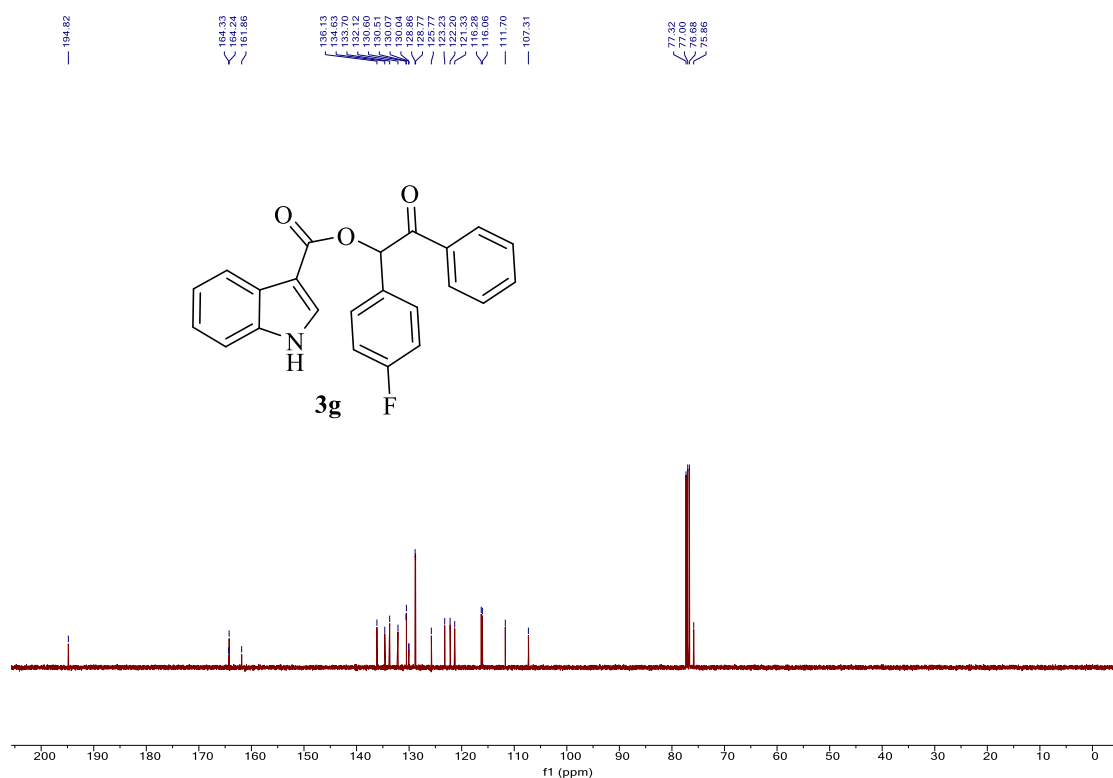
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3f** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **3g** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3g** (100 MHz, CDCl_3)



Chemical structure of **3h** is shown above the spectrum. The structure is a benzimidazole derivative with a 4-chlorophenyl group and a 2-oxo-1-phenylethyl group.

¹H NMR spectrum (CDCl₃) of compound **3h**. The spectrum shows peaks in the aromatic region (7.0-8.4 ppm) and a small peak in the aliphatic region (2.5 ppm). Integration values are provided below the baseline.

Chemical shift (ppm): 8.206, 8.198, 8.147, 8.144, 8.127, 8.123, 7.938, 7.935, 7.933, 7.731, 7.725, 7.714, 7.711, 7.695, 7.691, 7.670, 7.673, 7.673, 7.654, 7.650, 7.632, 7.588, 7.588, 7.557, 7.550, 7.537, 7.534, 7.523, 7.519, 7.502, 7.506, 7.440, 7.388, 7.388, 7.222, 7.218, 7.195, 7.195, 7.177, 7.175, 7.158, 7.154, 3.373, 2.510, 2.505, 2.495, 2.491.

Integration values: 0.97, 1.00, 1.00, 1.00, 1.07, 5.03, 1.00, 2.03.

Chemical structure of **3h** is shown above the spectrum. The structure is an indole-3-carboxylate derivative: 1H-indole-3-carboxylic acid 1-(4-chlorophenyl) 1-phenylethyl ester.

¹³C NMR spectrum (CDCl₃) of **3h**. The x-axis represents the chemical shift in ppm (f1), ranging from 0 to 200. The spectrum shows several peaks, with the following chemical shifts labeled above the spectrum:

- 194.23
- 163.49
- 136.48
- 134.08
- 133.89
- 133.43
- 130.46
- 128.10
- 125.59
- 121.54
- 120.28
- 112.53
- 105.43
- 75.20
- 40.15
- 39.94
- 39.73
- 39.52
- 39.31
- 39.10
- 38.89

Chemical structure of 3i: O=C1C=Cc2ccccc2N1C(=O)OC(c3ccccc3)C(=O)c4ccccc4

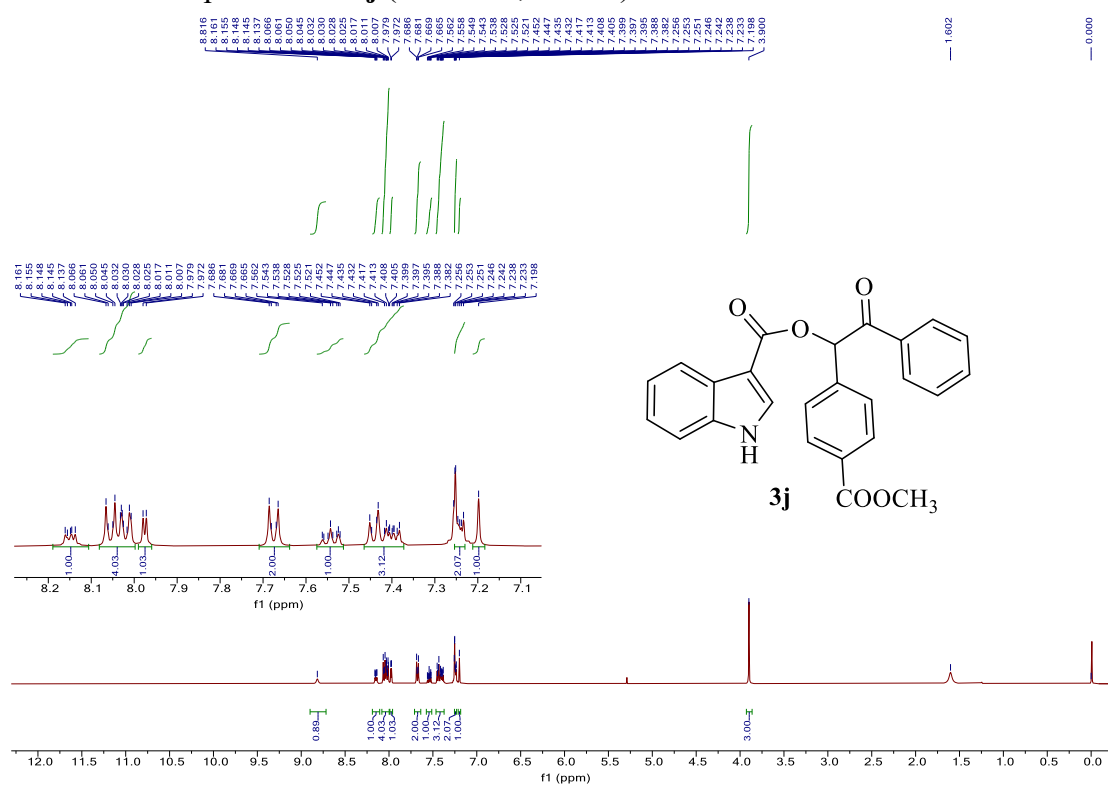
¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
8.142, 8.134, 8.125, 8.119, 8.103, 8.028, 8.022, 8.015, 8.010, 7.967, 7.916, 7.908, 7.853, 7.848, 7.834, 7.829, 7.813, 7.807, 7.776, 7.770, 7.742, 7.735, 7.725, 7.716, 7.711, 7.705, 7.695, 7.685, 7.678, 7.668, 7.658, 7.643, 7.628, 7.620, 7.615	1.07, 2.02, 1.02, 2.99, 4.05, 1.04, 2.04, 1.00

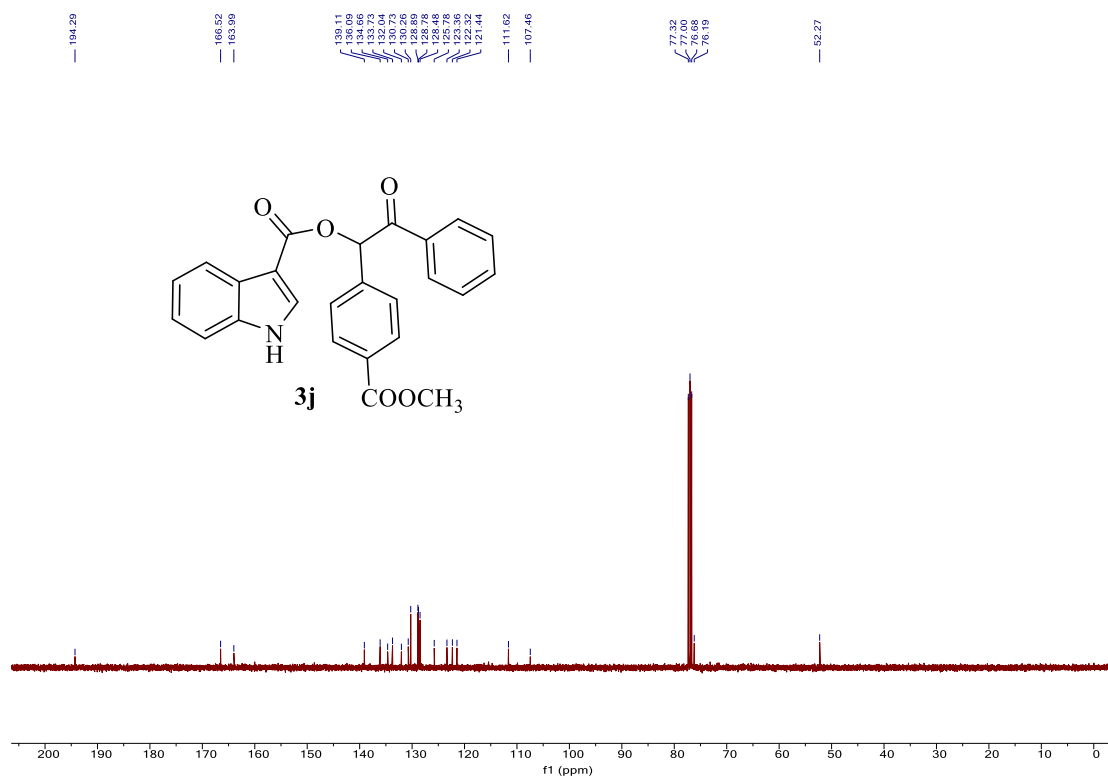
Chemical structure of compound **3i** is shown above the spectrum. The structure is a benzimidazole derivative with a benzoyl group and a 4-bromophenyl group attached to the imidazole ring. The spectrum displays the ¹³C NMR peaks for compound **3i** in CDCl₃, with the solvent peak (CDCl₃) visible at approximately 77.0 ppm. The x-axis represents the chemical shift in ppm, ranging from 0 to 200.

Chemical structure of compound **3i** is shown above the spectrum. The structure is a benzimidazole derivative with a benzoyl group and a 4-bromophenyl group attached to the imidazole ring. The spectrum displays the ¹³C NMR peaks for compound **3i** in CDCl₃, with the solvent peak (CDCl₃) visible at approximately 77.0 ppm. The x-axis represents the chemical shift in ppm, ranging from 0 to 200.

The ^1H NMR spectrum of **3j** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3j** (100 MHz, CDCl_3)



Chemical structure of **3k** is shown above the spectrum. The structure is a benzimidazole derivative with a methoxy group (OCH₃) and a benzoyl group.

¹H NMR spectrum (CDCl₃) of compound **3k**. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 12.0. The spectrum shows several peaks, with integration values provided below the peaks.

Integration values (from left to right): 1.00, 1.95, 1.00, 3.04, 2.00, 1.03, 2.03, 0.94, 1.98, 3.07.

Chemical shift values (ppm) are listed on the right side of the spectrum, ranging from 6.8 to 8.2.

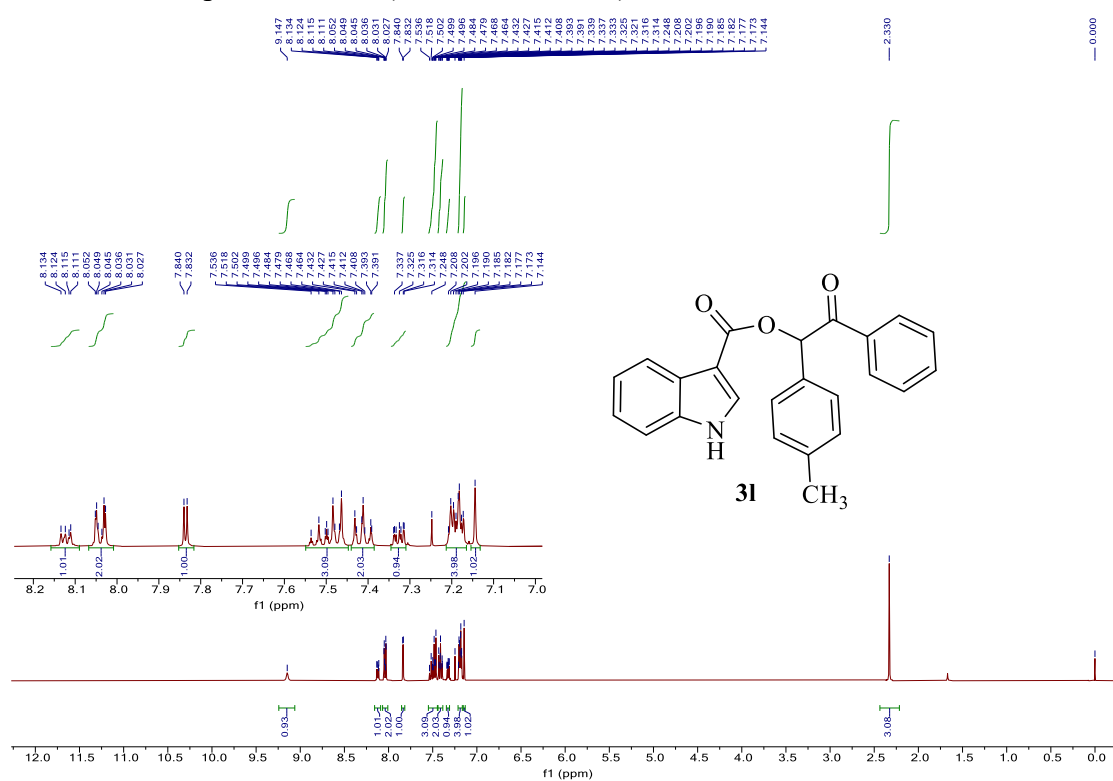
Chemical structure of **3k** is shown above the spectrum. The structure is a benzimidazole derivative with a methoxy group and a benzoyl group.

COc1ccc(cc1)C(=O)Oc2c[nH]c3ccccc23

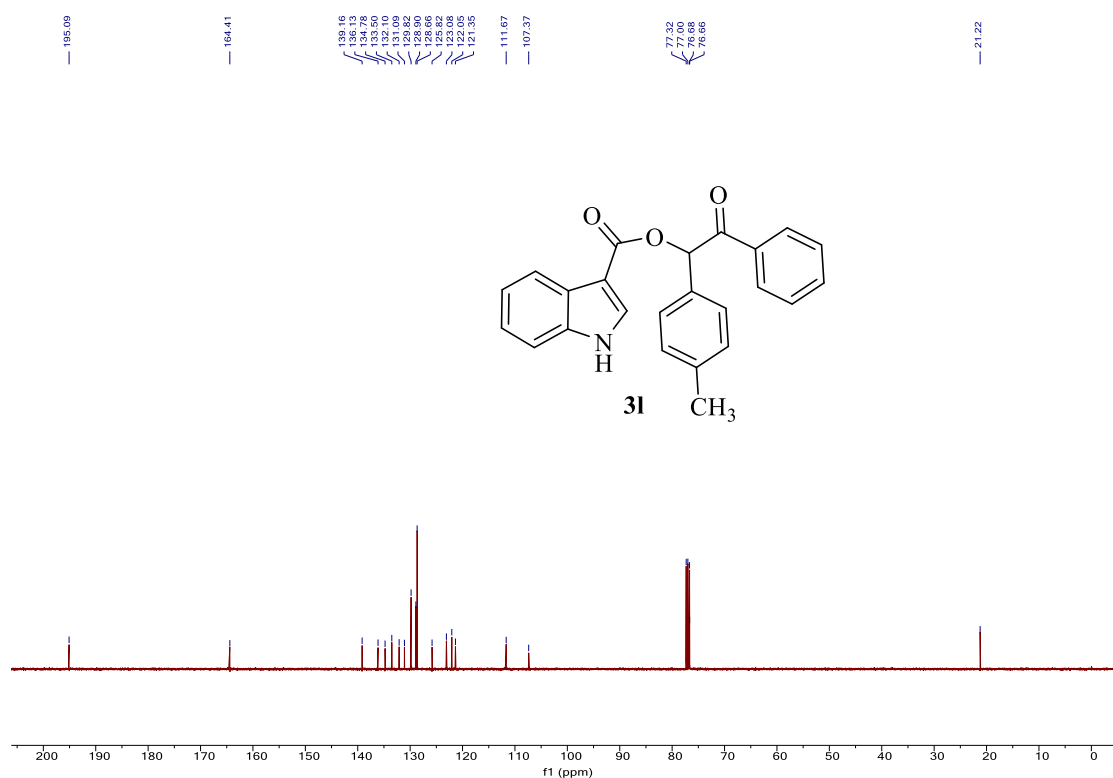
The spectrum displays the following chemical shifts (ppm):

- 195.00
- 164.46
- 160.20
- 136.13
- 134.80
- 133.47
- 132.20
- 130.20
- 128.87
- 127.60
- 126.05
- 125.83
- 123.57
- 122.07
- 114.53
- 111.66
- 107.45
- 77.32
- 77.00
- 76.85
- 76.39
- 55.26

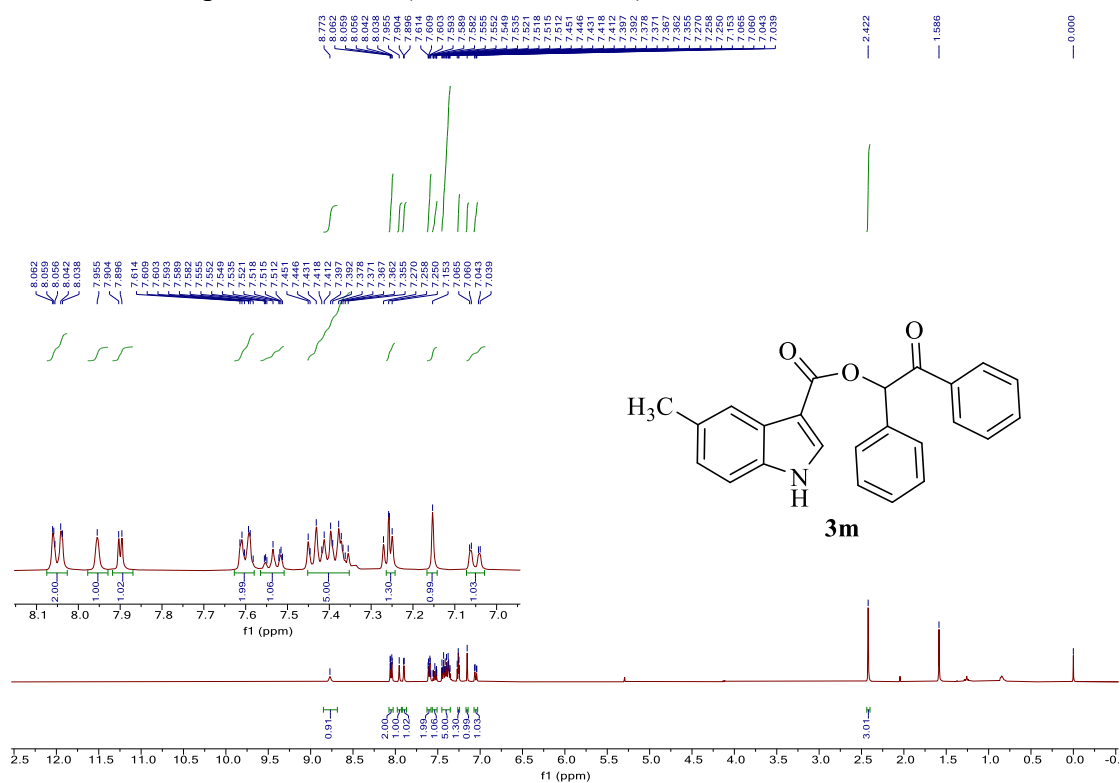
The ^1H NMR spectrum of **31** (400 MHz, CDCl_3)



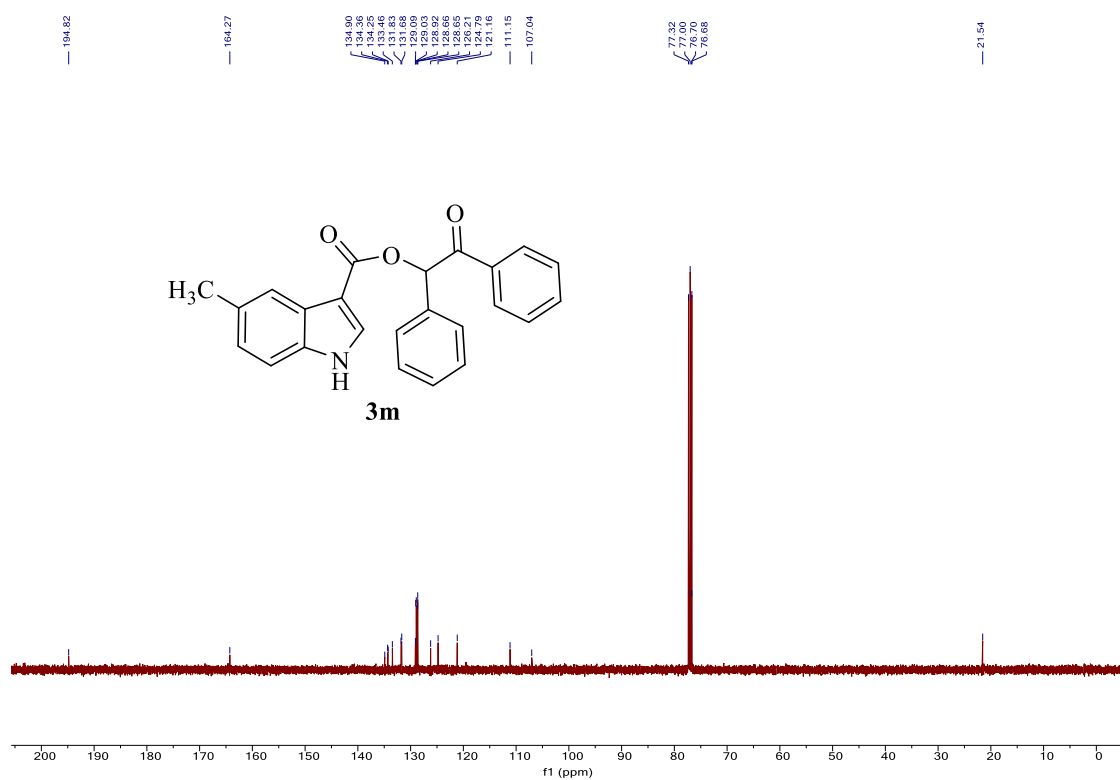
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **31** (100 MHz, CDCl_3)



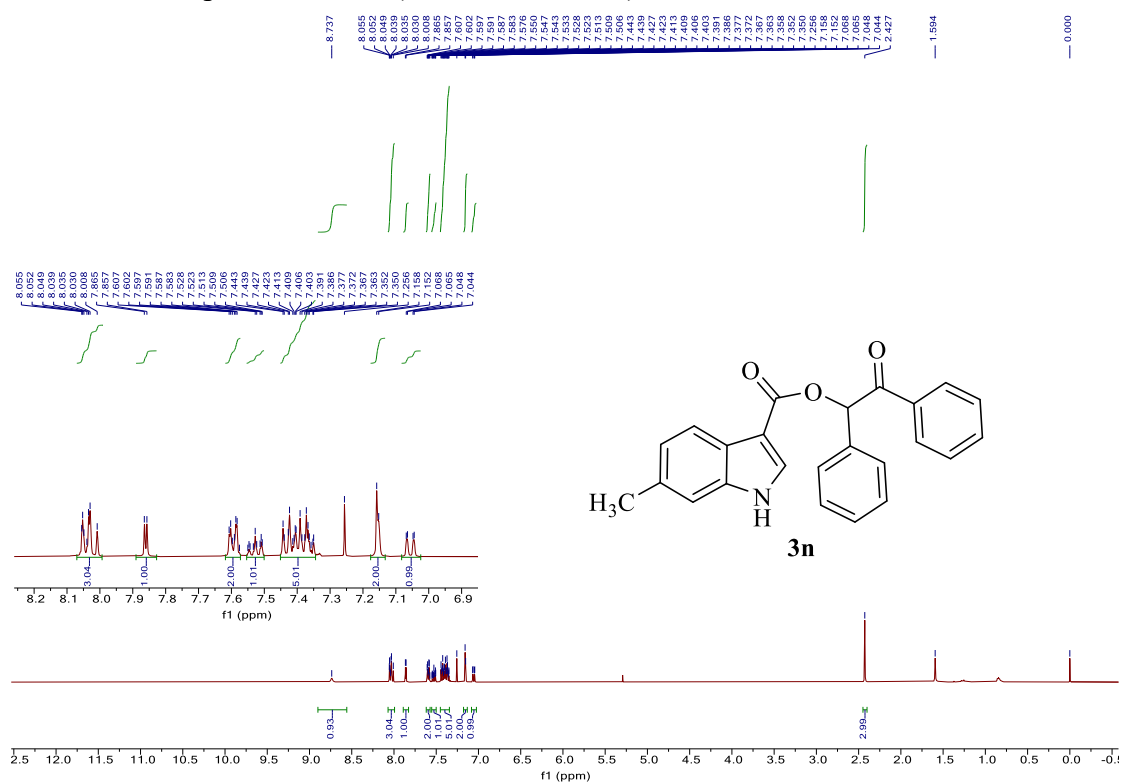
The ^1H NMR spectrum of **3m** (400 MHz, CDCl_3)



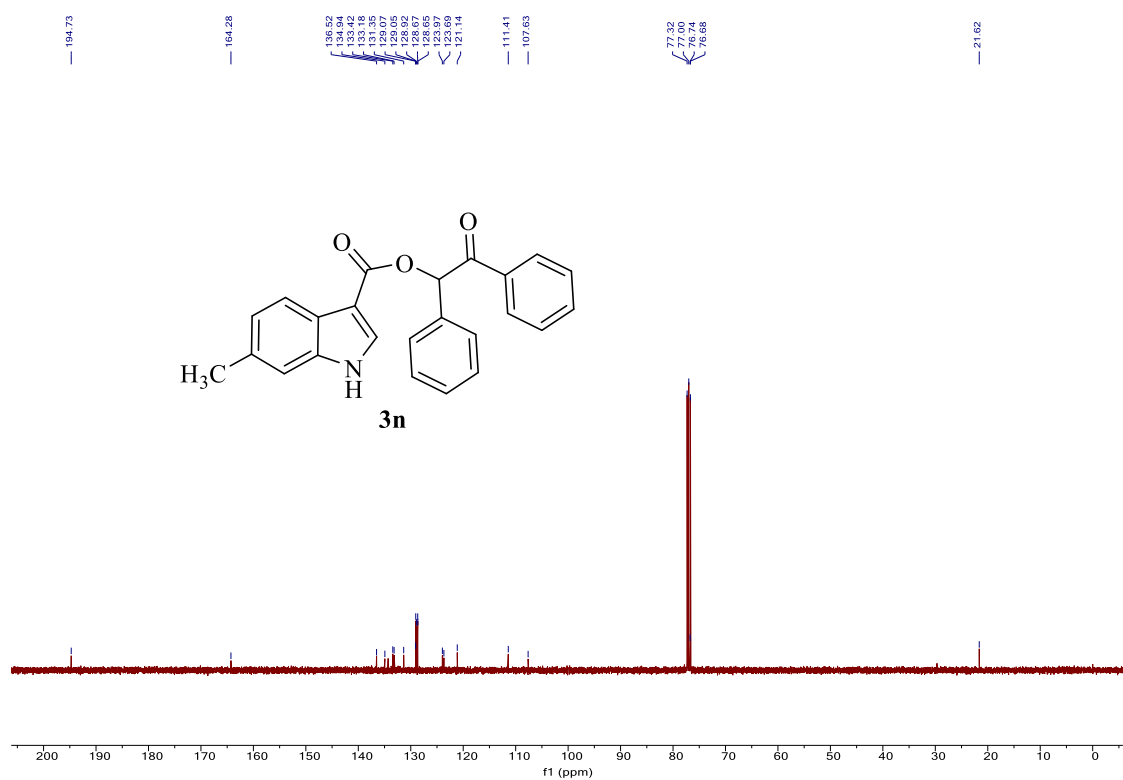
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3m** (100 MHz, CDCl_3)



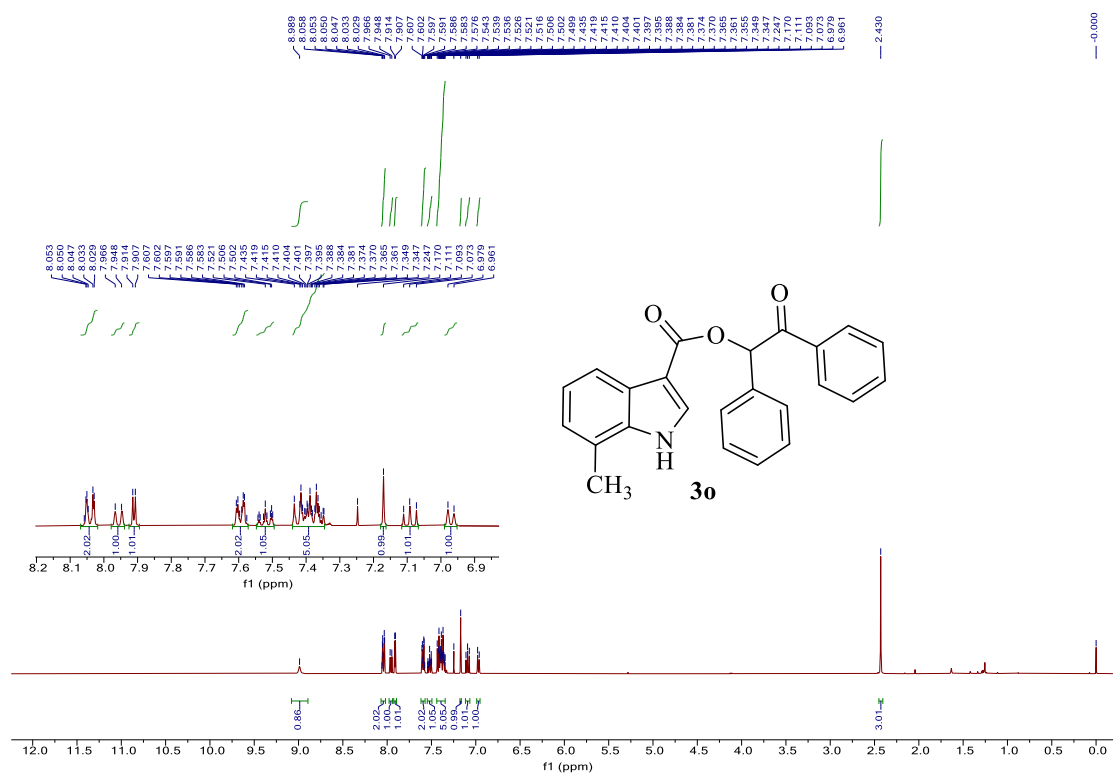
The ^1H NMR spectrum of **3n** (400 MHz, CDCl_3)



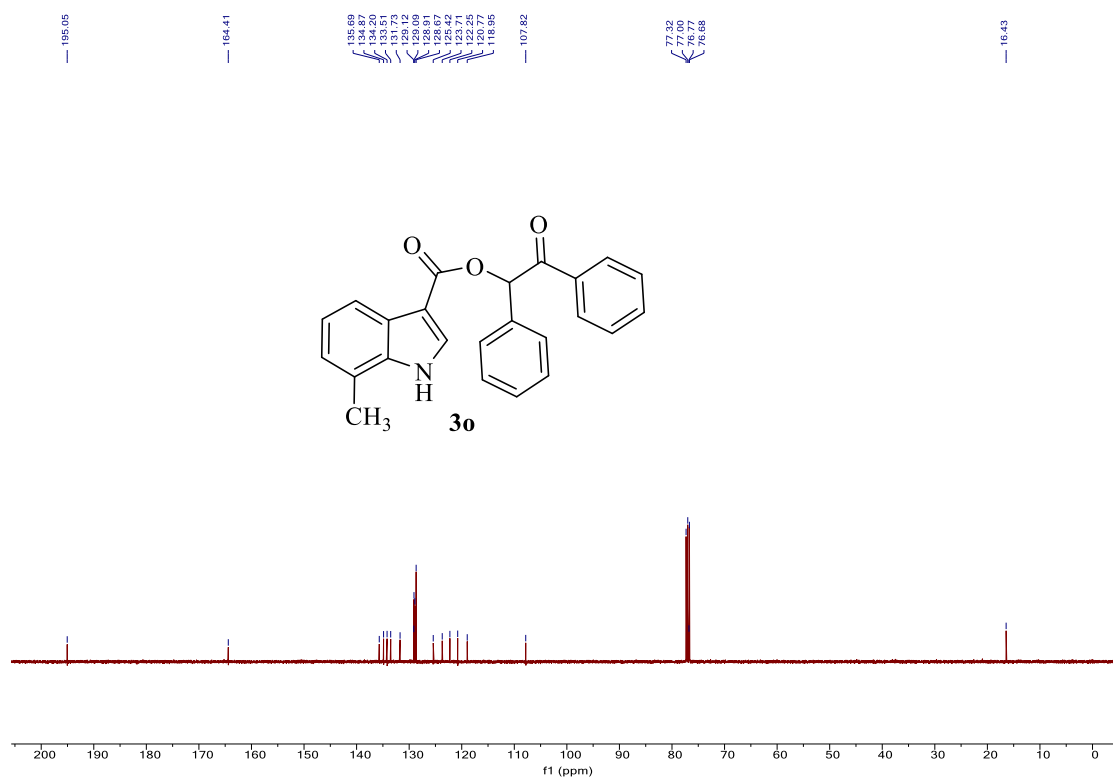
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3n** (100 MHz, CDCl_3)



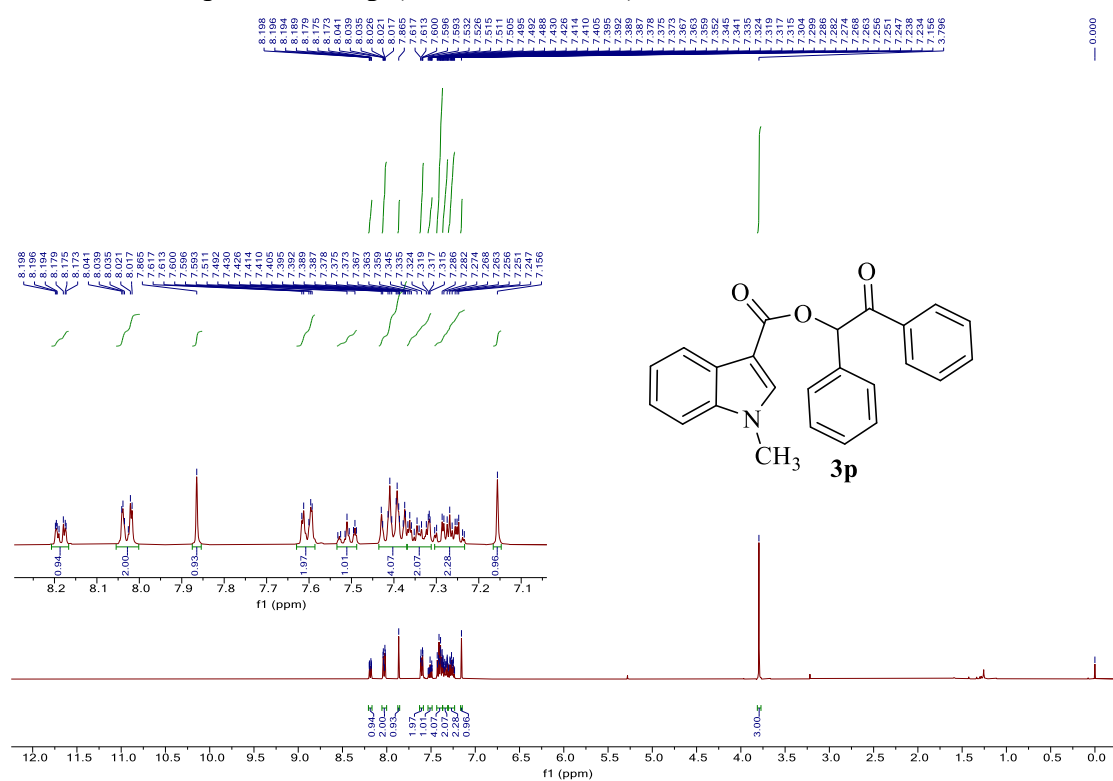
The ^1H NMR spectrum of **3o** (400 MHz, CDCl_3)



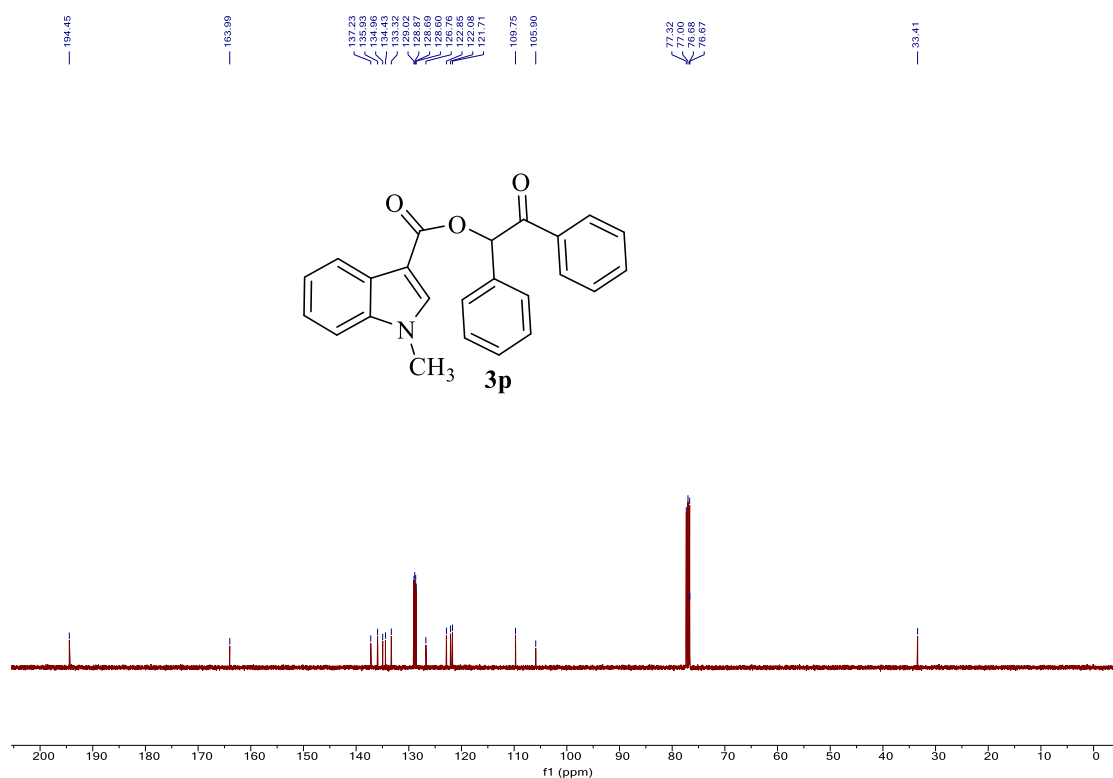
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3o** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **3p** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3p** (100 MHz, CDCl_3)



The figure displays two NMR spectra and the chemical structure of compound **3q**.

Chemical Structure: The structure of **3q** is shown as a benzimidazole derivative. It features a benzimidazole core substituted with a methoxy group (H_3CO) at position 6 and a 1-oxo-2-phenylpropan-1-yloxy group at position 3.

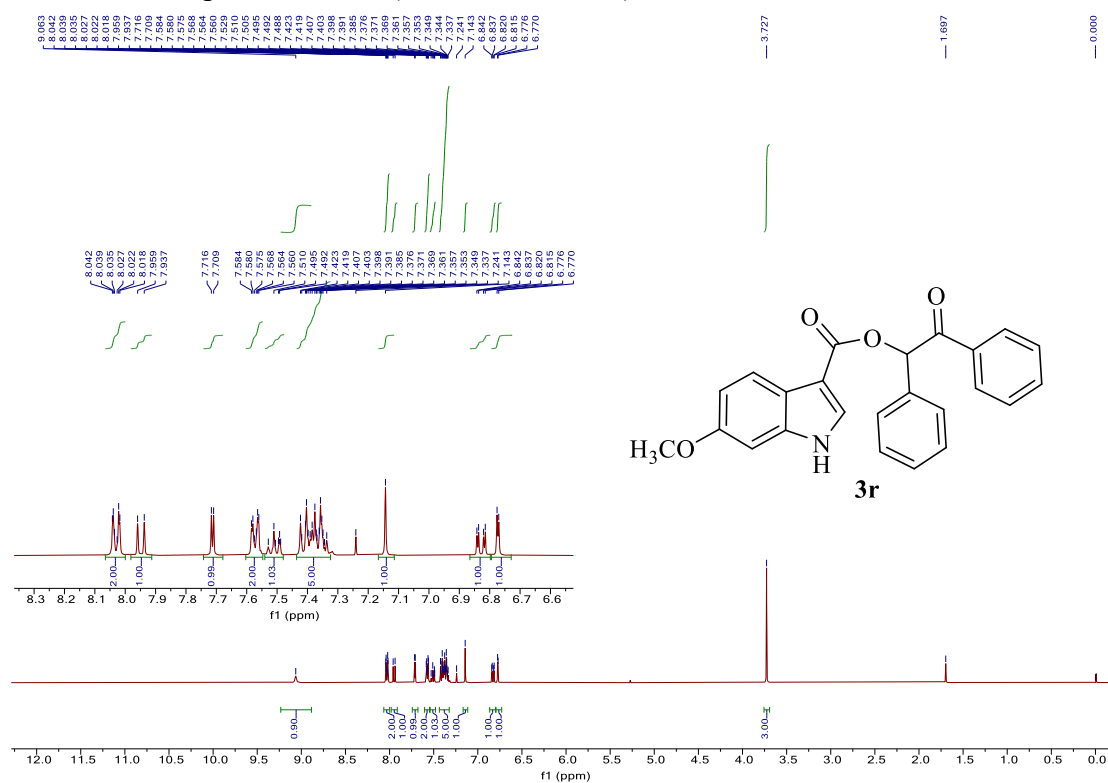
^1H NMR Spectrum (Top): The spectrum shows peaks from 6.7 to 8.2 ppm. Integration values are provided below the baseline: 0.97, 0.98, 1.00, 6.03, 1.03, 3.00, 1.00, 1.00, 2.00. A solvent peak for water is visible around 3.3 ppm.

^{13}C NMR Spectrum (Bottom): The spectrum shows peaks from 153.7 to 16.1 ppm. Key peaks include carbonyl carbons at approximately 163.4 and 153.4 ppm, aromatic carbons between 110 and 150 ppm, and aliphatic carbons at approximately 39.8, 37.7, and 16.1 ppm.

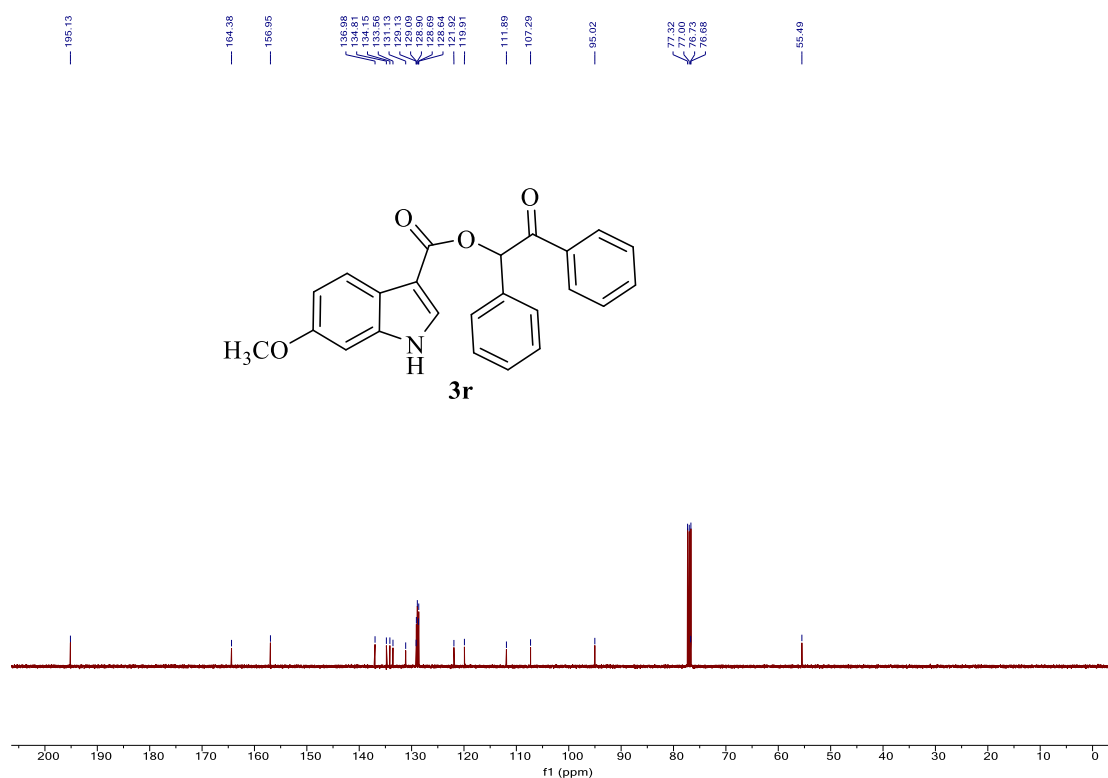
Chemical structure of **3q** is shown above the spectrum. The structure is a 5-methoxy-1H-indole-3-carboxylic acid derivative, specifically a 5-methoxy-1H-indole-3-carboxylic acid derivative, where the carboxylic acid group is esterified with a 1-phenylethyl group. The structure is labeled **3q**.

The ¹³C NMR spectrum (CDCl₃) shows the following chemical shifts (ppm): 194.86, 164.32, 155.81, 134.77, 134.24, 133.85, 132.05, 130.90, 130.65, 129.07, 128.93, 128.65, 126.72, 113.92, 112.44, 107.16, 102.38, 77.32, 77.00, 76.68, and 55.50. The spectrum displays a series of peaks corresponding to these chemical shifts, with a prominent peak at 77.00 ppm, likely representing the solvent (CDCl₃).

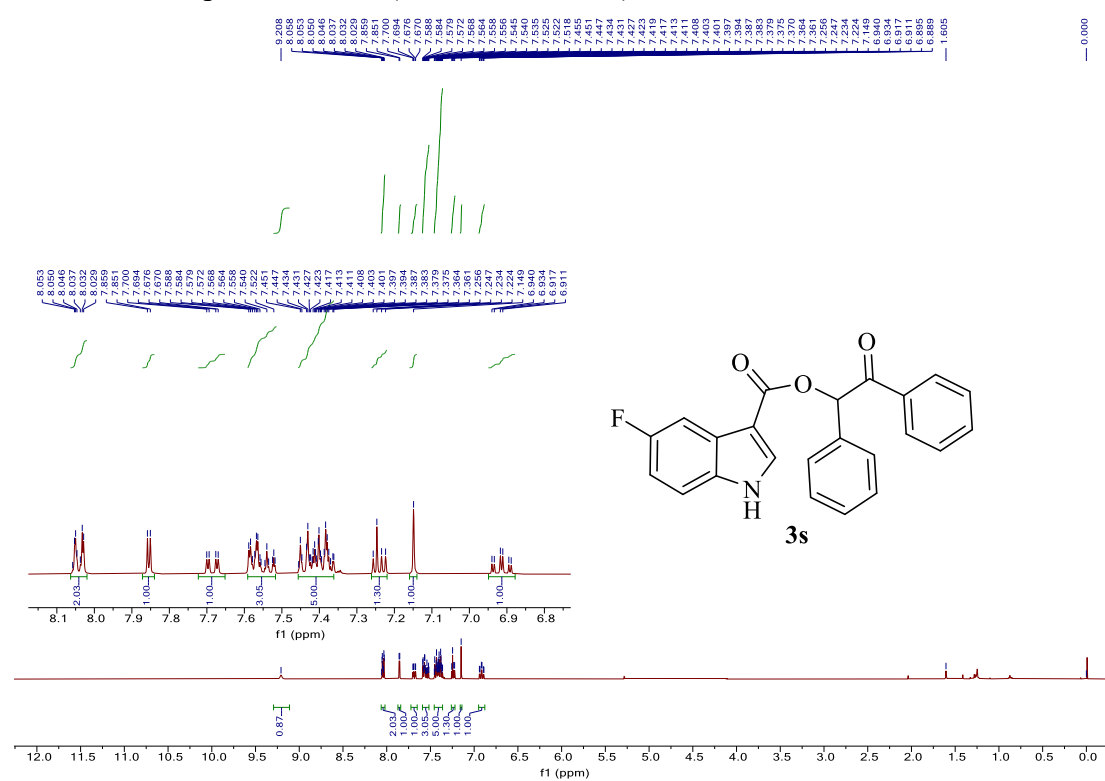
The ^1H NMR spectrum of **3r** (400 MHz, CDCl_3)



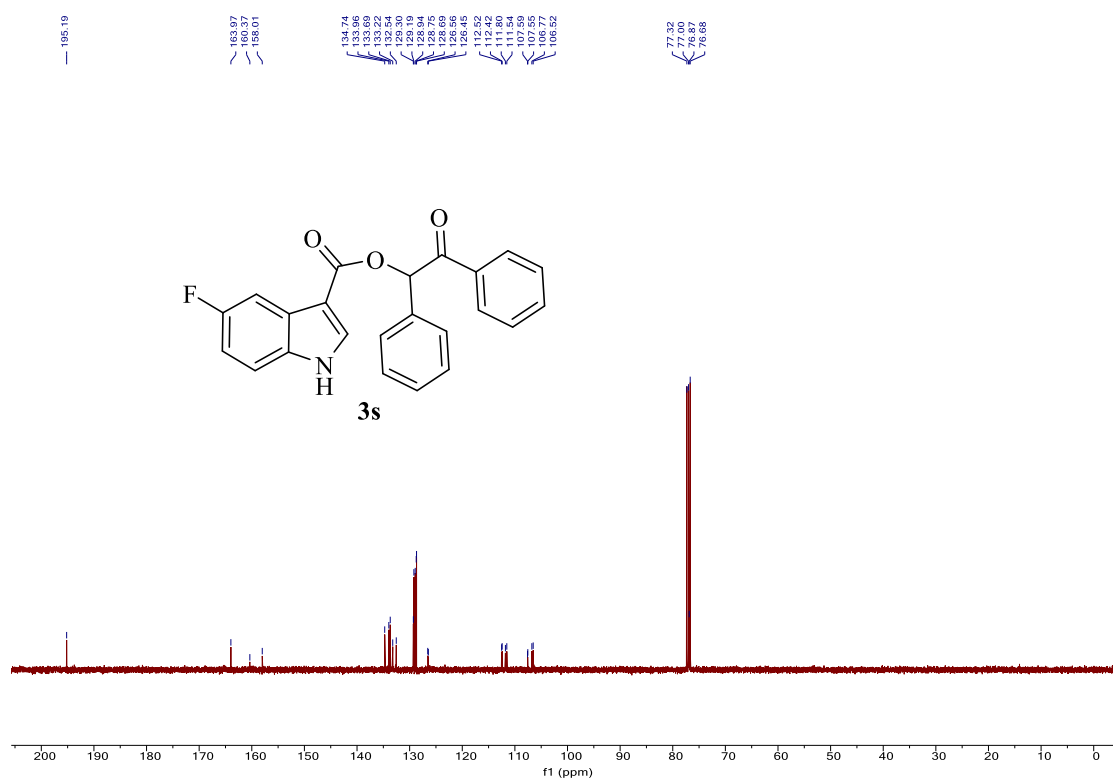
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3r** (100 MHz, CDCl_3)



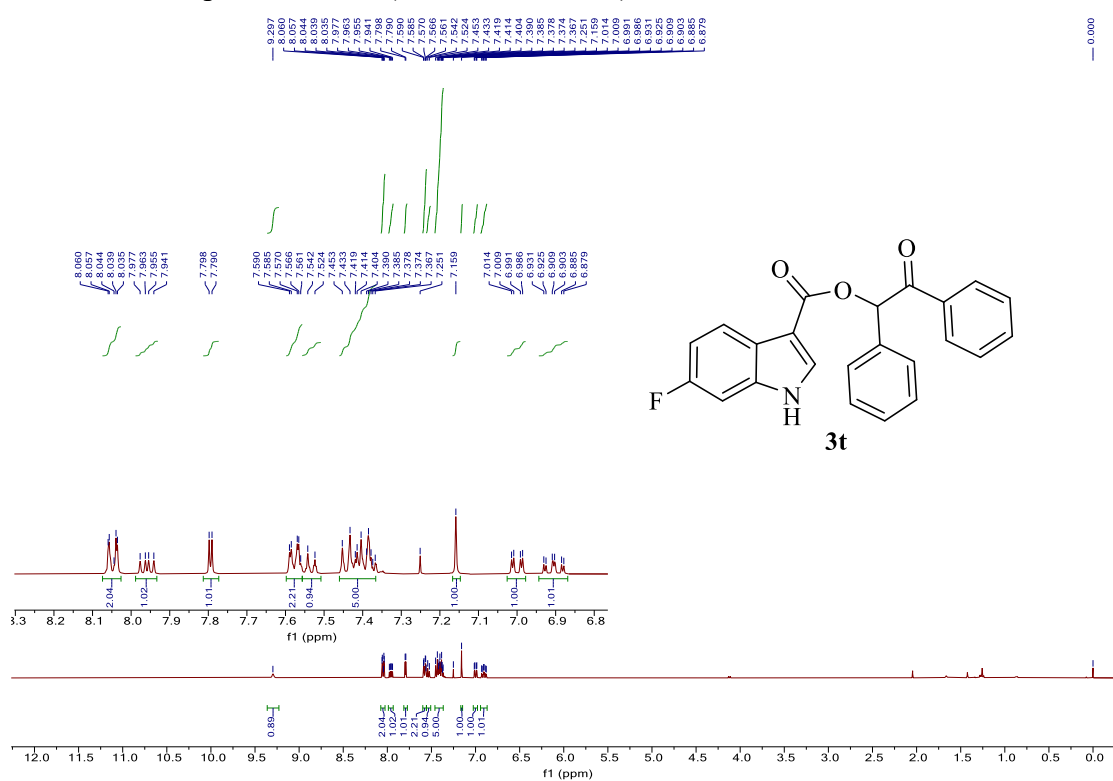
The ^1H NMR spectrum of **3s** (400 MHz, CDCl_3)



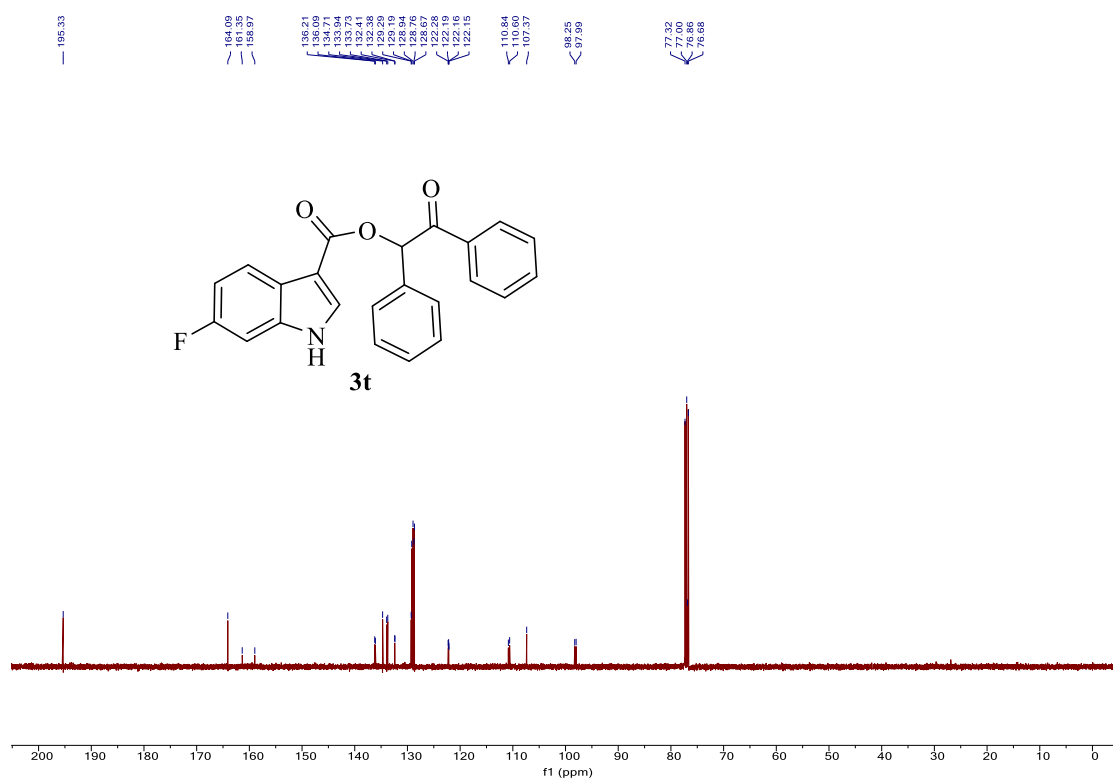
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3s** (100 MHz, CDCl_3)



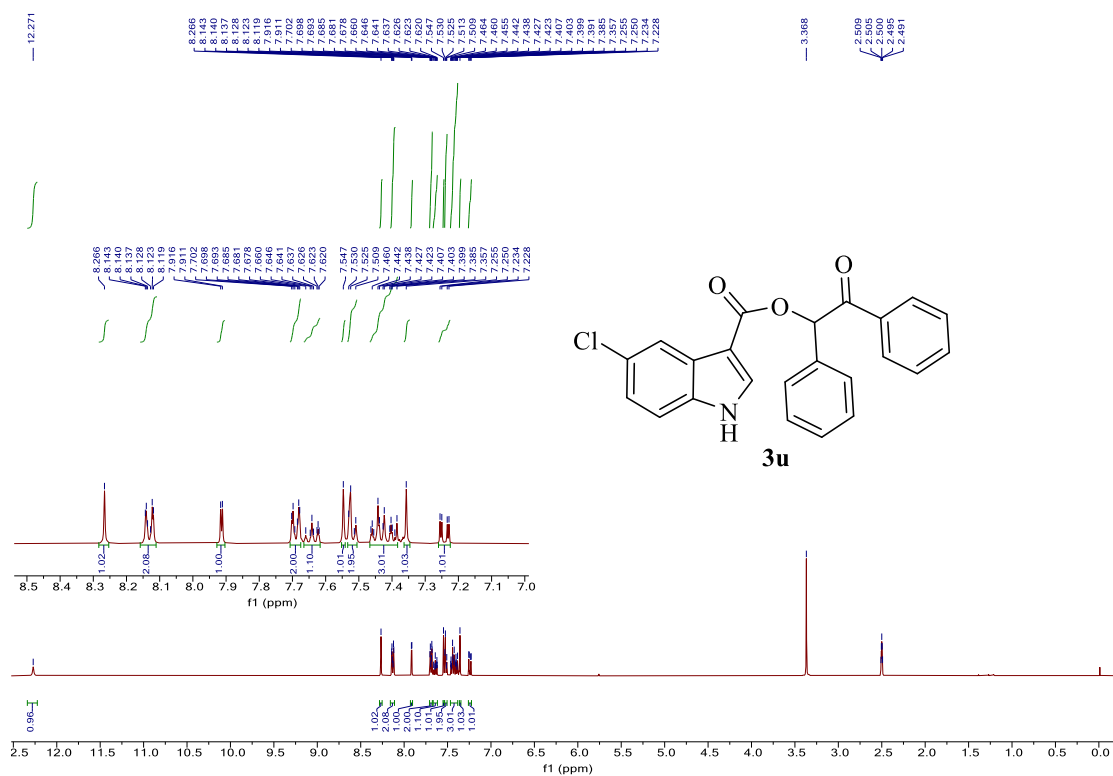
The ^1H NMR spectrum of **3t** (400 MHz, CDCl_3)



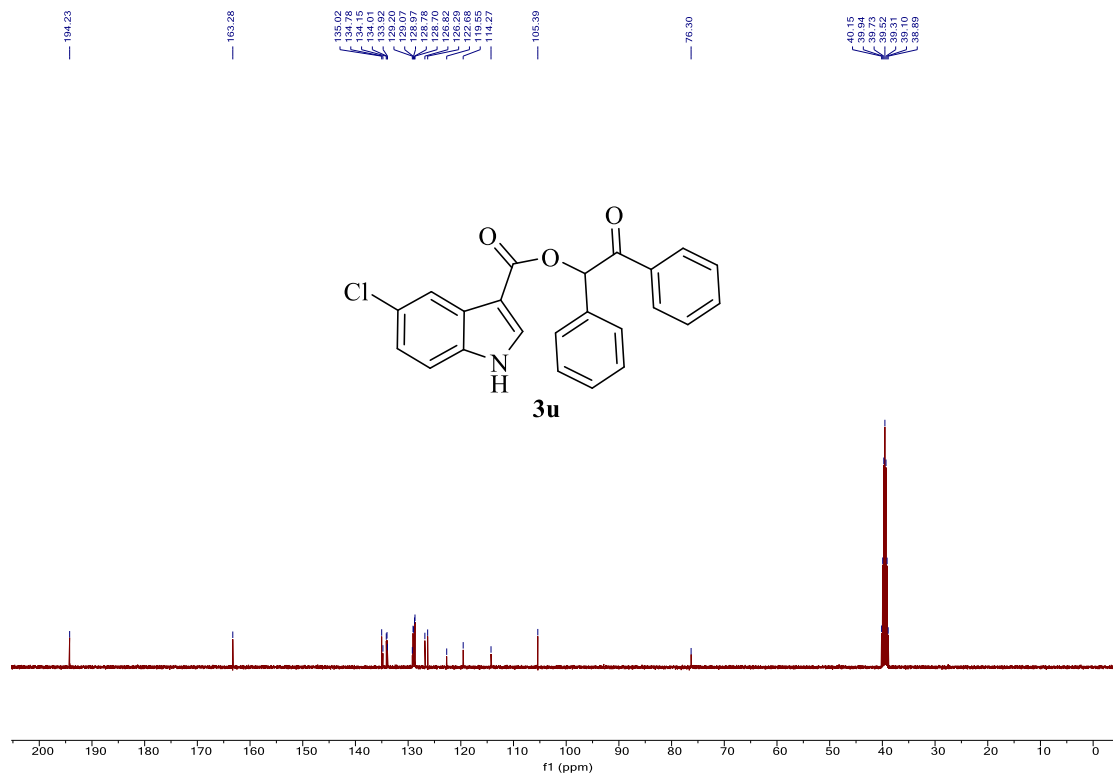
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3t** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **3u** (400 MHz, DMSO- d_6)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3u** (100 MHz, DMSO- d_6)



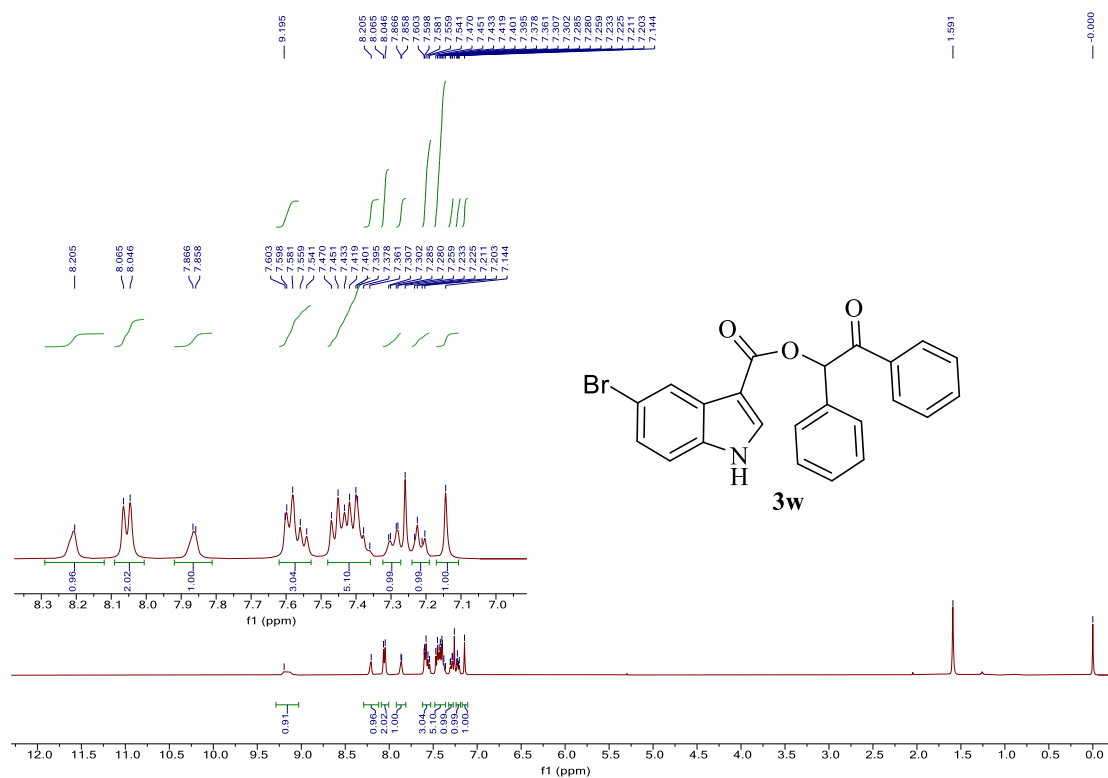
Chemical structure of **3v** is shown to the right of the spectrum.

Chemical structure of **3v** is shown above the spectrum.

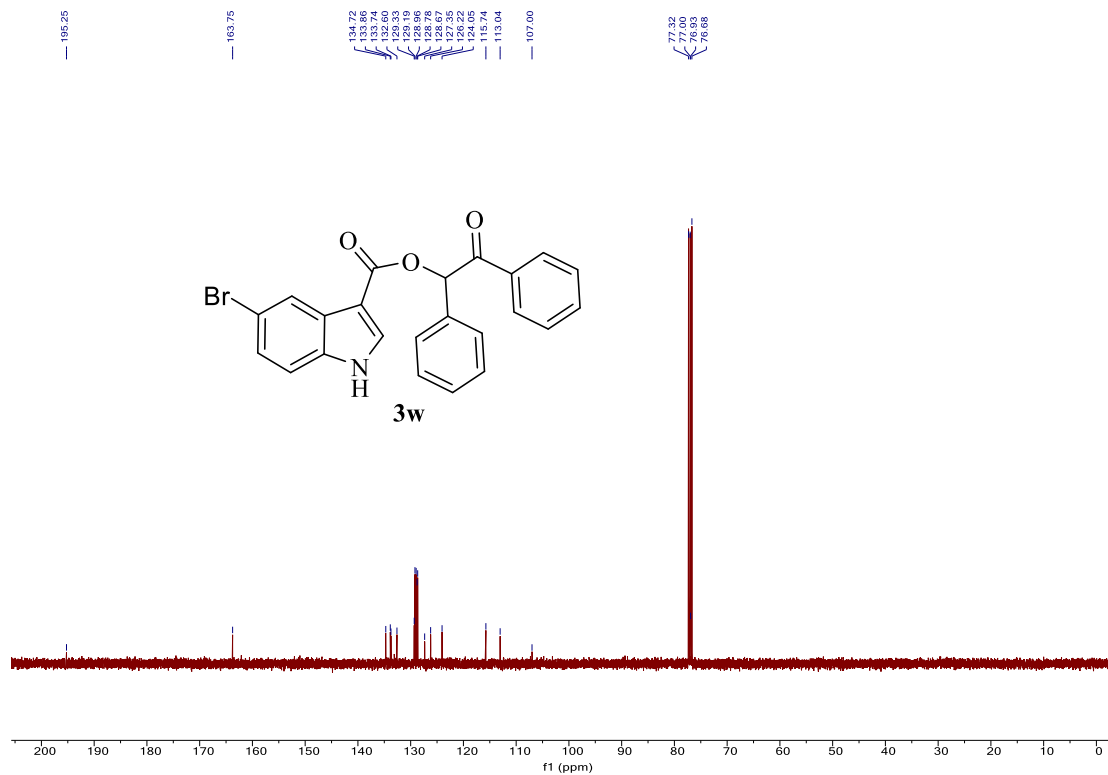
¹³C NMR spectrum (CDCl₃) of **3v**. The x-axis represents the chemical shift in ppm (f1), ranging from 0 to 200. The spectrum shows several peaks, with the following chemical shifts (ppm) labeled above the corresponding peaks:

- 194.24
- 163.28
- 136.90
- 134.31
- 134.17
- 133.82
- 133.66
- 128.10
- 128.02
- 128.71
- 128.05
- 124.39
- 124.38
- 121.88
- 121.85
- 112.23
- 105.81
- 76.27
- 40.15
- 39.94
- 39.73
- 39.72
- 39.31
- 39.40
- 39.05

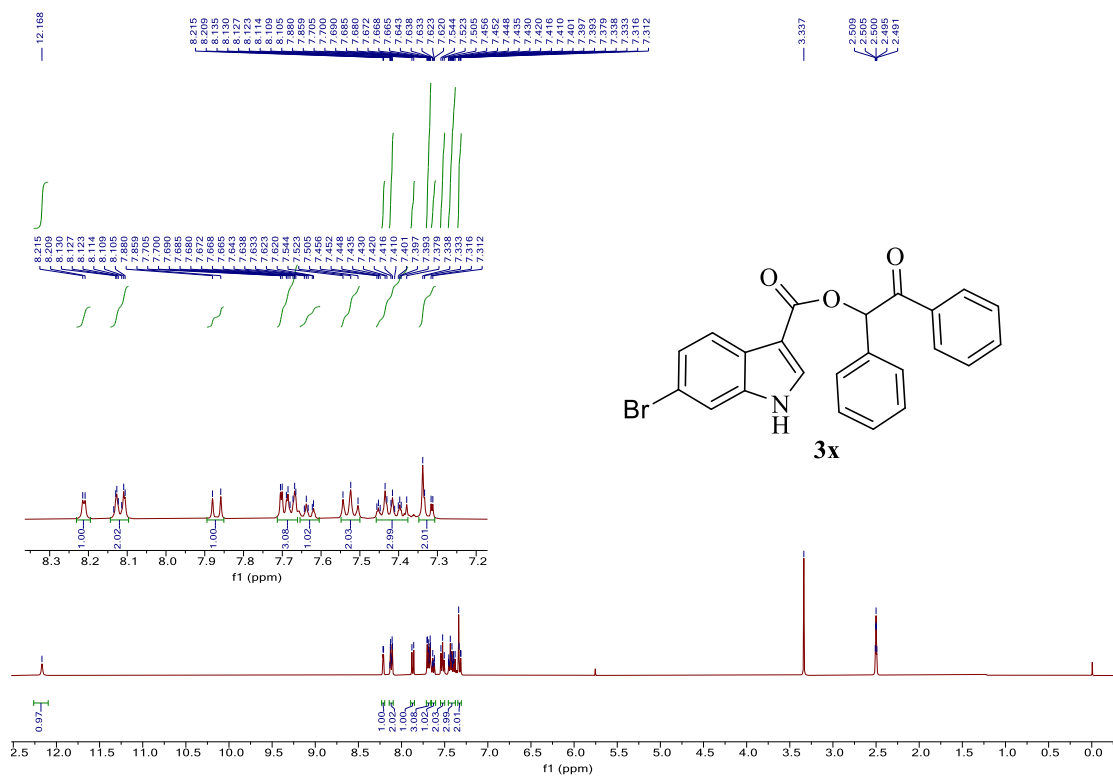
The ^1H NMR spectrum of **3w** (400 MHz, CDCl_3)



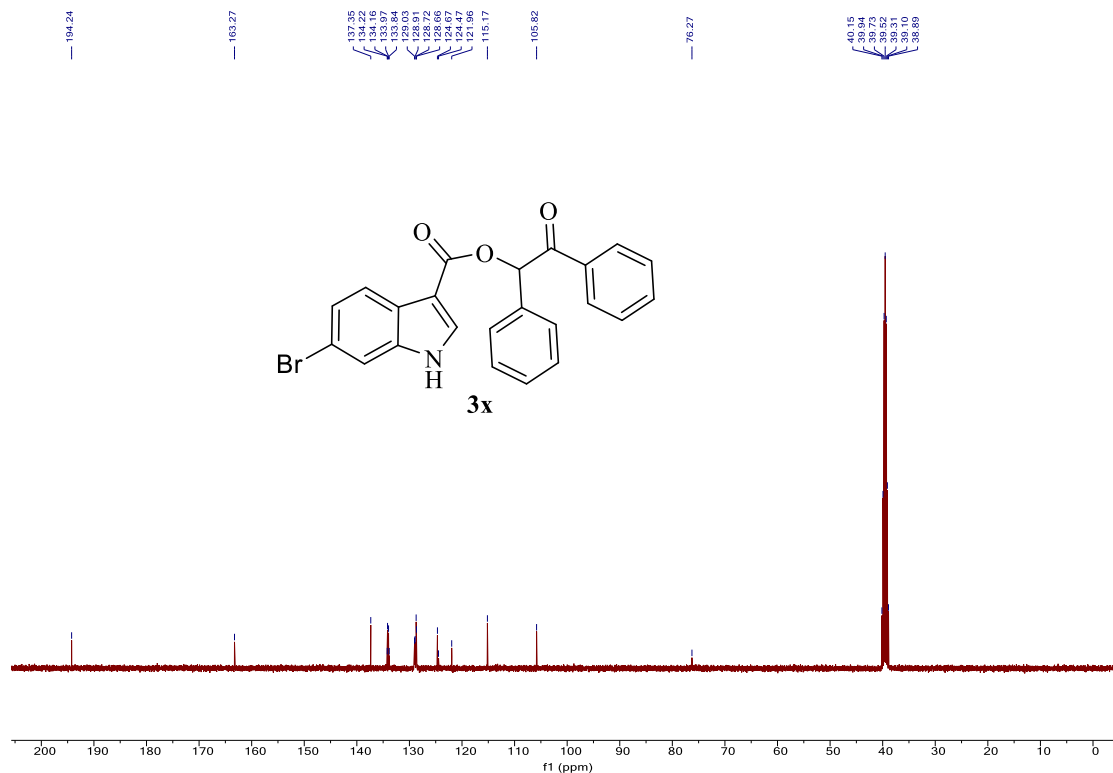
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3w** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **3x** (400 MHz, DMSO- d_6)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3x** (100 MHz, DMSO- d_6)



[illegible]

Chemical structure of **3y** is shown above the spectrum. The structure is a 5-nitro-1H-indole-3-carboxylic acid benzyl ester derivative, specifically (benzyloxy carbonyl) 5-nitro-L-tryptophan.

¹³C NMR spectrum (f1 (ppm)) showing peaks at:

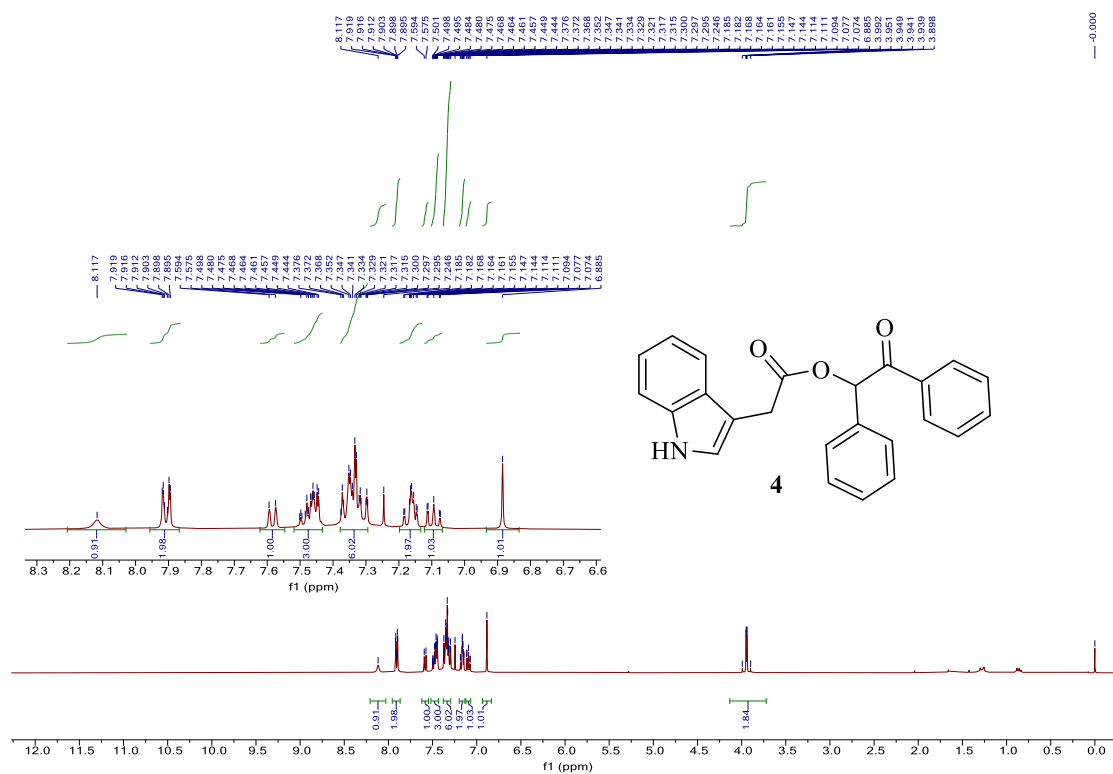
- 194.06
- 162.92
- 142.68
- 136.68
- 136.97
- 135.96
- 135.99
- 133.80
- 133.82
- 129.11
- 128.00
- 128.03
- 128.73
- 125.05
- 117.99
- 115.44
- 113.41
- 107.67
- 76.63
- 40.15
- 39.94
- 39.73
- 39.52
- 39.31
- 39.10
- 38.90

Chemical structure of **3z** is shown on the right. The structure is a benzimidazole derivative with a cyano group (NC) and a benzimidazole ring system. The structure is labeled **3z**.

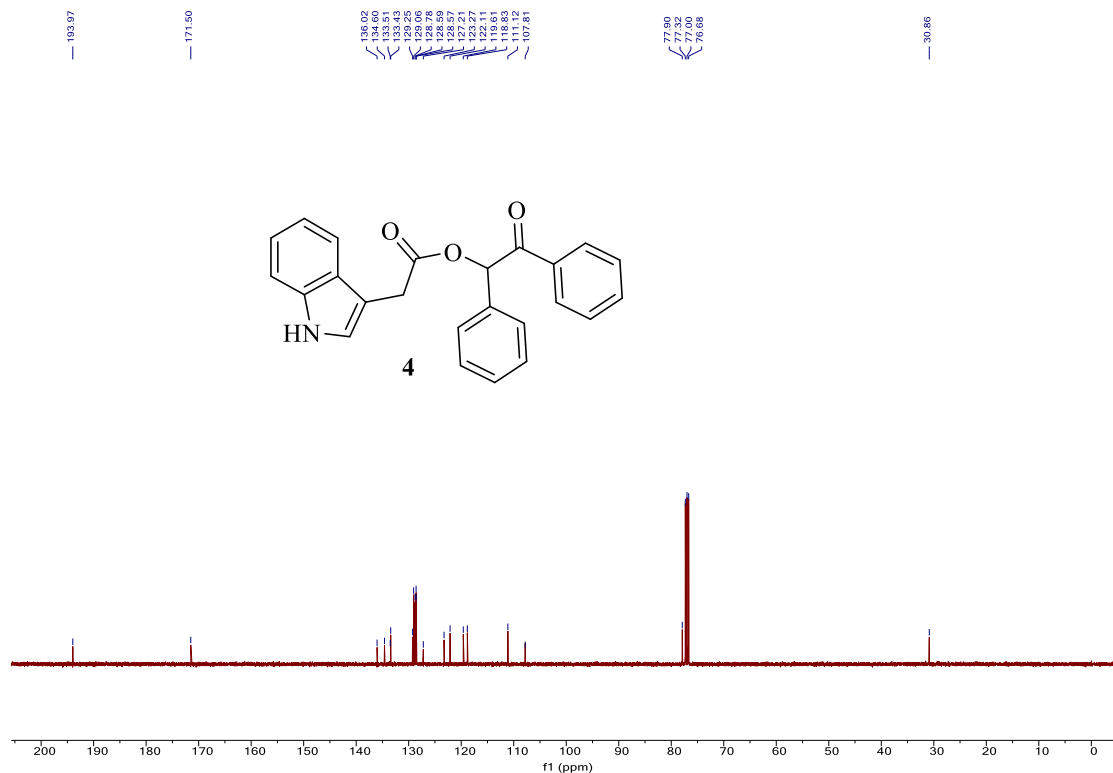
Chemical structure of **3z** is shown above the spectrum. The structure is a 4-cyano-1H-indole-3-carboxylic acid derivative, specifically 4-cyano-1H-indole-3-carboxylic acid, which is esterified with 1-phenylethanol and 1-phenylethanol. The structure is labeled **3z**.

Peak values (ppm): 195.693, 163.445, 135.025, 134.483, 134.483, 134.053, 133.565, 133.565, 129.596, 129.370, 129.370, 128.888, 128.888, 128.888, 128.888, 122.717, 122.047, 119.902, 116.683, 107.850, 106.775, 77.320, 77.191, 77.063, 76.884.

The ^1H NMR spectrum of **4** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4** (100 MHz, CDCl_3)



Chemical structure of compound **5**: O=C(Oc1ccccc1)C(=O)c2ccccc2

¹H NMR spectrum (CDCl₃) of compound **5**. The spectrum shows peaks in the aromatic region (6.9–8.1 ppm) and a small peak at 0.000 ppm (TMS). Integration values are provided below the peaks.

Chemical shift (ppm): 8.1, 8.0, 7.9, 7.8, 7.7, 7.6, 7.5, 7.4, 7.3, 7.2, 7.1, 7.0, 6.9.

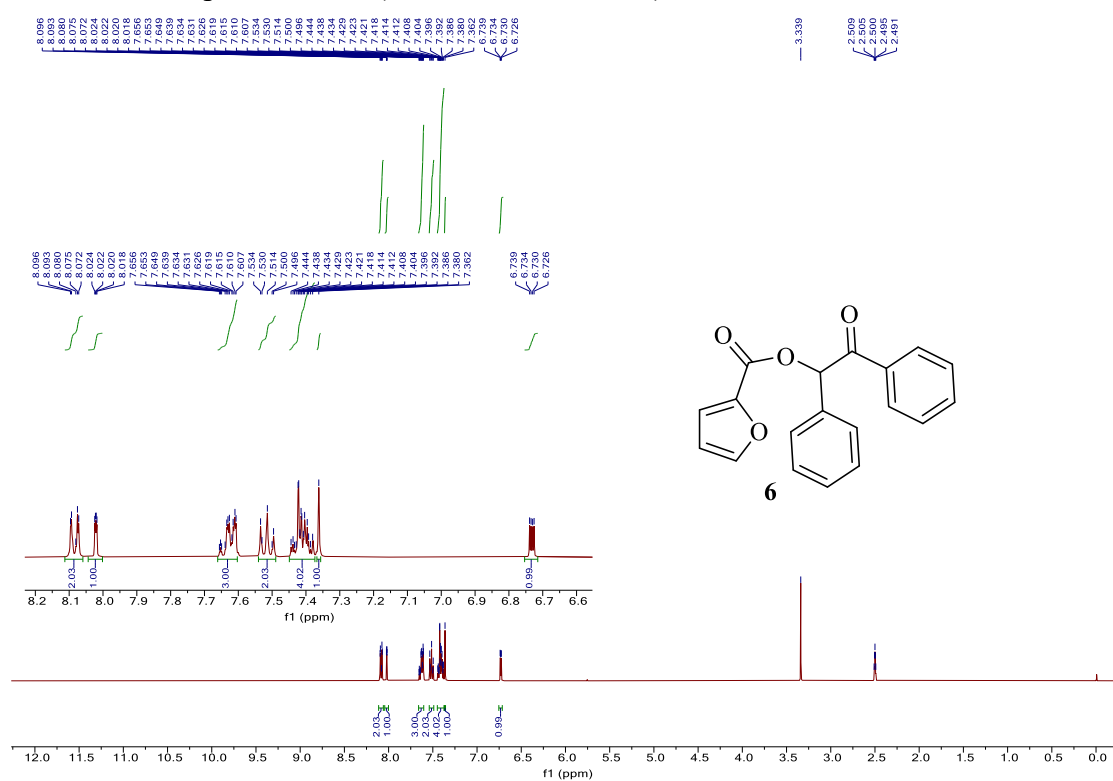
Integration values: 3.58, 1.04, 1.01, 1.13, 1.18, 7.03, 3.52, 2.00, 1.27, 2.21.

Chemical structure of compound **5** is shown above the spectrum. The structure is 1-(2-(2-oxo-1-phenylethan-1-yl)-2-oxo-1-phenylethan-1-yl)indole.

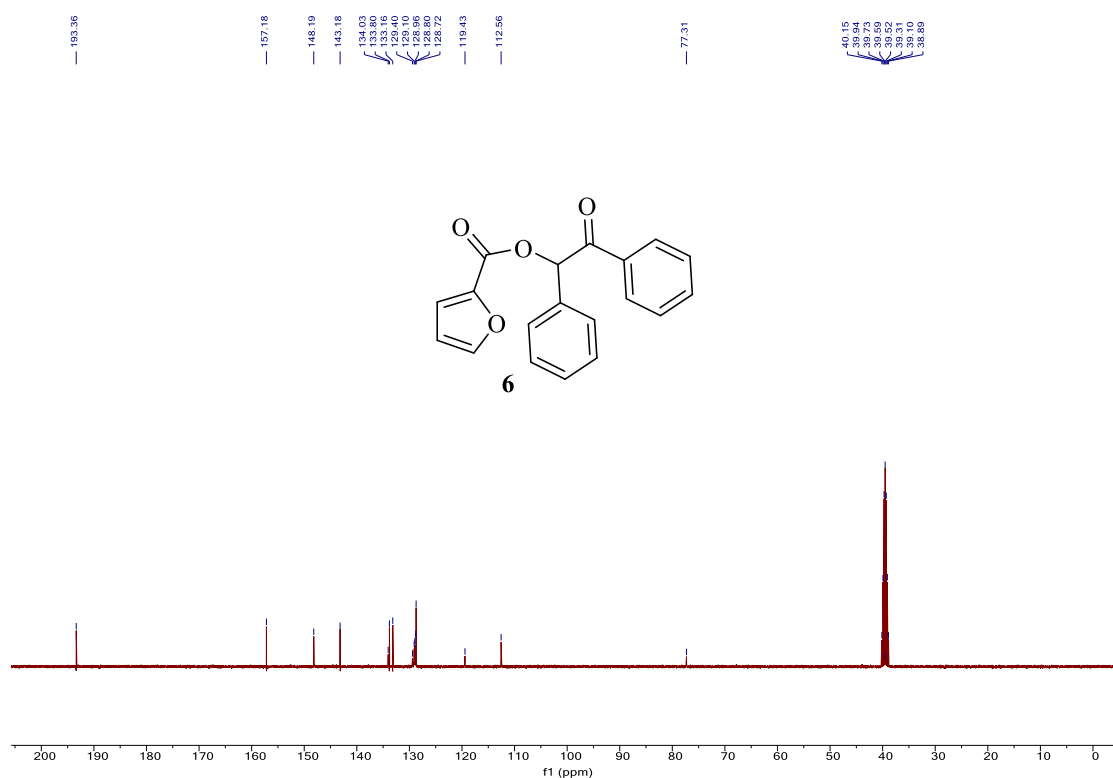
¹³C NMR spectrum (CDCl₃) of compound **5**. The x-axis represents the chemical shift in ppm, ranging from 0 to 200. The spectrum shows several peaks corresponding to the structure, with the following chemical shifts (ppm) listed on the right:

- 161.120
- 159.752
- 137.142
- 136.465
- 134.553
- 133.716
- 133.618
- 133.208
- 133.548
- 129.461
- 129.277
- 129.557
- 129.083
- 128.971
- 129.187
- 128.852
- 128.776
- 128.523
- 128.703
- 127.386
- 126.579
- 126.279
- 125.671
- 125.697
- 122.666
- 119.640
- 112.181
- 111.951
- 110.212
- 78.440
- 77.320
- 77.090
- 76.864

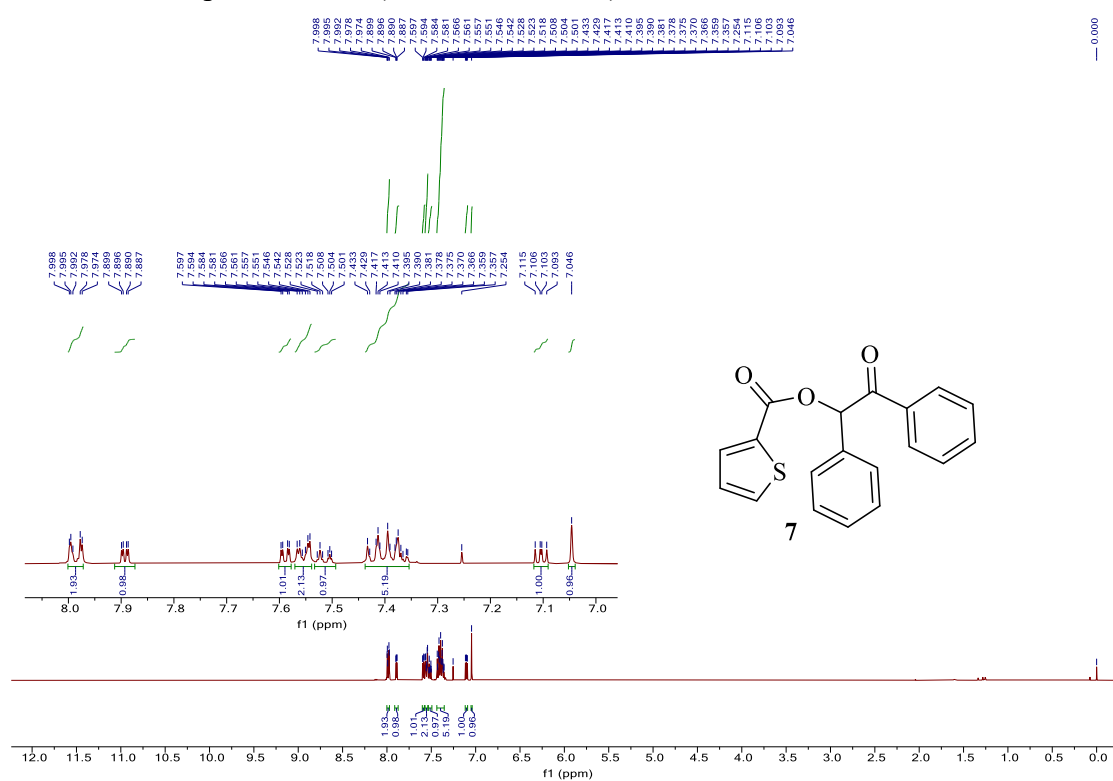
The ^1H NMR spectrum of **6** (400 MHz, DMSO-d_6)



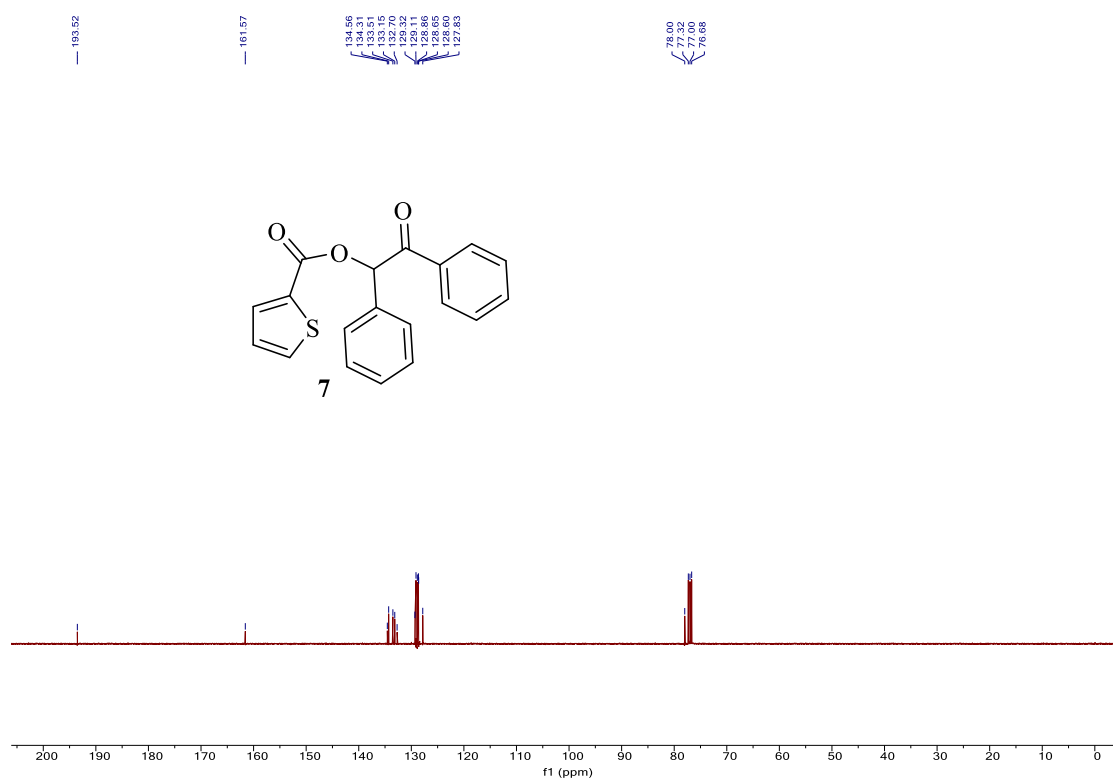
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** (100 MHz, DMSO-d_6)



The ^1H NMR spectrum of **7** (400 MHz, CDCl_3)



The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7** (100 MHz, CDCl_3)



Chemical structure of 1,1-diphenyl-2-phenylethan-1-one (chalcone): O=C(c1ccccc1)C(=O)c2ccccc2

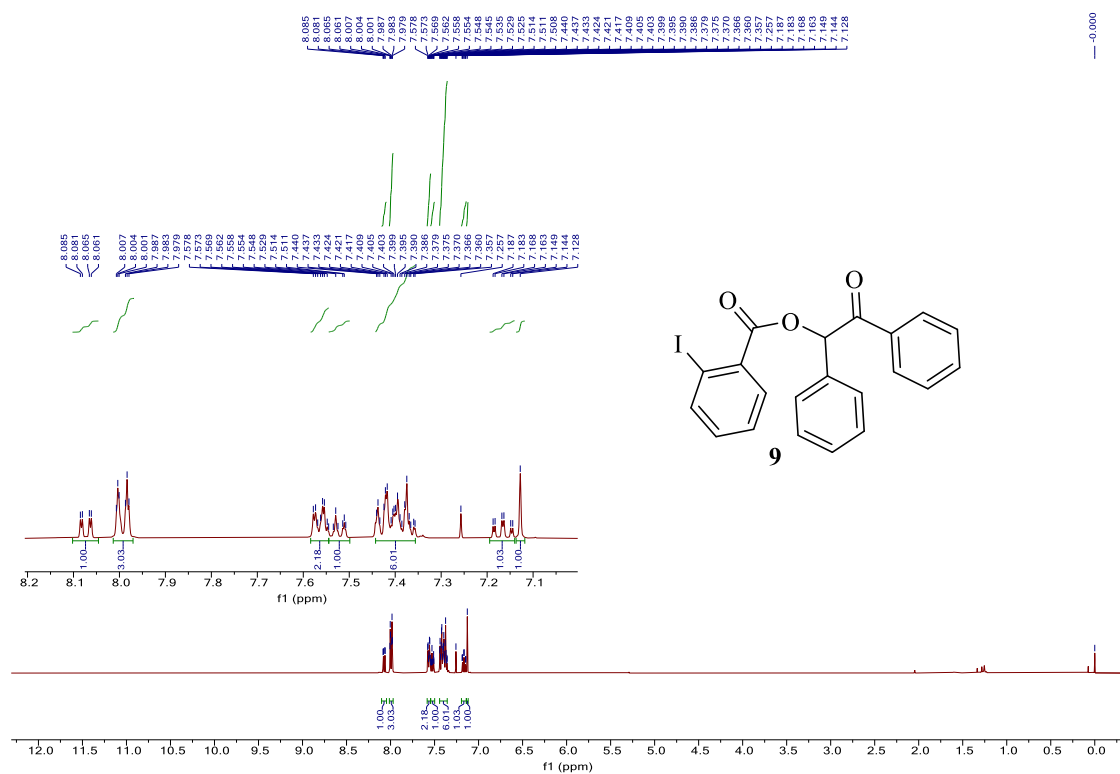
¹H NMR spectrum (CDCl₃) showing peaks and integration values:

Chemical Shift (ppm)	Integration
7.00	1.00
7.10	3.00
7.20	3.11
7.30	4.03
7.40	3.11
7.50	0.93
7.60	3.11
7.70	2.03
7.80	2.00

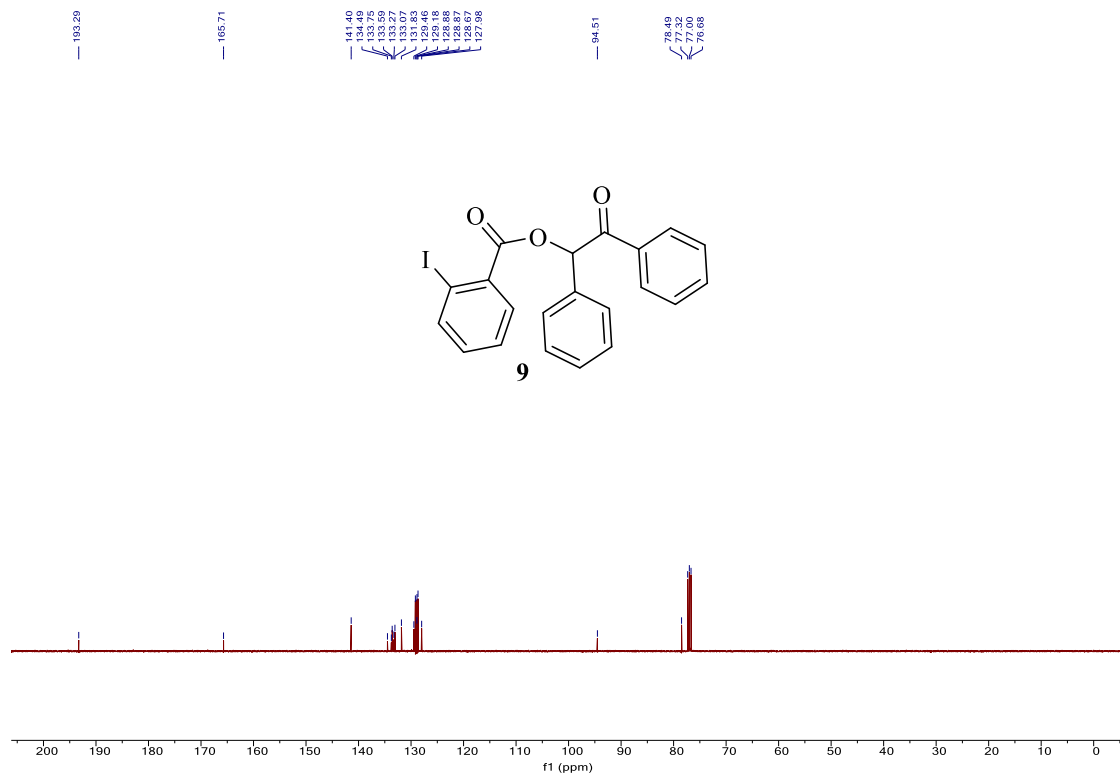
Chemical structure of **8** is shown above the spectrum. The structure is a benzophenone derivative with a central carbon atom bonded to two phenyl rings and a carbonyl group. The carbonyl group is further substituted with a phenyl ring. The spectrum shows peaks corresponding to the chemical shifts of the atoms in the molecule, with the following chemical shifts (ppm) listed above the peaks:

134.680, 133.595, 133.549, 133.356, 132.778, 129.308, 128.126, 128.051, 128.388, 77.511, 77.216, 76.880, 166.029, 193.694.

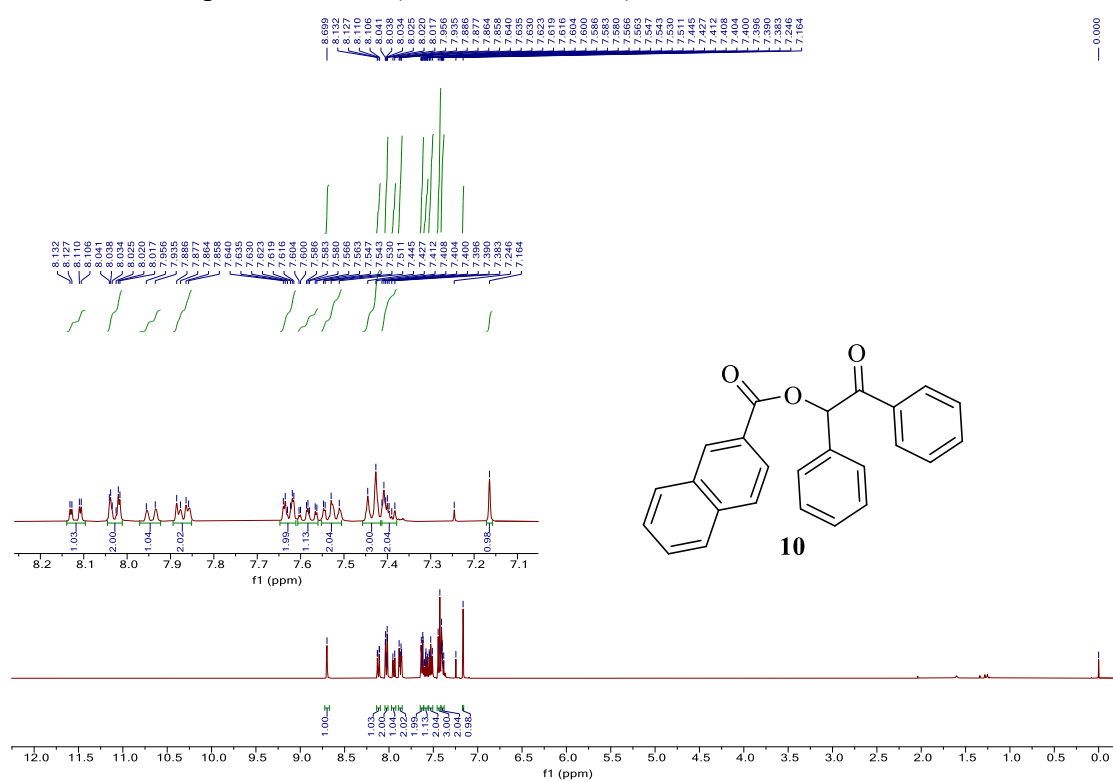
The ^1H NMR spectrum of **9** (400 MHz, CDCl_3)



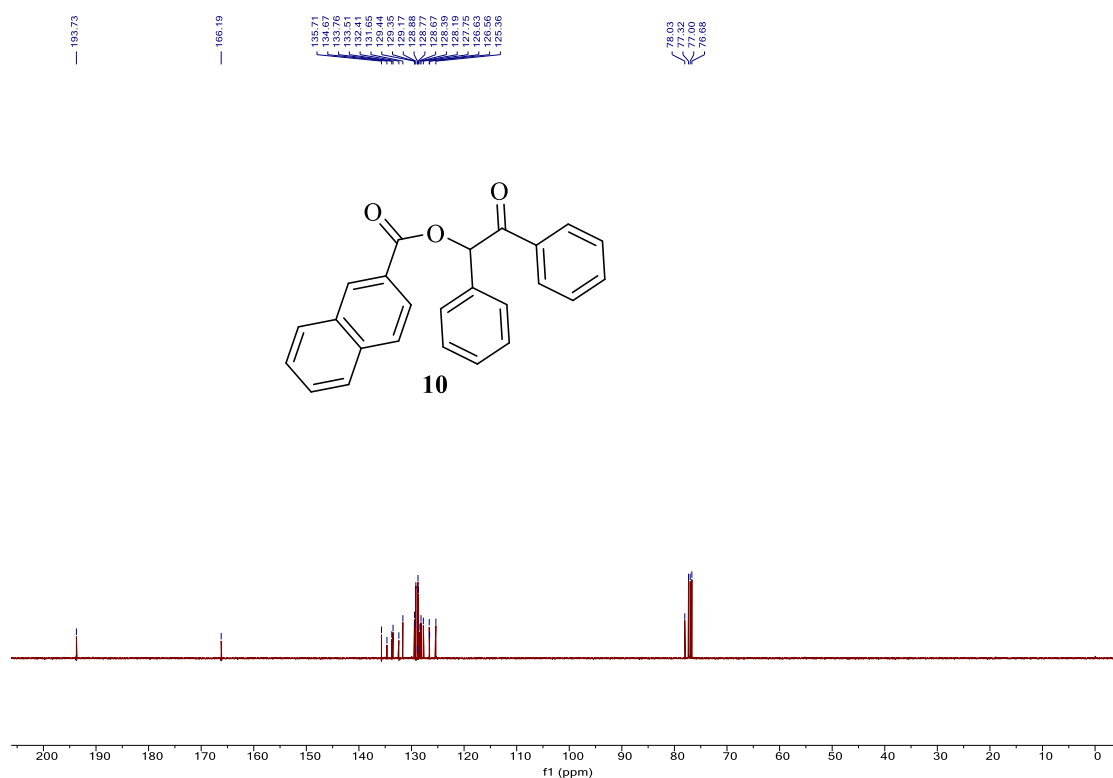
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **9** (100 MHz, CDCl_3)



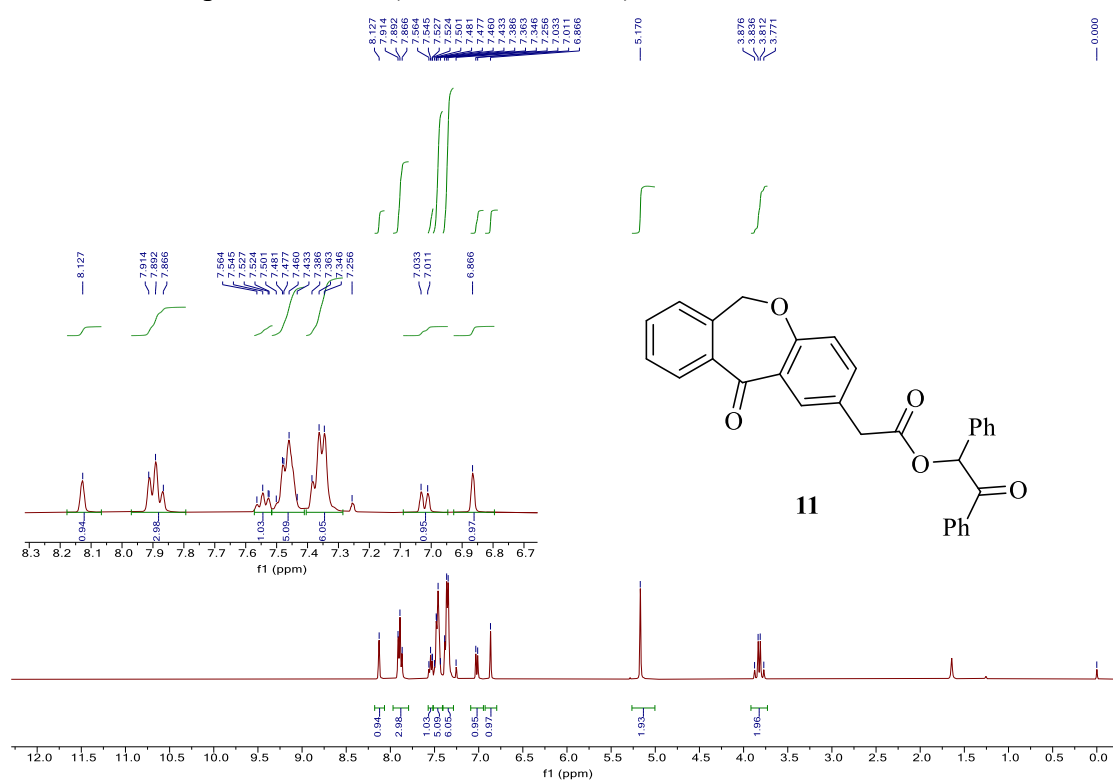
The ^1H NMR spectrum of **10** (400 MHz, CDCl_3)



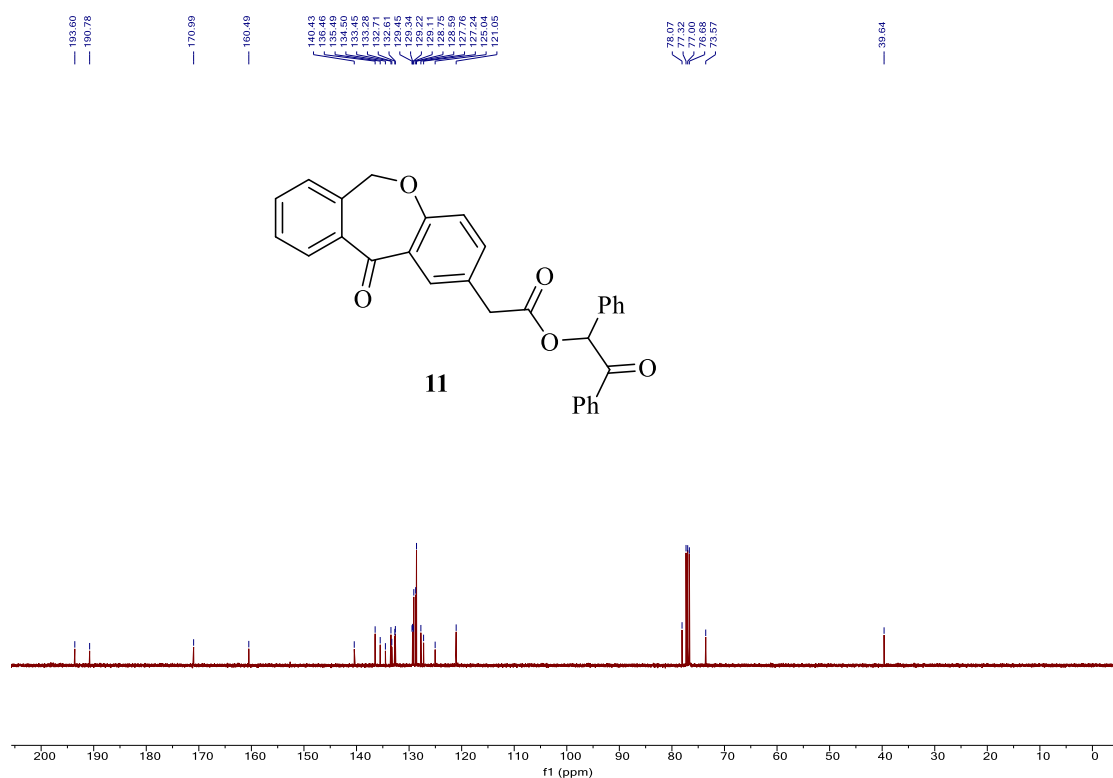
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **10** (100 MHz, CDCl_3)



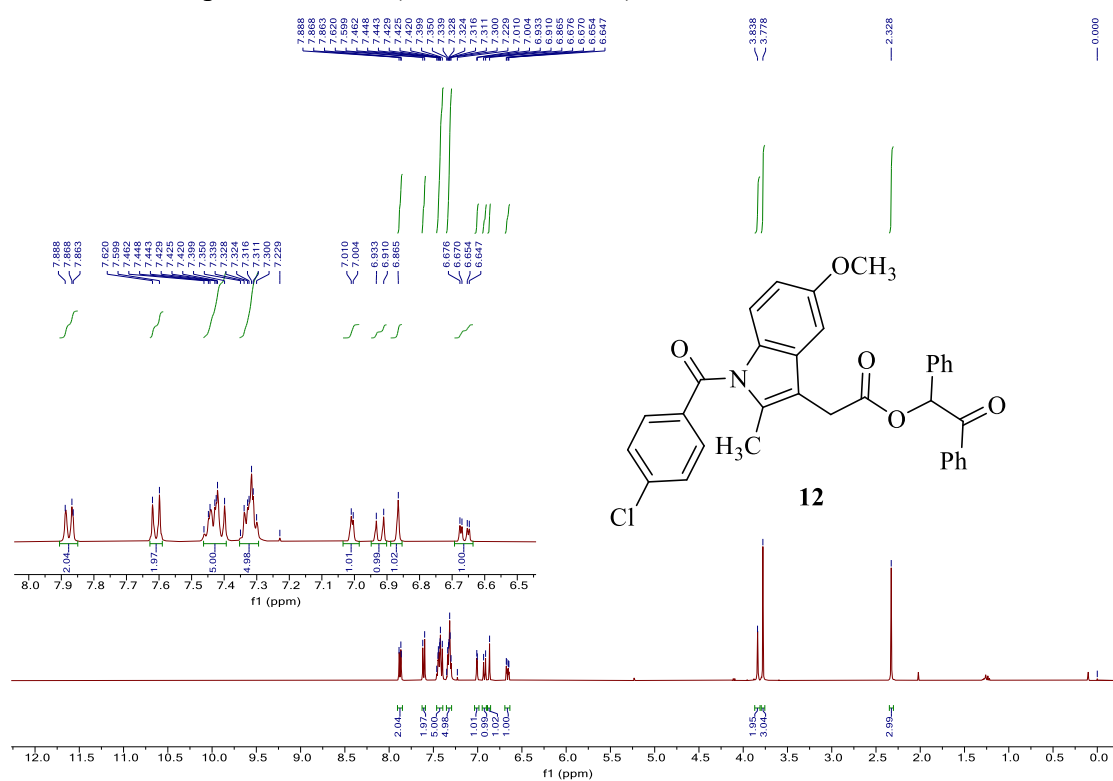
The ^1H NMR spectrum of **11** (400 MHz, CDCl_3)



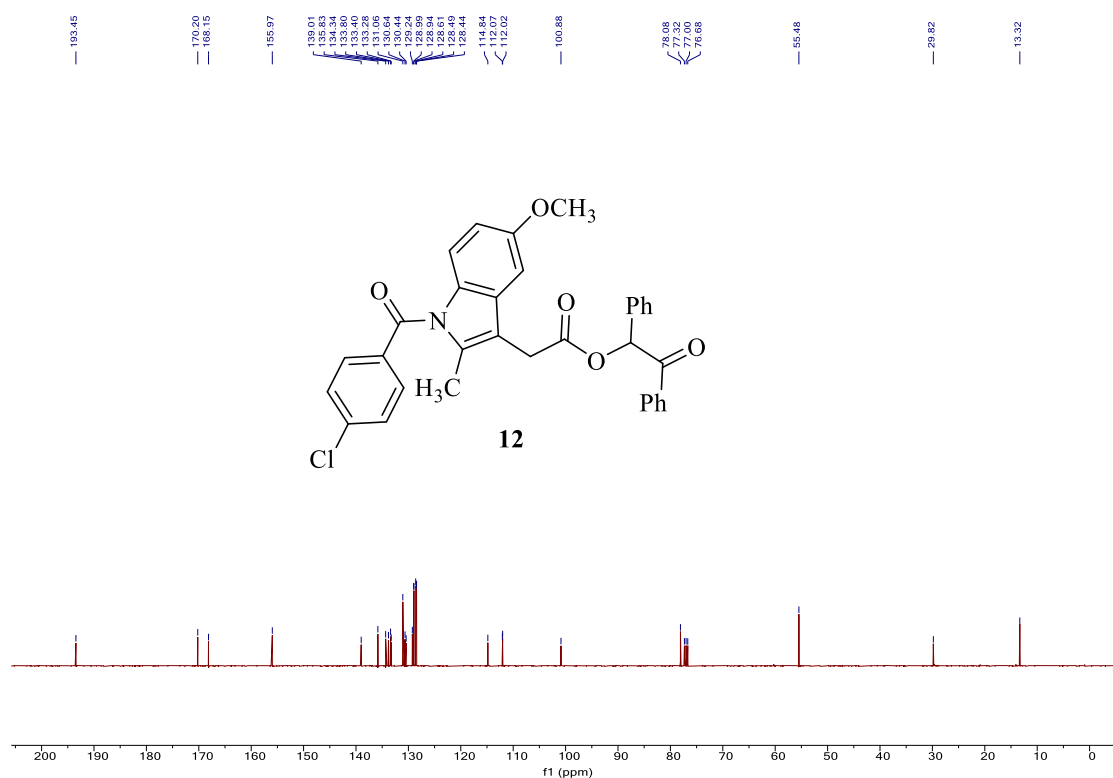
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **11** (100 MHz, CDCl_3)



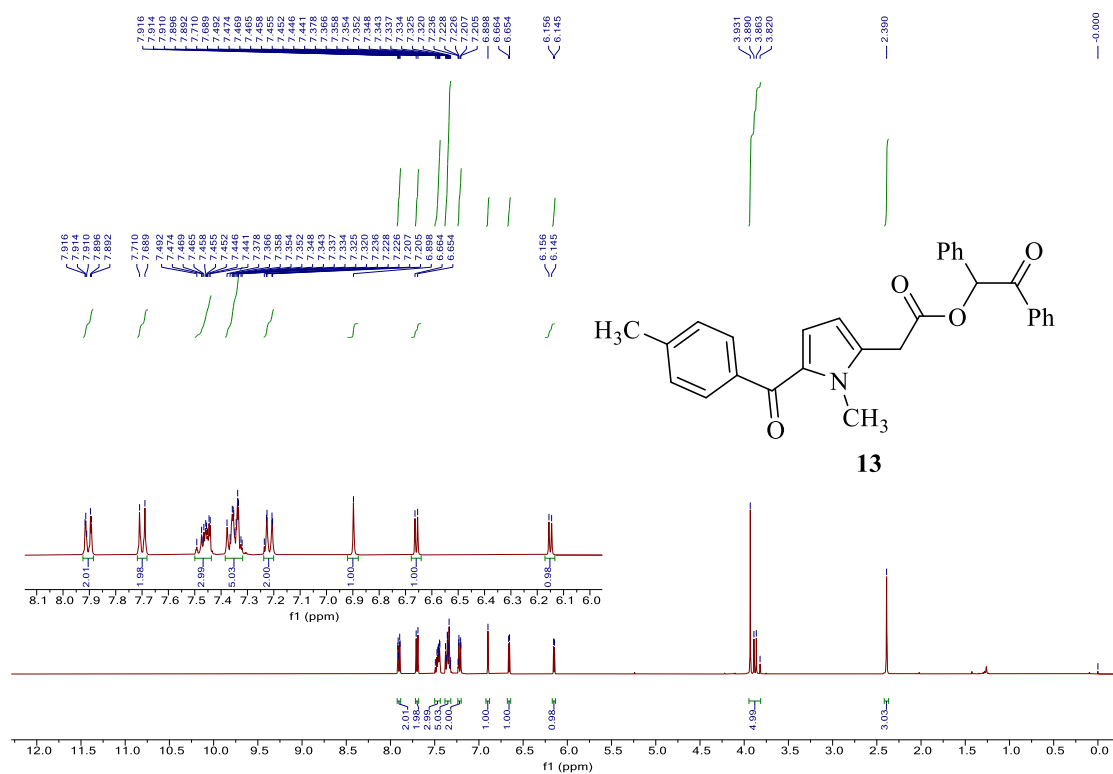
The ^1H NMR spectrum of **12** (400 MHz, CDCl_3)



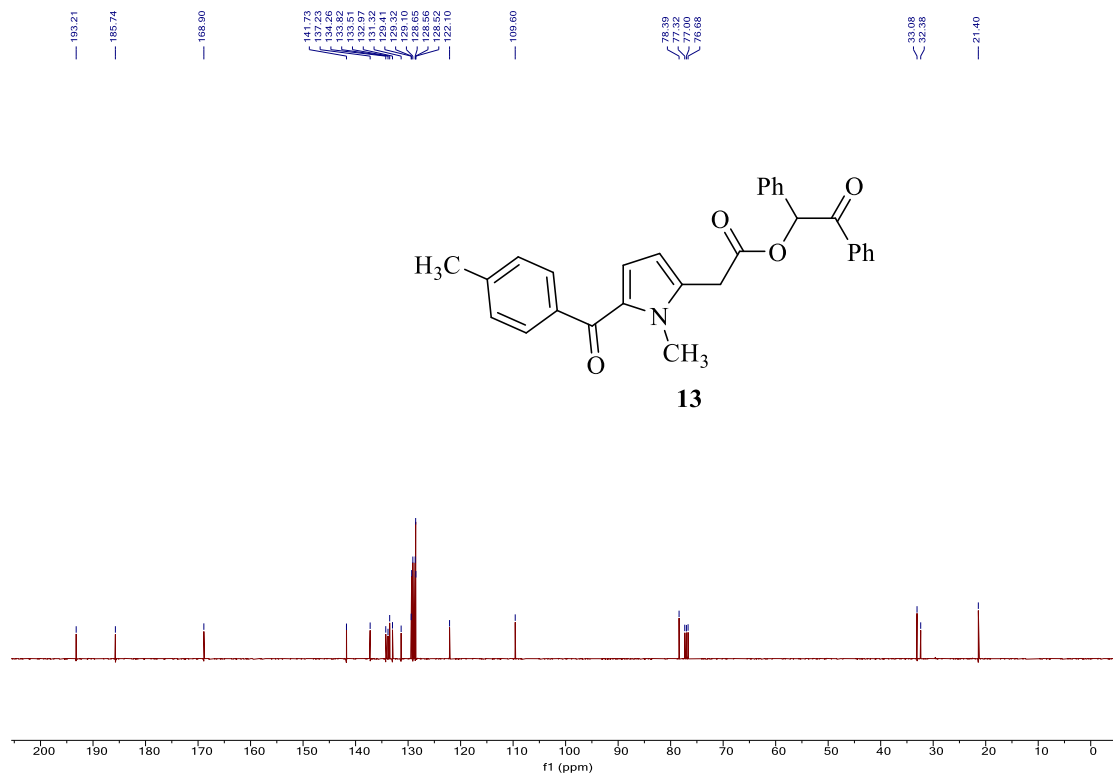
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **12** (100 MHz, CDCl_3)



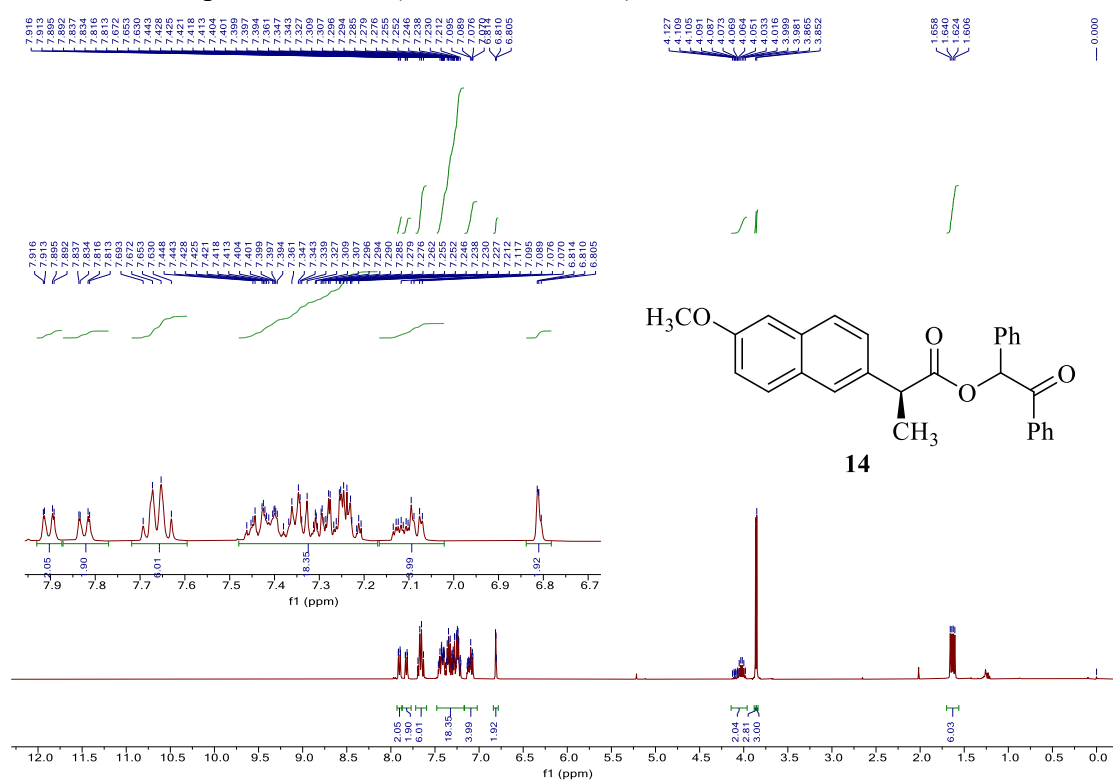
The ^1H NMR spectrum of **13** (400 MHz, CDCl_3)



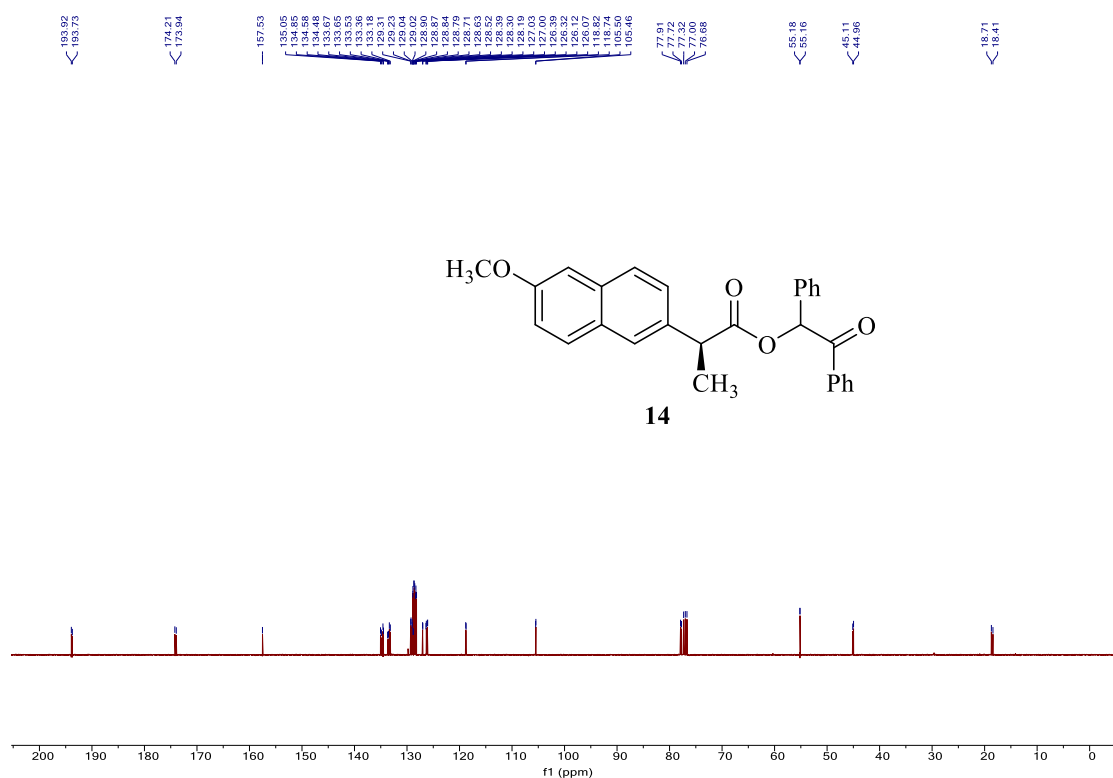
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **13** (100 MHz, CDCl_3)



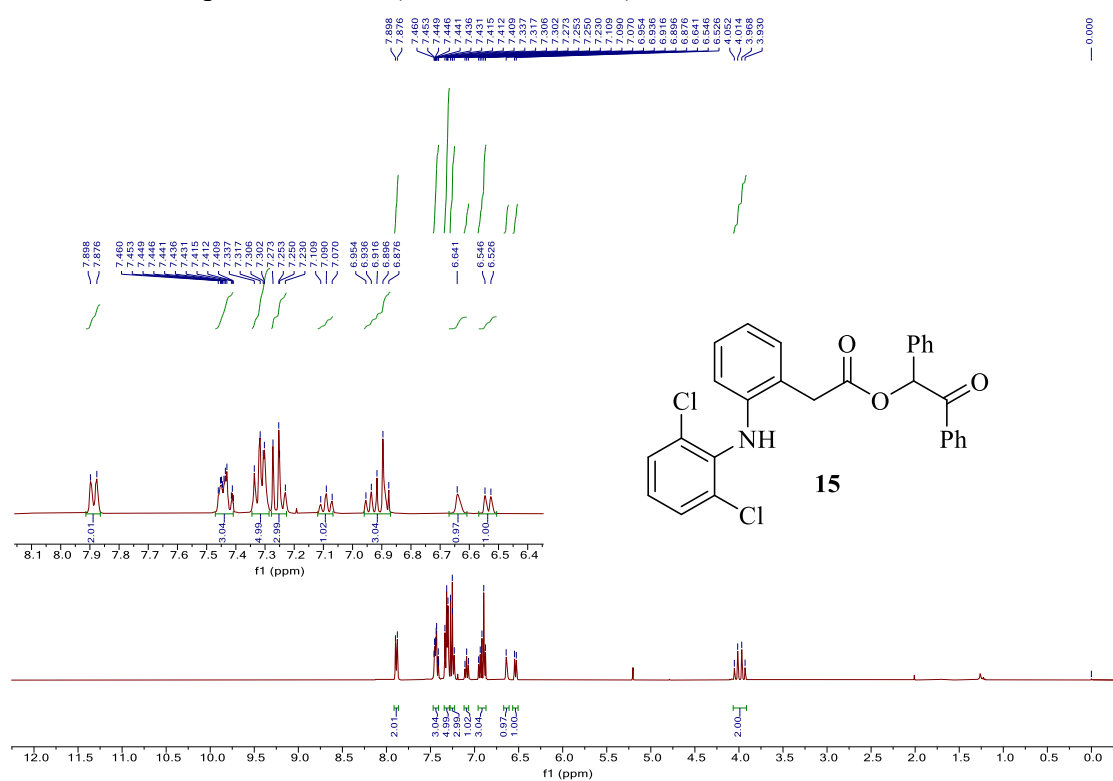
The ^1H NMR spectrum of **14** (400 MHz, CDCl_3)



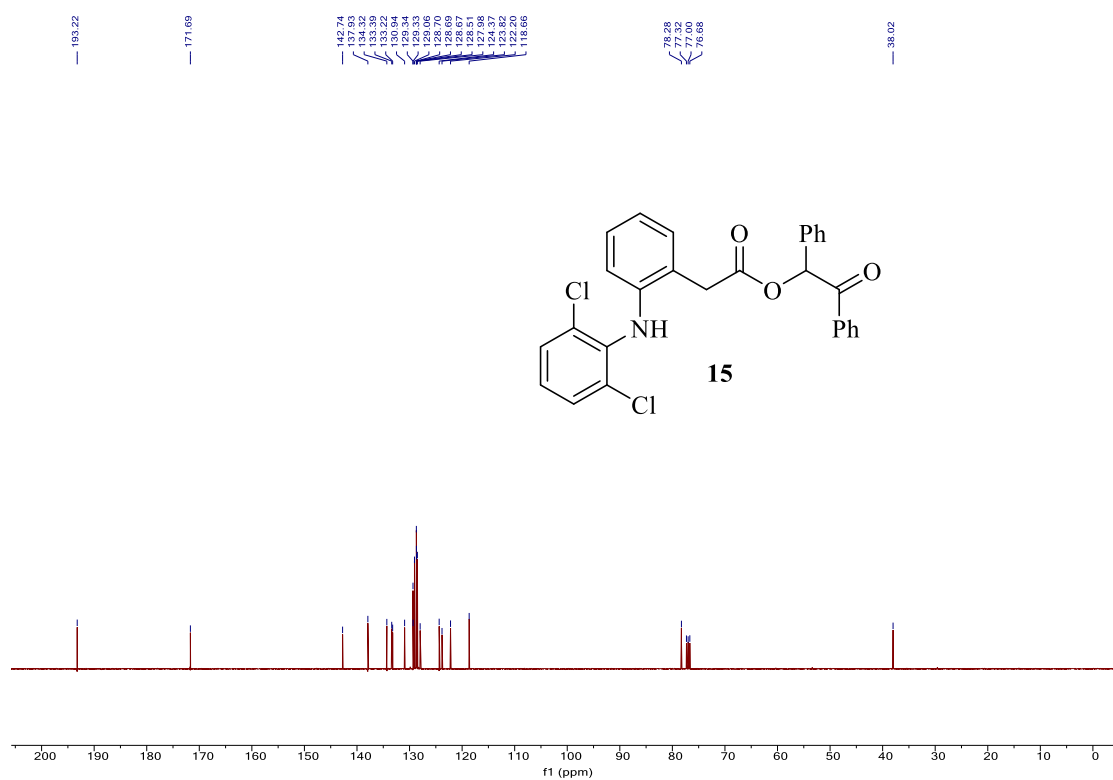
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **14** (100 MHz, CDCl_3)



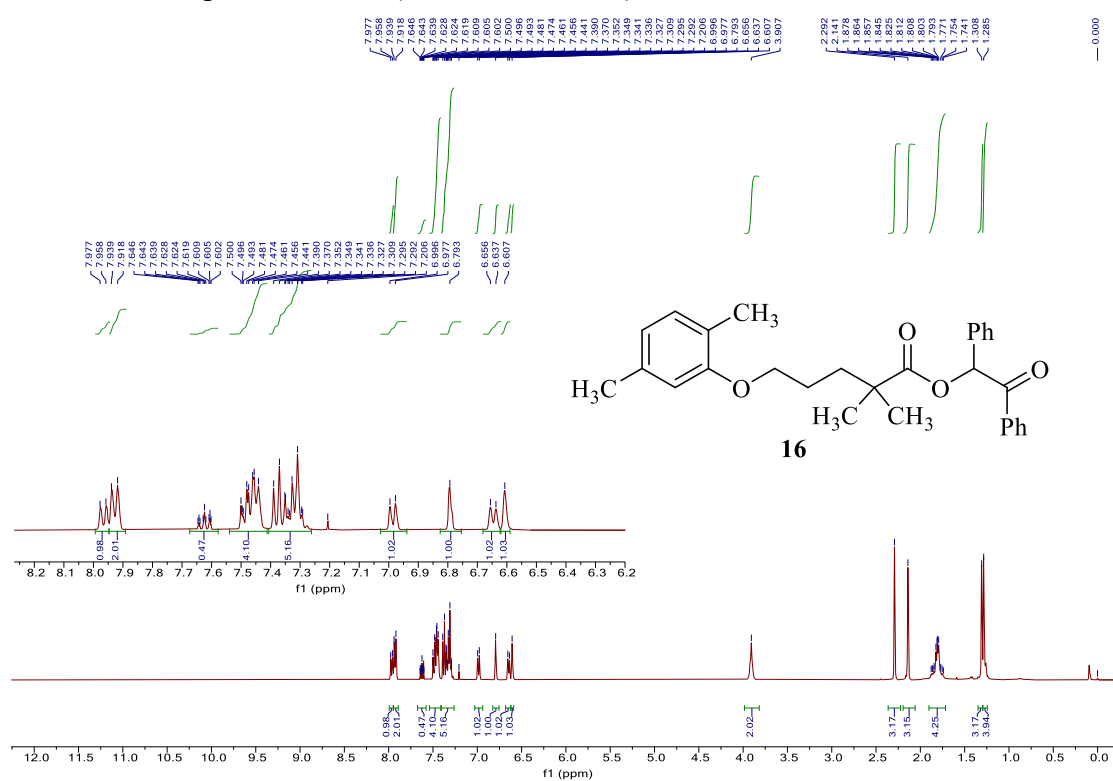
The ^1H NMR spectrum of **15** (400 MHz, CDCl_3)



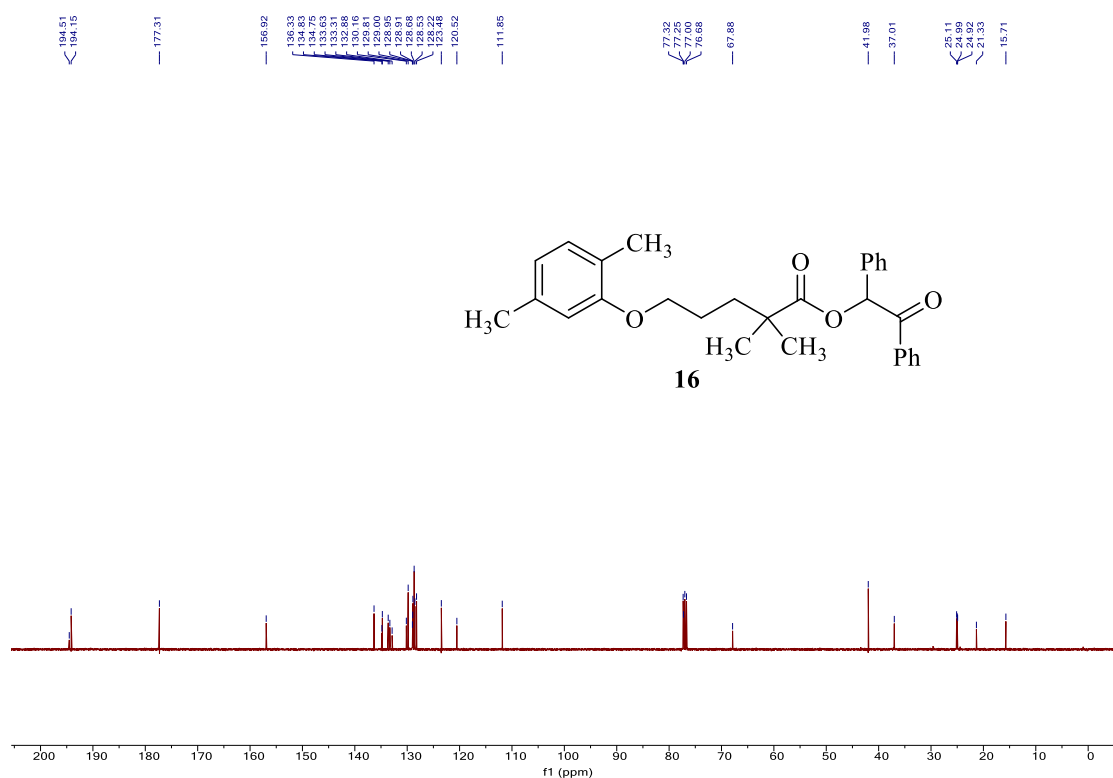
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **15** (100 MHz, CDCl_3)



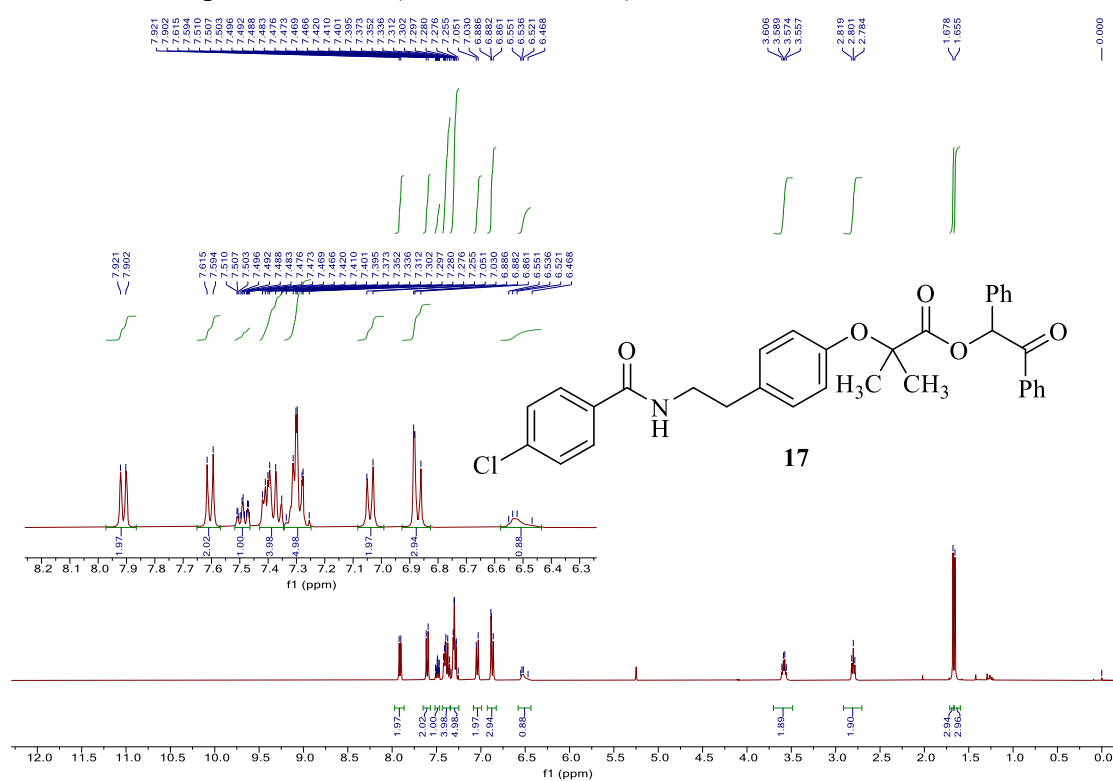
The ^1H NMR spectrum of **16** (400 MHz, CDCl_3)



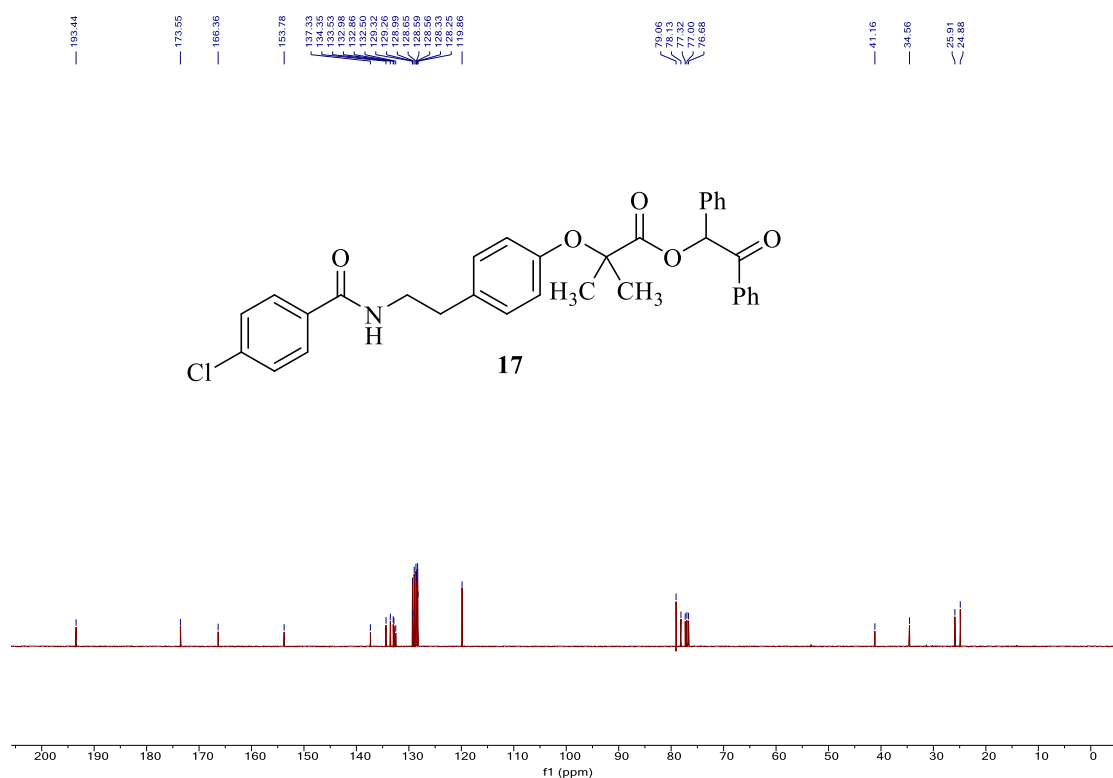
The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **16** (100 MHz, CDCl_3)



The ^1H NMR spectrum of **17** (400 MHz, CDCl_3)

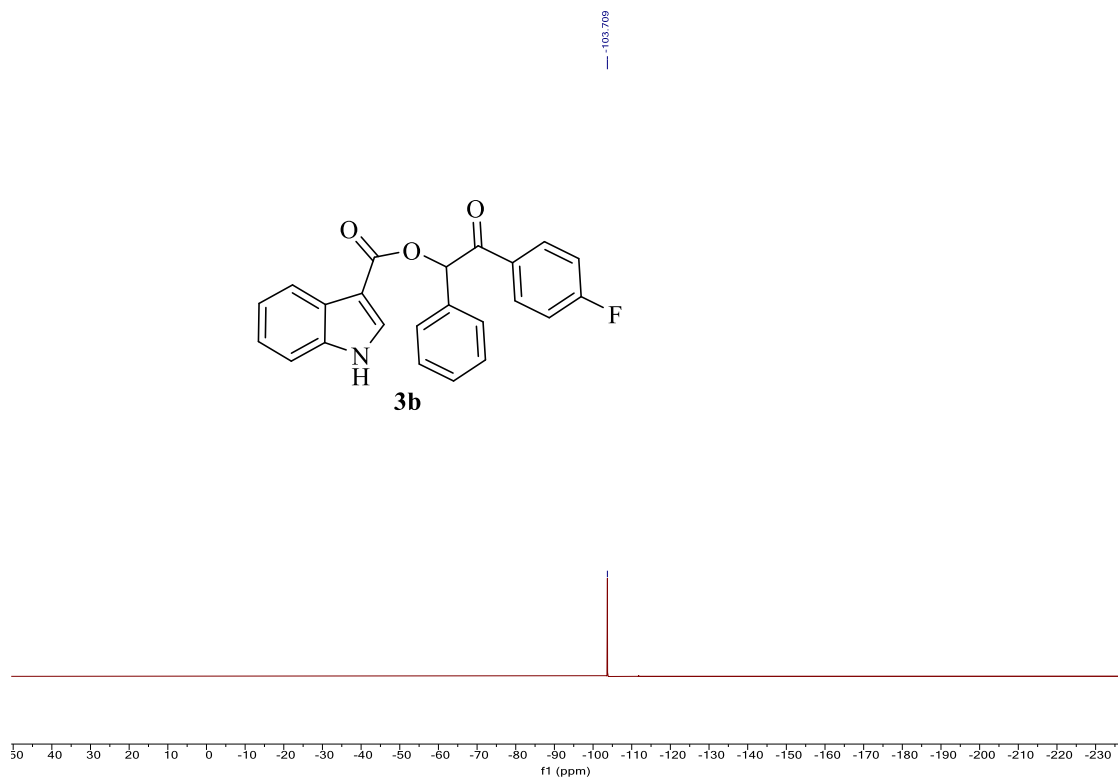


The $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **17** (100 MHz, CDCl_3)

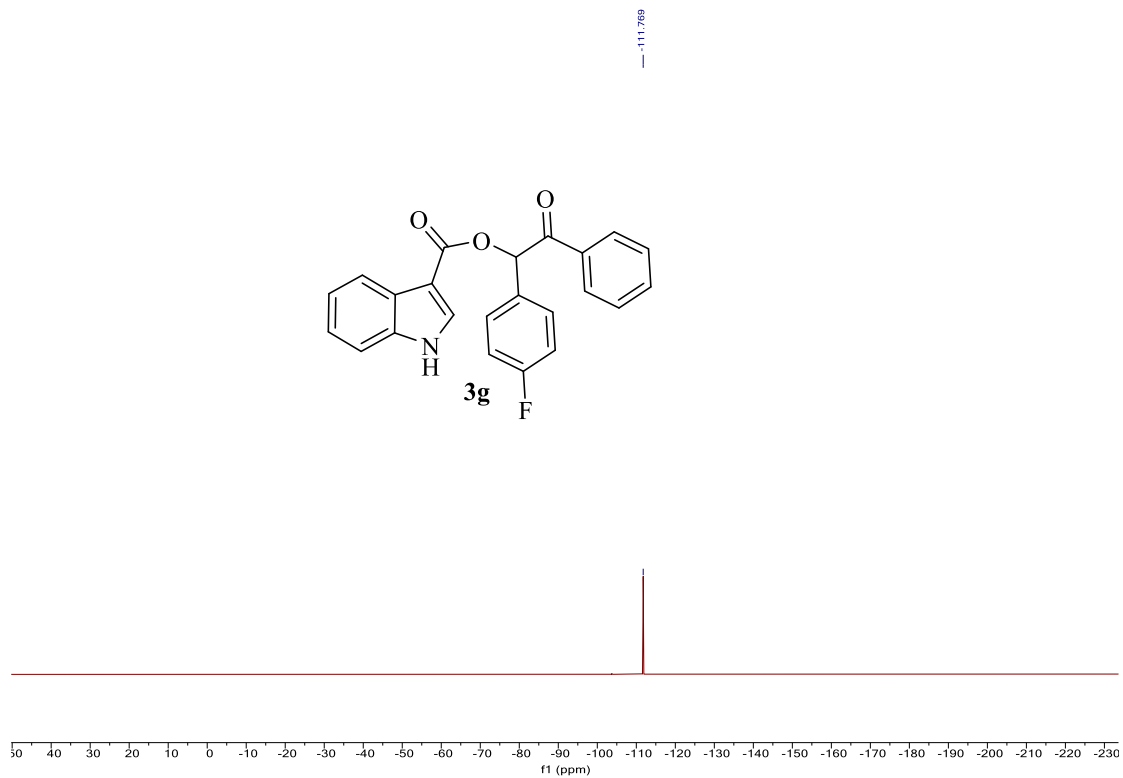


6. ^{19}F NMR Spectra of Products **3b**, **3g**, **3s**, **3t**

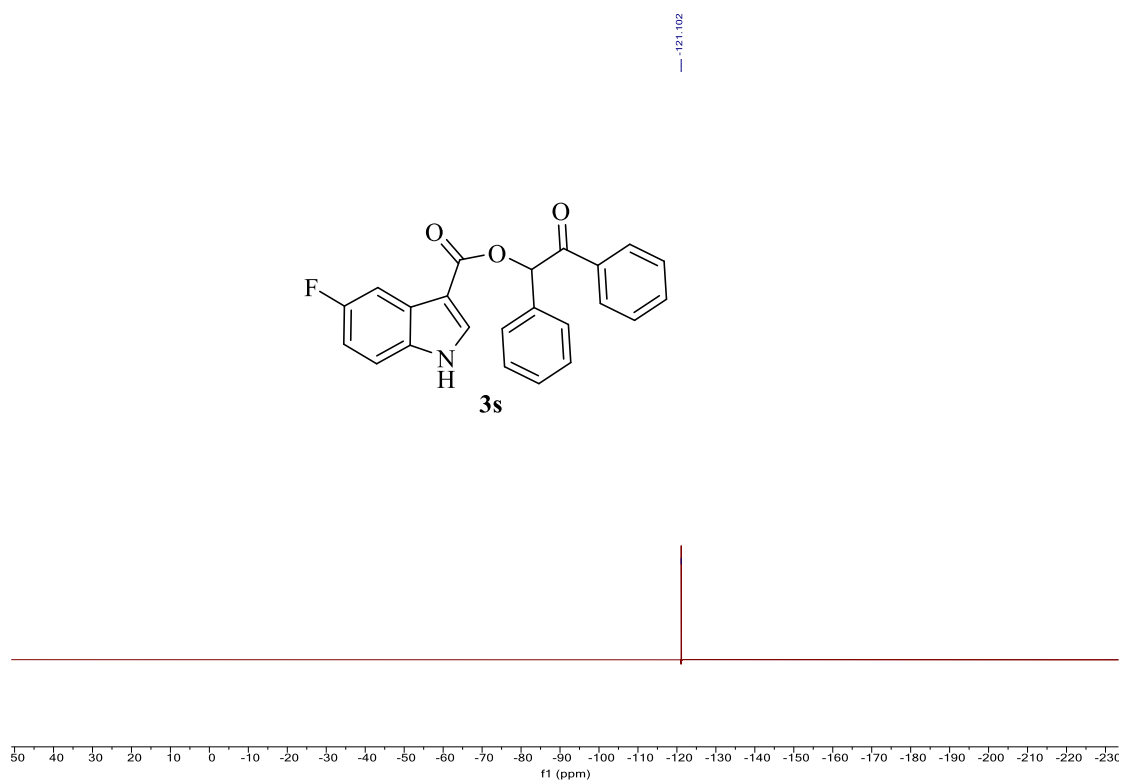
The ^{19}F NMR spectrum of **3b** (376 MHz, CDCl_3)



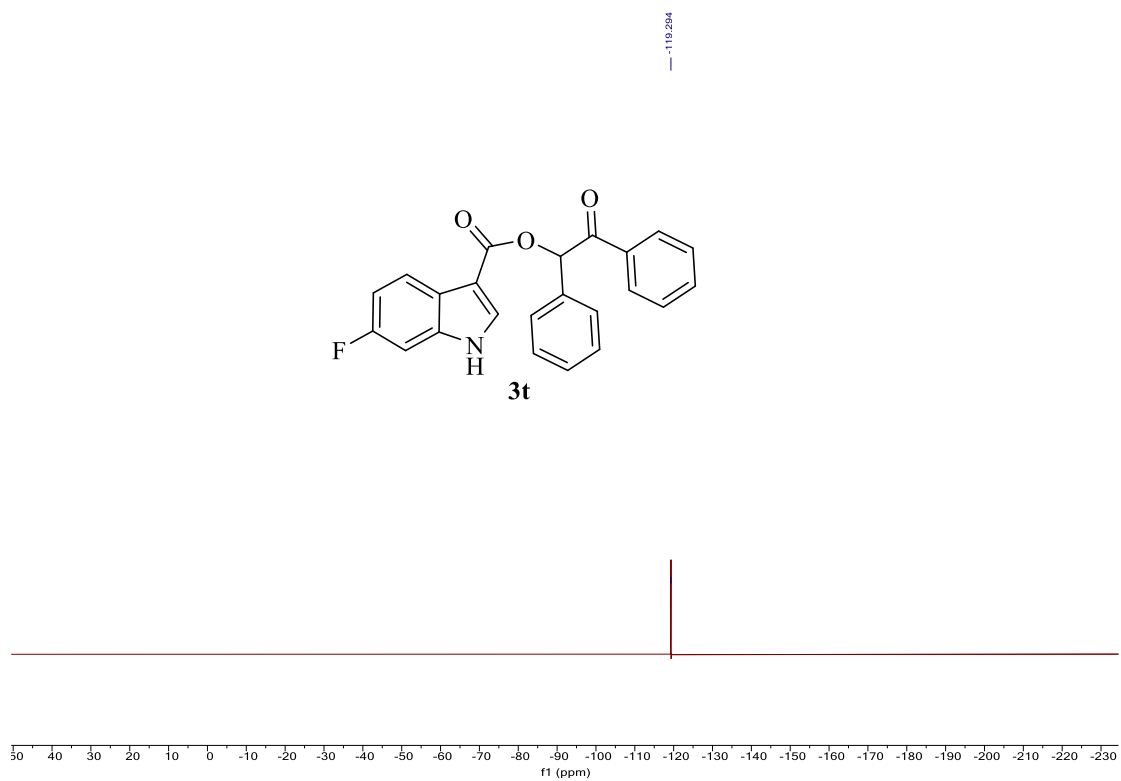
The ^{19}F NMR spectrum of **3g** (376 MHz, CDCl_3)



The ^{19}F NMR spectrum of **3s** (376 MHz, CDCl_3)



The ^{19}F NMR spectrum of **3t** (376 MHz, CDCl_3)



7. X-ray crystallography of compounds 3a

2-Oxo-1,2-diphenylethyl-1*H*-indole-3-carboxylate (3a, zz)

(Ortep ellipsoids are depicted at the 50% level)

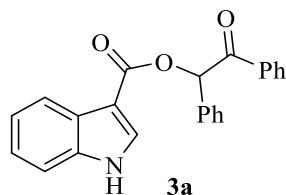


Table 1. Crystal data and structure refinement for **3a**

Identification code	3a
Empirical formula	C ₂₃ H ₁₇ NO ₃
Formula weight	355.39
Temperature	273 K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.222 (3) Å α = 92.926 (9)°. b = 10.291 (3) Å β = 110.642 (9)°. c = 12.395 (4) Å γ = 98.522 (9)°.
Volume	1081.8 (6) Å ³
Z, Calculated density	2, 1.221 g/cm ³
Absorption coefficient	0.199 mm ⁻¹
F(000)	414.0
Crystal size	0.08 x 0.06 x 0.03
Theta range for data collection	2.014 to 25.330°.
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -14 ≤ l ≤ 14
Reflections collected / Independent reflections	28182/3922 [R(int) = 0.0334]
Completeness to theta = 25.242°	99.5 %
Absorption correction	Multi-Scan
Max. and min. transmission	0.745 and 0.715
Data / restraints / parameters	3922 / 29 / 284
Goodness-of-fit on F ²	1.009
Final R indices [I > 2σ(I)]	R1 = 0.0614, wR2 = 0.1751
R indices (all data)	R1 = 0.0754, wR2 = 0.1918
Largest diff. peak and hole	0.405 and -0.218 e.Å ⁻³

