

Electrochemical dehydrogenative annulation for the synthesis of 4-oxo-oxazolines

Yong Yuan,* Xincong Liu, Feng Zhang, Chunyan Bai, Yuyan Tao, Xiazhen Bao,
Dongsheng Ji, and Congde Huo

College of Chemistry and Chemical Engineering, Northwest Normal University,
Lanzhou, Gansu 730070, China

*Email: yuanyong@nwnu.edu.cn

Table of Contents

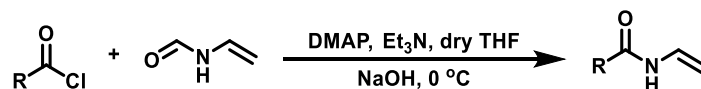
1. General Information	02
2. Experimental Details	06
3. Mechanistic Investigations	11
4. Characterization of Products	26
5. References	27
6. NMR Spectra of Products	70

1. General Information

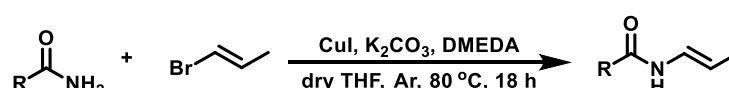
All glassware was oven dried at 110 °C for hours and cooled down under vacuum. Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. Flash column chromatography was performed with silica gel (200 - 300 mesh). Cyclic voltammograms were recorded on a CHI 660E potentiostat. ^1H NMR, ^{13}C NMR, and ^{19}F NMR experiments were carried out using Vnmr Mercury plus 400 MHz or Agilent DD2-600 MHz spectrometers. All chemical shifts (δ) are reported in ppm relative to internal tetramethyl silane (TMS, 0 ppm) for ^1H , CDCl_3 (77.16 ppm) or $\text{DMSO-}d_6$ (39.52 ppm) for ^{13}C . The abbreviations used for explaining the multiplicities were as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad. Coupling constants (J) are reported in Hz. High-resolution mass spectra (HRMS) spectra were obtained from the Thermo Fisher Q-Exactive mass spectrometer in electrospray ionization (ESI^+) mode. X-ray crystallographic analyses were performed on a Rigaku XtaL AB Synergy-DW diffractometer.

2. Experimental Details

2.1 General procedure for the synthesis of enamides¹



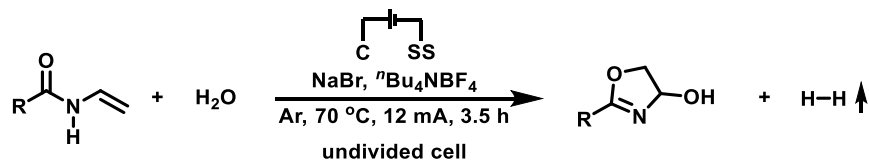
An oven-dried 100 mL two-neck glass tube was equipped with a stir bar was charged with freshly distilled *N*-vinylformamide (10 mmol) and dry THF (40 mL) under an argon atmosphere. Triethylamine (1.4 equiv., 1.9 mL) was added via syringe and the reaction mixture was then cooled to 0 °C. The corresponding acyl chloride (1.2 equiv.) was added dropwise via syringe followed by the slow addition of 4-dimethylamino pyridine (10 mol%, 0.12 g). The reaction was warmed to room temperature and let stir until the reaction was completed by TLC monitoring. After the reaction was cooled to 0 °C, 5 N NaOH was added. The reaction mixture was next stirred vigorously at room temperature until complete consumption of the imide (TLC). The reaction mixture was diluted with water (30 mL) and extracted with EtOAc (30 mL × 3). The combined organic layers were dried (Na₂SO₄), filtered, and concentrated. Target product was finally purified by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 15:1 to 10:1).



An oven-dried 100 mL two-neck glass tube was equipped with a stir bar was charged with freshly distilled (E)-1-bromoprop-1-ene (10 mmol, 1.2 g) and dry THF (40 mL) under an argon atmosphere. CuI (10% mol, 0.2 g), DMEDA (40 mol%, 0.35 g) and K₂CO₃ (2 equiv., 2.76 g) were added via syringe and the reaction mixture was then heat up to 80 °C. The corresponding amide (1.2 equiv.) was added dropwise via syringe. The reaction was warmed 18 h and let stir until the reaction was completed by TLC monitoring. The reaction mixture was diluted with water (30 mL) and extracted with EtOAc (30 mL × 3). The combined organic layers were dried (Na₂SO₄), filtered, and concentrated. Target product was finally purified by flash column chromatography

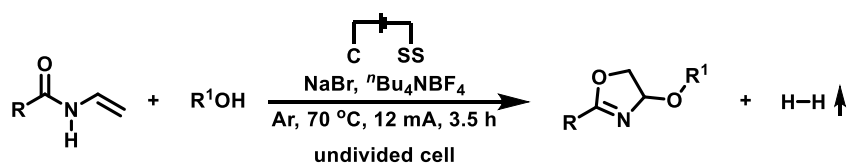
on silica gel (petroleum ether : ethyl acetate = 15:1 to 10:1).

2.2 General procedure for the electrochemical dehydrogenative annulation for the synthesis of 4-hydroxy substituted oxazolines



In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, enamides (0.5 mmol), water (1.5 mL), NaBr (1.0 mmol, 2.0 equiv., 102 mg) and $t\text{Bu}_4\text{NBF}_4$ (0.5 mmol, 1.0 equiv., 165 mg) were combined and added. The bottle was equipped with a carbon cloth (15 mm \times 15 mm \times 0.33 mm) anode and a stainless steel plate (15 mm \times 15 mm \times 1 mm) cathode and was then charged with argon. Under the protection of argon, MeCN (10.5 mL) was injected into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 12 mA at 70 °C for 3.5 h. After the reaction was completed, the reaction mixture was concentrated under reduced pressure. The pure product was obtained by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 2:1 to 1:1).

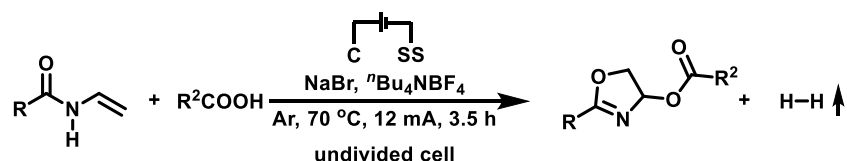
2.3 General procedure for the electrochemical dehydrogenative annulation for the synthesis of 4-alkoxy substituted oxazolines



In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, enamides (0.5 mmol), alcohols (0.5 mL), NaBr (1.0 mmol, 2.0 equiv., 102 mg) and $t\text{Bu}_4\text{NBF}_4$ (0.5 mmol, 1.0 equiv., 165 mg) were combined and added. The bottle was equipped with a carbon cloth (15 mm \times 15 mm \times 0.33 mm) anode and a stainless steel plate (15 mm \times 15 mm \times 1 mm) cathode and was then charged with argon. Under the protection of argon, MeCN (10.5 mL) was injected into the tubes via syringes. The

reaction mixture was stirred and electrolyzed at a constant current of 12 mA at 70 °C for 3.5 h. After the reaction was completed, the reaction mixture was concentrated under reduced pressure. The pure product was obtained by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 10:1 to 4:1).

2.4 General procedure for the electrochemical dehydrogenative annulation for the synthesis of 4- acyloxy substituted oxazolines

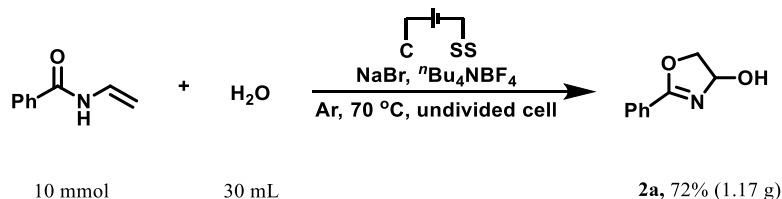


In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, enamides (0.5 mmol), acids (2 equiv.), NaBr (1.0 mmol, 2.0 equiv., 102 mg) and $t\text{Bu}_4\text{NBF}_4$ (0.5 mmol, 1.0 equiv., 165 mg) were combined and added. The bottle was equipped with a carbon cloth (15 mm × 15 mm × 0.33 mm) anode and a stainless steel plate (15 mm × 15 mm × 1 mm) cathode and was then charged with argon. Under the protection of argon, MeCN (10.5 mL) was injected into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 12 mA at 70 °C for 3.5 h. After the reaction was completed, the reaction mixture was concentrated under reduced pressure. The pure product was obtained by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 10:1 to 4:1).

2.5 The experimental setup for electrolysis



2.6 Procedure for the gram scale synthesis of 2a



In an oven-dried undivided three-necked bottle equipped with a stir bar, N-vinylbenzamide (10.0 mmol, 1.5 g), water (30 mL), NaBr (10.0 mmol, 1.0 equiv., 2.1 g) and $t\text{Bu}_4\text{NBF}_4$ (1.0 mmol, 0.1 equiv., 0.33 g) were combined and added. The bottle was equipped with two carbon cloths (15 mm \times 30 mm \times 0.33 mm) as the anodes and two stainless steel plates (15 mm \times 30 mm \times 1 mm) as the cathodes and was then charged with argon. Under the protection of argon, MeCN (80 mL) was injected into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 48 mA at 70 °C for 8.75 h. After the reaction was completed, the reaction mixture was concentrated under reduced pressure. The pure product was obtained by flash column chromatography on silica gel (petroleum ether : ethyl acetate = 1:1) with 72% as a white solid.

3. Mechanistic Investigations

3.1 Cyclic voltammetry study

Cyclic voltammetry (CV) experiments were conducted in an electrolyte of $n\text{Bu}_4\text{NPF}_6$ (0.01 M) in MeCN and H_2O using a glassy carbon disk working electrode (diameter, 1 mm), a Pt wire auxiliary electrode and a Ag/AgCl reference electrode. The scan rate is 100 mV/s.

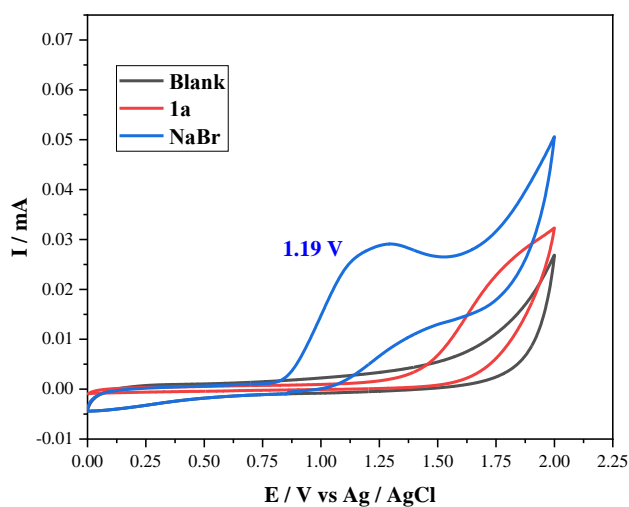
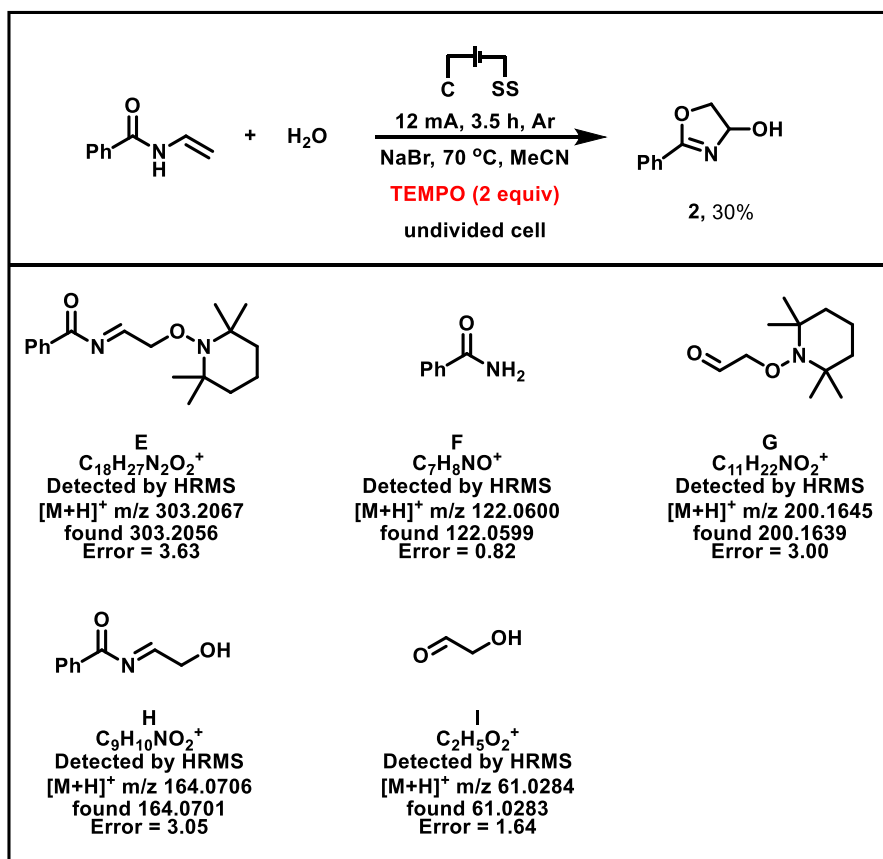


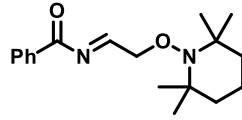
Fig. S1. Cyclic voltammogram of **1a**, **NaBr**, and their mixture in MeCN and H_2O . Conditions: $n\text{Bu}_4\text{NPF}_6$ (0.1 M in MeCN), and with (a) **1a** (2.0 mM), (b) **NaBr** (2.0 mM), or. Scan rate: 100 mV/s.

3.2 Radical trapping by TEMPO

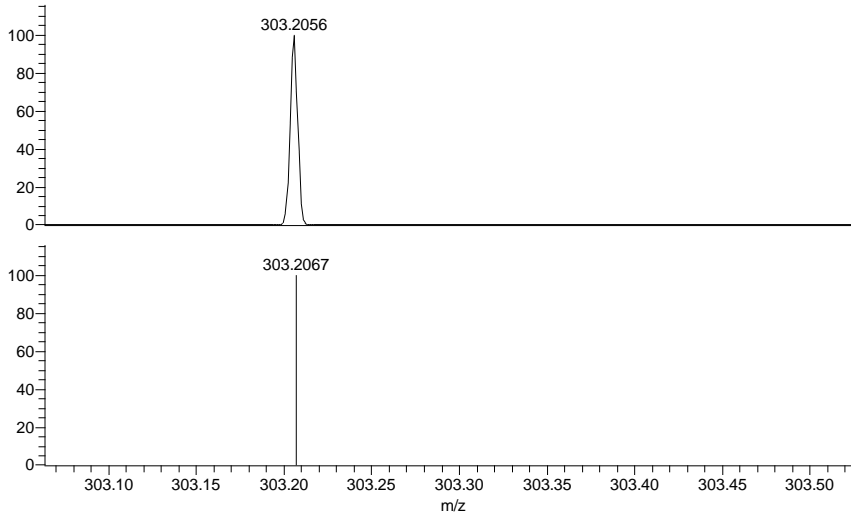
In an oven-dried undivided three-necked bottle (25 mL) equipped with a stir bar, N-vinylbenzamide (0.5 mmol, 1.0 equiv., 73 mg), water (1.5 mL), NaBr (1.0 mmol, 2.0 equiv., 102 mg) and 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) (1.0 mmol, 2.0 equiv., 156 mg) were combined and added. The bottle was equipped with a carbon cloth (15 mm \times 15 mm \times 0.33 mm) anode and a stainless steel plate (15 mm \times 15 mm \times 1 mm) cathode and was then charged with argon. Under the protection of argon, MeCN (11.5 mL) was injected into the tubes via syringes. The reaction mixture was stirred and electrolyzed at a constant current of 12 mA at 70 $^\circ\text{C}$ for 3.5 h. After the reaction was

completed, the reaction mixture was concentrated under reduced pressure. Pure product obtained by silica gel rapid column chromatography with a yield of 30%. Other intermediate products were detected by HRMS analysis of the reaction mixture.



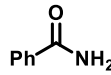


E
C₁₈H₂₇N₂O₂⁺
Detected by HRMS
[M+H]⁺ m/z 303.2067
found 303.2056
Error = 3.63

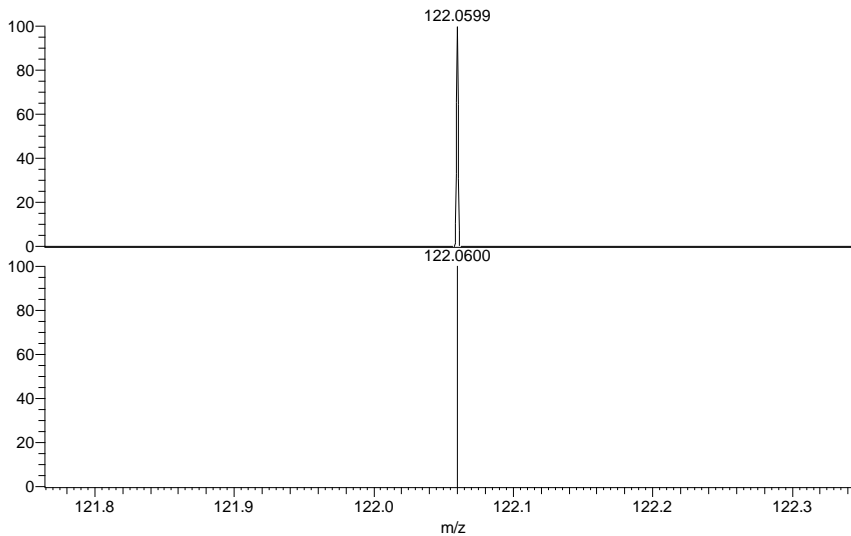


NL:
3.84E7
LIUXINCONG-Q7
(1)#1 RT: 0.00 AV:
1 T: FTMS + p ESI
Full ms
[50.0000-750.0000]

NL:
8.11E5
C₁₈H₂₆N₂O₂+H:
C₁₈H₂₇N₂O₂
pa Chrg 1

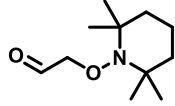


F
C₇H₈NO⁺
Detected by HRMS
[M+H]⁺ m/z 122.0600
found 122.0599
Error = 0.82

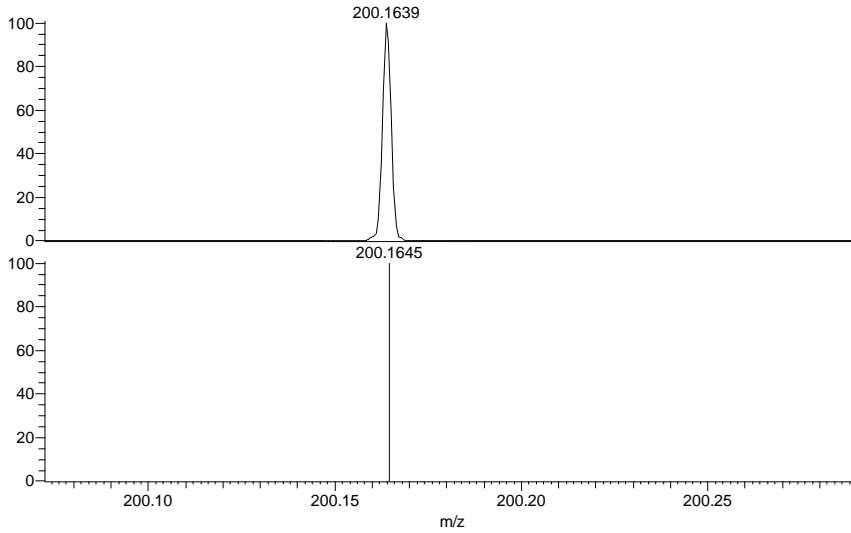


NL:
2.44E7
LIUXINCONG-Q7
(1)#1 RT: 0.00 AV:
1 T: FTMS + p ESI
Full ms
[50.0000-750.0000]

NL:
9.21E5
C₇H₇NO+H:
C₇H₈N₁O₁
pa Chrg 1

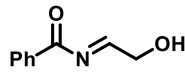


G
 $C_{11}H_{22}NO_2^+$
Detected by HRMS
[M+H]⁺ m/z 200.1645
found 200.1639
Error = 3.00

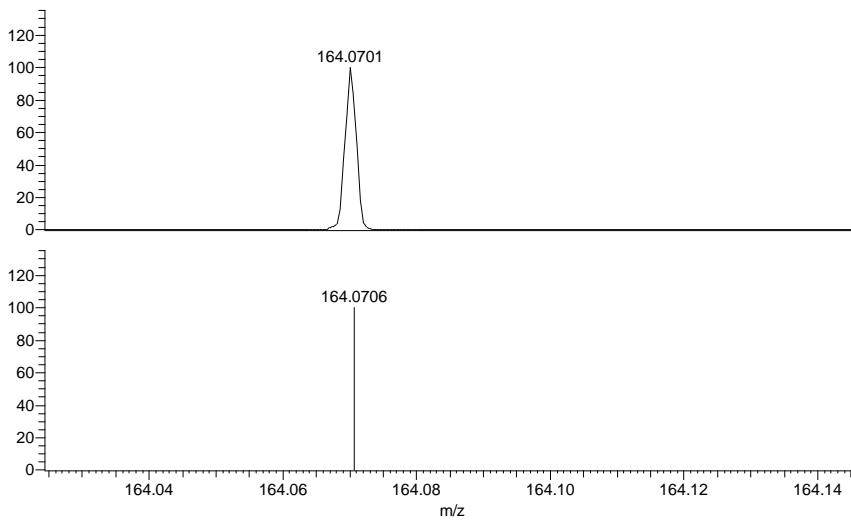


NL:
9.71E8
LIUXINCONG-Q7
(1)#59 RT: 0.26
AV: 1 T: FTMS + p
ESI Full ms
[50.0000-750.0000]

NL:
8.79E5
 $C_{11}H_{21}NO_2 + H:$
 $C_{11}H_{22}N_1O_2$
pa Chrg 1

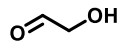


H
 $C_9H_{10}NO_2^+$
Detected by HRMS
[M+H]⁺ m/z 164.0706
found 164.0701
Error = 3.05

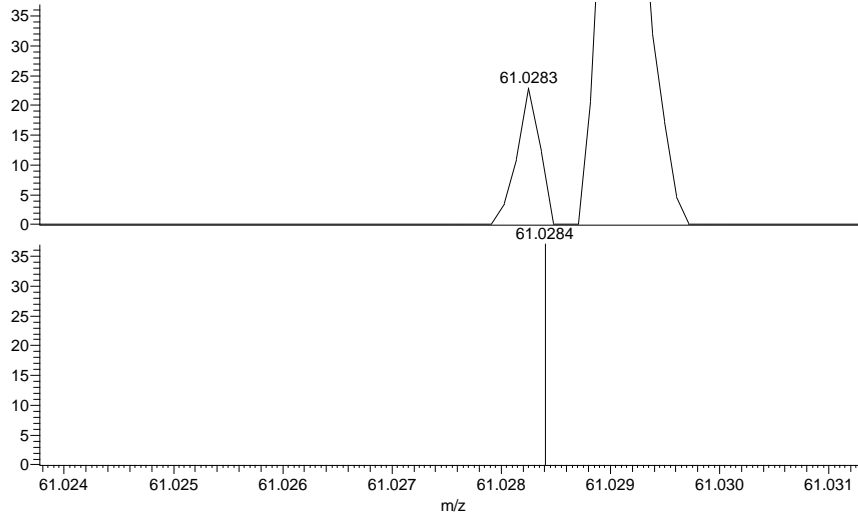


NL:
9.81E8
LIUXINCONG-Q7
(1)#59 RT: 0.26
AV: 1 T: FTMS + p
ESI Full ms
[50.0000-750.0000]

NL:
8.99E5
 $C_9H_9NO_2 + H:$
 $C_9H_{10}N_1O_2$
pa Chrg 1



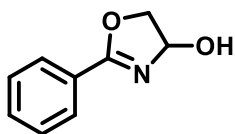
$C_2H_5O_2^+$
Detected by HRMS
[M+H]⁺ m/z 61.0284
found 61.0283
Error = 1.64



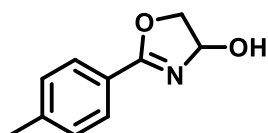
NL:
8.57E6
LIUXINCONG-Q7
(1)#62 RT: 0.28
AV: 1 T: FTMS + p
ESI Full ms
[50.0000-750.0000]

NL:
9.73E5
 $C_2H_4O_2 + H$:
 $C_2H_5O_2$
pa Chrg 1

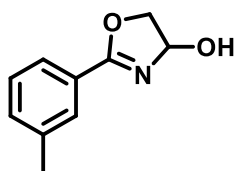
4. Characterization of the products



2-Phenyl-4,5-dihydrooxazol-4-ol (2a). The desired pure product was obtained in 89% yield (73 mg) as a white solid. M.P. = 88 °C - 90 °C. ^1H NMR (400 MHz, DMSO- d_6) δ 7.90 (d, J = 6.4 Hz, 2H), 7.55 - 7.53 (m, 1H), 7.48 - 7.45 (m, 2H), 6.18 (s, 1H), 5.74 - 5.73 (m, 1H), 4.40 - 4.04 (m, 2H). ^{13}C NMR (151 MHz, DMSO- d_6) δ 164.3, 132.2, 129.1, 128.5, 127.8, 90.0, 74.4. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_9\text{H}_{10}\text{NO}_2$ 164.0706; found 164.0706.

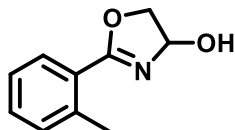


2-(*p*-Tolyl)-4,5-dihydrooxazol-4-ol (2b). The desired pure product was obtained in 78% yield (69 mg) as a white solid. M.P. = 103 °C - 105 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.84 (d, J = 8.2 Hz, 2H), 7.22 (d, J = 8.0 Hz, 2H), 6.01 (dd, J = 7.0, 4.4 Hz, 1H), 4.47 - 4.33 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.8, 142.7, 129.2, 128.6, 124.0, 89.2, 74.2, 21.6. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_2$ 178.0863; found 178.0862.

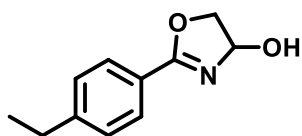


2-(*m*-Tolyl)-4,5-dihydrooxazol-4-ol (2c). The desired pure product was obtained in 71% yield (63 mg) as a white solid. M.P. = 107 °C - 109 °C. ^1H NMR (600 MHz, CDCl_3) δ 7.77 (s, 2H), 7.32 - 7.30 (m, 2H), 6.02 (dd, J = 7.0, 4.4 Hz, 1H), 4.47 - 4.34 (m, 2H), 2.39 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.9, 138.2, 132.9, 129.2, 128.4, 126.8,

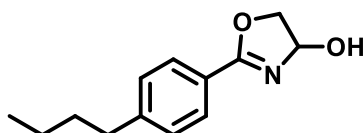
125.8, 89.3, 74.2, 21.3. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{10}H_{12}NO_2$ 178.0863; found 178.0862.



2-(*o*-Tolyl)-4,5-dihydrooxazol-4-ol (2d). The desired pure product was obtained in 74% yield (66 mg) as a white solid. M.P. = 117 °C - 119 °C. 1H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, $J = 7.4$ Hz, 1H), 7.36 (t, $J = 7.5$ Hz, 1H), 7.24 (d, $J = 7.4$ Hz, 2H), 5.99 (dd, $J = 7.1, 4.5$ Hz, 1H), 4.42 - 4.27 (m, 2H), 2.57 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.7, 138.8, 131.3, 131.2, 130.1, 126.5, 125.7, 89.5, 73.6, 21.5. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{10}H_{12}NO_2$ 178.0863; found 178.0860.

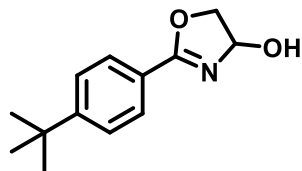


2-(4-Ethylphenyl)-4,5-dihydrooxazol-4-ol (2e). The desired pure product was obtained in 85% yield (82 mg) as a white solid. M.P. = 93 °C - 95 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, $J = 8.0$ Hz, 2H), 7.25 (d, $J = 7.7$ Hz, 2H), 6.03 - 6.00 (m, 1H), 4.48 - 4.34 (m, 2H), 2.68 (dd, $J = 15.1, 7.6$ Hz, 2H), 1.23 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.9, 148.9, 128.7, 128.0, 124.2, 89.3, 74.2, 28.9, 15.2. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{11}H_{14}NO_2$ 192.1019; found 192.1019.

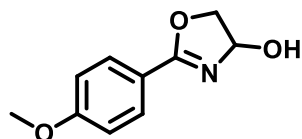


2-(4-Butylphenyl)-4,5-dihydrooxazol-4-ol (2f). The desired pure product was obtained in 96% yield (112 mg) as a white solid. M.P. = 115 °C - 117 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, $J = 8.3$ Hz, 2H), 7.23 (d, $J = 7.9$ Hz, 2H), 6.01 (dd, $J = 7.0, 4.3$ Hz, 1H), 4.48 - 4.33 (m, 2H), 2.65 (t, $J = 7.7$ Hz, 2H), 1.64 - 1.56 (m, 2H), 1.40 - 1.30 (m, 2H), 0.92 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.9, 147.6, 128.6,

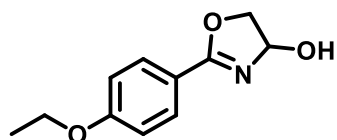
128.6, 124.2, 89.2, 74.2, 35.6, 33.2, 22.3, 13.9. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{13}H_{18}NO_2$ 220.1332; found 220.1333.



2-(4-(*tert*-Butyl) phenyl)-4,5-dihydrooxazol-4-ol (2g). The desired pure product was obtained in 84% yield (92 mg) as a white solid. M.P. = 110 °C - 112 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.4 Hz, 2H), 7.45 (d, J = 8.3 Hz, 2H), 6.02 (dd, J = 7.1, 4.4 Hz, 1H), 4.48 - 4.34 (m, 2H), 1.32 (s, 9H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.8, 155.7, 128.5, 125.5, 124.0, 89.2, 74.2, 35.0, 31.1. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{13}H_{18}NO_2$ 220.1332; found 220.1331.

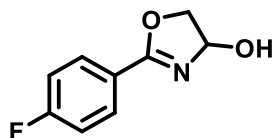


2-(4-Methoxyphenyl)-4,5-dihydrooxazol-4-ol (2h). The desired pure product was obtained in 66% yield (63 mg) as a white solid. M.P. = 128 °C - 130 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 5.99 (dd, J = 7.0, 4.3 Hz, 1H), 4.46 - 4.31 (m, 2H), 3.82 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.5, 162.7, 130.5, 119.2, 113.9, 89.2, 74.2, 55.3. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{10}H_{12}NO_3$ 194.0812; found 194.0813.

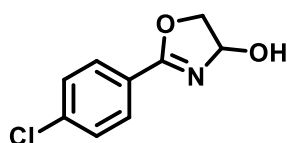


2-(4-Ethoxyphenyl)-4,5-dihydrooxazol-4-ol (2i). The desired pure product was obtained in 87% yield (90 mg) as a white solid. M.P. = 143 °C - 145 °C. 1H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 8.8 Hz, 2H), 6.91 (d, J = 8.8 Hz, 2H), 6.01 (dd, J = 6.9, 4.3 Hz, 1H), 4.48 - 4.33 (m, 2H), 4.06 (q, J = 7.0 Hz, 2H), 1.42 (t, J = 7.0 Hz, 3H). ^{13}C

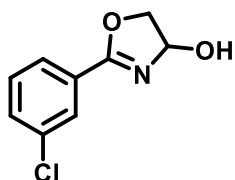
NMR (151 MHz, CDCl₃) δ 166.6, 162.1, 130.5, 119.0, 114.3, 89.3, 74.2, 63.6, 14.7.
HRMS (ESI) m/z: [M + H]⁺ calcd for C₁₁H₁₄NO₃ 208.0968; found 208.0968.



2-(4-Fluorophenyl)-4,5-dihydrooxazol-4-ol (2j). The desired pure product was obtained in 80% yield (73 mg) as a white solid. M.P. = 127 °C - 129 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.99 - 7.96 (m, 2H), 7.14 - 7.09 (m, 2H), 6.01 (dd, *J* = 7.0, 4.3 Hz, 1H), 4.51 - 4.34 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 165.9, 131.1 (d, *J* = 15.1 Hz), 115.8 (d, *J* = 15.1 Hz), 89.4, 74.4. ¹⁹F NMR (376 MHz, CDCl₃) δ -106.47. HRMS (ESI) m/z: [M + H]⁺ calcd for C₉H₉FNO₂ 182.0612; found 182.0611.

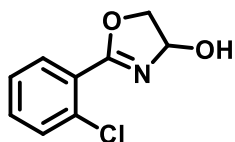


2-(4-Chlorophenyl)-4,5-dihydrooxazol-4-ol (2k). The desired pure product was obtained in 78% yield (77 mg) as a white solid. M.P. = 112 °C - 114 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.91 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 6.00 (dd, *J* = 6.9, 4.4 Hz, 1H), 4.51 - 4.34 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 166.0, 138.5, 130.0, 128.8, 125.4, 89.7, 74.4. HRMS (ESI) m/z: [M + H]⁺ calcd for C₉H₉ClNO₂ 198.0316; found 198.0317.

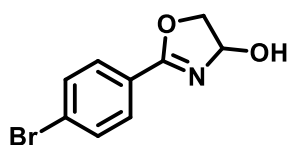


2-(3-Chlorophenyl)-4,5-dihydrooxazol-4-ol (2l). The desired pure product was obtained in 68% yield (67 mg) as a white solid. M.P. = 114 °C - 116 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.94 (s, 1H), 7.86 (d, *J* = 7.8 Hz, 1H), 7.51 - 7.48 (m, 1H), 7.40 - 7.36 (m, 1H), 6.01 (dd, *J* = 7.0, 4.4 Hz, 1H), 4.52 - 4.35 (m, 2H). ¹³C NMR (151 MHz,

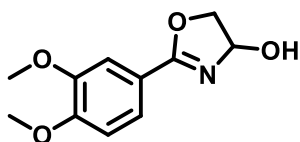
CDCl₃) δ 165.7, 132.2, 129.8, 128.7, 127.7, 126.8, 125.4, 89.5, 74.4. HRMS (ESI) m/z : [M + H]⁺ calcd for C₉H₁₀ClNO₂ 198.0316; found 198.0314.



2-(2-Chlorophenyl)-4,5-dihydrooxazol-4-ol (2m). The desired pure product was obtained in 72% yield (71 mg) as a white solid. M.P. = 105 °C - 106 °C. ¹H NMR (400 MHz, CDCl₃) δ 7.82 - 7.79 (m, 1H), 7.48 - 7.39 (m, 2H), 7.35 - 7.31 (m, 1H), 6.05 (dd, J = 7.2, 4.5 Hz, 1H), 4.49 - 4.31 (m, 2H). ¹³C NMR (151 MHz, CDCl₃) δ 165.3, 133.6, 132.2, 131.4, 130.9, 126.7, 126.6, 89.7, 73.9. HRMS (ESI) m/z : [M + H]⁺ calcd for C₉H₁₀ClNO₂ 198.0316; found 198.0316.

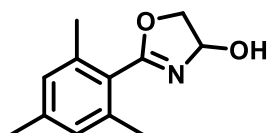


2-(4-Bromophenyl)-4,5-dihydrooxazol-4-ol (2n). The desired pure product was obtained in 82% yield (99 mg) as a white solid. M.P. = 152 °C - 154 °C. ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.81 (d, J = 8.6 Hz, 2H), 7.69 (d, J = 8.6 Hz, 2H), 6.20 - 6.19 (m, 1H), 5.75 - 5.70 (m, 1H), 4.42 - 4.02 (m, 2H). ¹³C NMR (151 MHz, DMSO-*d*₆) δ 163.6, 132.3, 130.5, 127.0, 126.0, 90.0, 74.6. HRMS (ESI) m/z : [M + H]⁺ calcd for C₉H₉BrNO₂ 241.9811; found 241.9812.

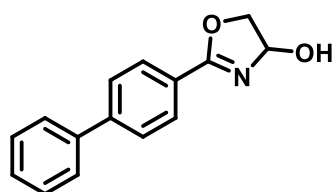


2-(3,4-Dimethoxyphenyl)-4,5-dihydrooxazol-4-ol (2o). The desired pure product was obtained in 86% yield (117 mg) as a white solid. M.P. = 138 °C - 140 °C. ¹H NMR (400 MHz, CHCl₃) δ 7.59 (d, J = 8.5 Hz, 1H), 7.51 (s, 1H), 6.89 (d, J = 8.3 Hz, 1H), 5.98 (s, 1H), 4.46 - 4.32 (m, 2H), 3.93 (s, 6H). ¹³C NMR (151 MHz, CDCl₃) δ 166.8, 152.3,

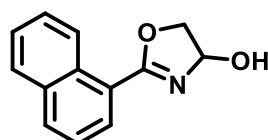
148.7, 122.4, 119.3, 111.2, 110.5, 89.5, 74.4, 56.0, 55.9. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{11}H_{14}NO_4$ 224.0917; found 224.0917.



2,4,6-Trimethyl-4,5-dihydrooxazol-4-ol (2p). The desired pure product was obtained in 68% yield (70 mg) as a white solid. M.P. = 135 °C - 137 °C. 1H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 2H), 5.92 (dd, $J = 7.0, 4.2$ Hz, 1H), 4.37 - 4.21 (m, 2H), 2.30 (s, 6H), 2.28 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.7, 139.6, 136.7, 128.3, 125.1, 89.3, 73.7, 21.1, 19.5. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{12}H_{16}NO_2$ 206.1176; found 206.1176.

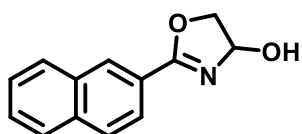


2-([1,1'-Biphenyl]-4-yl)-4,5-dihydrooxazol-4-ol (2q). The desired pure product was obtained in 70% yield (84 mg) as a white solid. M.P. = 175 °C - 177 °C. 1H NMR (600 MHz, $DMSO-d_6$) δ 7.97 - 7.95 (m, 2H), 7.78 (d, $J = 2.0$ Hz, 2H), 7.72 - 7.69 (m, 3H), 7.48 - 7.44 (m, 2H), 6.19 (d, $J = 6.0$ Hz, 1H), 5.77 - 5.74 (m, 1H), 4.42 - 4.39 (m, 2H). ^{13}C NMR (151 MHz, $DMSO-d_6$) δ 164.1, 143.7, 139.4, 129.5, 128.6, 127.3, 127.2, 126.9, 126.8, 90.0, 74.4. HRMS (ESI) m/z : $[M + H]^+$ calcd for $C_{15}H_{14}NO_2$ 240.1019; found 240.1023.

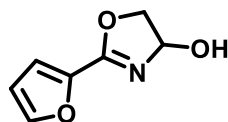


2-(Naphthalen-1-yl)-4,5-dihydrooxazol-4-ol (2r). The desired pure product was obtained in 78% yield (85 mg) as a white solid. M.P. = 120 °C - 122 °C. 1H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, $J = 8.5$ Hz, 1H), 8.08 (d, $J = 7.3$ Hz, 1H), 7.98 (d, $J = 8.2$ Hz,

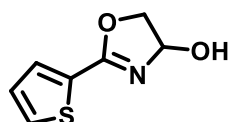
1H), 7.88 (d, $J = 8.0$ Hz, 1H), 7.63 - 7.47 (m, 3H), 6.08 (dd, $J = 7.1, 4.4$ Hz, 1H), 5.93 (s, 1H), 4.48 - 4.32 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 167.3, 133.7, 132.5, 130.9, 129.4, 128.5, 127.4, 126.3, 125.9, 124.7, 124.2, 90.0, 73.7. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{12}\text{NO}_2$ 214.0863; found 214.0861.



2-(Naphthalen-2-yl)-4,5-dihydrooxazol-4-ol (2s). The desired pure product was obtained in 86% yield (92 mg) as a white solid. M.P. = 143 °C - 145 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.49 (s, 1H), 8.04 (d, $J = 8.6$ Hz, 1H), 7.94 - 7.85 (m, 3H), 7.60 - 7.51 (m, 2H), 6.13 - 6.10 (m, 1H), 4.58 - 4.43 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.9, 135.1, 132.6, 129.7, 129.1, 128.4, 128.0, 127.8, 126.7, 124.7, 124.2, 89.6, 74.4. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{12}\text{NO}_2$ 214.0863; found 214.0862.

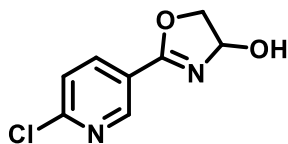


2-(Furan-2-yl)-4,5-dihydrooxazol-4-ol (2t). The desired pure product was obtained in 57% yield (44 mg) as a white solid. M.P. = 100 °C - 102 °C. ^1H NMR (600 MHz, CDCl_3) δ 7.59 - 7.58 (m, 1H), 7.06 (d, $J = 3.5$ Hz, 1H), 6.50 - 6.49 (m, 1H), 6.01 (dd, $J = 6.8, 4.2$ Hz, 1H), 4.44 - 4.32 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 158.7, 146.1, 142.2, 116.2, 111.7, 89.3, 74.4. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_7\text{H}_8\text{NO}_3$ 154.0499; found 154.0501.

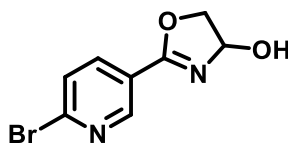


2-(Thiophen-2-yl)-4,5-dihydrooxazol-4-ol (2u). The desired pure product was obtained in 87% yield (74 mg) as a white solid. M.P. = 88 °C - 90 °C. ^1H NMR (400 MHz, CDCl_3) δ 7.70 (d, $J = 3.7$ Hz, 1H), 7.52 (d, $J = 4.7$ Hz, 1H), 7.11 - 7.09 (m, 1H),

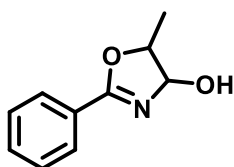
6.00 (dd, $J = 6.9, 4.2$ Hz, 1H), 4.49 - 4.35 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 162.4, 131.8, 131.1, 129.3, 127.9, 89.4, 74.7. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_7\text{H}_8\text{NO}_2\text{S}$ 170.0270; found 170.0271.



2-(6-Chloropyridin-3-yl)-4,5-dihydrooxazol-4-ol (2v). The desired pure product was obtained in 74% yield (73 mg) as a white solid. M.P. = 135 °C - 137 °C. ^1H NMR (600 MHz, CDCl_3) δ 8.96 (d, $J = 1.8$ Hz, 1H), 8.19 (dd, $J = 8.3, 2.4$ Hz, 1H), 7.42 (d, $J = 8.3$ Hz, 1H), 6.01 (dd, $J = 7.0, 4.4$ Hz, 1H), 4.53 - 4.37 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 164.2, 155.0, 150.0, 138.5, 124.3, 122.1, 89.4, 74.6. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{ClN}_2\text{O}_2$ 199.0269; found 199.0269.

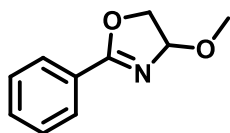


2-(6-Bromopyridin-3-yl)-4,5-dihydrooxazol-4-ol (2w). The desired pure product was obtained in 64% yield (68 mg) as a white solid. M.P. = 140 °C - 142 °C. ^1H NMR (400 MHz, CDCl_3) δ 8.96 (d, $J = 1.6$ Hz, 1H), 8.19 (dd, $J = 8.3, 2.4$ Hz, 1H), 7.42 (d, $J = 8.4$ Hz, 1H), 6.01 (dd, $J = 7.0, 4.4$ Hz, 1H), 5.75 (s, 1H), 4.54 - 4.36 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 164.2, 155.0, 150.0, 138.5, 124.3, 122.1, 89.5, 74.6. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_8\text{H}_8\text{BrN}_2\text{O}_2$ 242.9764; found 242.9764.

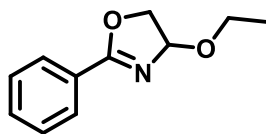


5-Methyl-2-phenyl-4,5-dihydrooxazol-4-ol (2x). The desired pure product was obtained in 57% yield (51 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.96 (d, $J = 7.3$ Hz, 2H), 7.54 - 7.42 (m, 3H), 5.84 - 5.53 (m, 1H), 4.77 - 4.65 (m, 1H), 1.56 -

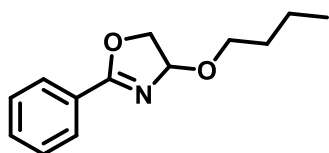
1.43 (m, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 161.3, 127.3, 127.2, 123.9, 123.8, 123.7, 123.7, 122.5, 122.4, 90.5, 84.1, 78.2, 75.3, 14.0, 13.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_2$ 178.0863; found 178.0863.



4-Methoxy-2-phenyl-4,5-dihydrooxazole (4a). The desired pure product was obtained in 90% yield (80 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, $J = 7.4$ Hz, 2H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.41 (t, $J = 7.5$ Hz, 2H), 5.53 (dd, $J = 7.2, 4.4$ Hz, 1H), 4.42 - 4.22 (m, 2H), 3.53 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 167.0, 131.9, 128.7, 128.3, 127.4, 97.9, 72.4, 55.4. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{10}\text{H}_{12}\text{NO}_2$ 178.0863; found 178.0862.

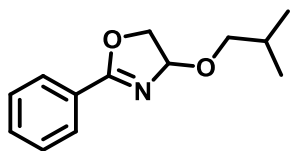


4-Ethoxy-2-phenyl-4,5-dihydrooxazole (4b). The desired pure product was obtained in 92% yield (88 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, $J = 7.6$ Hz, 2H), 7.49 (t, $J = 7.6$ Hz, 1H), 7.41 (t, $J = 7.5$ Hz, 2H), 5.63 - 5.60 (m, 1H), 4.44 - 4.25 (m, 2H), 4.00 - 3.61 (m, 2H), 1.25 (t, $J = 7.0$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.8, 131.8, 128.7, 128.3, 127.5, 96.7, 72.6, 63.6, 15.3. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_2$ 192.1019; found 192.1019.

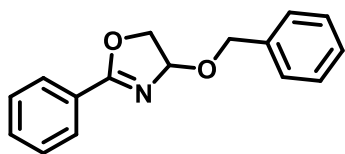


4-Butoxy-2-phenyl-4,5-dihydrooxazole (4c). The desired pure product was obtained in 82% yield (90 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, $J = 7.0$ Hz, 2H), 7.50 - 7.47 (m, 1H), 7.42 - 7.39 (m, 2H), 5.61 - 5.58 (m, 1H), 4.42 - 4.23 (m, 2H), 3.92 - 3.53 (m, 2H), 1.61 - 1.56 (m, 2H), 1.41 - 1.35 (m, 2H), 0.92 (t, $J = 6.7$ Hz,

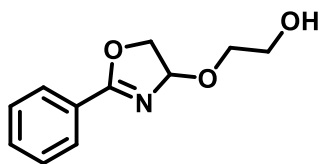
3H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.7, 131.8, 128.7, 128.3, 127.5, 96.8, 72.6, 68.0, 31.9, 19.3, 13.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_2$ 220.1332; found 220.1331.



4-Isobutoxy-2-phenyl-4,5-dihydrooxazole (4d). The desired pure product was obtained in 80% yield (88 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, $J = 7.3$ Hz, 2H), 7.52 - 7.47 (m, 1H), 7.41 (t, $J = 7.6$ Hz, 2H), 5.60 (dd, $J = 7.2, 4.5$ Hz, 1H), 4.43 - 4.25 (m, 2H), 3.70 - 3.29 (m, 2H), 1.92 - 1.86 (m, 1H), 0.93 - 0.91 (m, 6H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.6, 131.8, 128.7, 128.3, 127.5, 97.0, 74.9, 72.6, 28.6, 19.4, 19.3. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{18}\text{NO}_2$ 220.1332; found 220.1332.

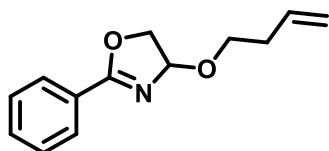


4-(Benzyloxy)-2-phenyl-4,5-dihydrooxazole (4e). The desired pure product was obtained in 79% yield (100 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, $J = 7.2$ Hz, 2H), 7.55 - 7.23 (m, 8H), 5.74 (dd, $J = 7.2, 4.5$ Hz, 1H), 4.86 (dd, $J = 104.9, 11.7$ Hz, 2H), 4.45 - 4.33 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 167.1, 138.0, 131.9, 128.8, 128.4, 128.3, 128.0, 127.7, 127.5, 96.2, 72.7, 69.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{16}\text{NO}_2$ 254.1176; found 254.1176.

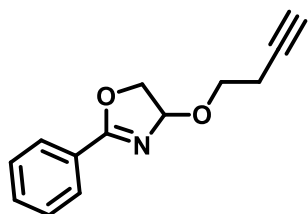


2-((2-Phenyl-4,5-dihydrooxazol-4-yl)oxy)ethan-1-ol (4f). The desired pure product was obtained in 90% yield (94 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ

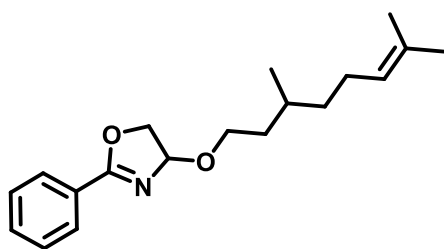
7.97 (d, $J = 7.8$ Hz, 2H), 7.53 (t, $J = 7.1$ Hz, 1H), 7.43 (t, $J = 7.6$ Hz, 2H), 5.60 (dd, $J = 7.4, 4.7$ Hz, 1H), 4.54 - 4.30 (m, 2H), 4.00 - 3.84 (m, 2H), 3.80 - 3.67 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 167.1, 132.3, 128.8, 128.5, 126.7, 97.7, 73.1, 73.0, 62.9. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{11}\text{H}_{14}\text{NO}_3$ 208.0968; found 208.0969.



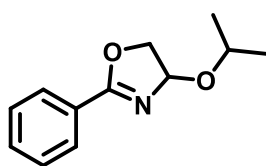
4-(But-3-en-1-yloxy)-2-phenyl-4,5-dihydrooxazole (4g). The desired pure product was obtained in 60% yield (65 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.01 - 7.98 (m, 2H), 7.52 - 7.48 (m, 1H), 7.44 - 7.39 (m, 2H), 5.89 - 5.79 (m, 1H), 5.62 (dd, $J = 7.2, 4.5$ Hz, 1H), 5.14 - 5.02 (m, 2H), 4.43 - 4.26 (m, 2H), 3.99 - 3.61 (m, 2H), 2.42 - 2.36 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.8, 135.1, 131.9, 128.7, 128.3, 127.4, 116.4, 96.9, 72.6, 67.4, 34.3. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{16}\text{NO}_2$ 218.1176; found 218.1176.



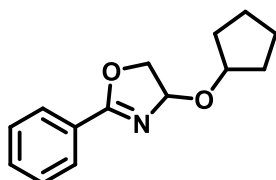
4-(But-3-yn-1-yloxy)-2-phenyl-4,5-dihydrooxazole (4h). The desired pure product was obtained in 63% yield (67 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.99 (d, $J = 7.4$ Hz, 2H), 7.50 (t, $J = 7.3$ Hz, 1H), 7.41 (t, $J = 7.6$ Hz, 2H), 5.66 (dd, $J = 7.2, 4.3$ Hz, 1H), 4.44 - 4.29 (m, 2H), 4.03 - 3.71 (m, 2H), 2.55 - 2.48 (m, 2H), 1.99 (t, $J = 2.6$ Hz, 1H). ^{13}C NMR (151 MHz, CDCl_3) δ 167.0, 131.9, 128.7, 128.4, 127.3, 97.0, 81.3, 72.6, 69.3, 66.1, 20.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{13}\text{H}_{14}\text{NO}_2$ 216.1019; found 216.1019.



4-((3,7-Dimethyloct-6-en-1-yl) oxy)-2-phenyl-4,5-dihydrooxazole (4i). The desired pure product was obtained in 81% yield (122 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, $J = 7.3$ Hz, 2H), 7.50 (t, $J = 7.4$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 2H), 5.60 (dd, $J = 7.2, 4.5$ Hz, 1H), 5.12 - 5.06 (m, 1H), 4.43 - 4.25 (m, 2H), 3.98 - 3.58 (m, 2H), 2.02 - 1.95 (m, 2H), 1.67 (s, 4H), 1.59 (s, 3H), 1.46 - 1.18 (m, 4H), 0.91 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.7, 131.8, 128.7, 128.3, 124.8, 96.9, 72.6, 66.6, 66.5, 37.2, 36.8, 36.7, 29.5, 25.7, 25.4, 19.5, 17.6. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{19}\text{H}_{28}\text{NO}_2$ 302.2115; found 302.2113.

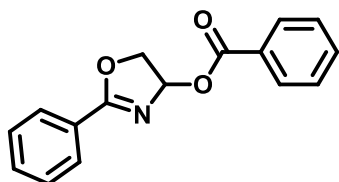


4-Isopropoxy-2-phenyl-4,5-dihydrooxazole (4j). The desired pure product was obtained in 83% yield (84 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.01 - 7.98 (m, 2H), 7.51 - 7.47 (m, 1H), 7.43 - 7.38 (m, 2H), 5.69 (dd, $J = 7.3, 4.4$ Hz, 1H), 4.44 - 4.20 (m, 2H), 4.16 - 4.08 (m, 1H), 1.28 - 1.22 (m, 6H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.4, 131.7, 128.7, 128.3, 127.6, 94.9, 73.1, 70.0, 23.5, 22.0. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{16}\text{NO}_2$ 206.1176; found 206.1167.

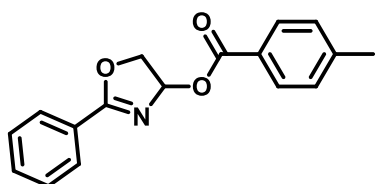


4-(Cyclopentyloxy)-2-phenyl-4,5-dihydrooxazole (4k). The desired pure product was obtained in 86% yield (100 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.05 - 7.96 (m, 2H), 7.54 - 7.46 (m, 1H), 7.45 - 7.37 (m, 2H), 5.66 (dd, $J = 7.3, 4.6$ Hz, 1H), 4.50 - 4.35 (m, 2H), 4.22 (dd, $J = 9.8, 4.6$ Hz, 1H), 1.93 - 1.78 (m, 2H), 1.76 - 1.65 (m,

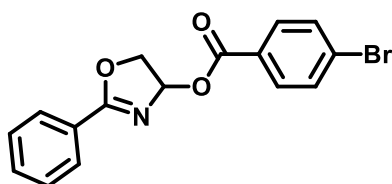
4H), 1.60 - 1.49 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 166.4, 131.7, 128.7, 128.3, 127.6, 95.5, 79.6, 73.0, 33.4, 32.3, 23.42, 23.39. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{14}\text{H}_{18}\text{NO}_2$ 232.1332; found 232.1332.



2-Phenyl-4,5-dihydrooxazol-4-yl benzoate (4l). The desired pure product was obtained in 75% yield (100 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.14 – 8.03 (m, 4H), 7.61 – 7.51 (m, 2H), 7.49 – 7.40 (m, 4H), 6.92 (dd, $J = 7.1, 4.2$ Hz, 1H), 4.75 – 4.46 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.3, 165.9, 133.4, 132.5, 129.9, 129.5, 129.0, 128.5, 128.4, 126.7, 92.5, 73.2. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{14}\text{NO}_3$ 268.0968; found 268.0966.

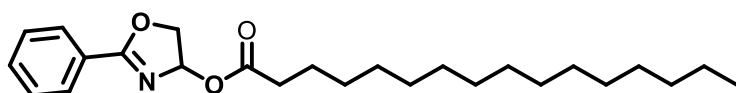


2-Phenyl-4,5-dihydrooxazol-4-yl 4-methylbenzoate (4m). The desired pure product was obtained in 70% yield (99 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.09 - 7.96 (m, 4H), 7.57 - 7.43 (m, 3H), 7.22 (d, $J = 1.8$ Hz, 2H), 6.90 (dd, $J = 7.1, 4.1$ Hz, 1H), 4.72 - 4.46 (m, 2H), 2.40 (s, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.2, 165.9, 144.1, 132.4, 129.9, 129.1, 128.9, 128.4, 126.7, 126.6, 92.4, 73.2, 21.7. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{17}\text{H}_{16}\text{NO}_3$ 282.1125; found 282.1126.

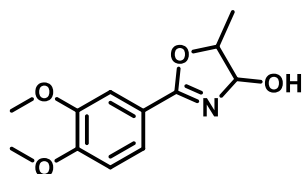


2-Phenyl-4,5-dihydrooxazol-4-yl 4-bromobenzoate (4n). The desired pure product was obtained in 55% yield (95 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ

8.03 (d, $J = 7.7$ Hz, 2H), 7.60 - 7.39 (m, 6H), 6.53 (dd, $J = 8.6, 5.5$ Hz, 1H), 6.29 - 6.28 (m, 1H), 4.79 - 4.70 (m, 2H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.3, 165.9, 133.4, 132.5, 129.9, 129.5, 129.0, 128.5, 128.4, 126.6, 92.5, 73.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{16}\text{H}_{13}\text{BrNO}_3$ 346.0073; found 346.0071.



2-Phenyl-4,5-dihydrooxazol-4-yl palmitate (4o). The desired pure product was obtained in 60% yield (120 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 8.04 (d, $J = 7.2$ Hz, 2H), 7.54 - 7.42 (m, 3H), 6.66 (dd, $J = 7.1, 4.2$ Hz, 1H), 4.63 - 4.31 (m, 2H), 2.35 (dd, $J = 7.6, 2.7$ Hz, 2H), 1.66 - 1.62 (m, 2H), 1.24 (s, 24H), 0.87 (t, $J = 6.7$ Hz, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 173.2, 169.1, 132.4, 128.9, 128.4, 126.6, 91.8, 73.2, 34.2, 31.9, 29.7, 29.7, 29.6, 29.6, 29.6, 29.6, 29.4, 29.3, 29.2, 29.1, 24.7, 22.7, 14.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{25}\text{H}_{40}\text{NO}_3$ 402.3003; found 402.3003.



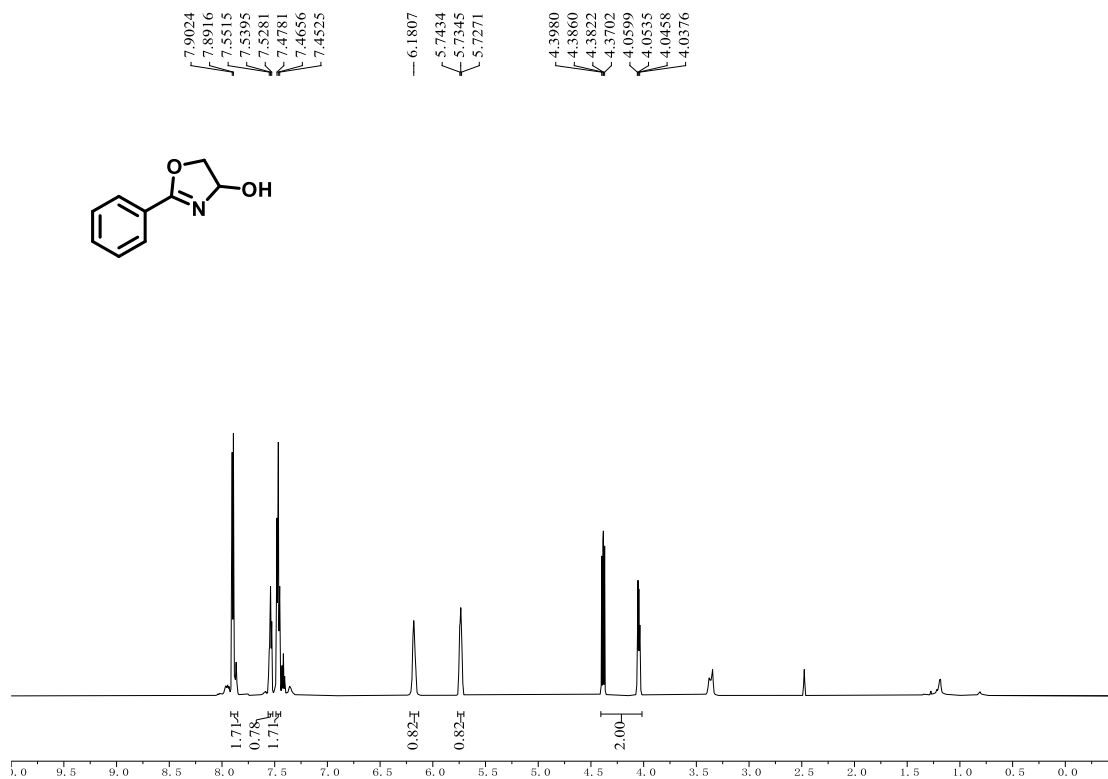
2-(3,4-Dimethoxyphenyl)-5-methyl-4,5-dihydrooxazol-4-ol (2y). The desired pure product was obtained in 81% yield (96 mg) as a colorless oil. ^1H NMR (400 MHz, CDCl_3) δ 7.57- 7.26 (m, 2H), 6.86 (dd, $J = 9.5, 8.4$ Hz, 1H), 5.77- 5.46 (m, 1H), 4.72- 4.56 (m, 1H), 3.91 (s, 6H), 1.52- 1.24 (m, 3H). ^{13}C NMR (151 MHz, CDCl_3) δ 169.1, 166.0, 152.2, 152.2, 148.9, 148.7, 125.9, 122.3, 120.1, 119.7, 111.1, 110.8, 110.5, 110.2, 95.5, 88.9, 83.1, 80.2, 56.0, 55.9, 55.9, 55.9, 18.7, 13.1. HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calcd for $\text{C}_{12}\text{H}_{16}\text{NO}_4$ 238.1074; found 238.1074.

5. References

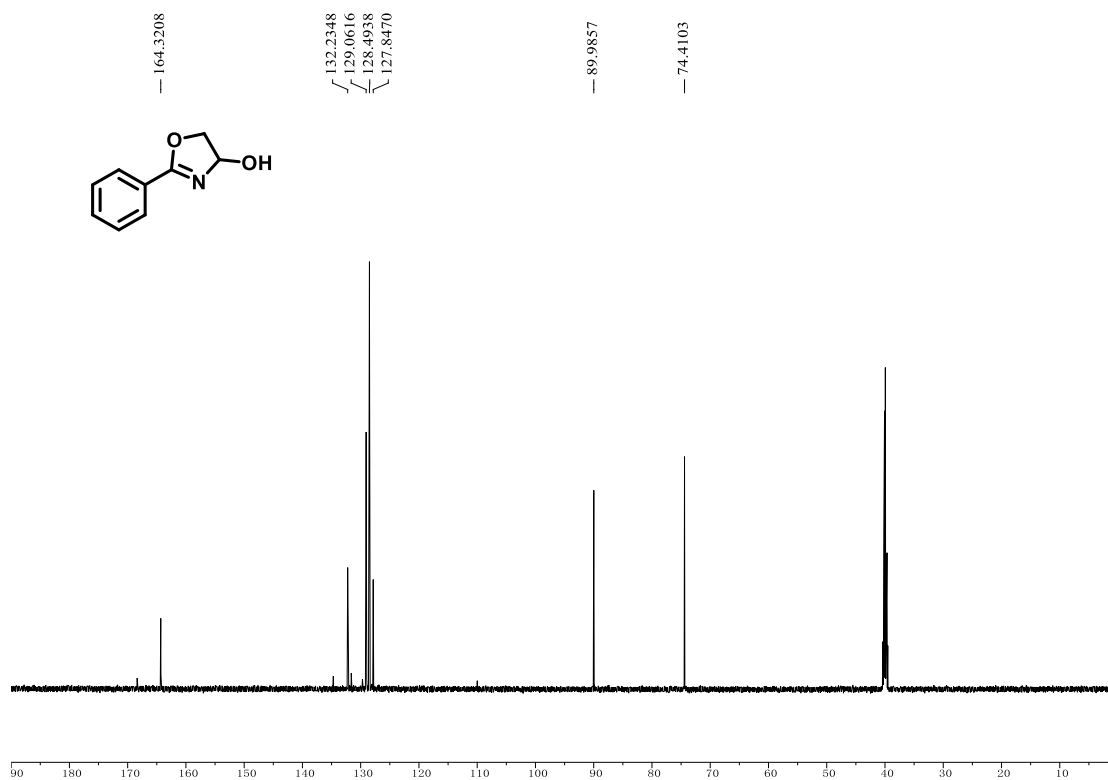
1. Boyington, A. J.; Seath, C. P.; Zearfoss, A. M.; Xu, Z.; Jui, N. T. Catalytic Strategy for Regioselective Arylethylamine Synthesis. *J. Am. Chem. Soc.* **2019**, *141*, 4147-4153.

6. NMR Spectra of Products

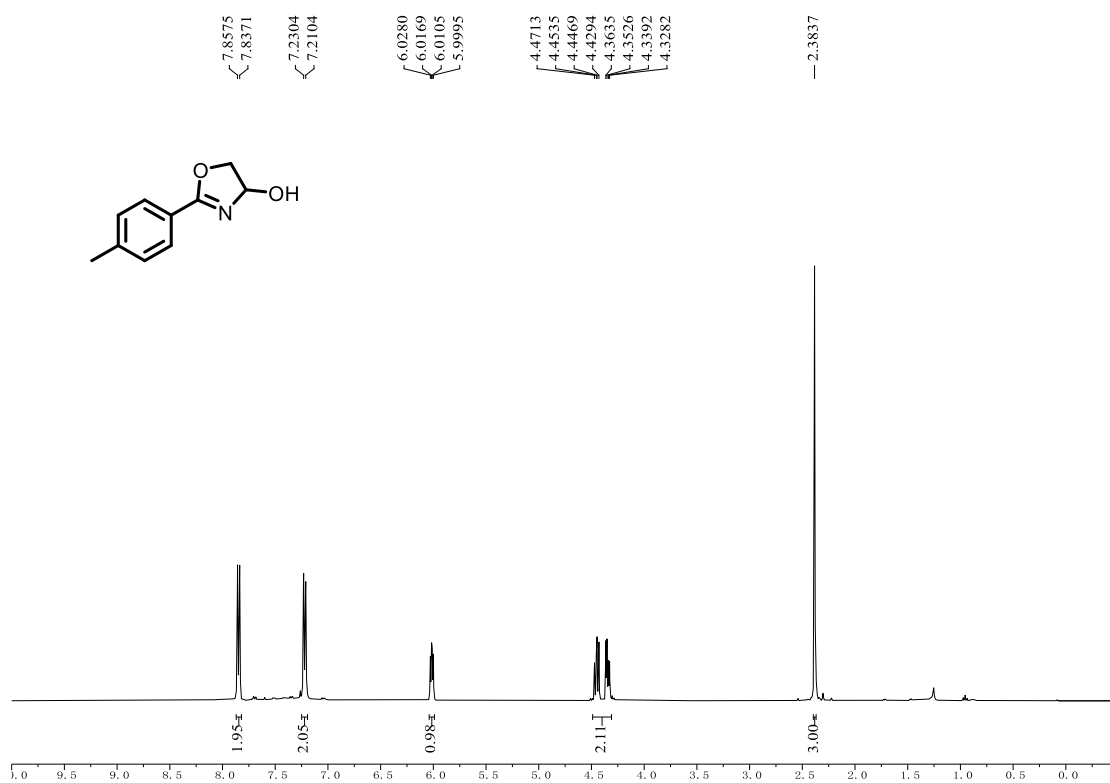
^1H NMR (400 MHz, $\text{DMSO-}d_6$) of compound **2a**



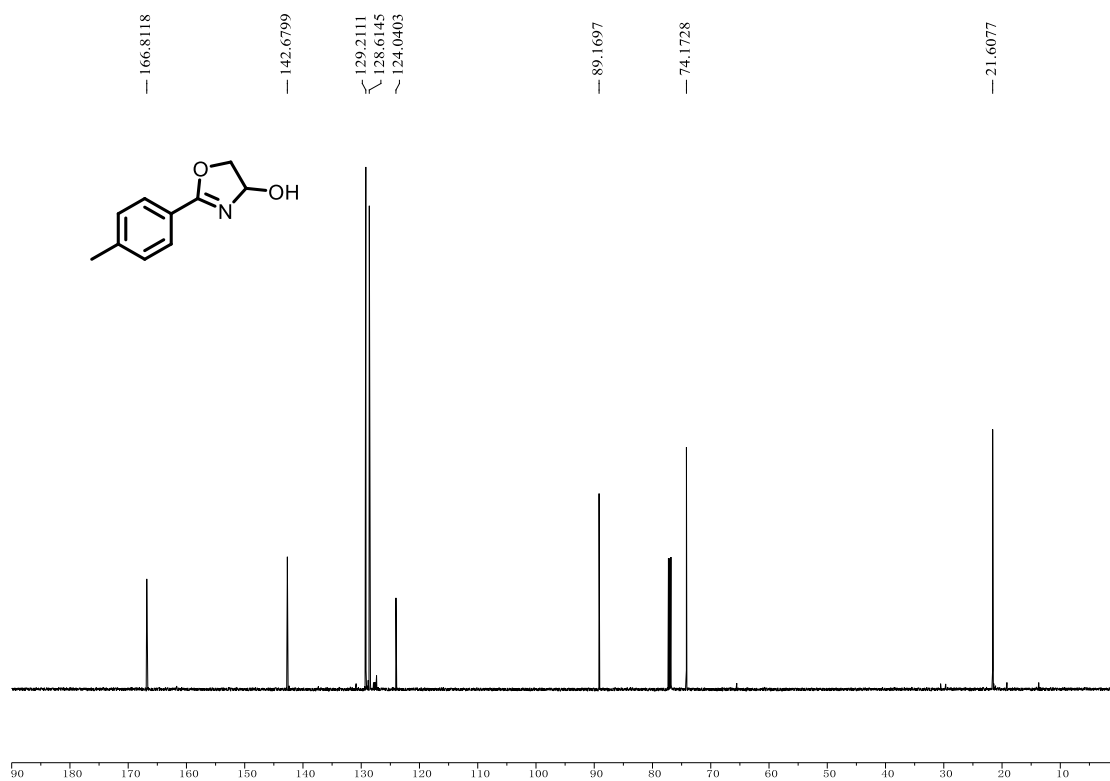
^{13}C NMR (151 MHz, $\text{DMSO-}d_6$) of compound **2a**



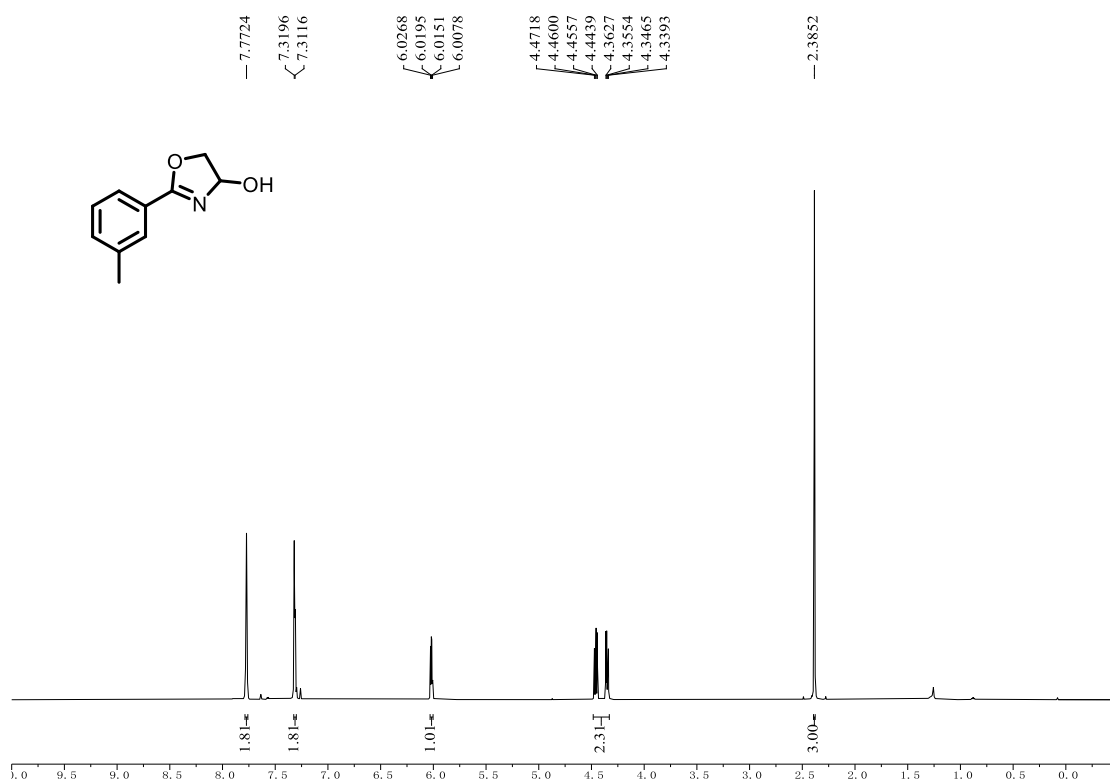
¹H NMR (400 MHz, CDCl₃) of compound **2b**



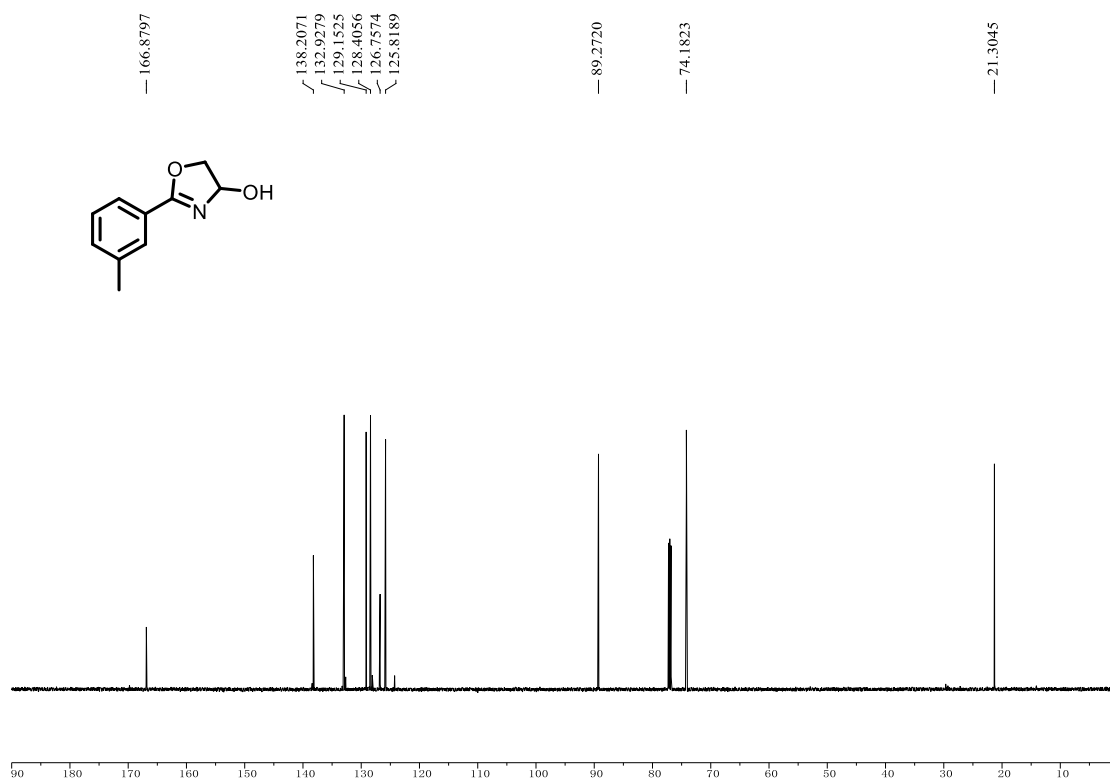
¹³C NMR (151 MHz, CDCl₃) of compound **2b**



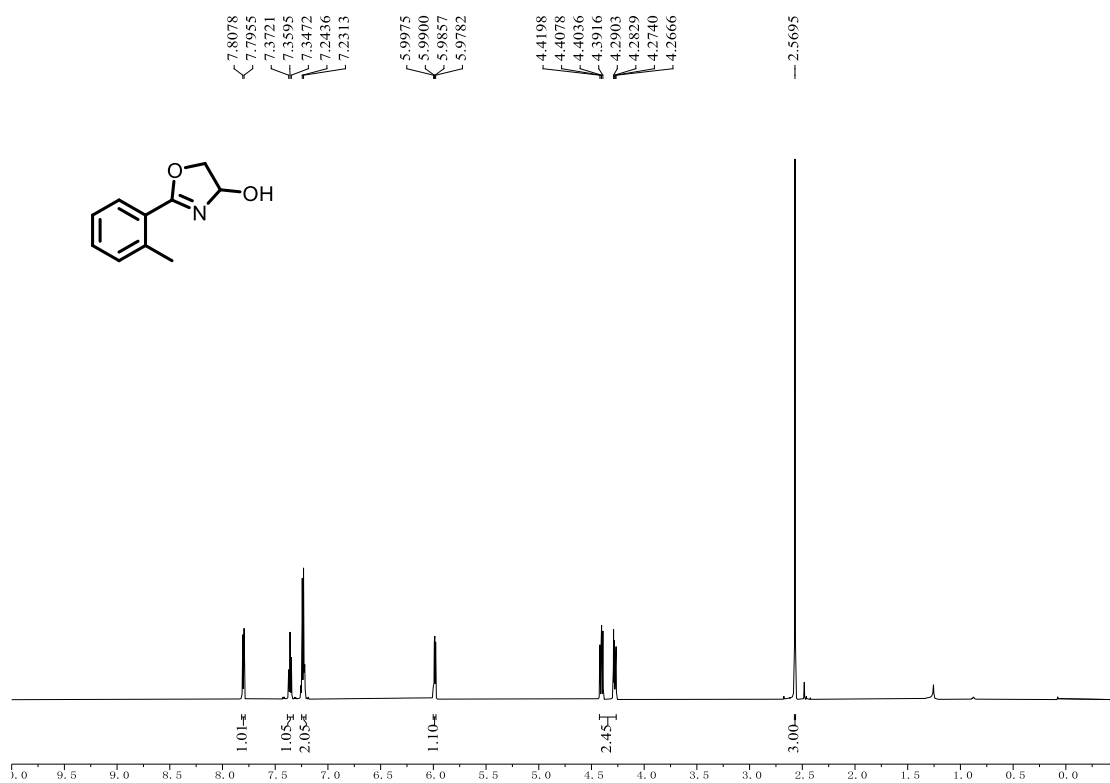
¹H NMR (600 MHz, CDCl₃) of compound 2c



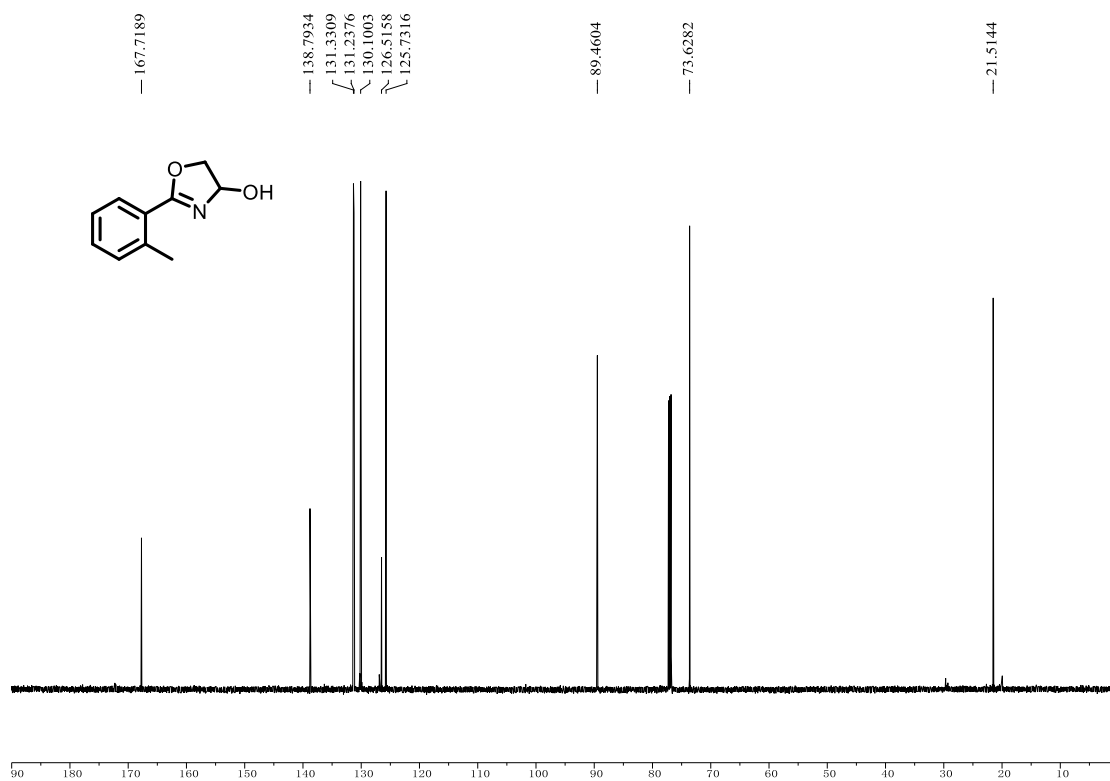
¹³C NMR (151 MHz, CDCl₃) of compound 2c



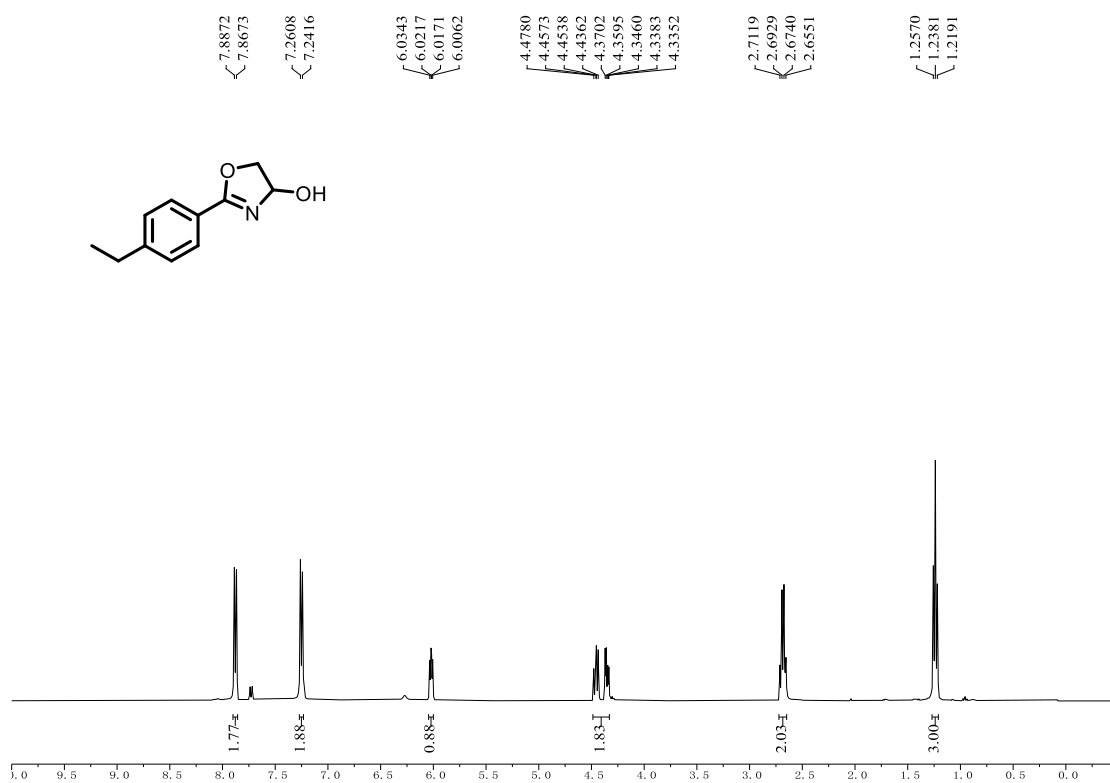
¹H NMR (600 MHz, CDCl₃) of compound **2d**



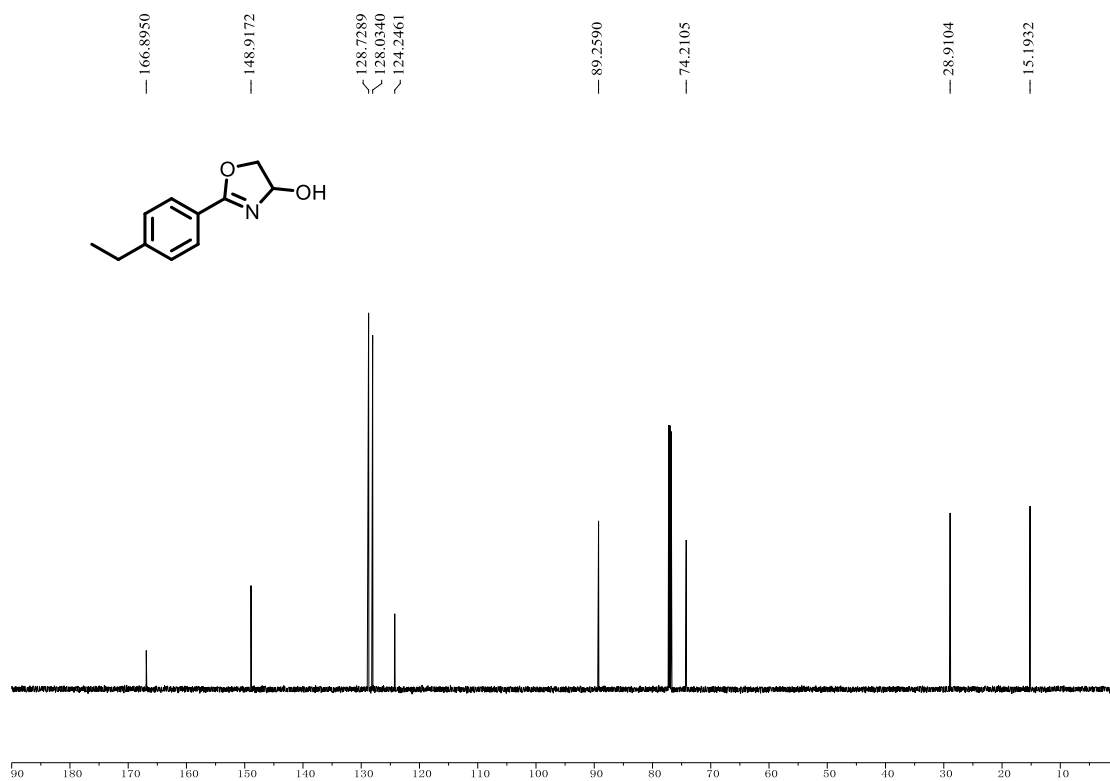
¹³C NMR (151 MHz, CDCl₃) of compound **2d**



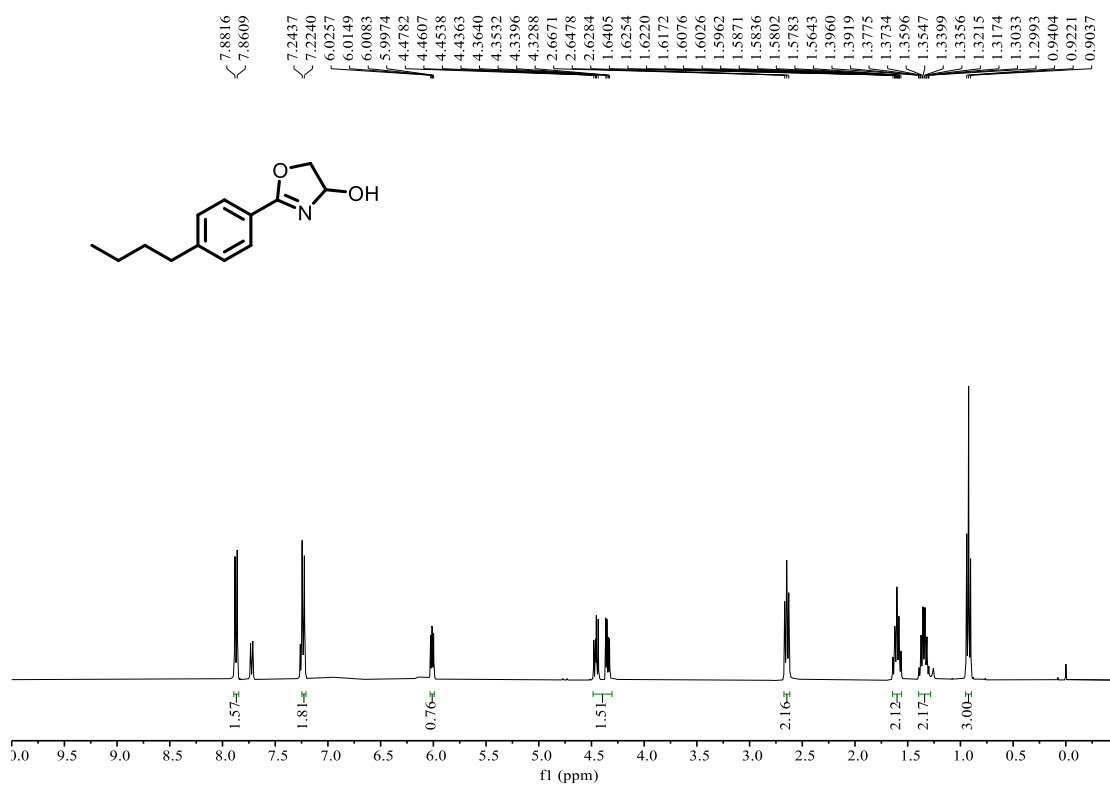
¹H NMR (400 MHz, CDCl₃) of compound **2e**



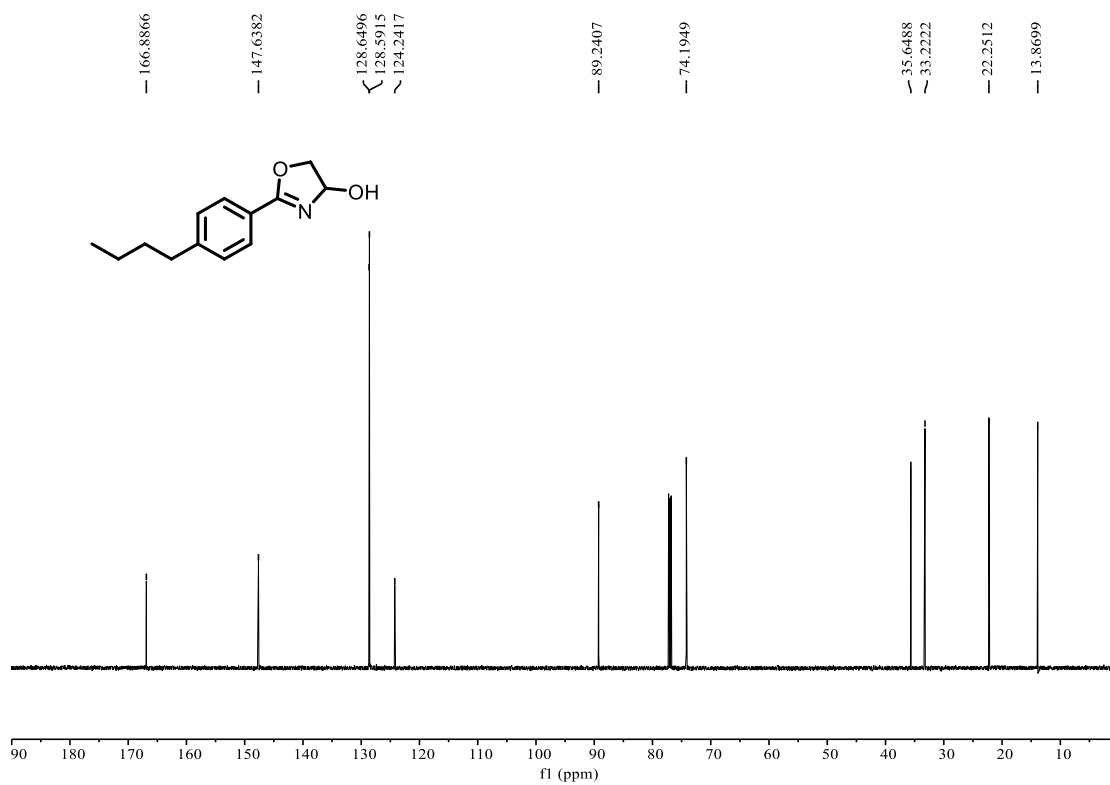
¹³C NMR (151 MHz, CDCl₃) of compound **2e**



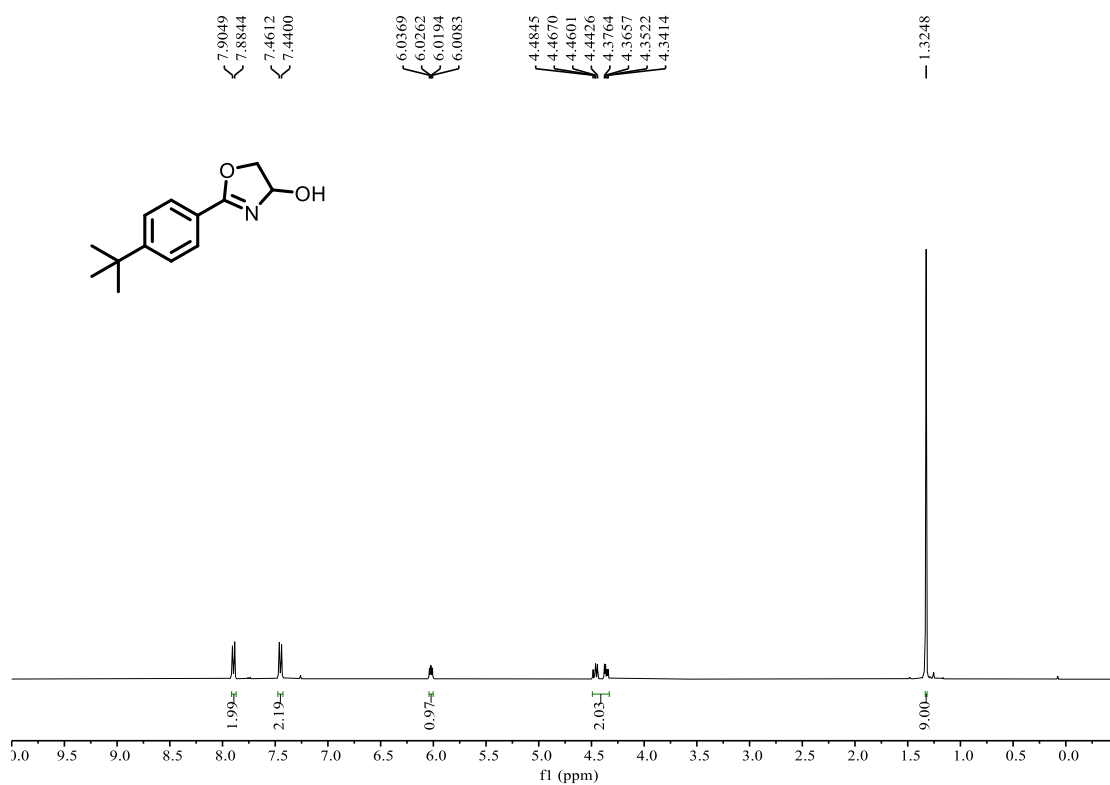
¹H NMR (400 MHz, CDCl₃) of compound **2f**



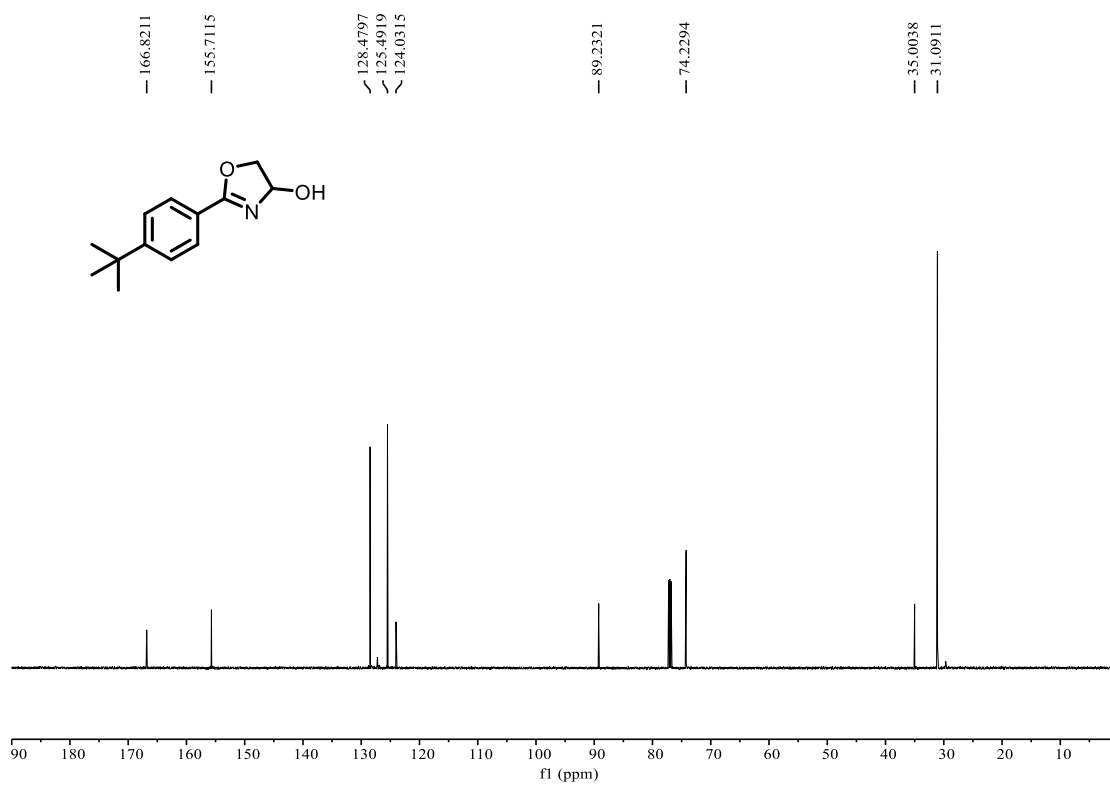
¹³C NMR (151 MHz, CDCl₃) of compound **2f**



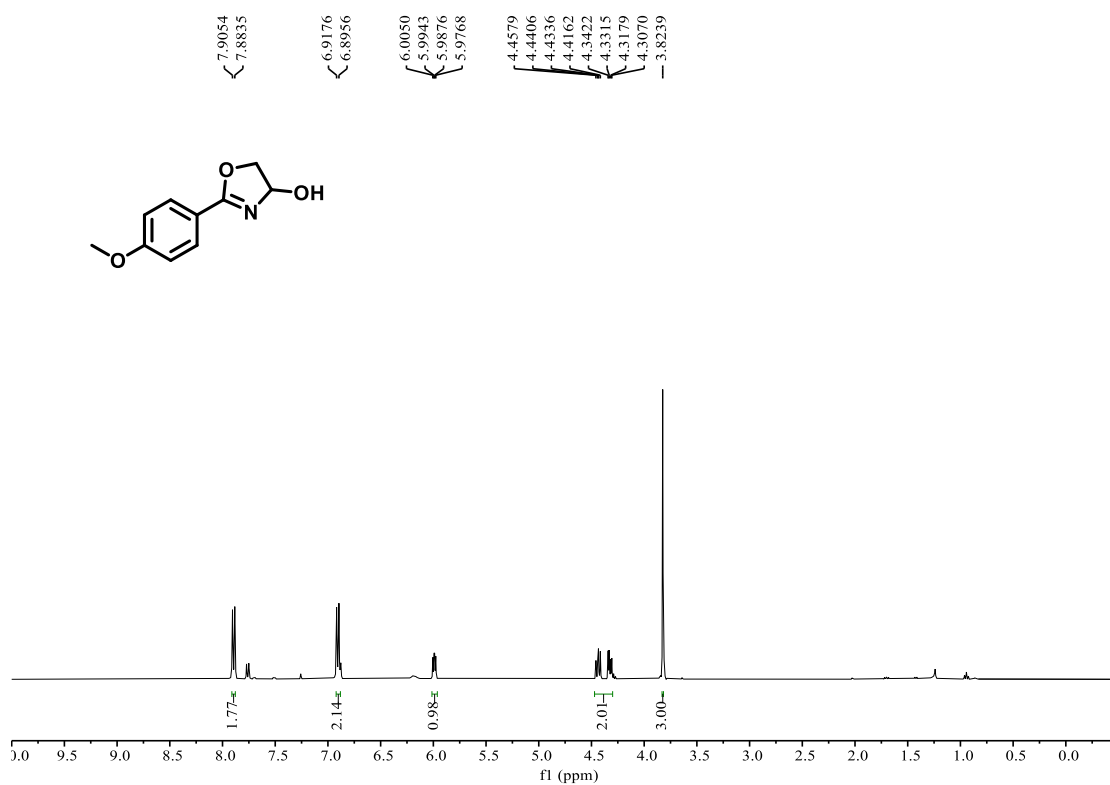
¹H NMR (400 MHz, CDCl₃) of compound **2g**



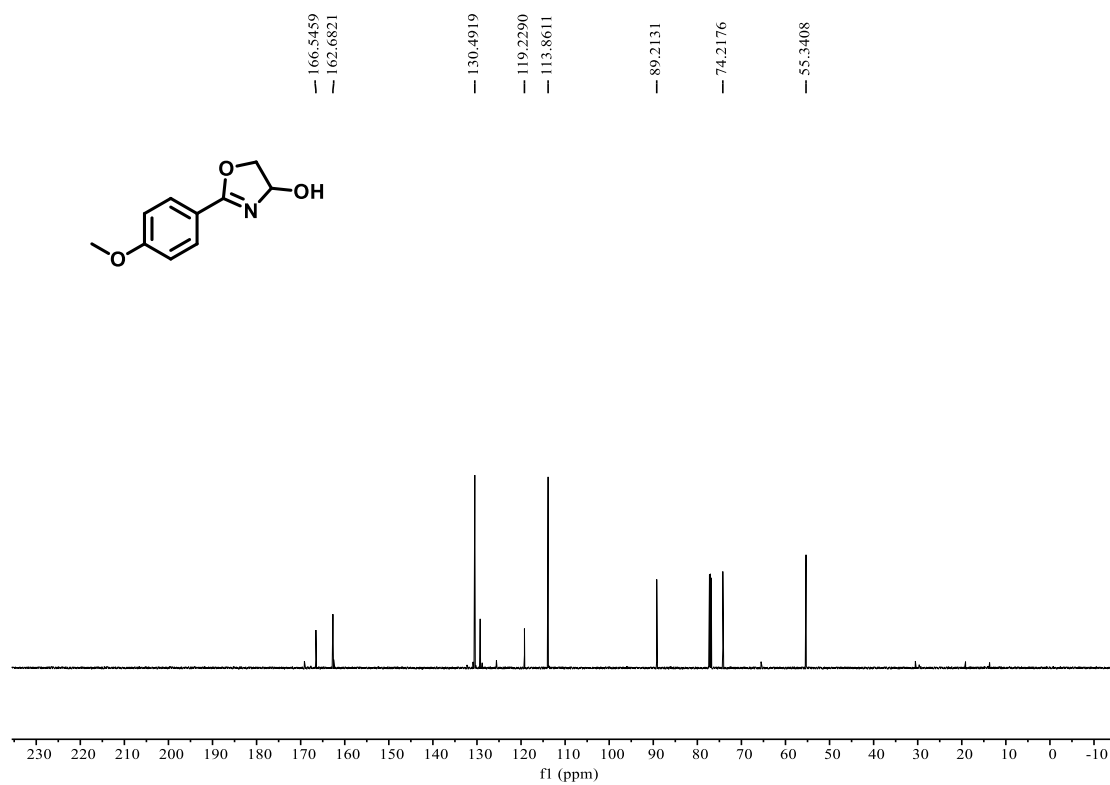
¹³C NMR (151 MHz, CDCl₃) of compound **2g**



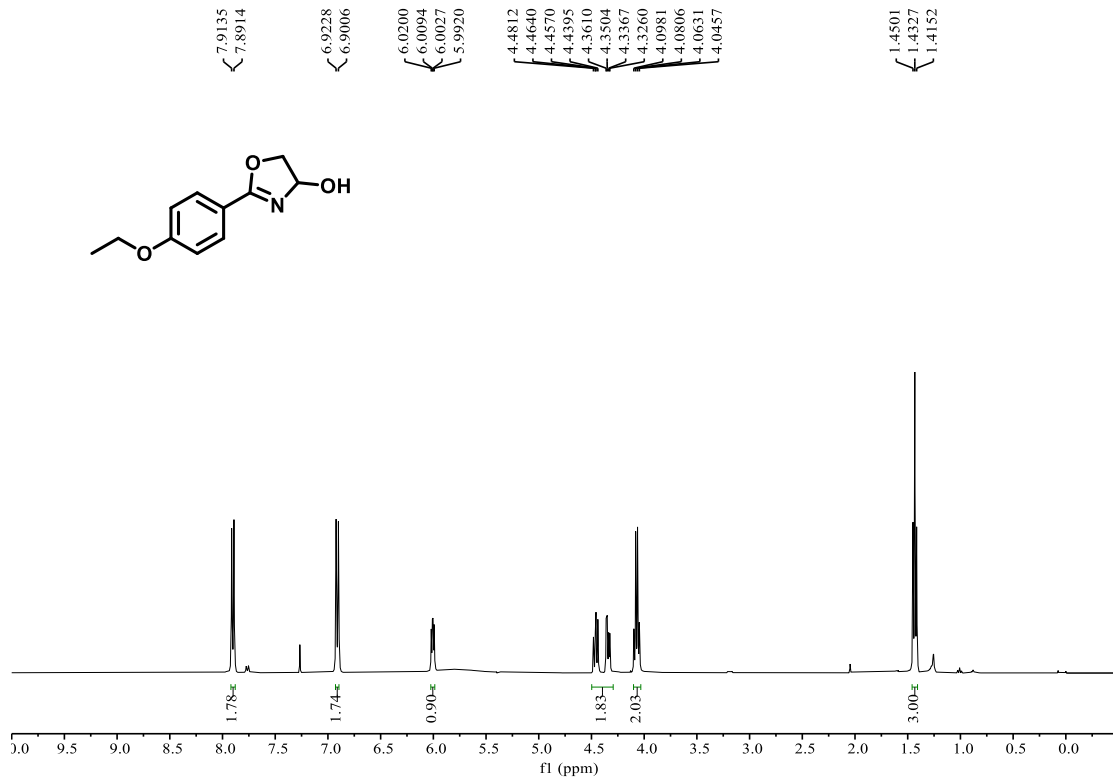
¹H NMR (400 MHz, CDCl₃) of compound **2h**



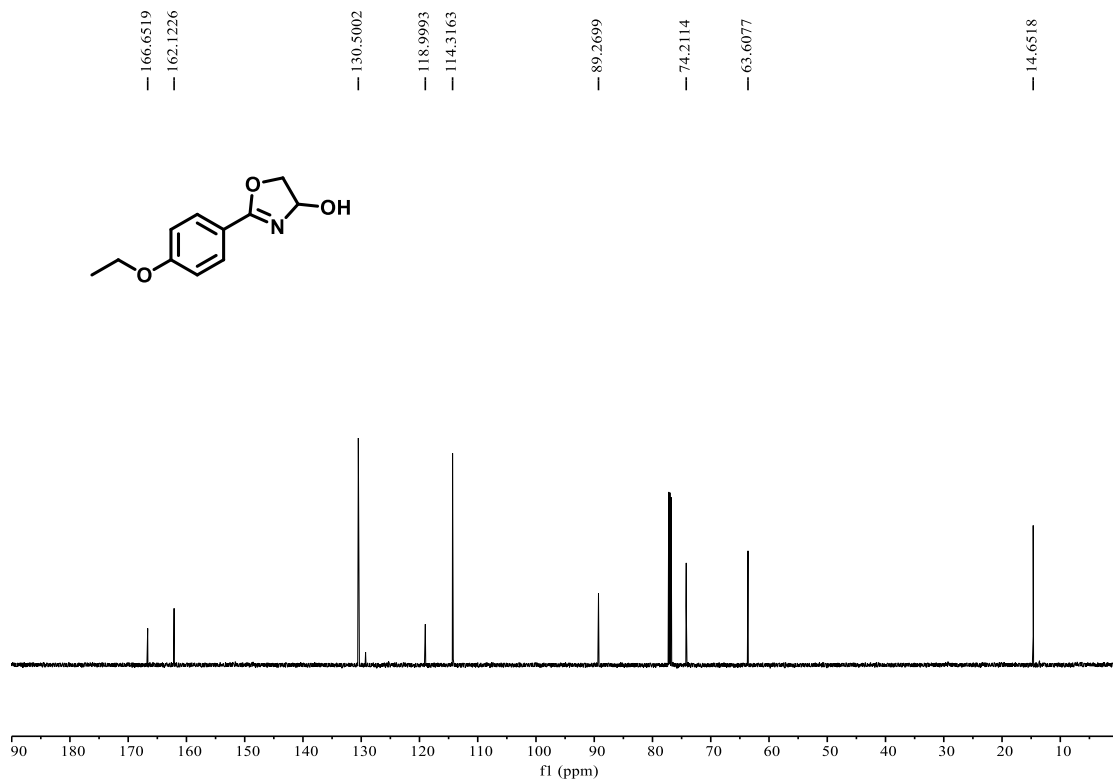
¹³C NMR (151 MHz, CDCl₃) of compound **2h**



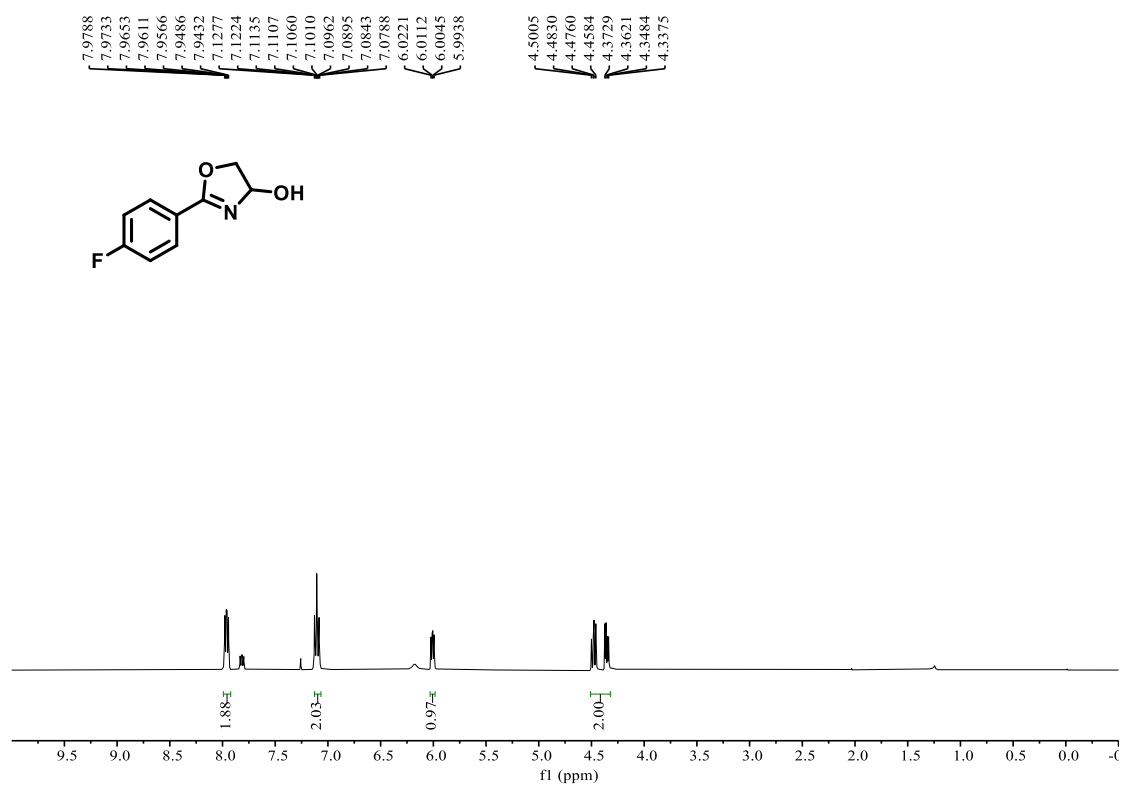
¹H NMR (400 MHz, CDCl₃) of compound **2i**



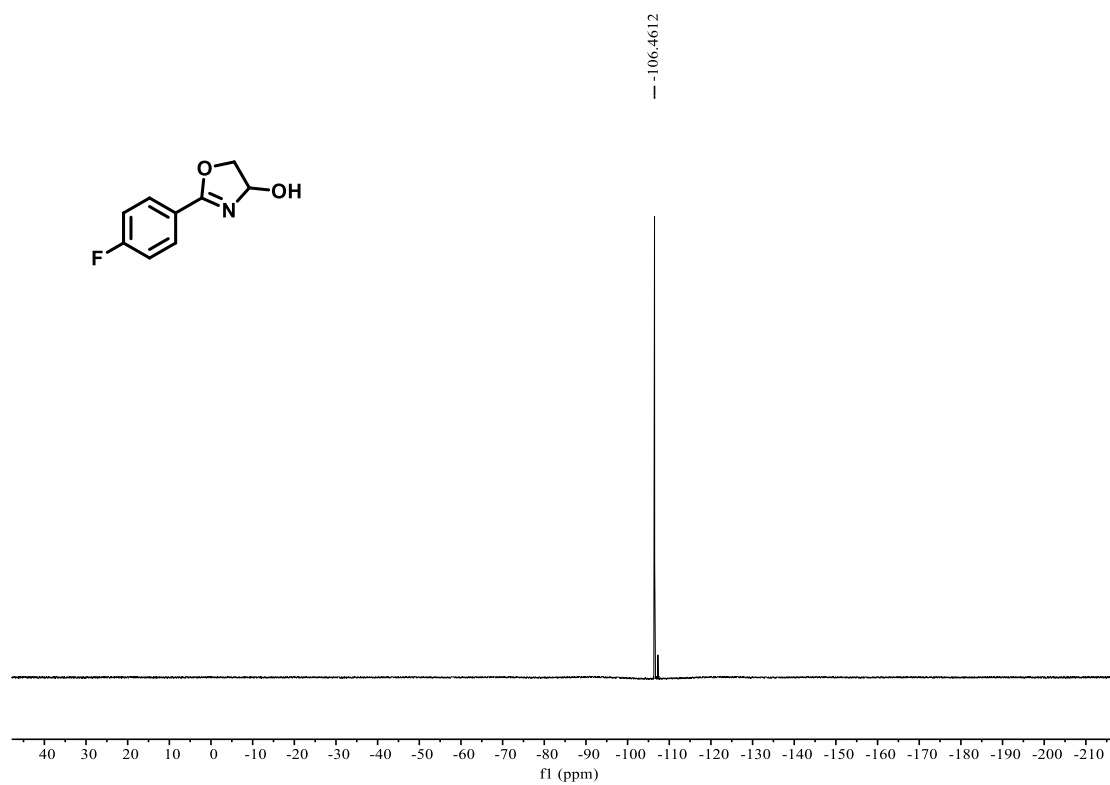
¹³C NMR (151 MHz, CDCl₃) of compound **2i**



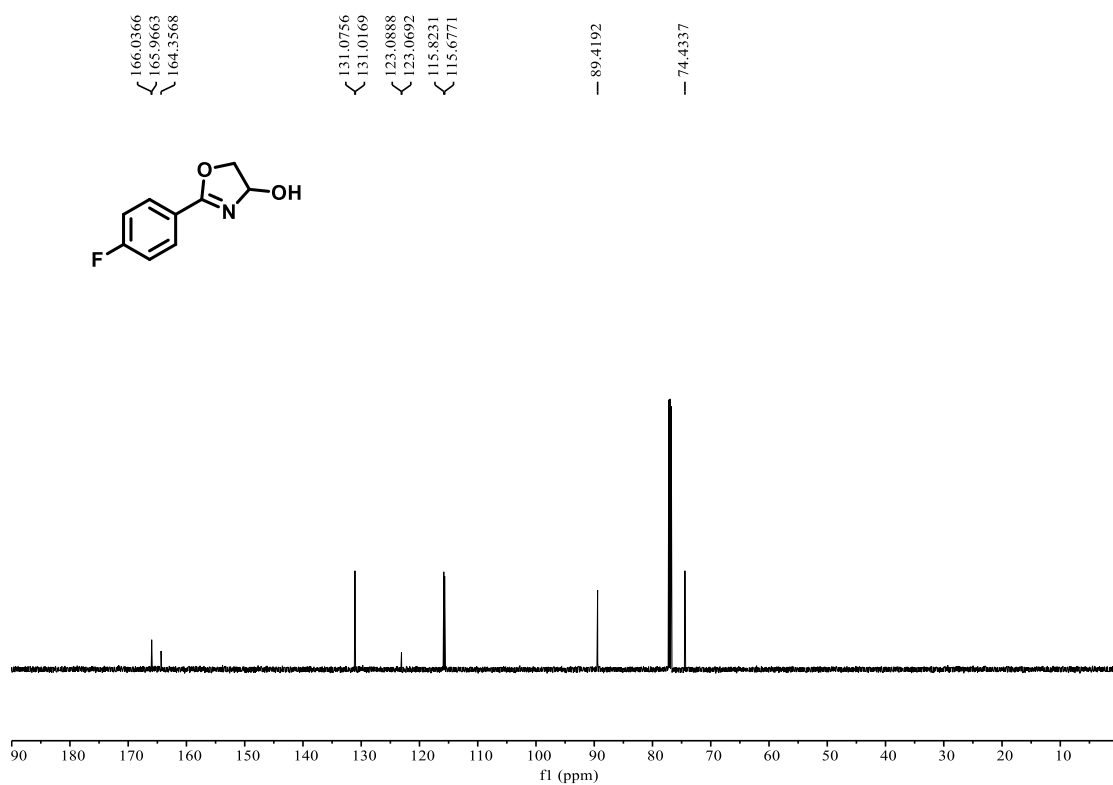
¹H NMR (400 MHz, CDCl₃) of compound **2j**



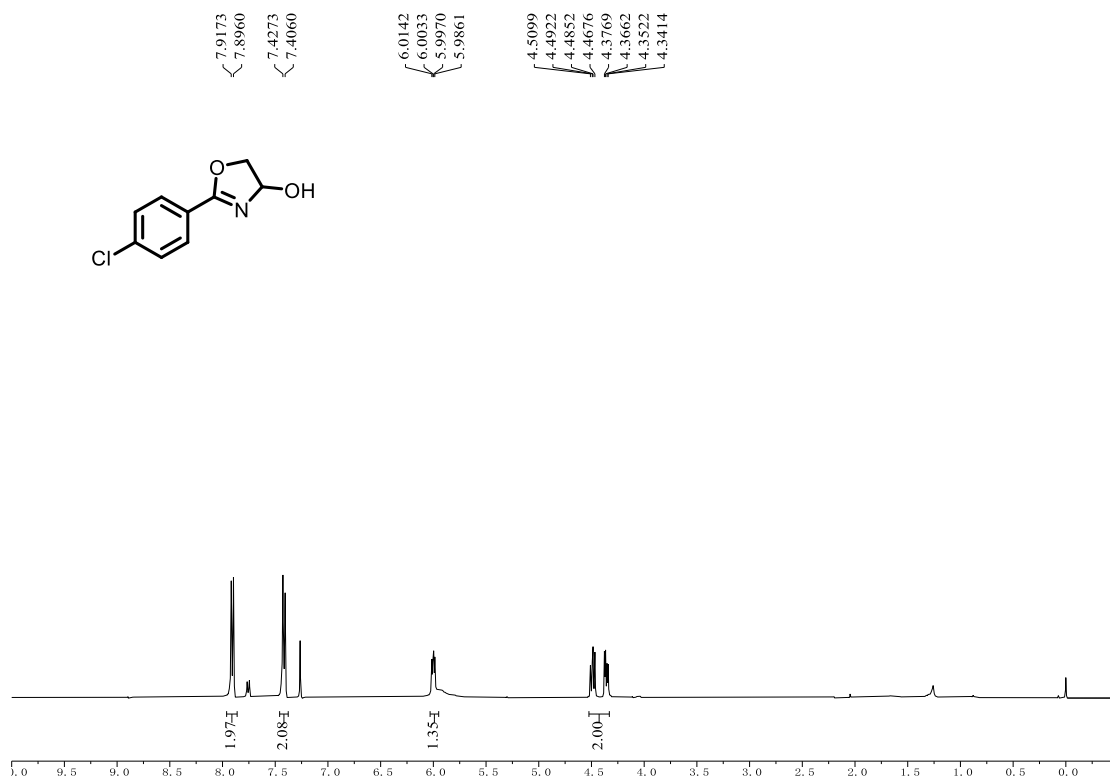
¹⁹F NMR (376 MHz, CDCl₃) of compound **2j**



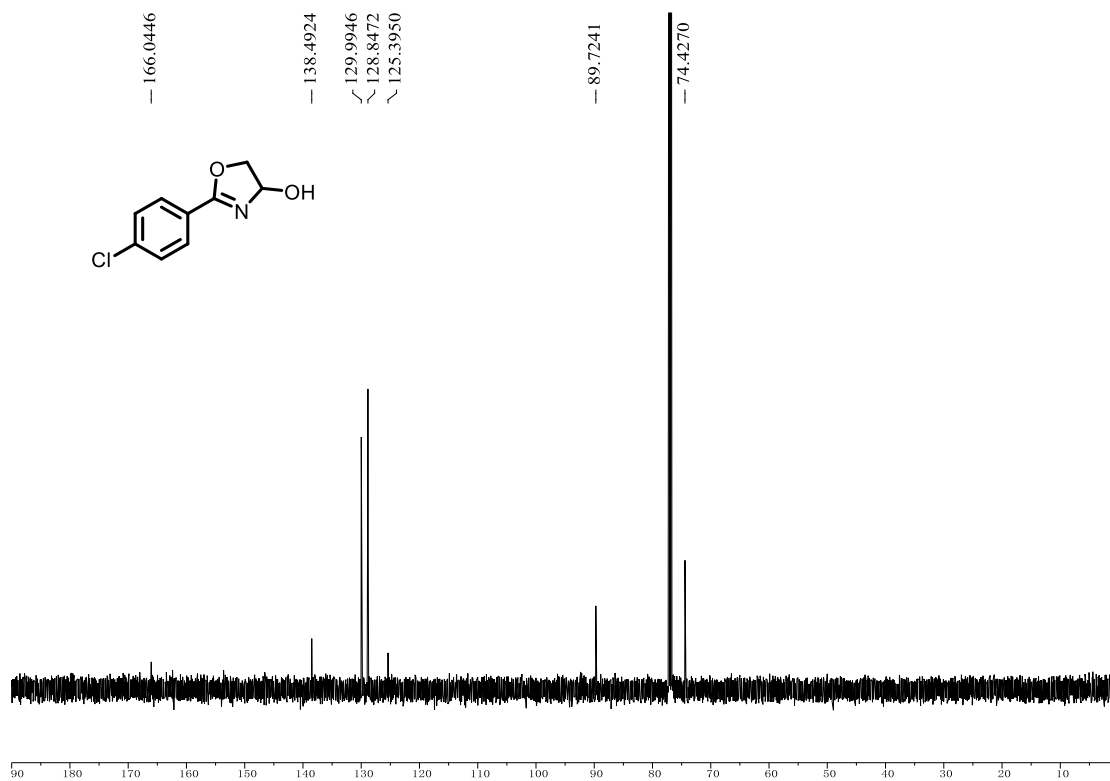
¹³C NMR (151 MHz, CDCl₃) of compound **2j**



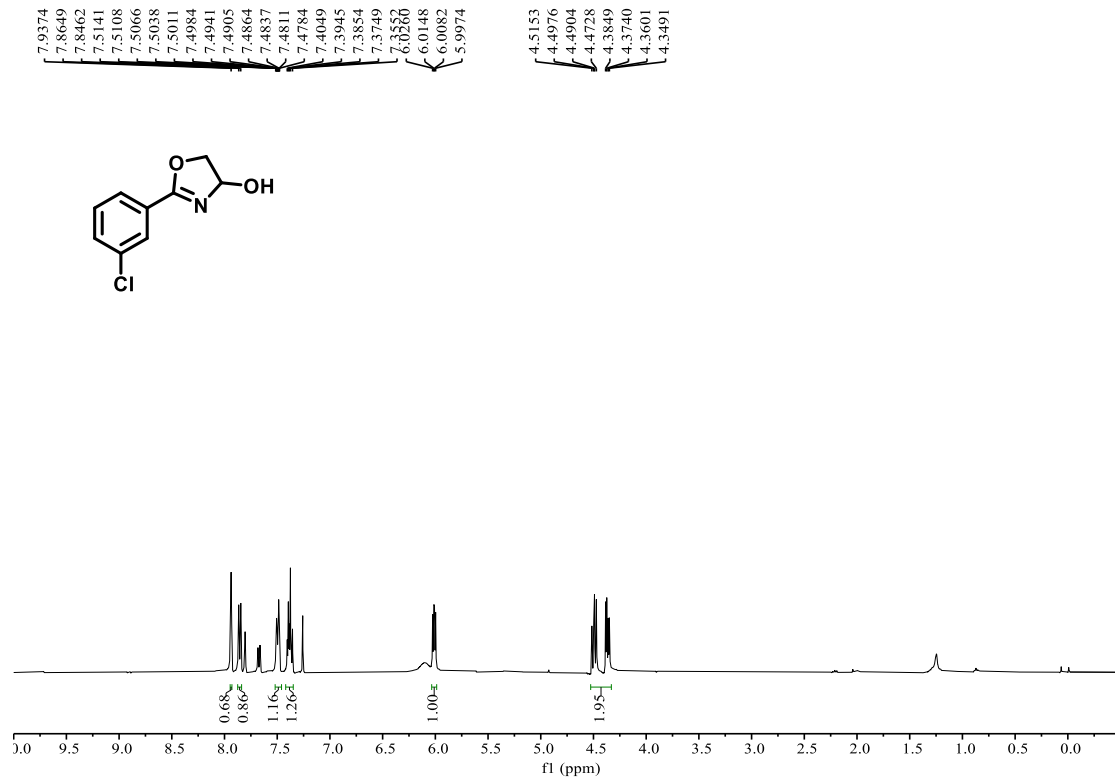
¹H NMR (400 MHz, CDCl₃) of compound **2k**



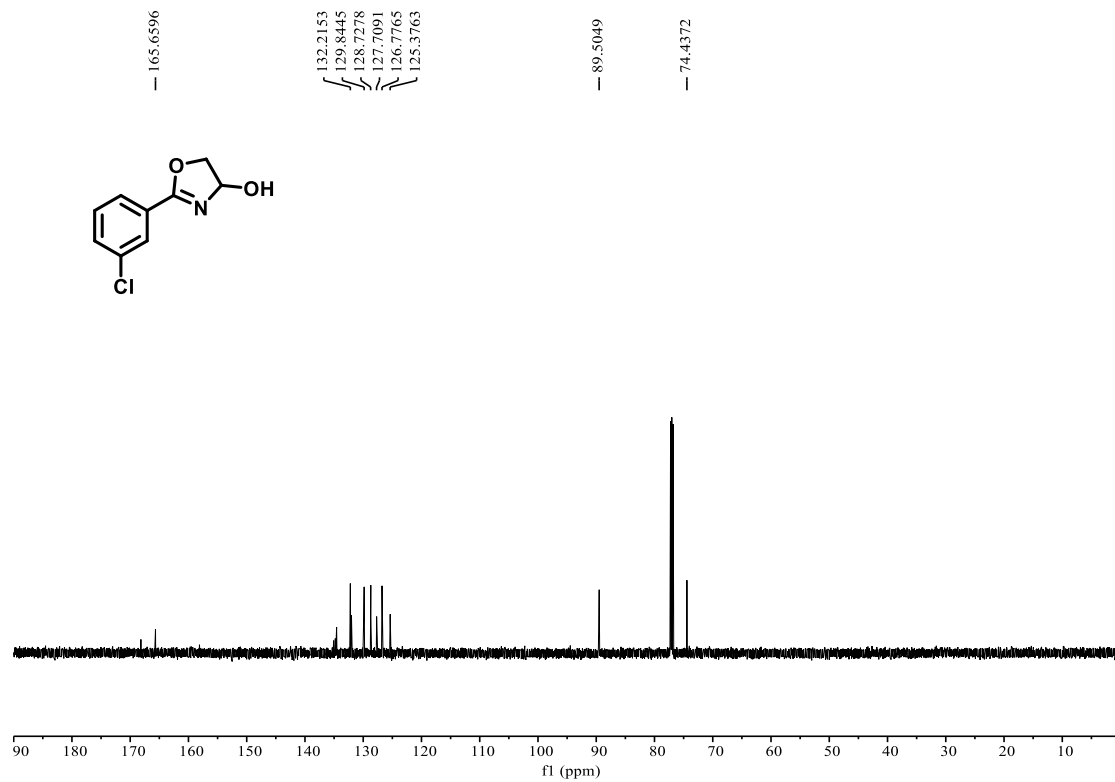
¹³C NMR (151 MHz, CDCl₃) of compound **2k**



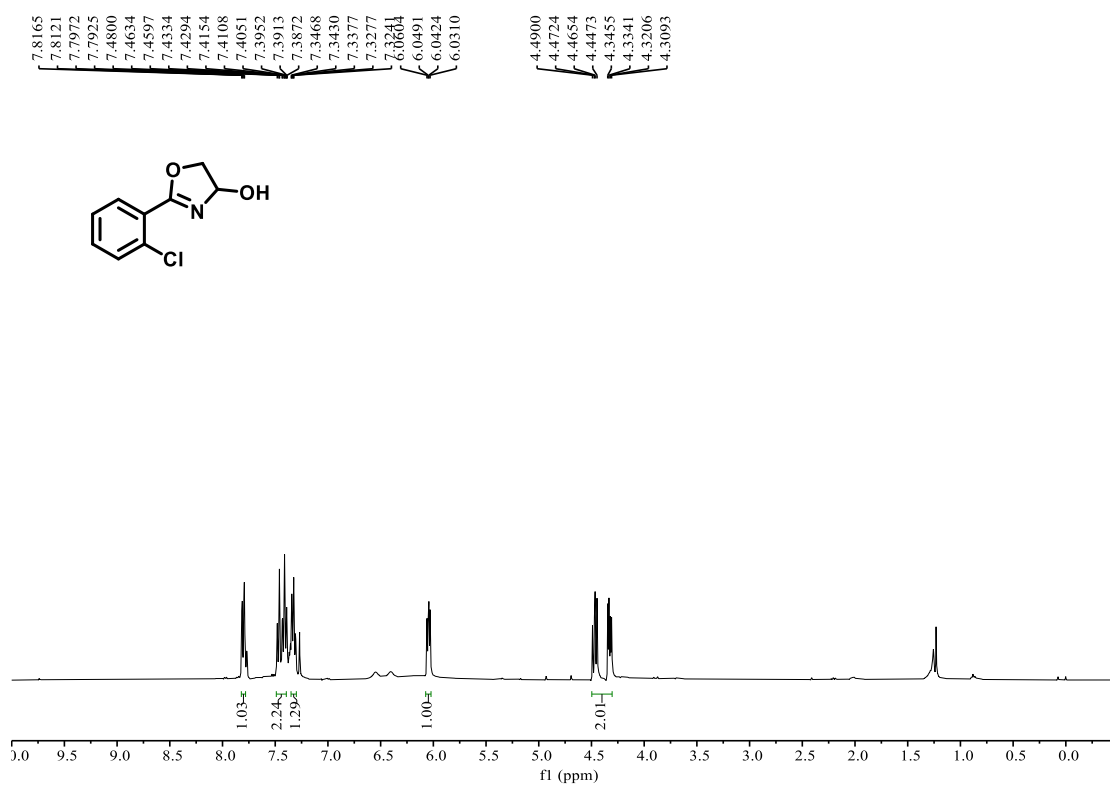
¹H NMR (400 MHz, CDCl₃) of compound **21**



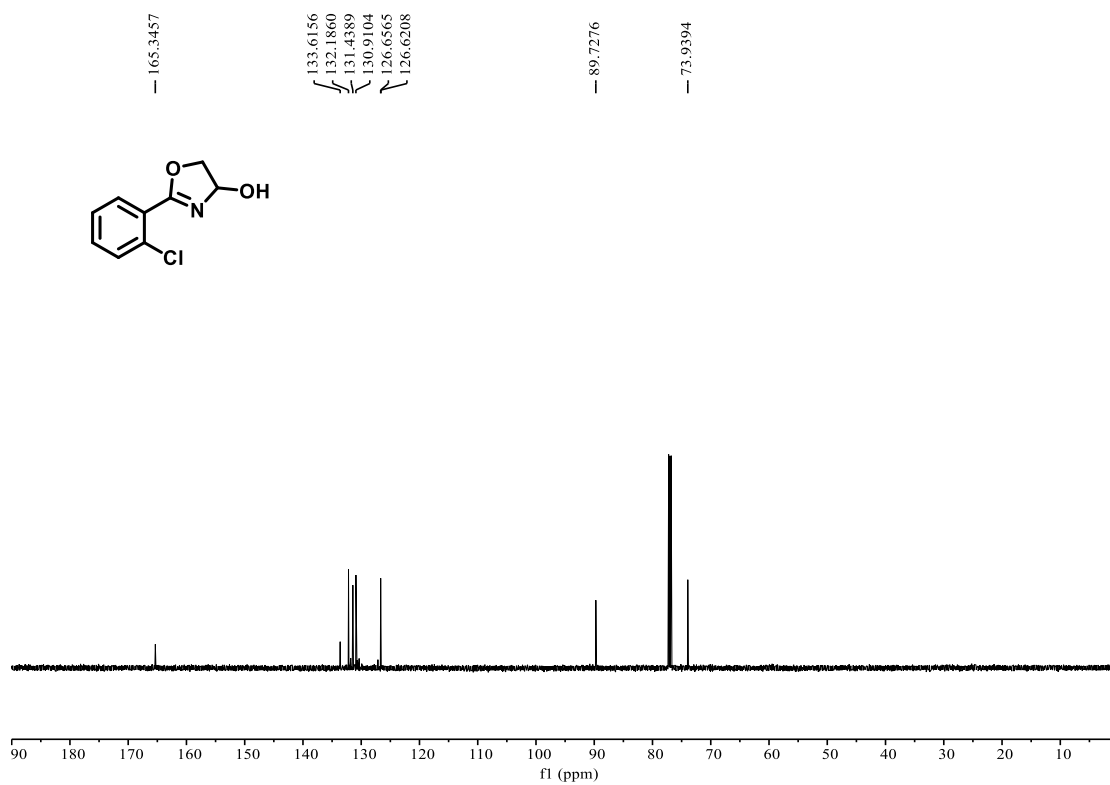
¹³C NMR (151 MHz, CDCl₃) of compound **21**



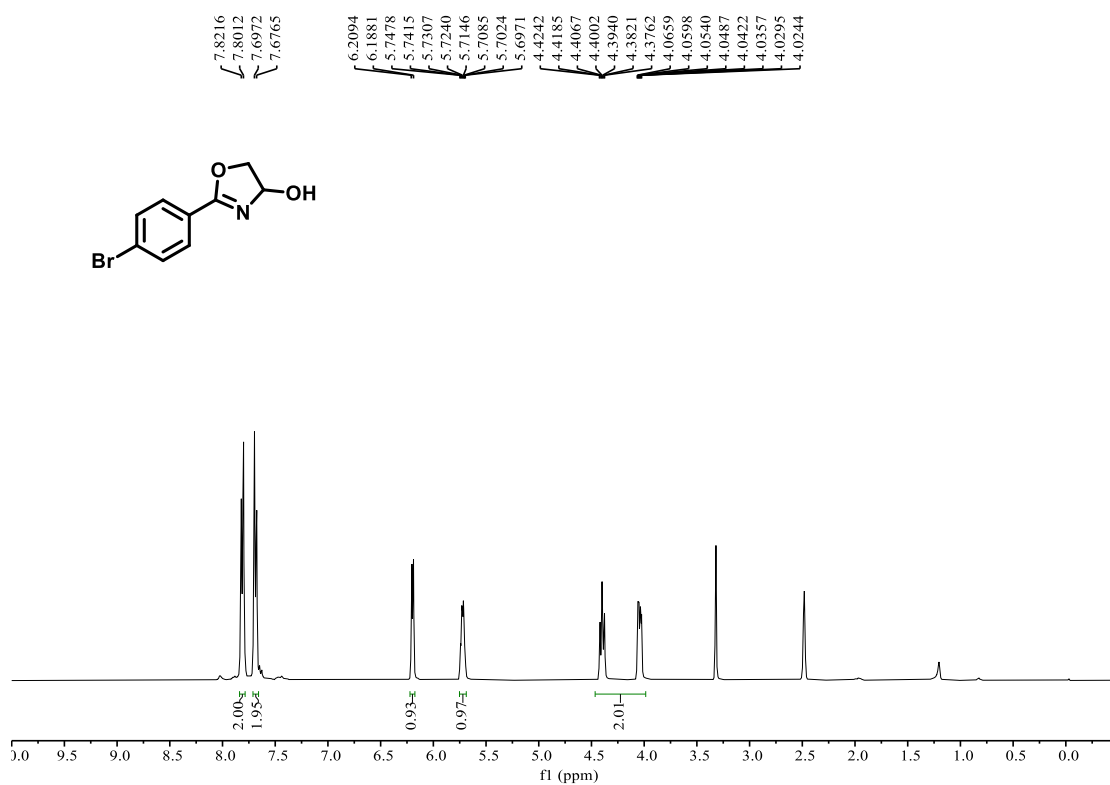
¹H NMR (400 MHz, CDCl₃) of compound **2m**



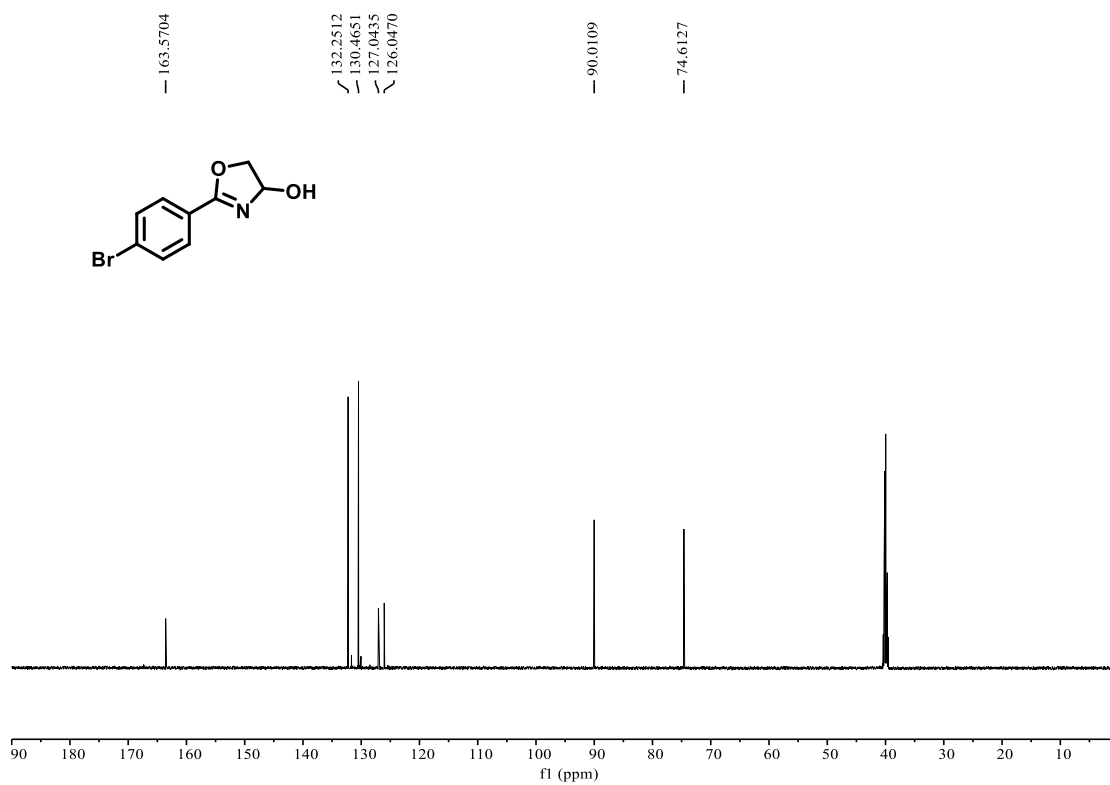
¹³C NMR (151 MHz, CDCl₃) of compound **2m**



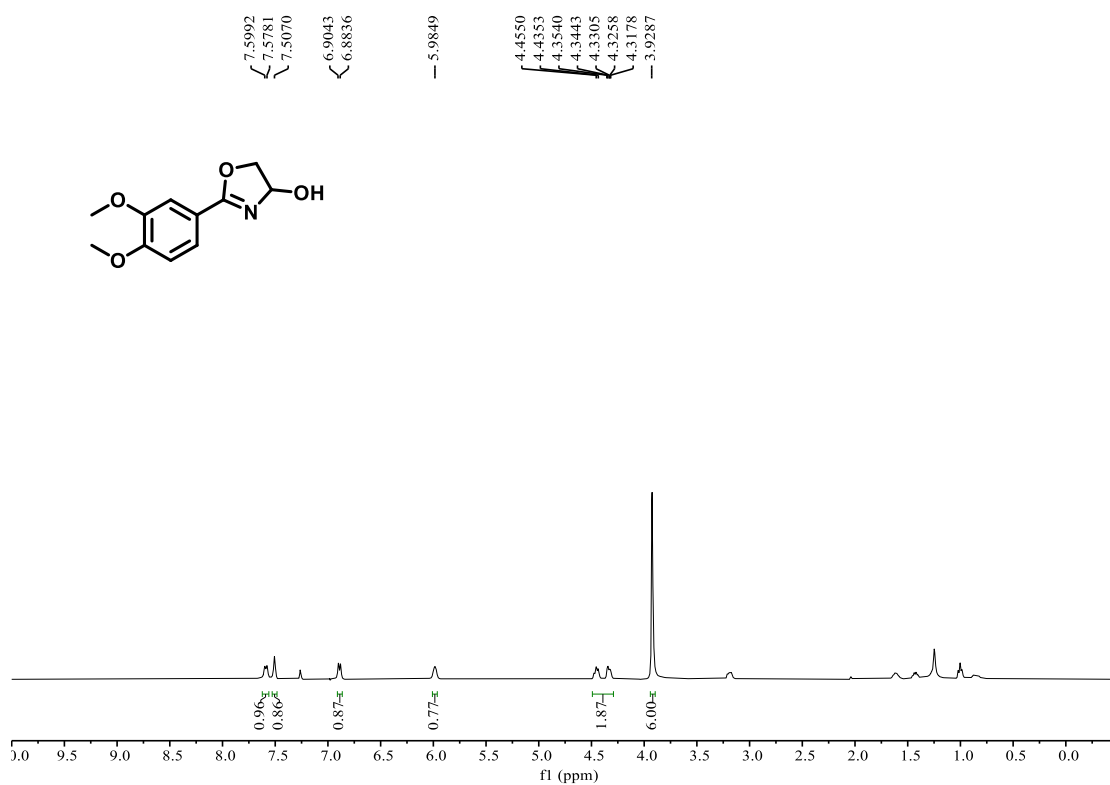
¹H NMR (400 MHz, DMSO-*d*₆) of compound **2n**



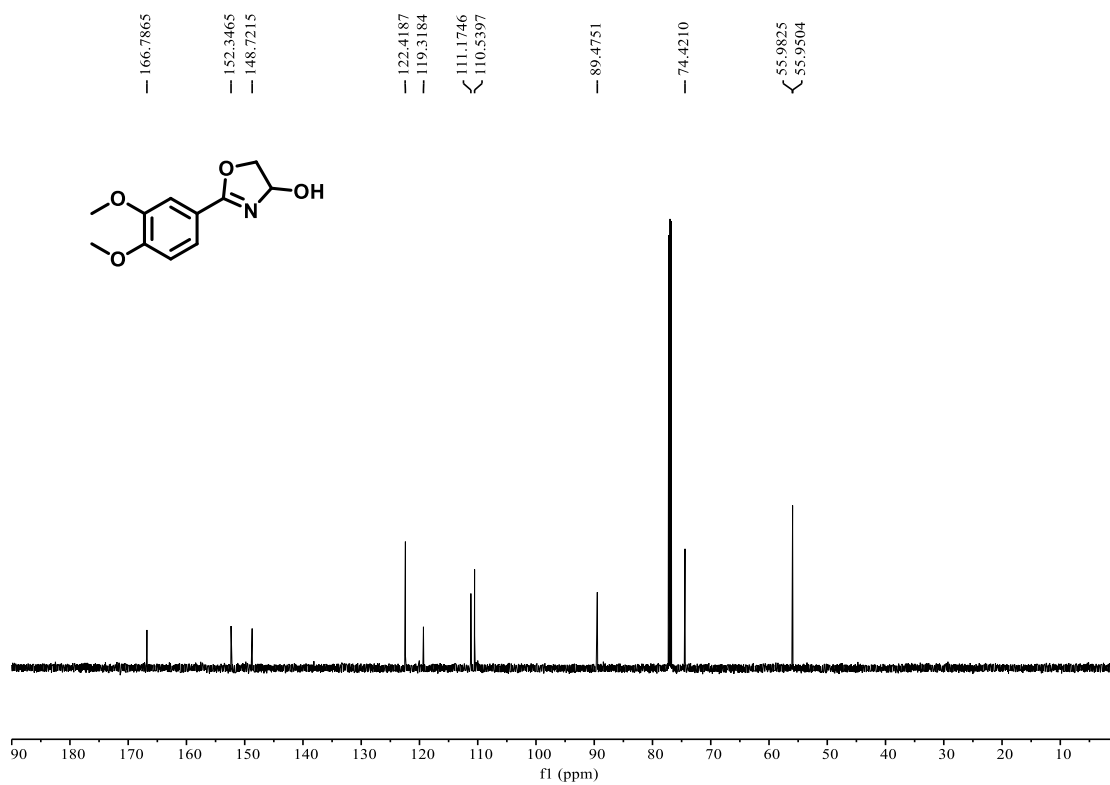
¹³C NMR (151 MHz, DMSO-*d*₆) of compound **2n**



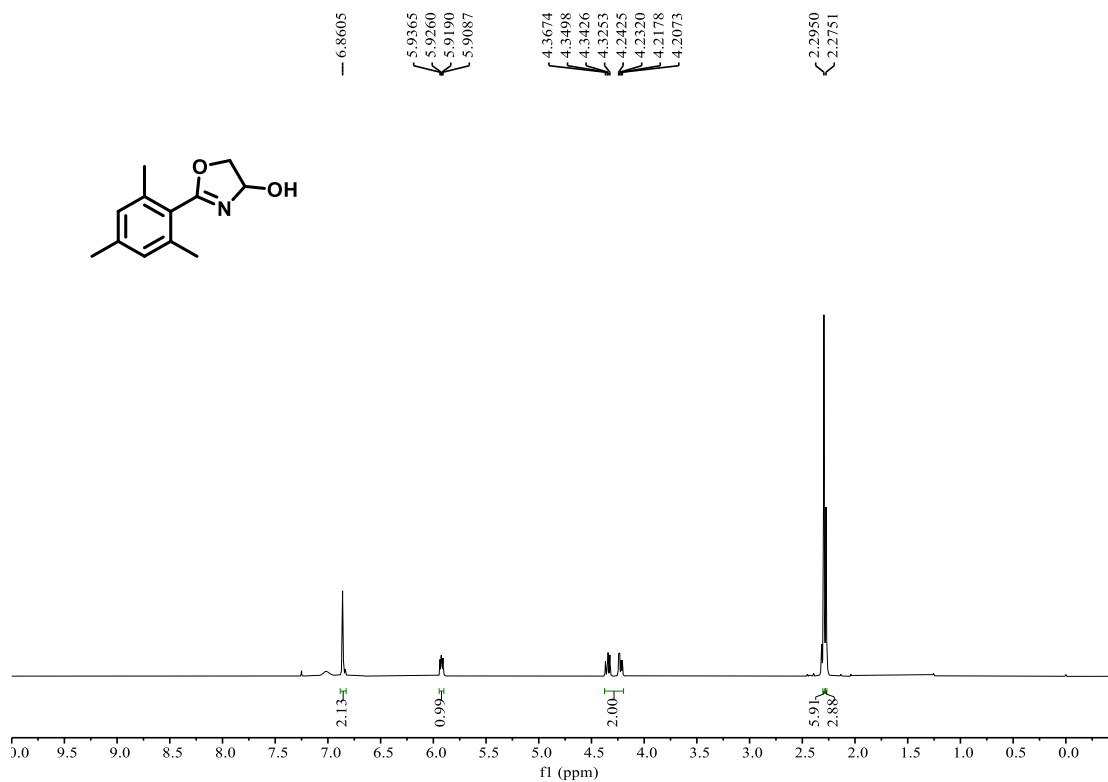
¹H NMR (400 MHz, CDCl₃) of compound **2o**



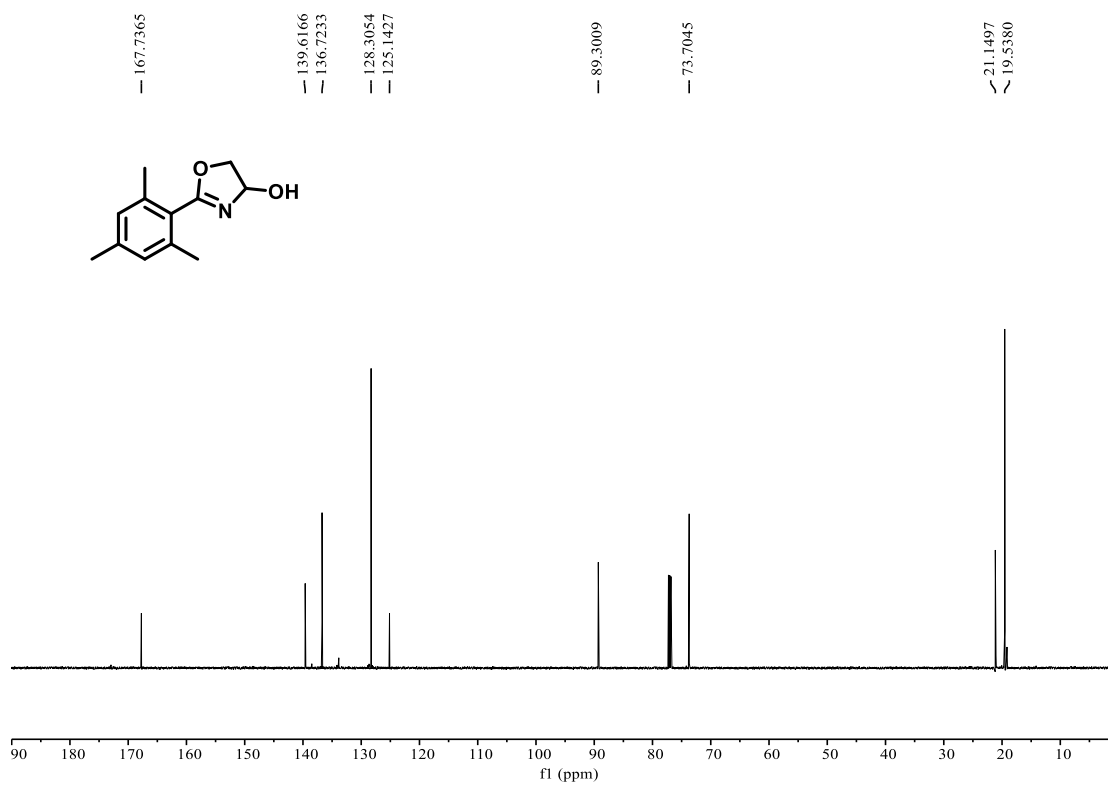
¹³C NMR (151 MHz, CDCl₃) of compound **2o**



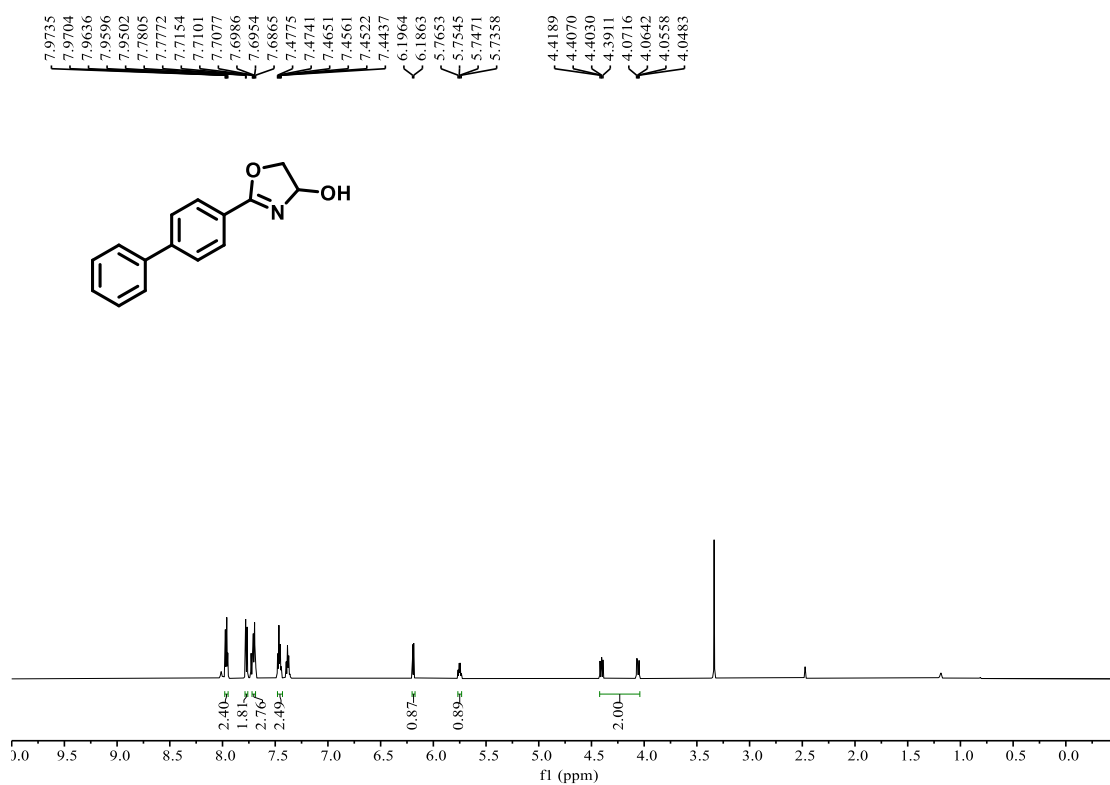
¹H NMR (400 MHz, CDCl₃) of compound **2p**



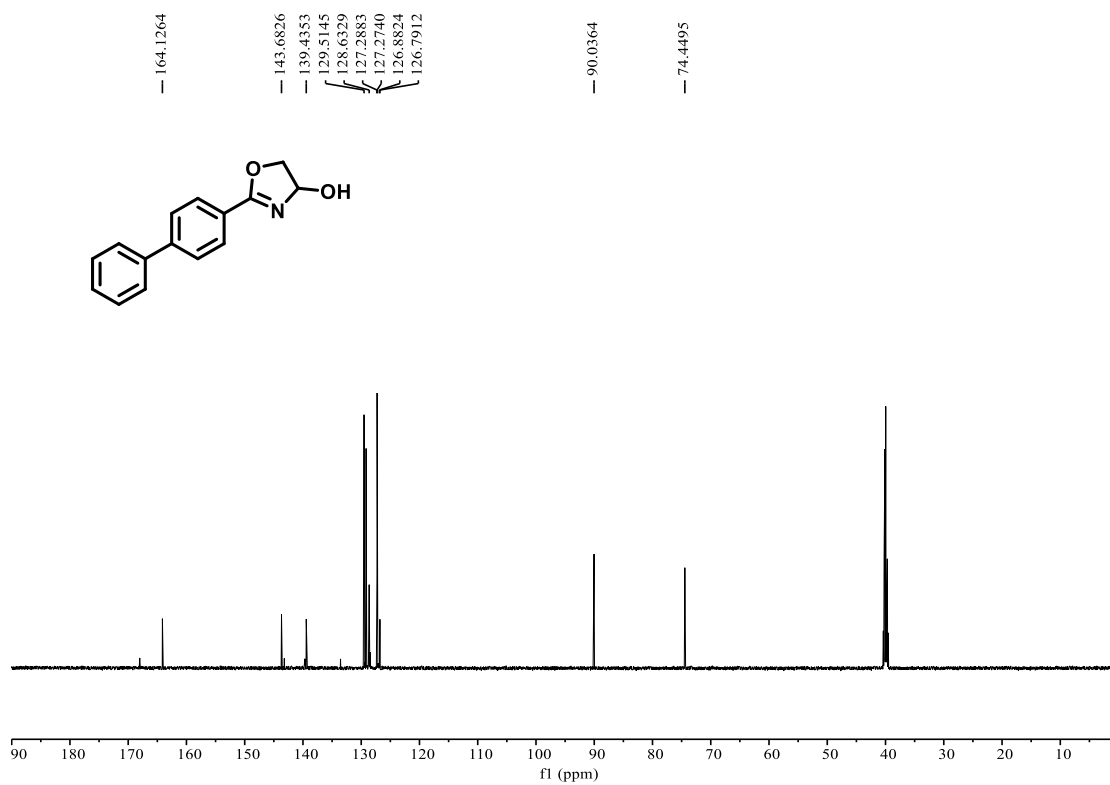
¹³C NMR (151 MHz, CDCl₃) of compound **2p**



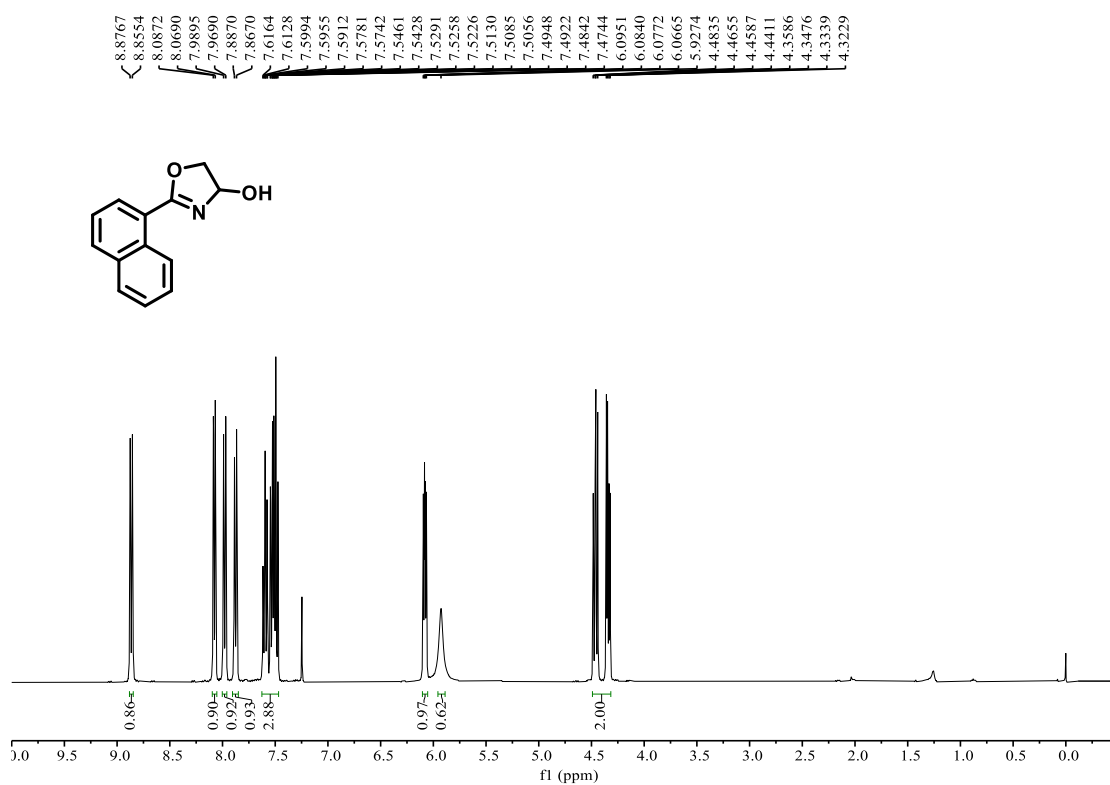
¹H NMR (400 MHz, DMSO-*d*₆) of compound **2q**



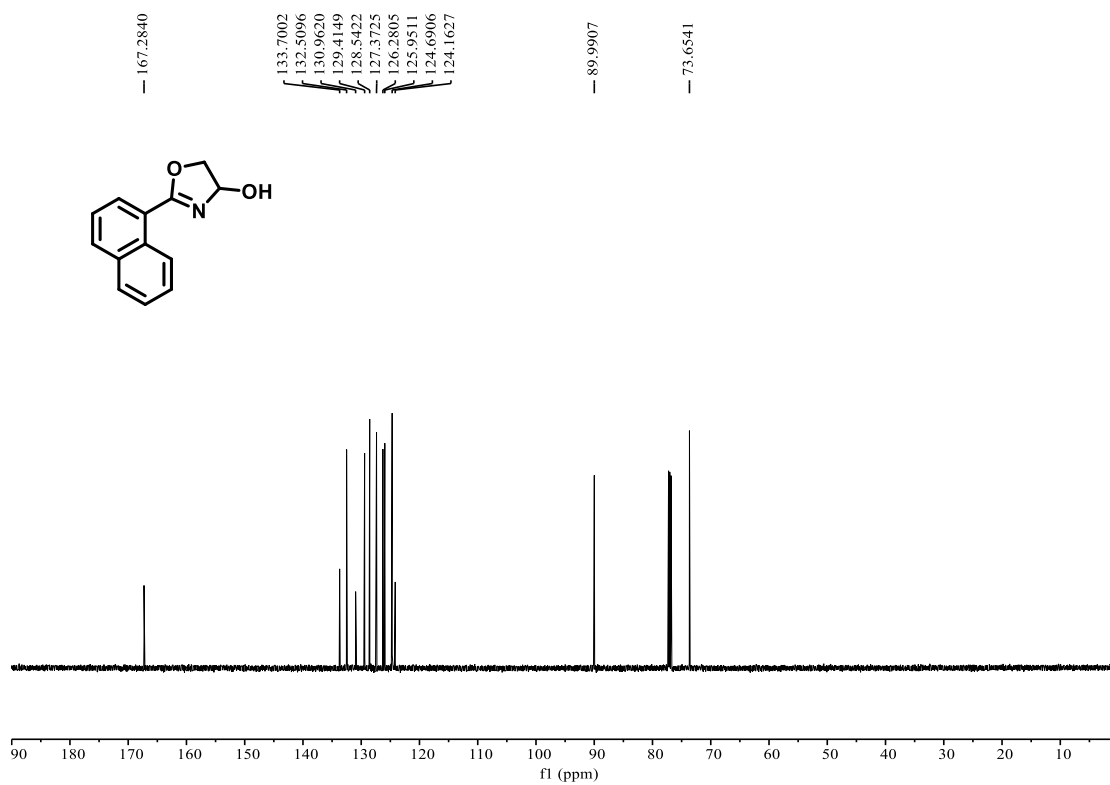
¹³C NMR (151 MHz, DMSO-*d*₆) of compound **2q**



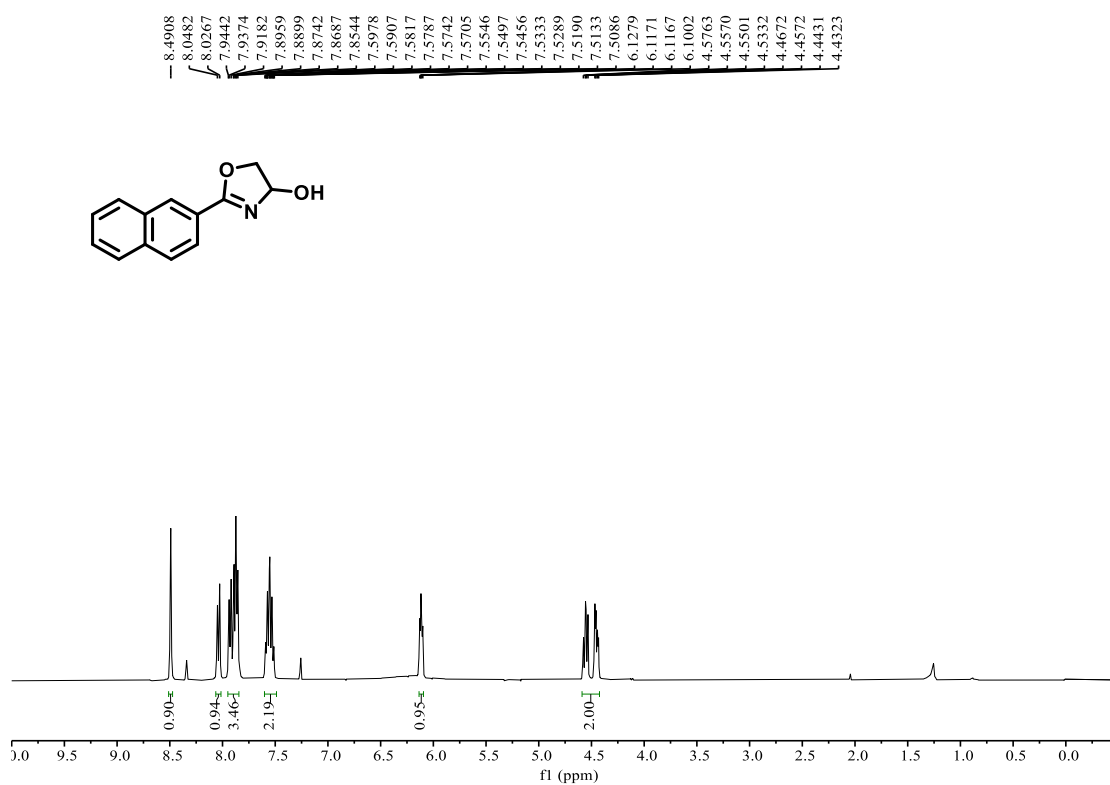
¹H NMR (400 MHz, CDCl₃) of compound **2r**



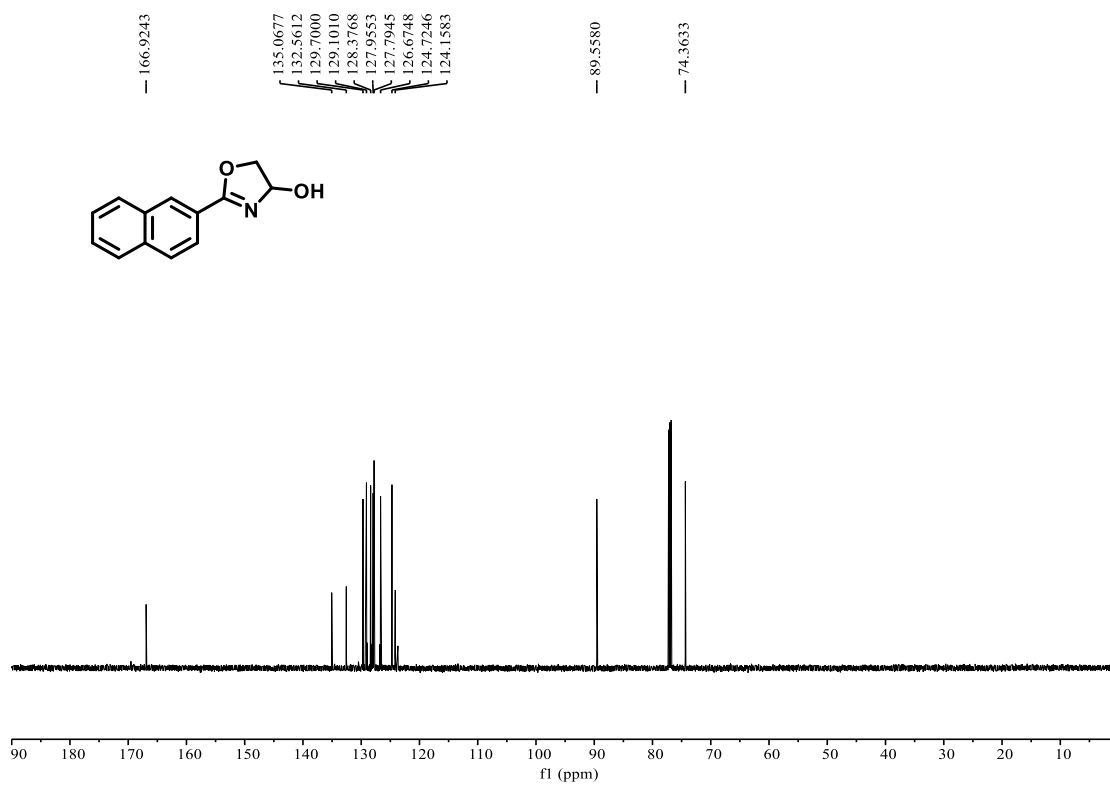
¹³C NMR (151 MHz, CDCl₃) of compound **2r**



¹H NMR (400 MHz, CDCl₃) of compound **2s**

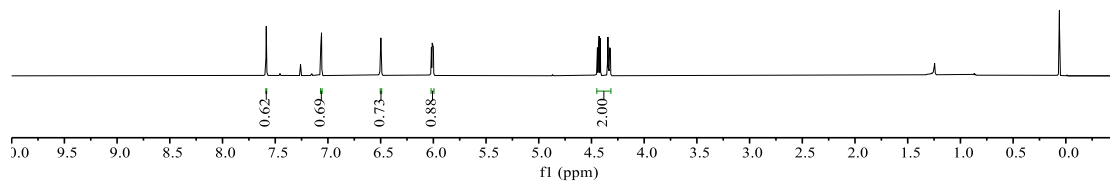
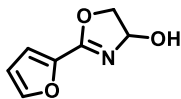


¹³C NMR (151 MHz, CDCl₃) of compound **2s**



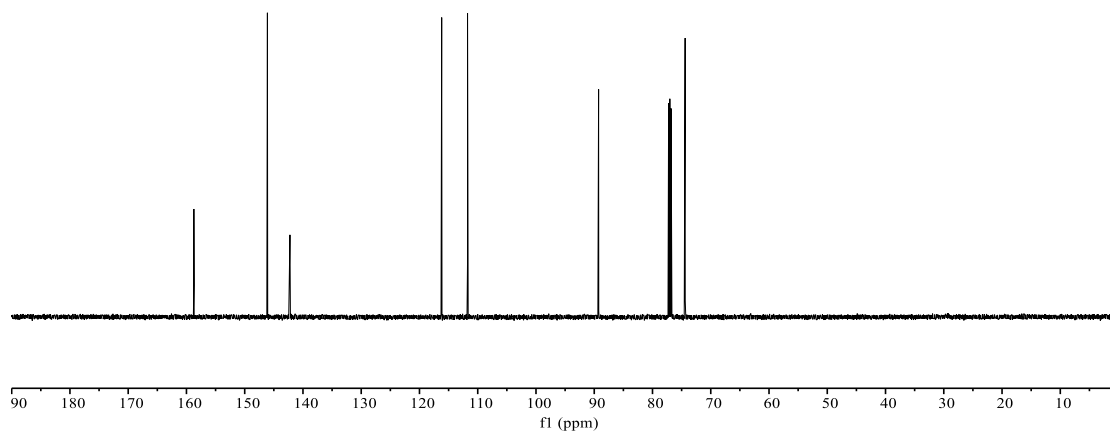
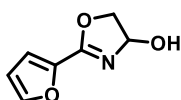
¹H NMR (600 MHz, CDCl₃) of compound **2t**

7.5866
7.5851
7.5836
7.5821
7.0667
7.0609
6.5009
6.4979
6.4950
6.4921
6.0183
6.0112
6.0068
5.9999
4.4438
4.4322
4.4276
4.4163
4.3440
4.3370
4.3279
4.3209



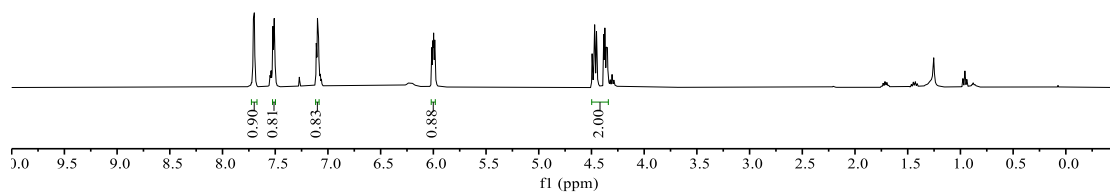
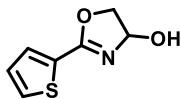
¹³C NMR (151 MHz, CDCl₃) of compound **2t**

158.7272
146.1043
142.2346
116.1871
111.7499
89.2513
74.3972



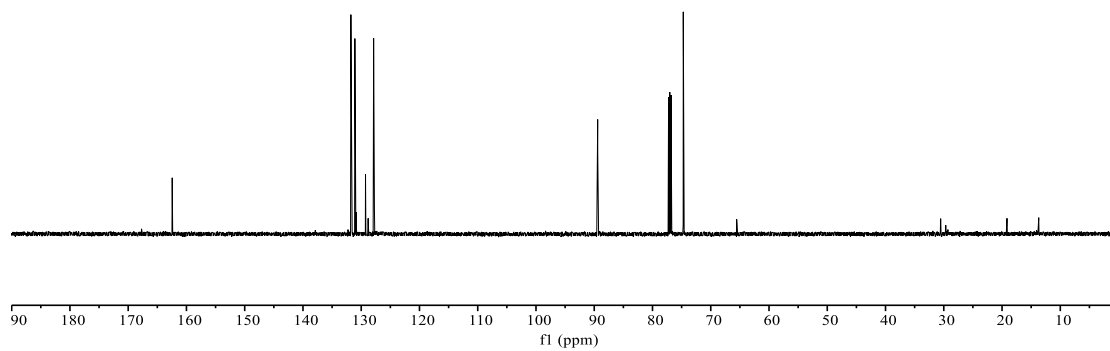
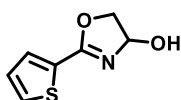
¹H NMR (400 MHz, CDCl₃) of compound **2u**

7.7073
7.6980
7.5217
7.5099
7.1102
7.0995
7.0883
6.0142
6.0037
5.9971
5.9863
4.4935
4.4763
4.4692
4.4520
4.3833
4.3728
4.3592
4.3484



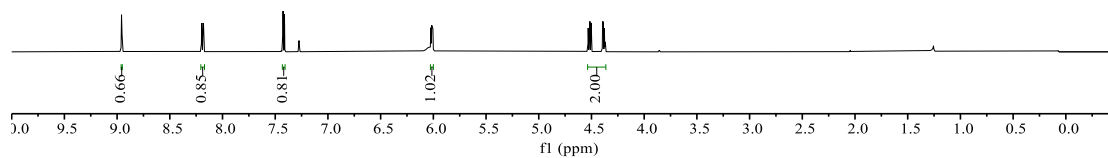
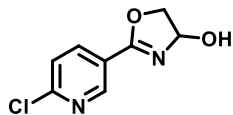
¹³C NMR (151 MHz, CDCl₃) of compound **2u**

162.4445
131.7759
131.0904
129.2603
127.8720
89.4123
74.7193



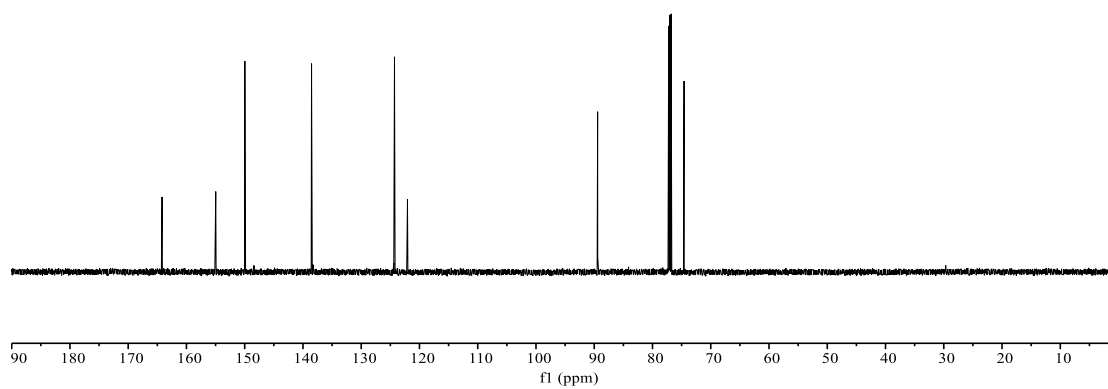
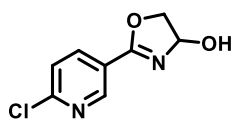
¹H NMR (600 MHz, CDCl₃) of compound **2v**

8.9580
8.9551
8.1984
8.1944
8.1845
8.1805
7.4264
7.4126
6.0231
6.0159
6.0114
6.0041
4.5312
4.5194
4.5147
4.5031
4.3943
4.3869
4.3777
4.3705



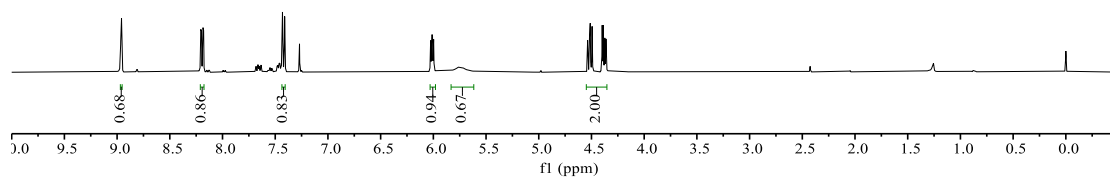
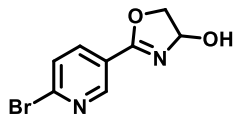
¹³C NMR (151 MHz, CDCl₃) of compound **2v**

164.1886
154.9719
149.9747
138.5282
124.2883
122.0576
89.4159
74.5815



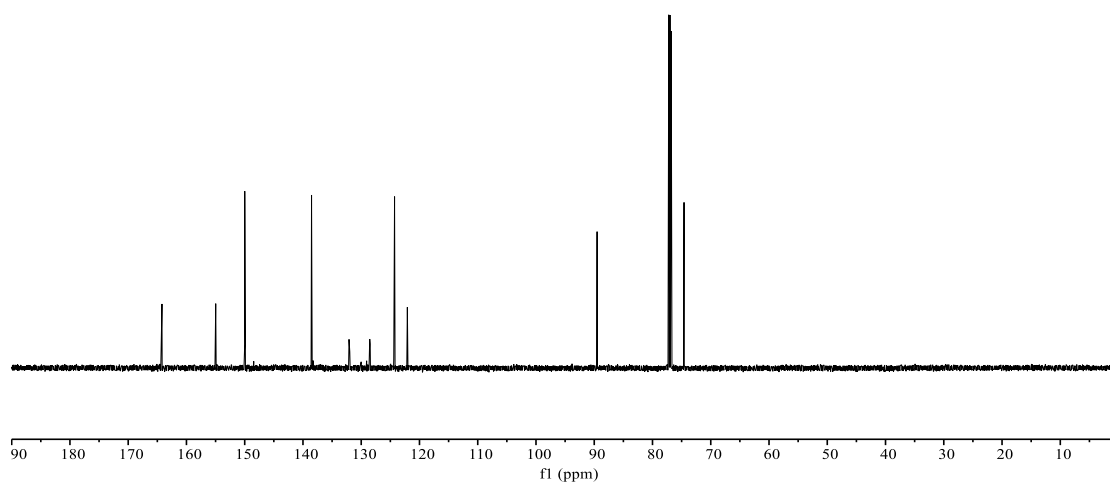
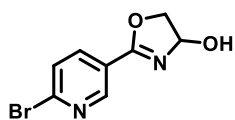
¹H NMR (400 MHz, CDCl₃) of compound **2w**

8.9624
8.9584
8.2060
8.2000
8.1852
8.1792
7.4310
7.4102
6.0259
6.0147
6.0082
5.9975
5.7455
4.5366
4.5190
4.5116
4.4941
4.3985
4.3875
4.3735
4.3626

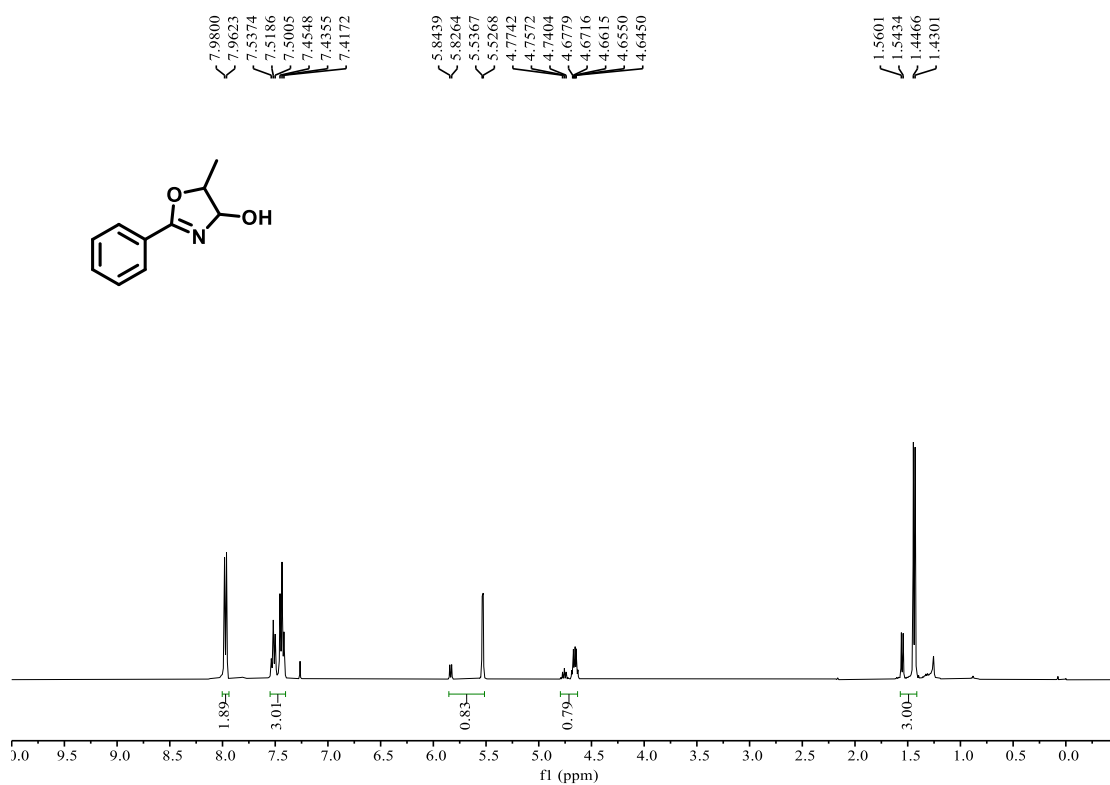


¹³C NMR (151 MHz, CDCl₃) of compound **2w**

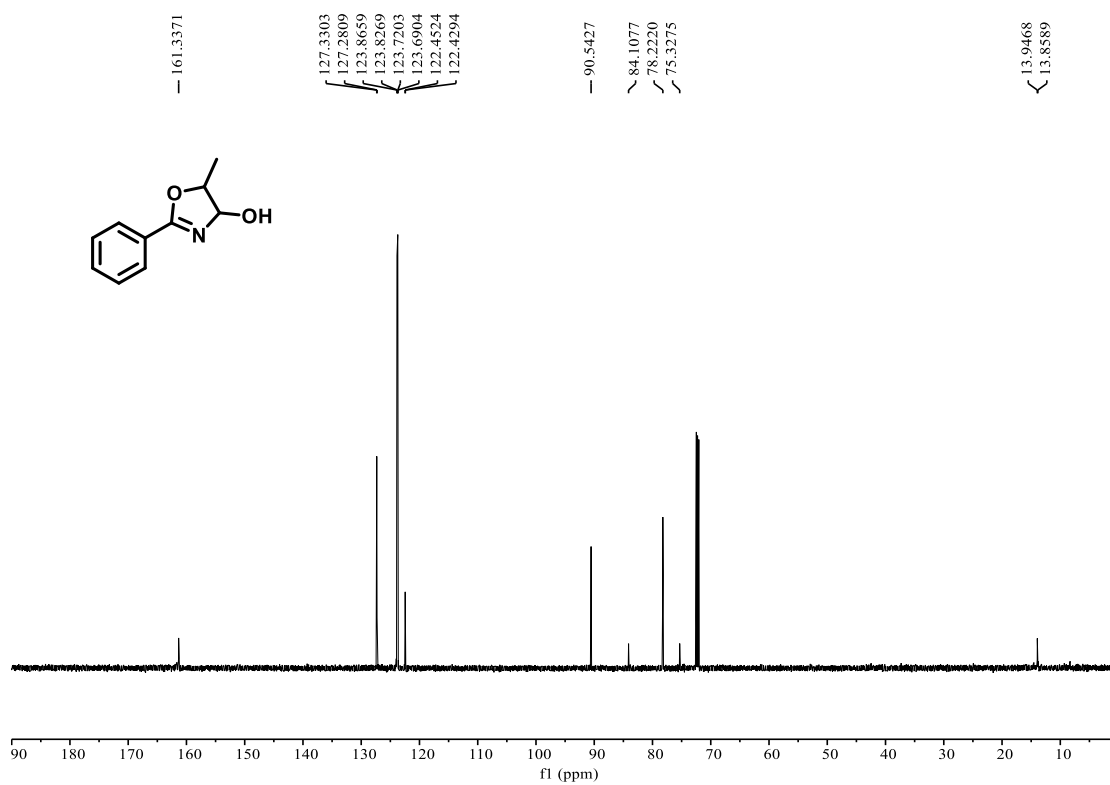
164.2037
154.9756
149.9907
138.5282
124.2770
122.0820
89.5117
74.5855



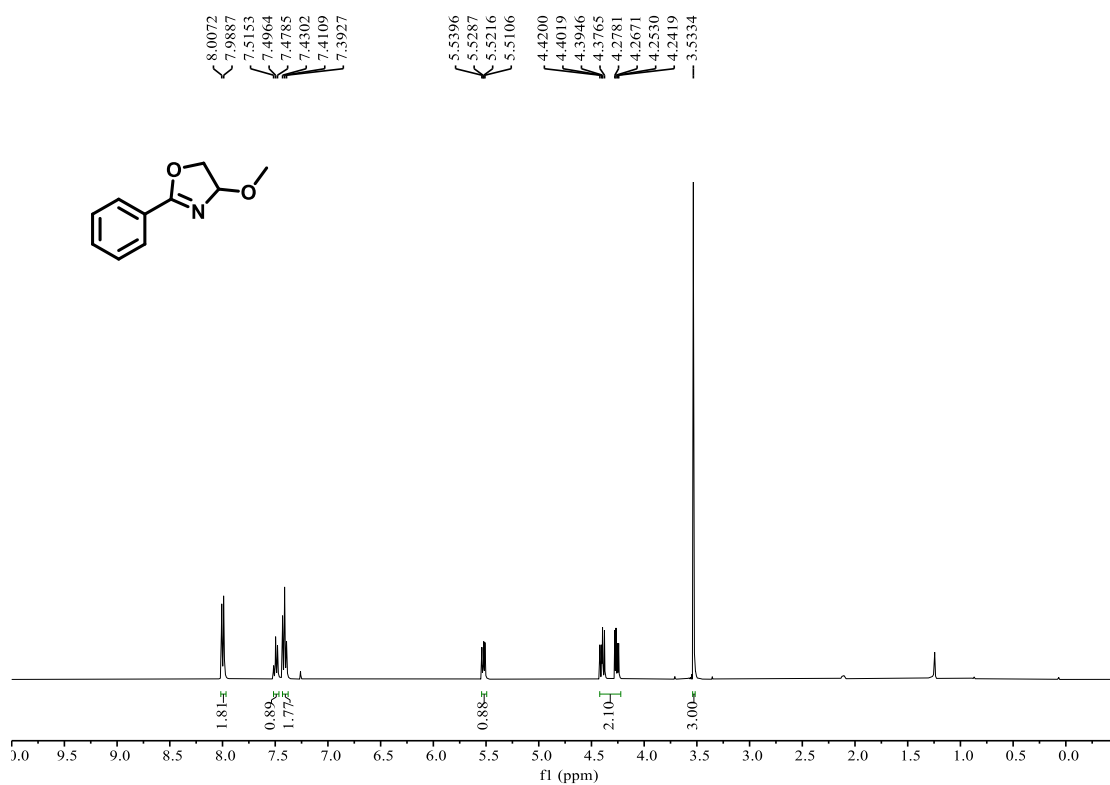
¹H NMR (400 MHz, CDCl₃) of compound **2x**



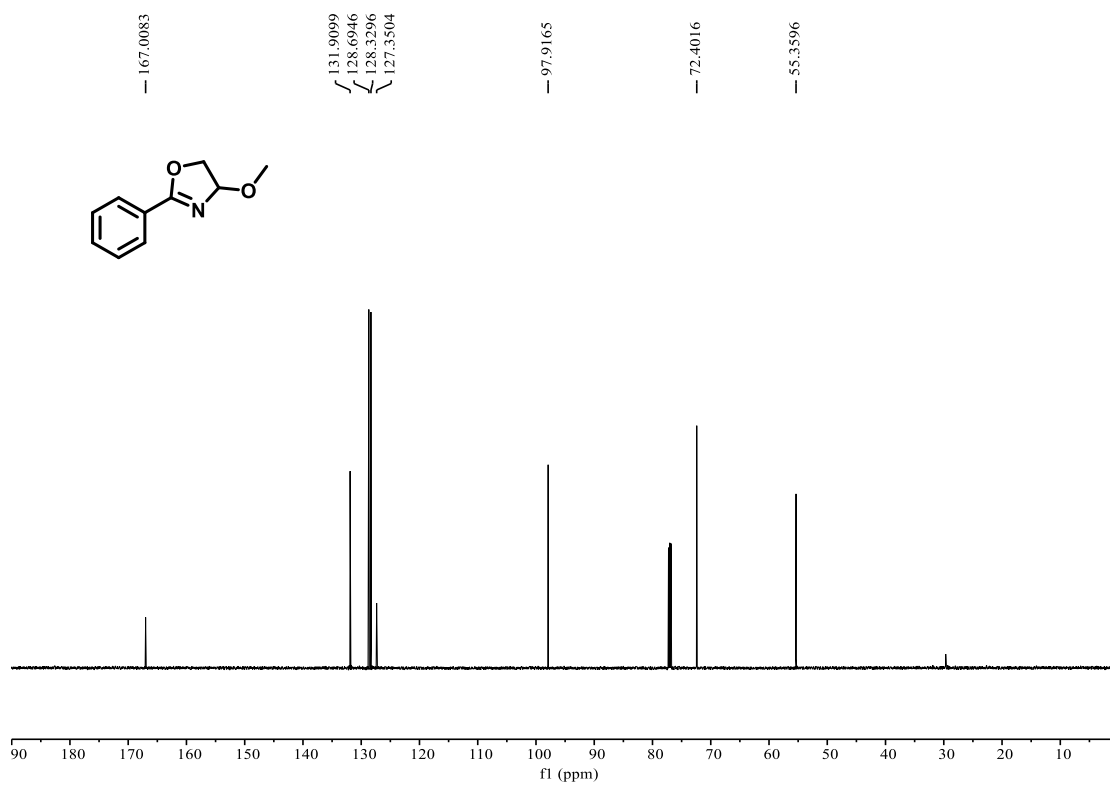
¹³C NMR (151 MHz, CDCl₃) of compound **2x**



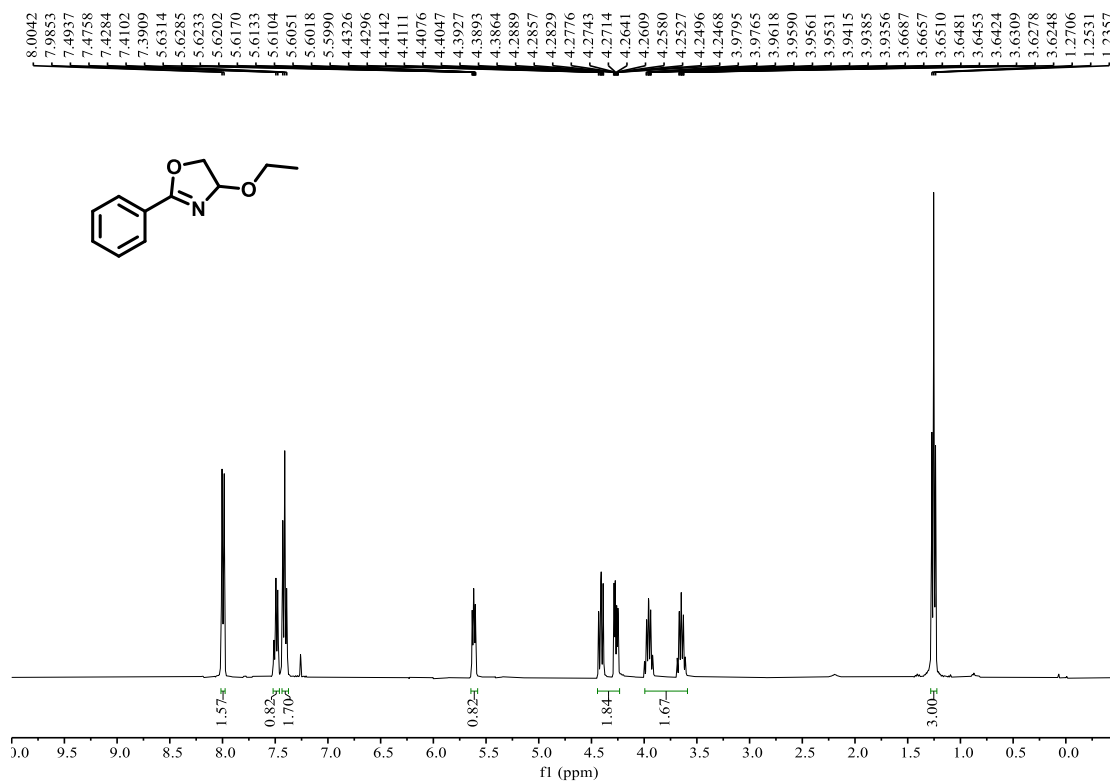
¹H NMR (400 MHz, CDCl₃) of compound **4a**



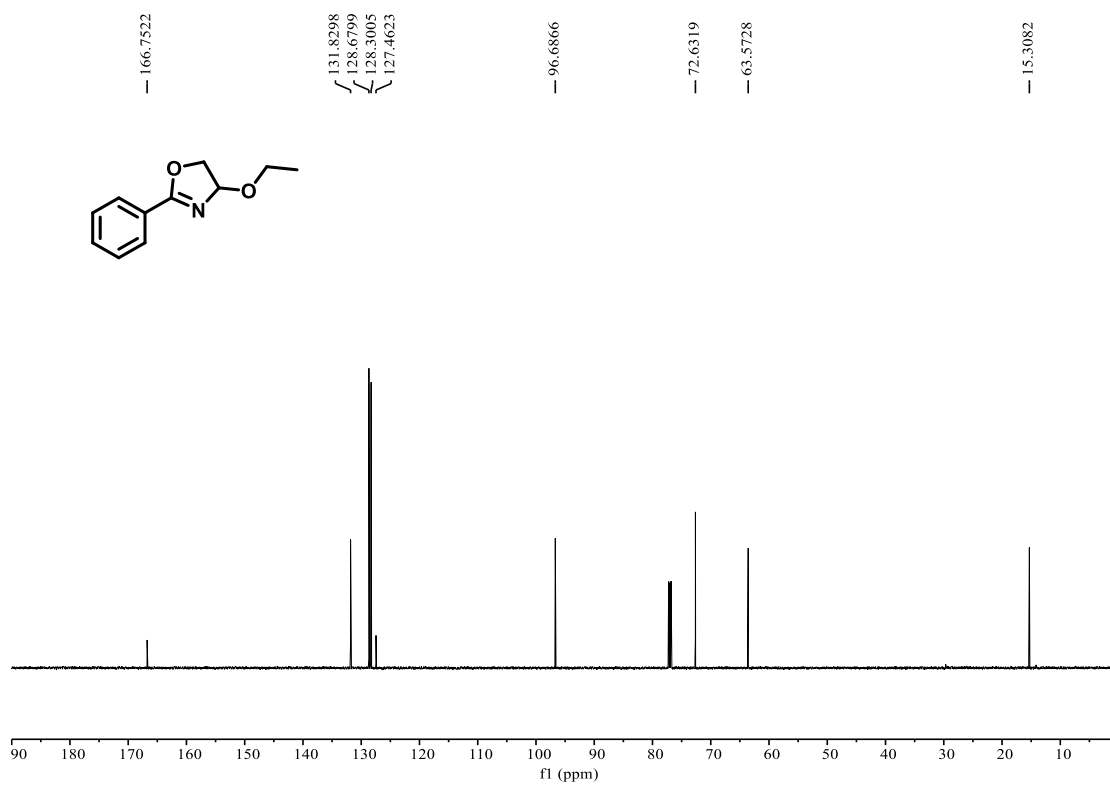
¹³C NMR (151 MHz, CDCl₃) of compound **4a**



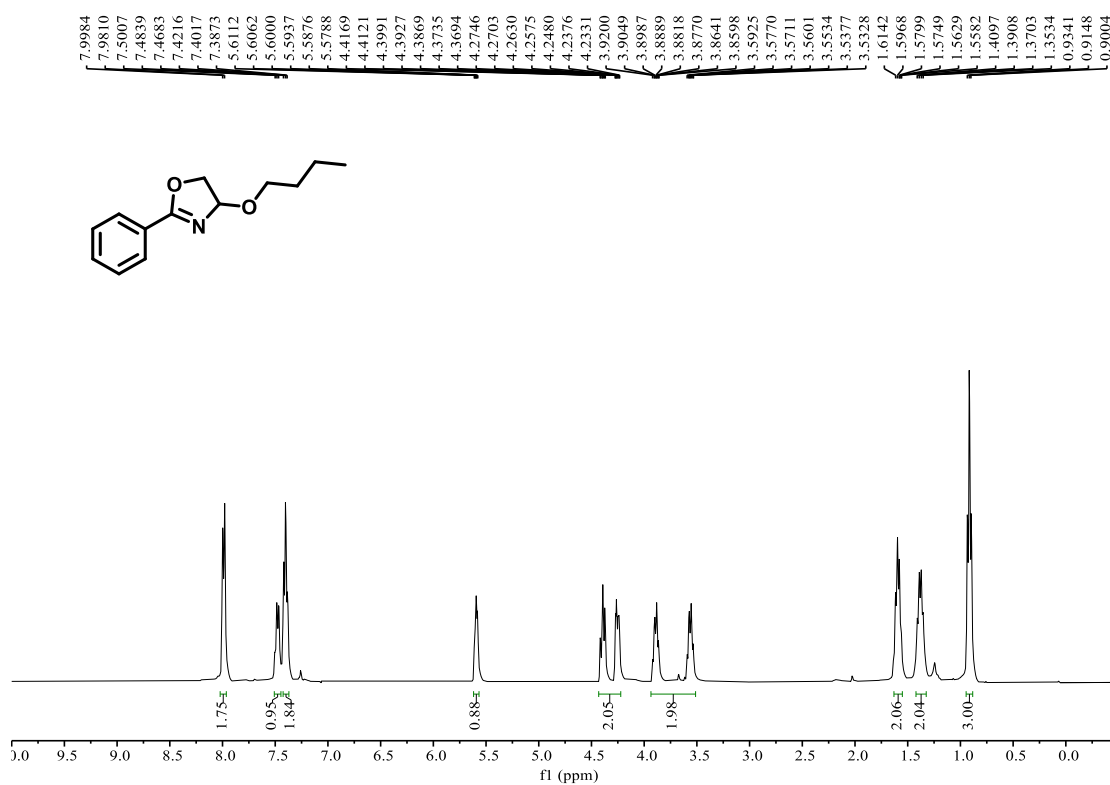
¹H NMR (400 MHz, CDCl₃) of compound **4b**



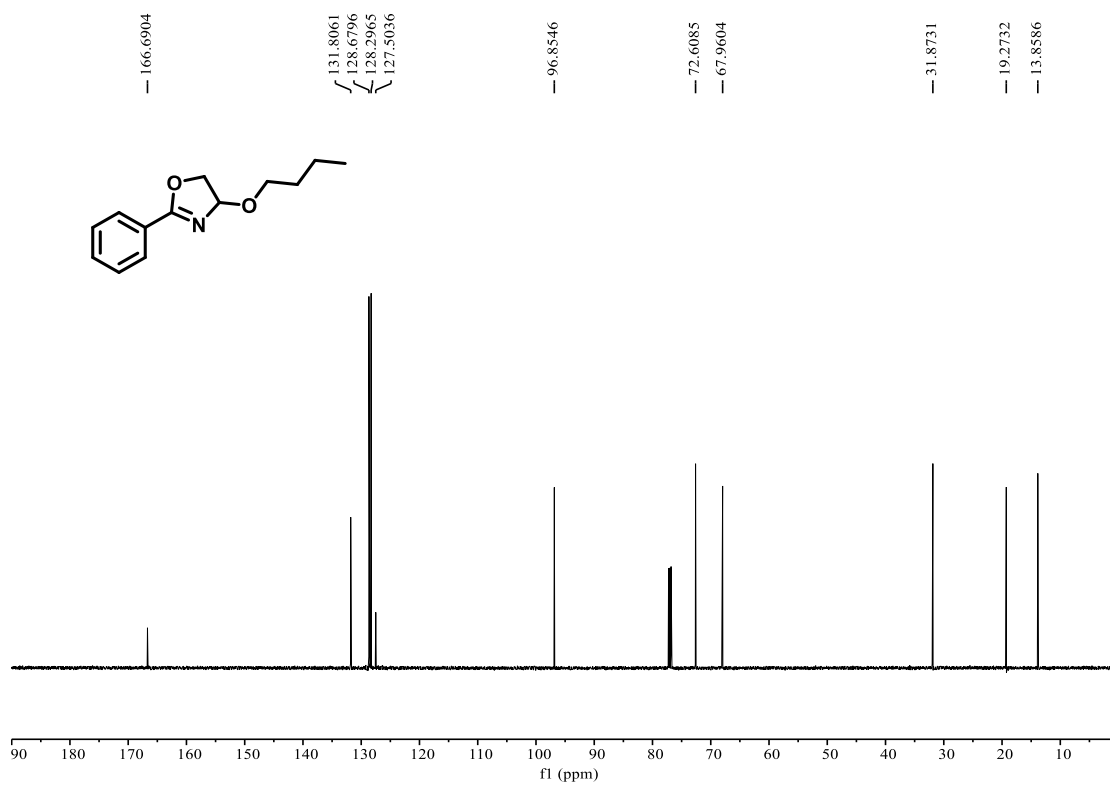
¹³C NMR (151 MHz, CDCl₃) of compound **4b**



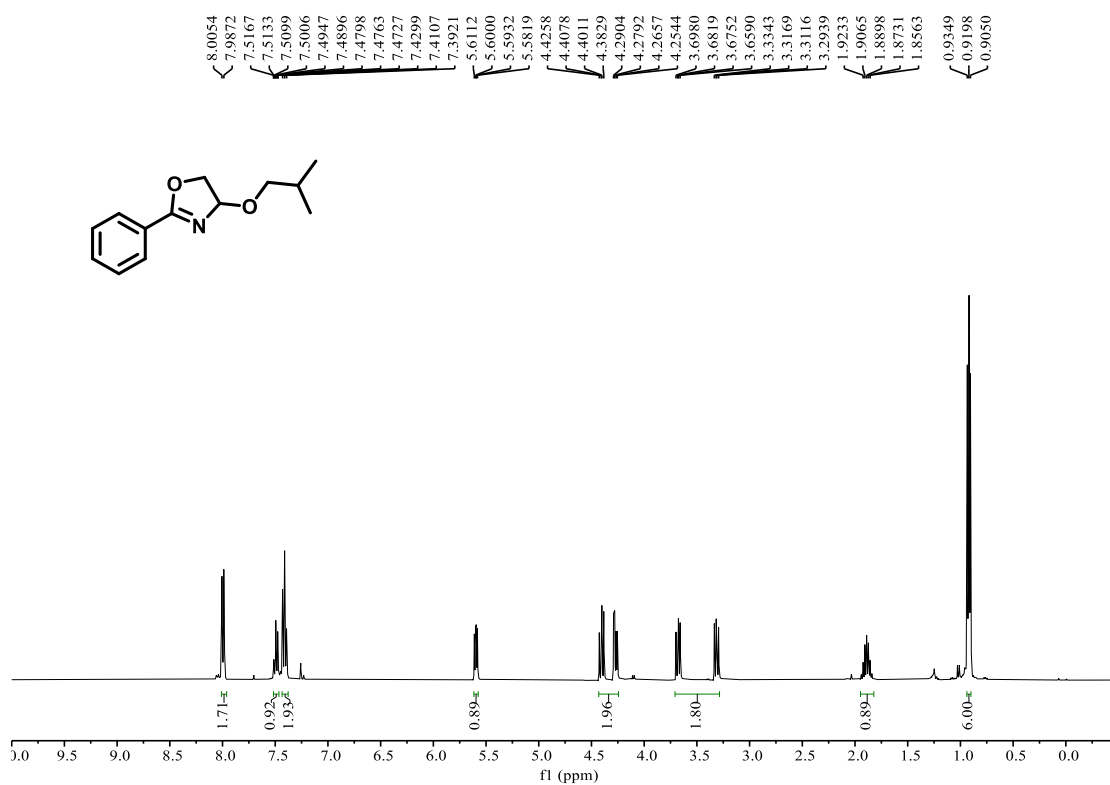
¹H NMR (400 MHz, CDCl₃) of compound 4c



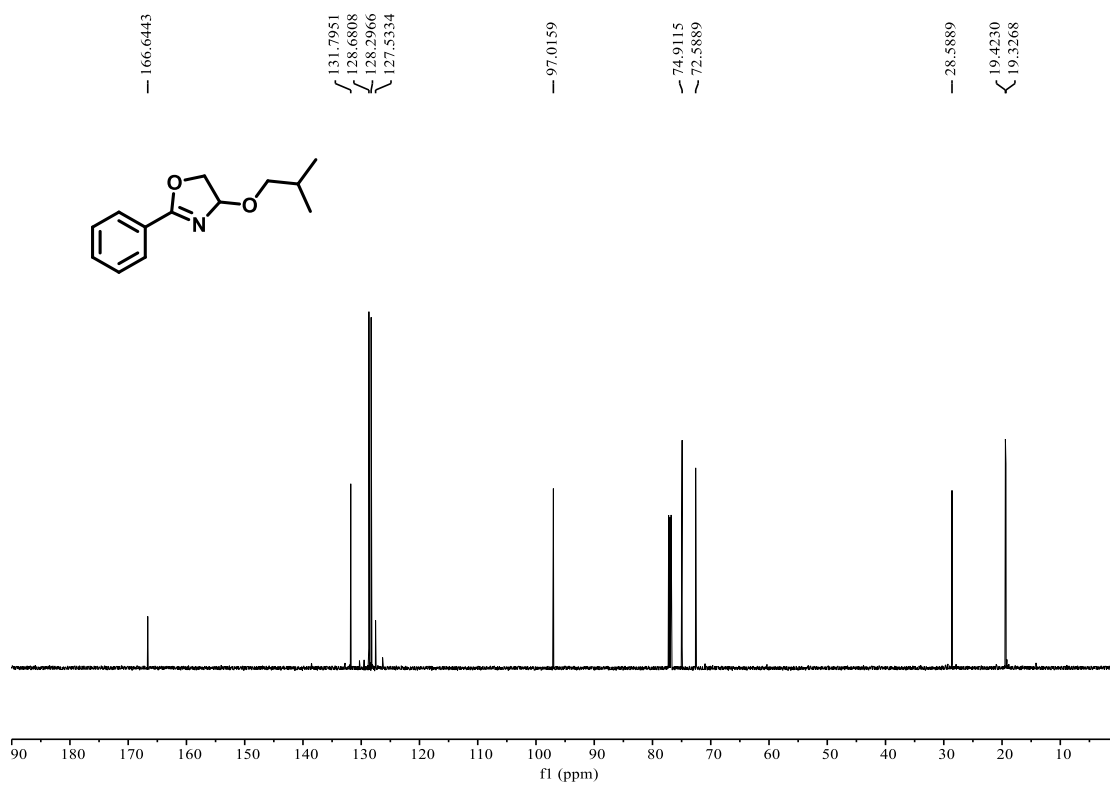
¹³C NMR (151 MHz, CDCl₃) of compound 4c



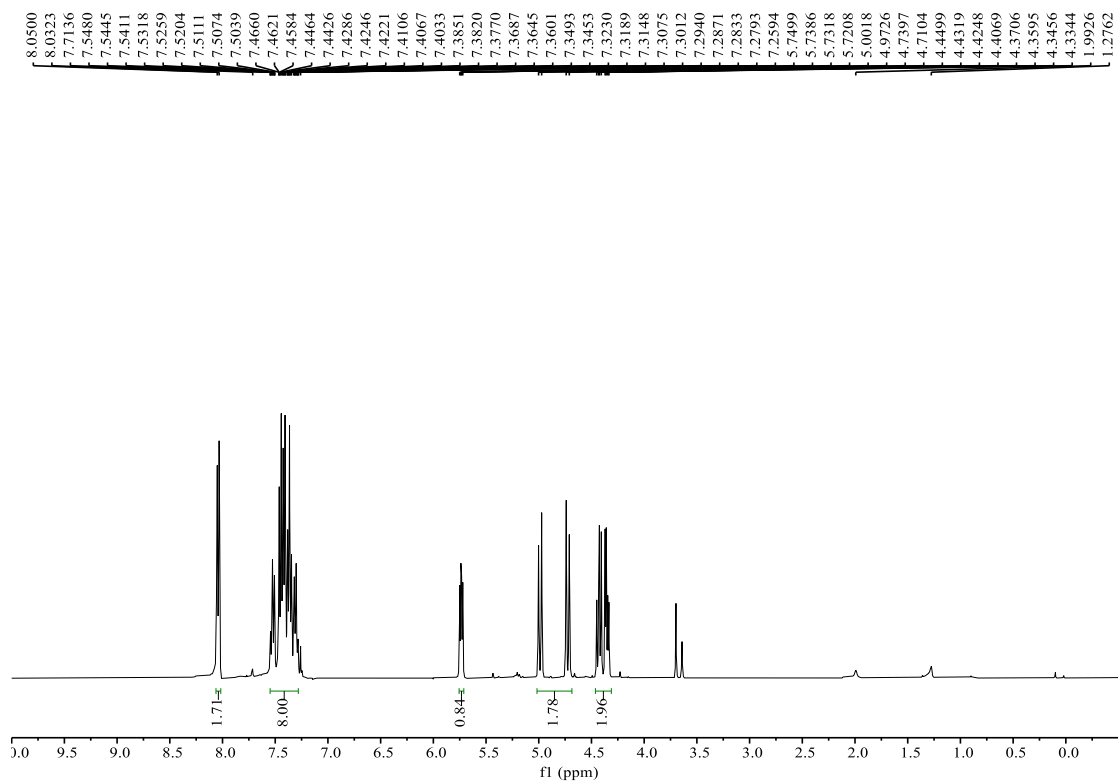
¹H NMR (400 MHz, CDCl₃) of compound **4d**



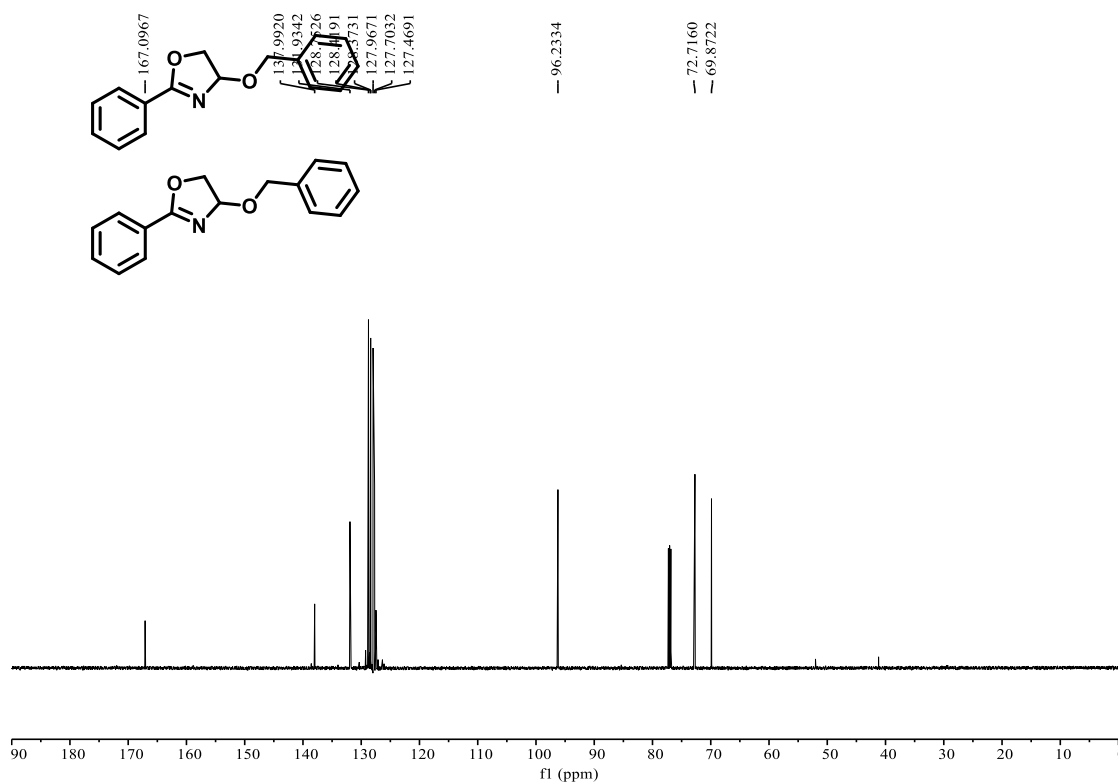
¹³C NMR (151 MHz, CDCl₃) of compound **4d**



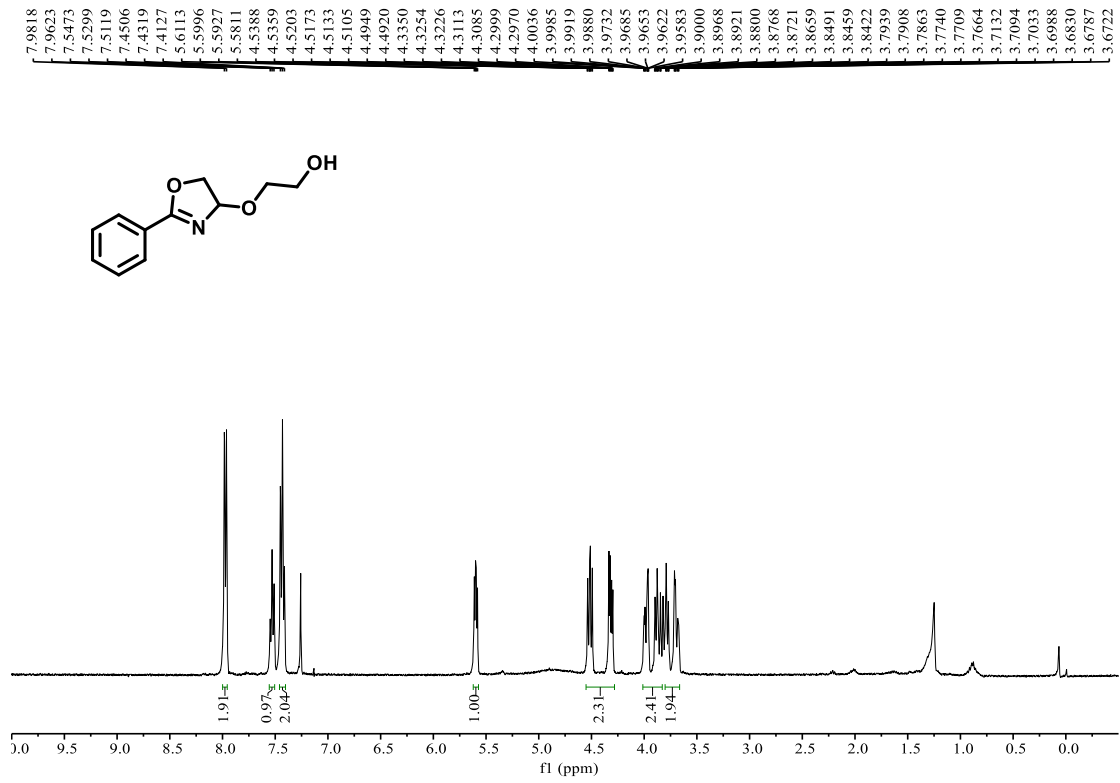
¹H NMR (400 MHz, CDCl₃) of compound 4e



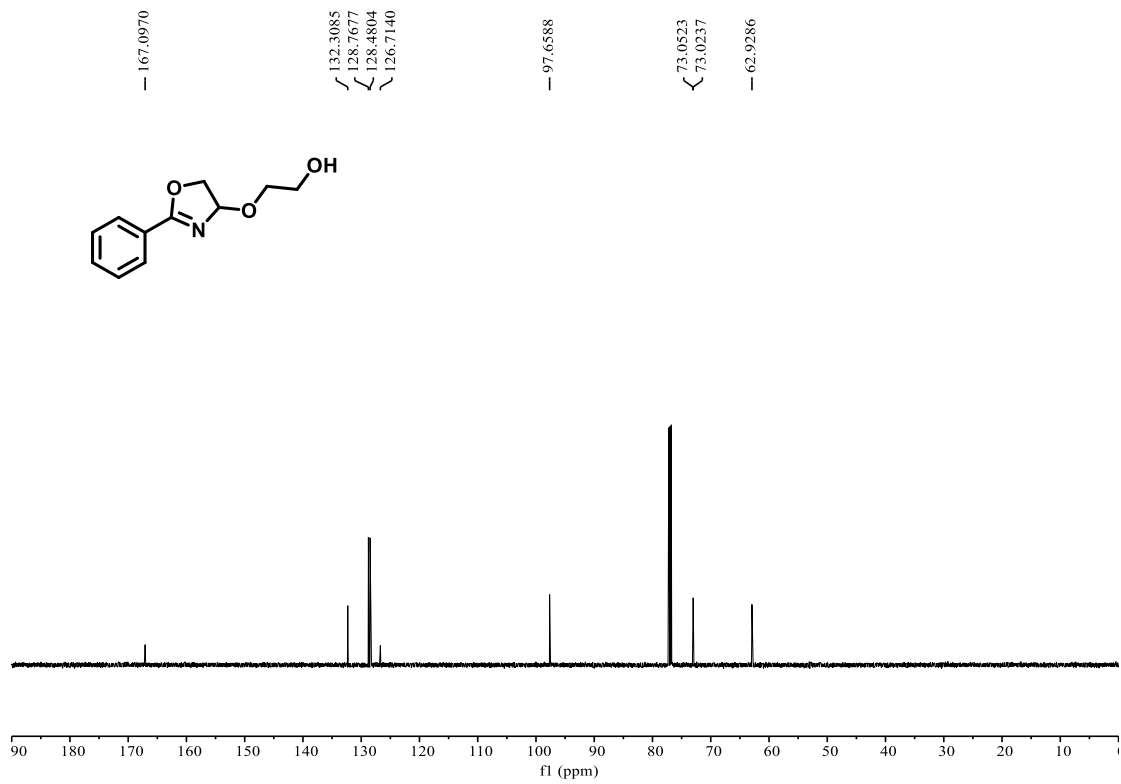
¹³C NMR (151 MHz, CDCl₃) of compound 4e



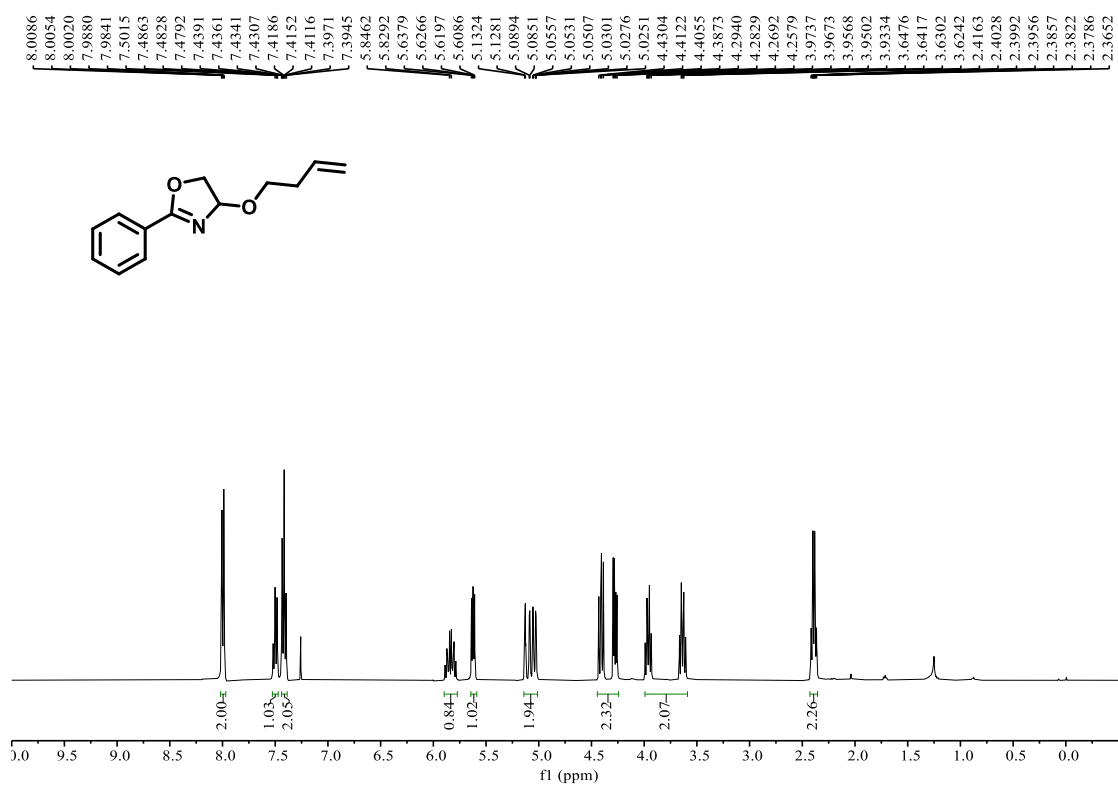
¹H NMR (400 MHz, CDCl₃) of compound **4f**



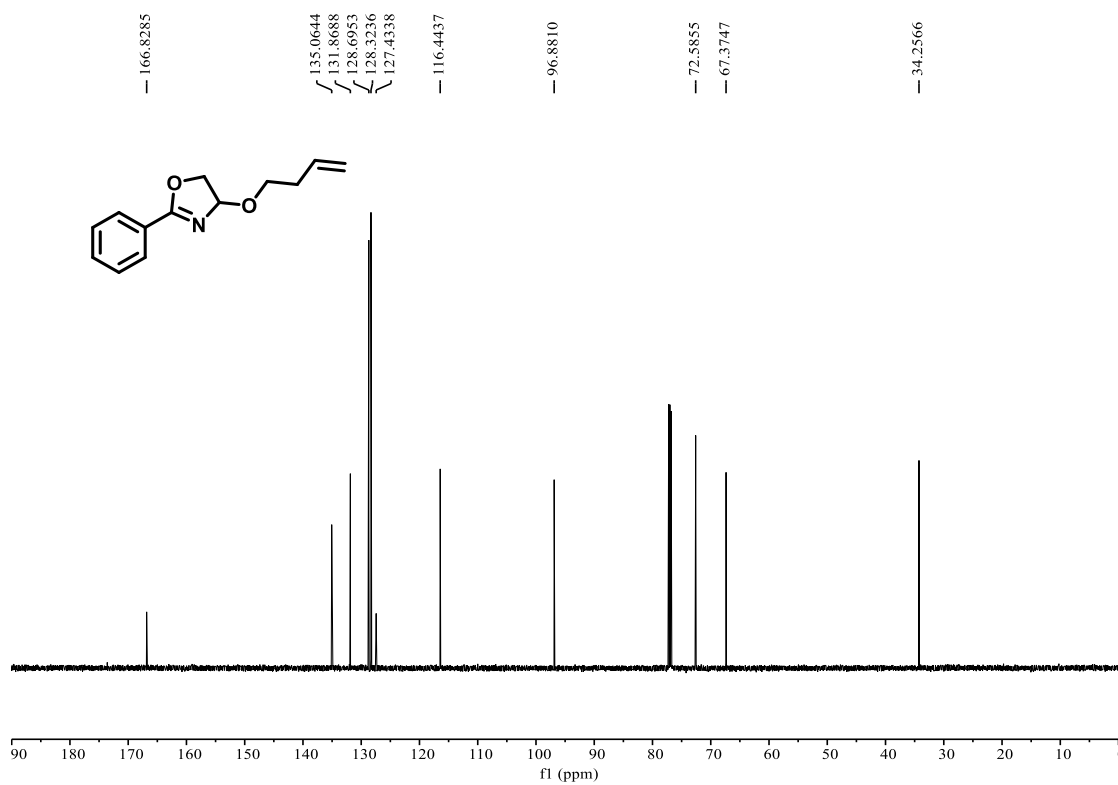
¹³C NMR (151 MHz, CDCl₃) of compound **4f**



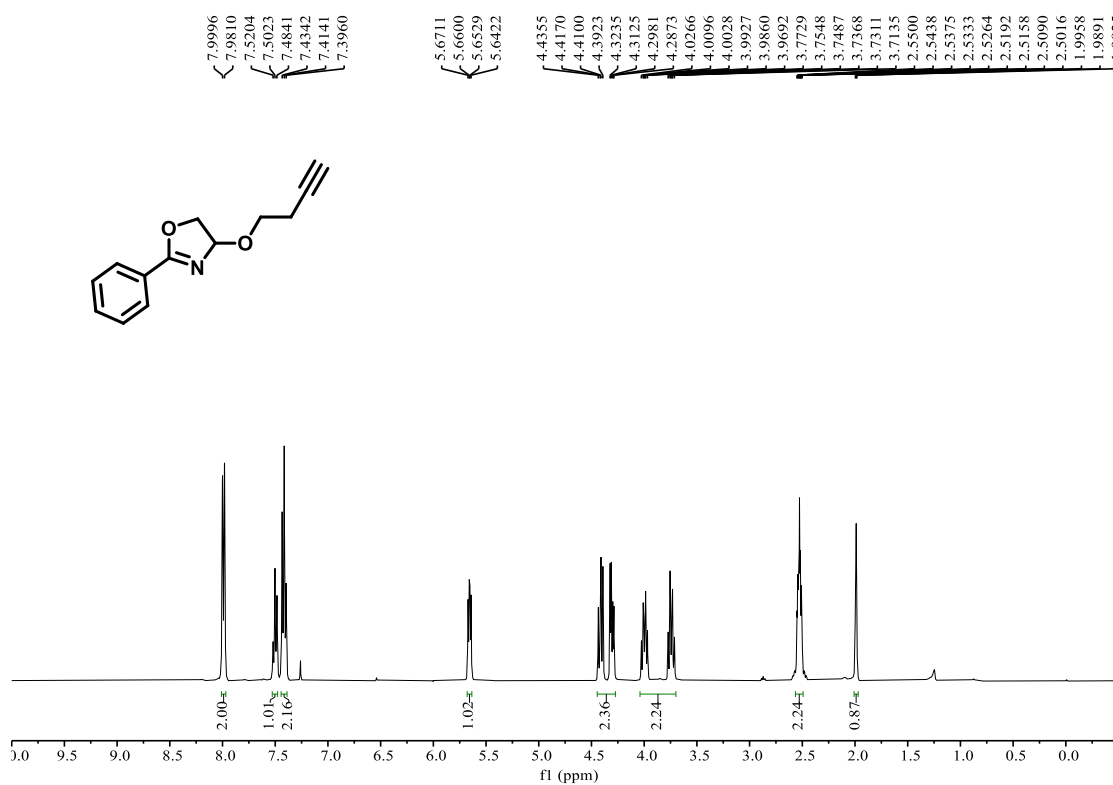
¹H NMR (400 MHz, CDCl₃) of compound **4g**



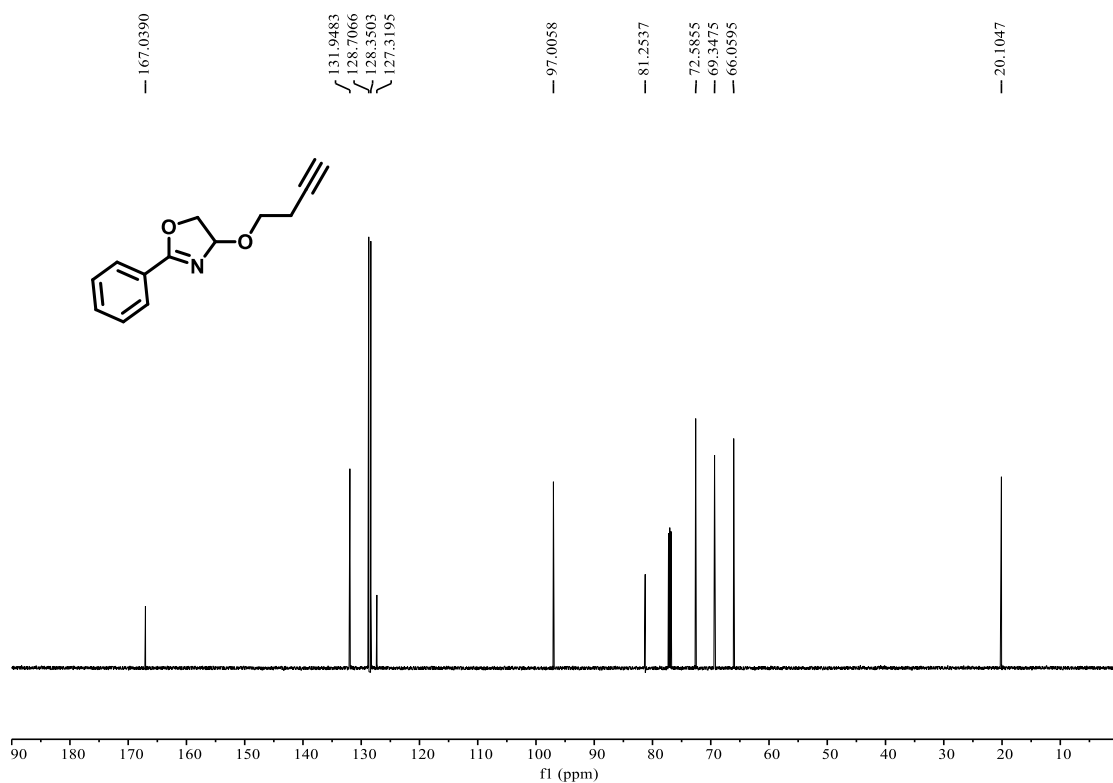
¹³C NMR (151 MHz, CDCl₃) of compound **4g**



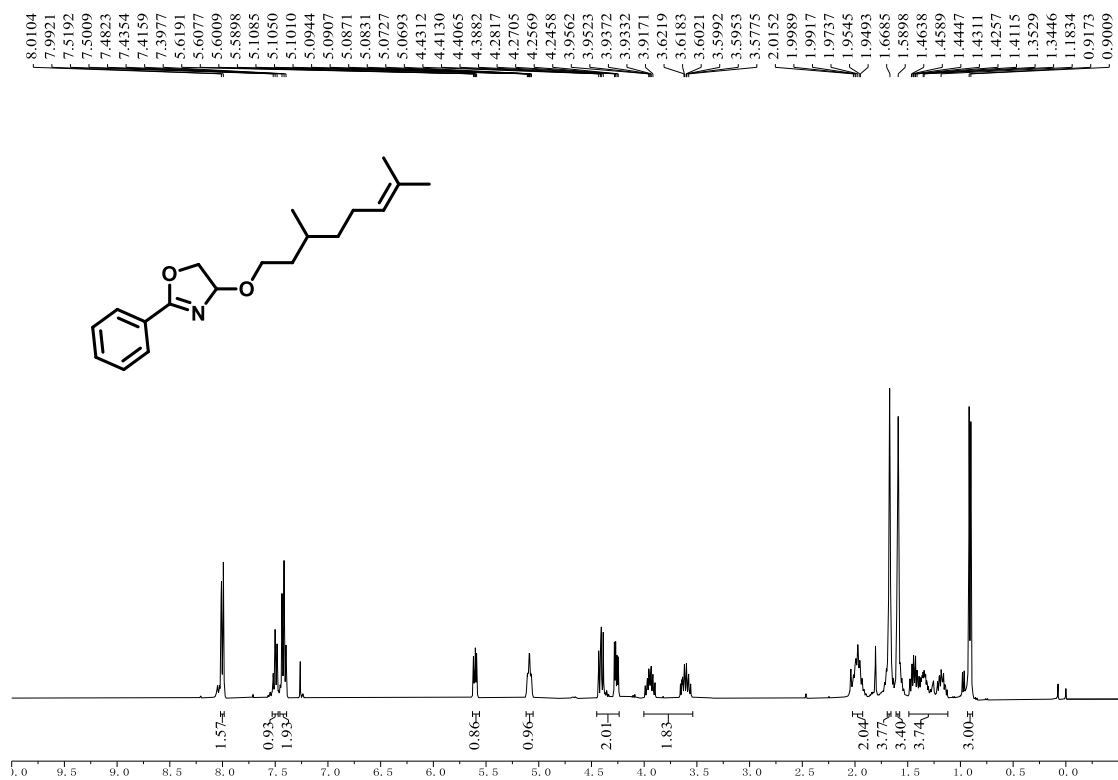
¹H NMR (400 MHz, CDCl₃) of compound **4h**



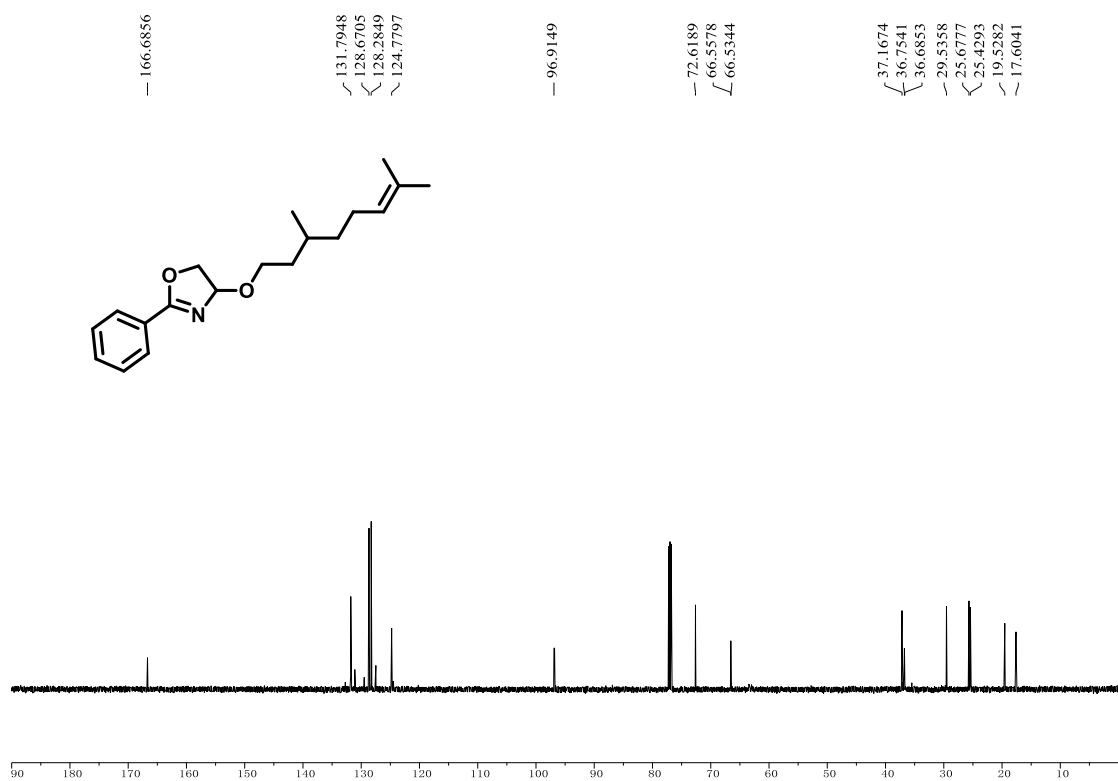
¹³C NMR (151 MHz, CDCl₃) of compound **4h**



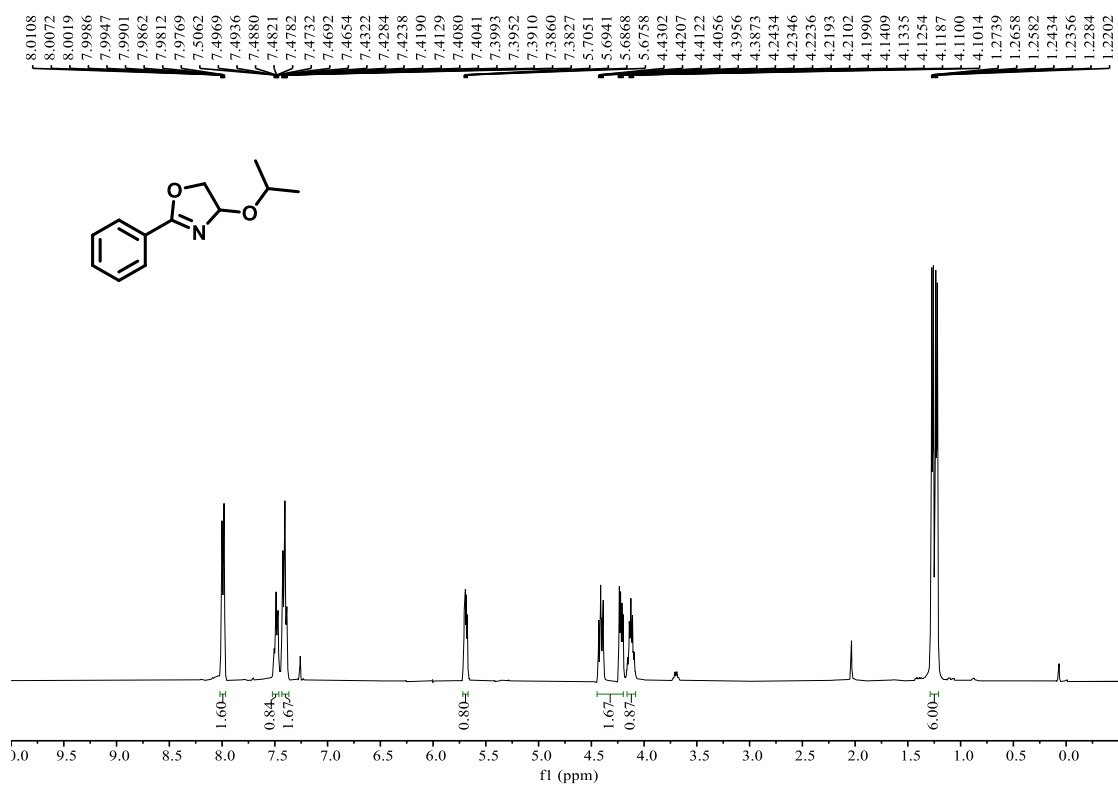
¹H NMR (400 MHz, CDCl₃) of compound **4i**



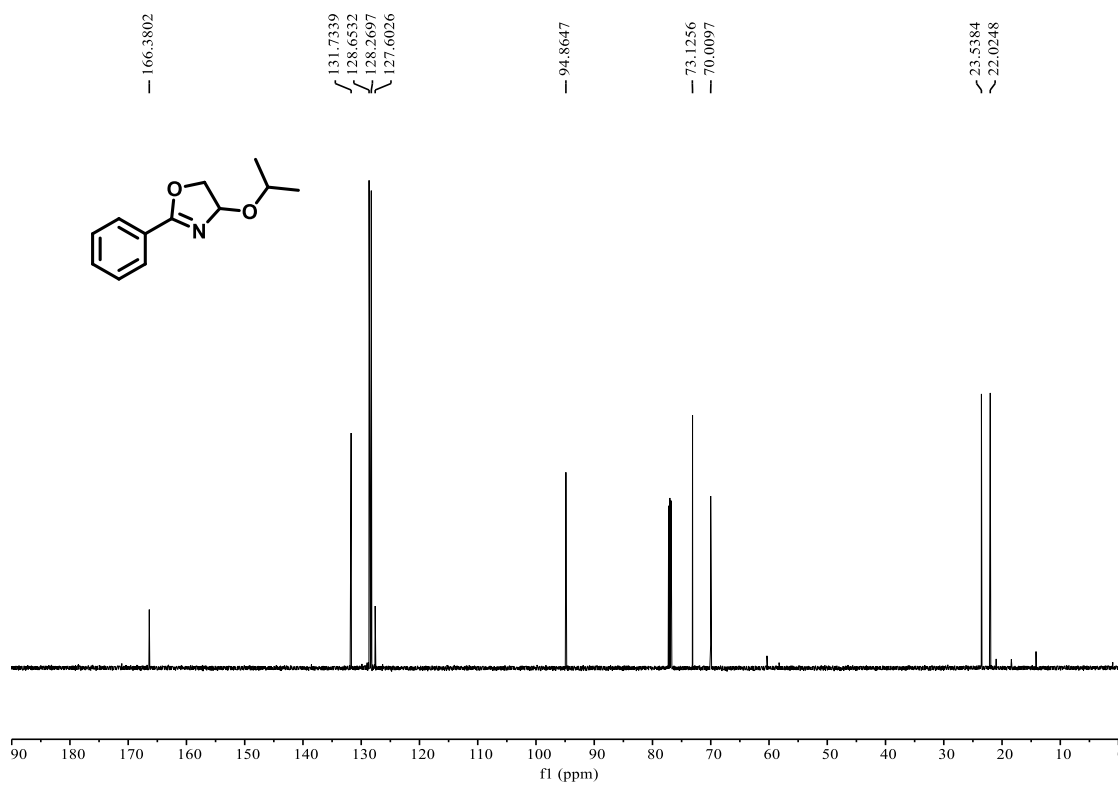
¹³C NMR (151 MHz, CDCl₃) of compound **4i**



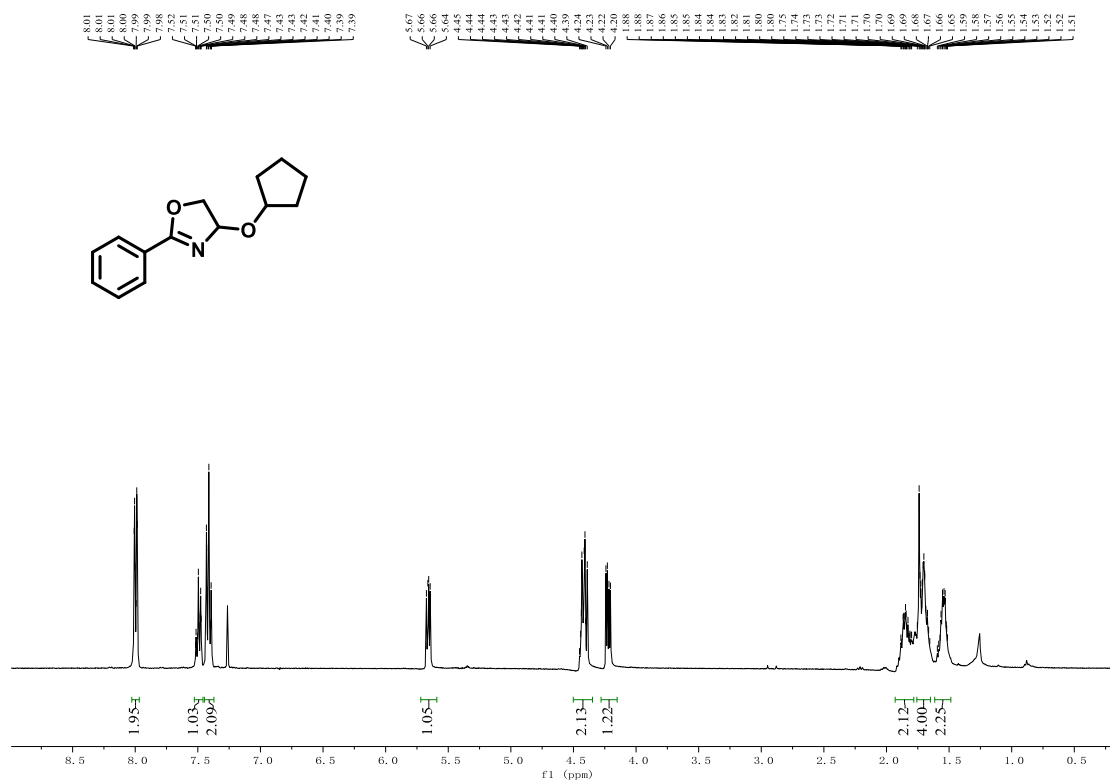
¹H NMR (400 MHz, CDCl₃) of compound **4j**



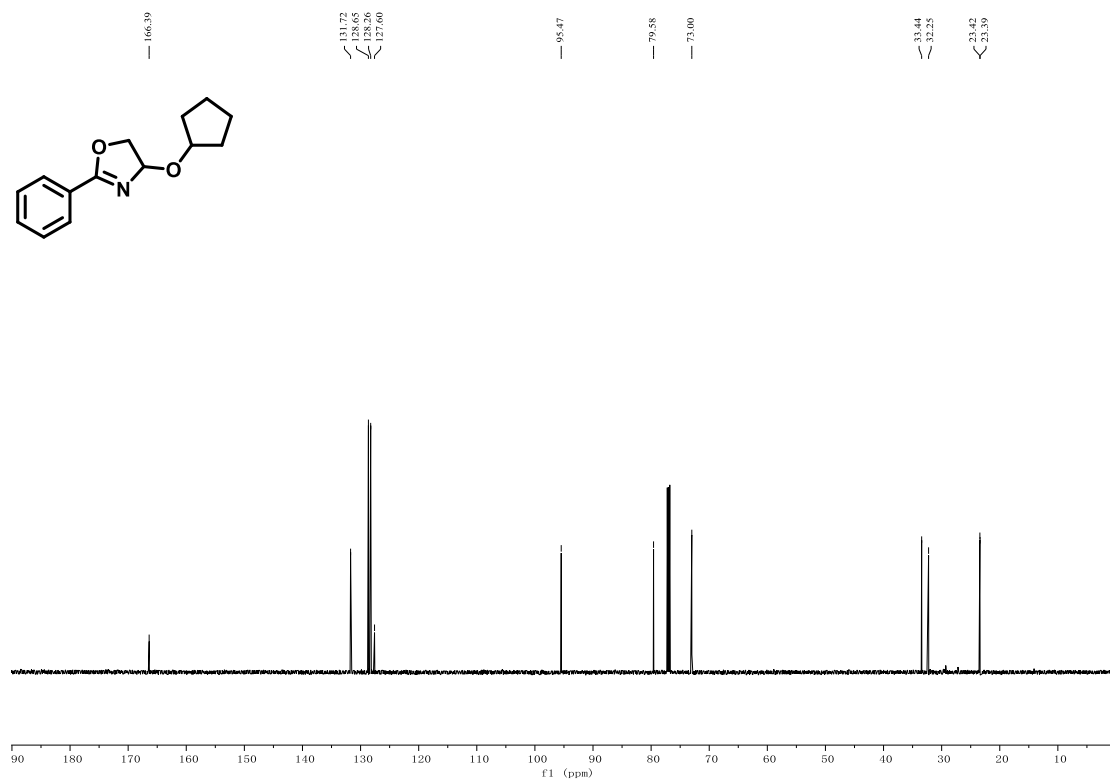
¹³C NMR (151 MHz, CDCl₃) of compound **4j**



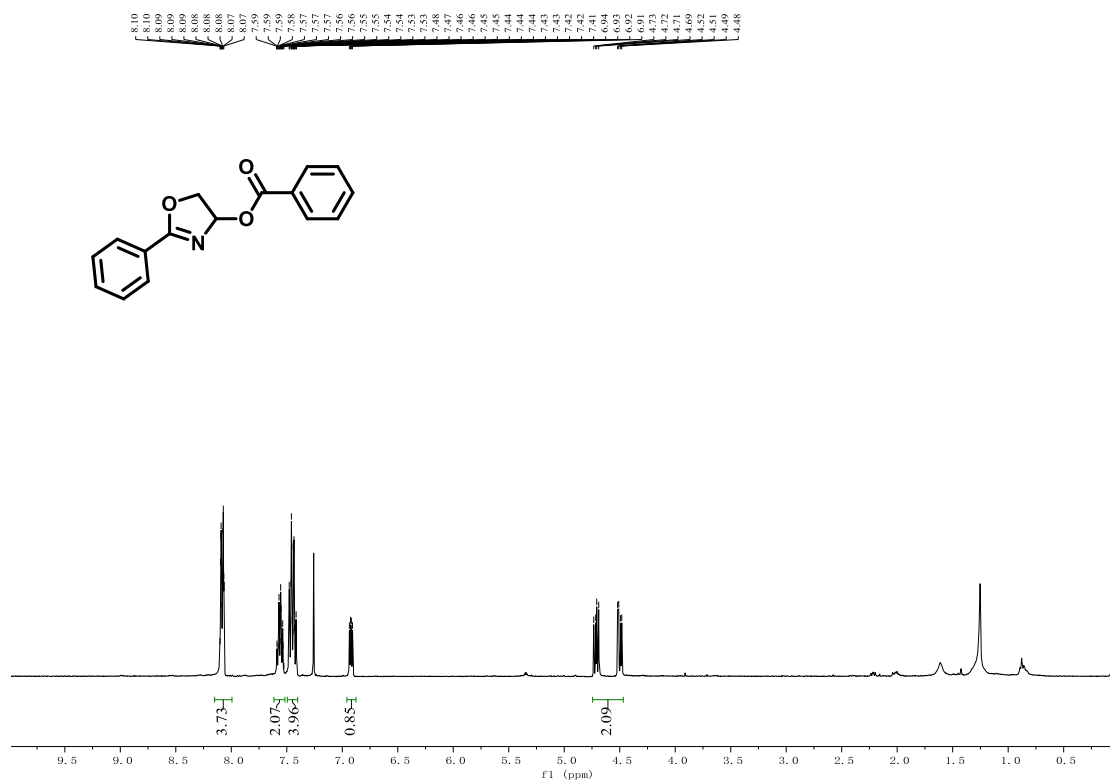
¹H NMR (400 MHz, CDCl₃) of compound 4k



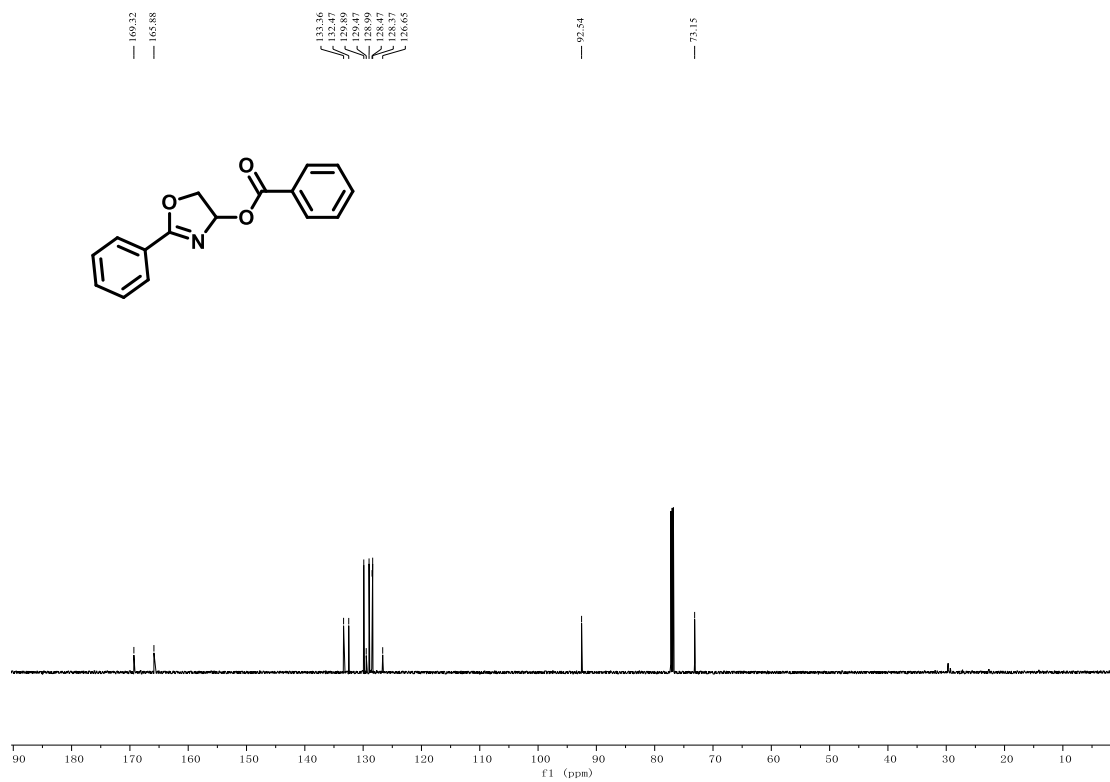
¹³C NMR (151 MHz, CDCl₃) of compound 4k



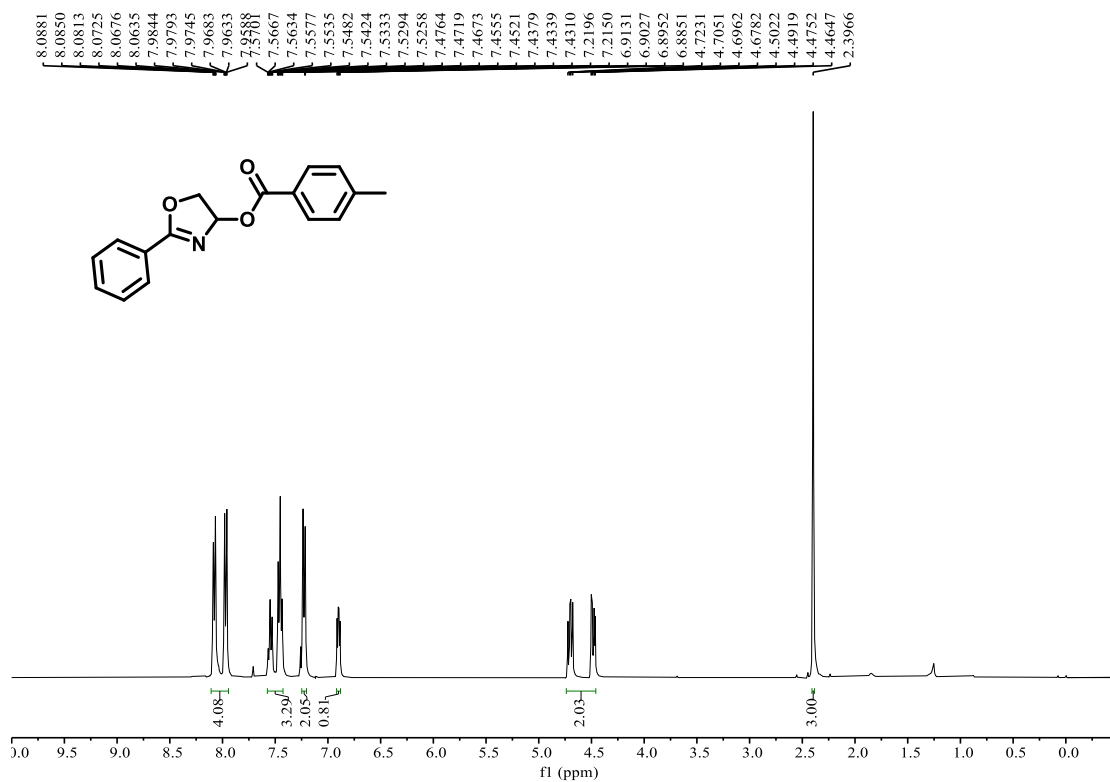
¹H NMR (400 MHz, CDCl₃) of compound **4l**



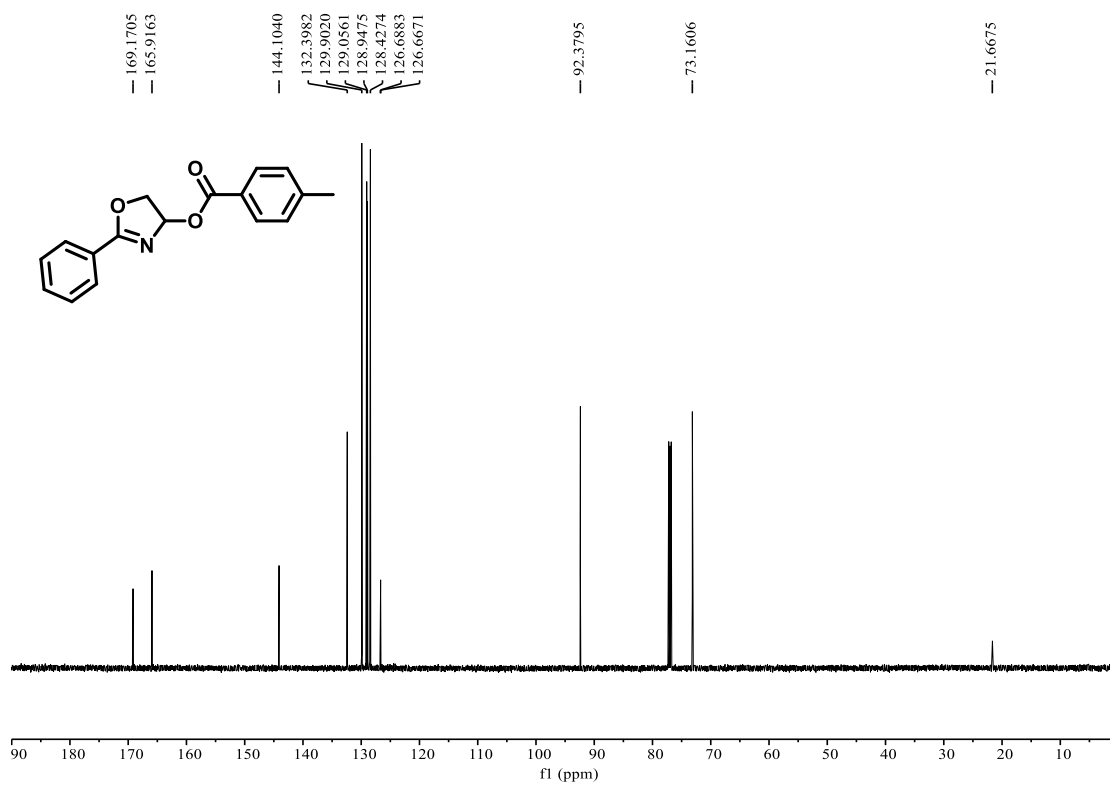
¹³C NMR (151 MHz, CDCl₃) of compound **4l**



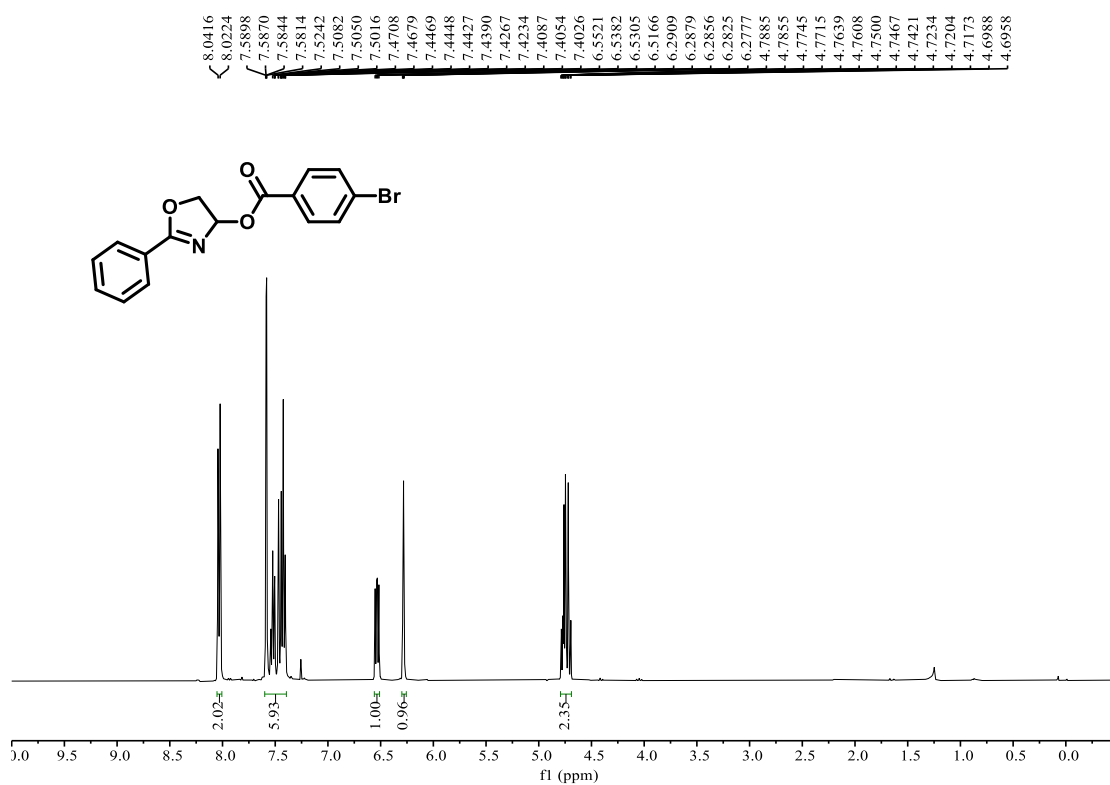
¹H NMR (400 MHz, CDCl₃) of compound **4m**



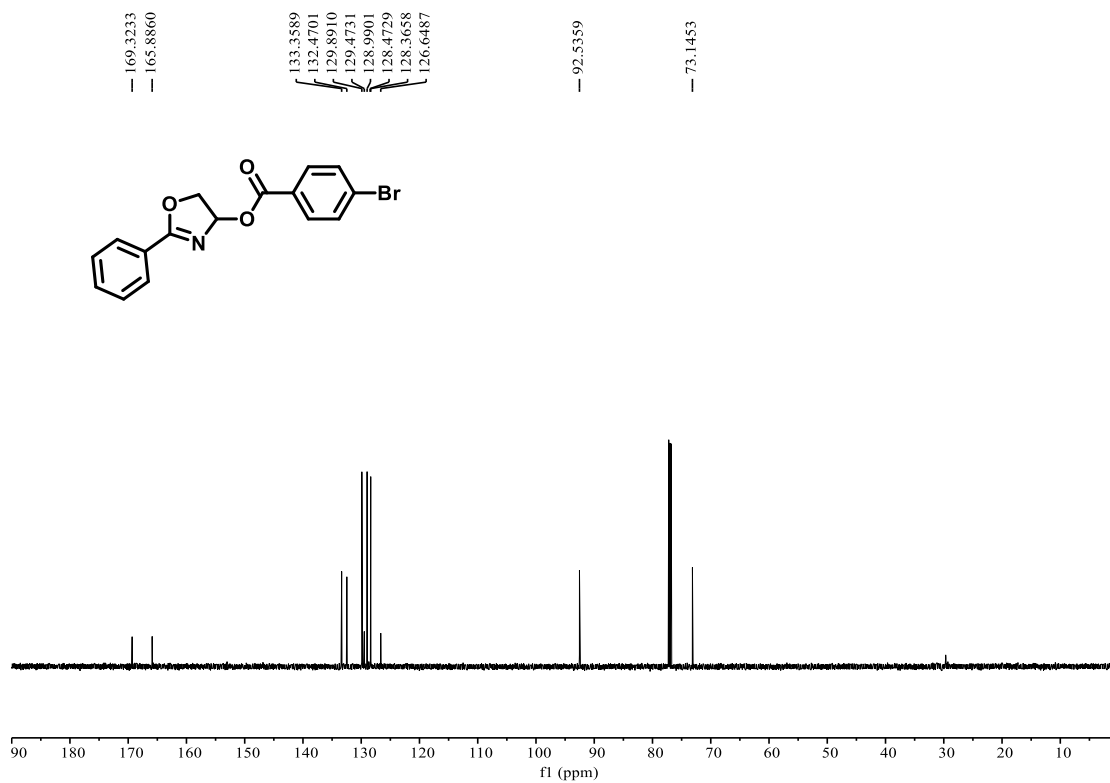
¹³C NMR (151 MHz, CDCl₃) of compound **4m**



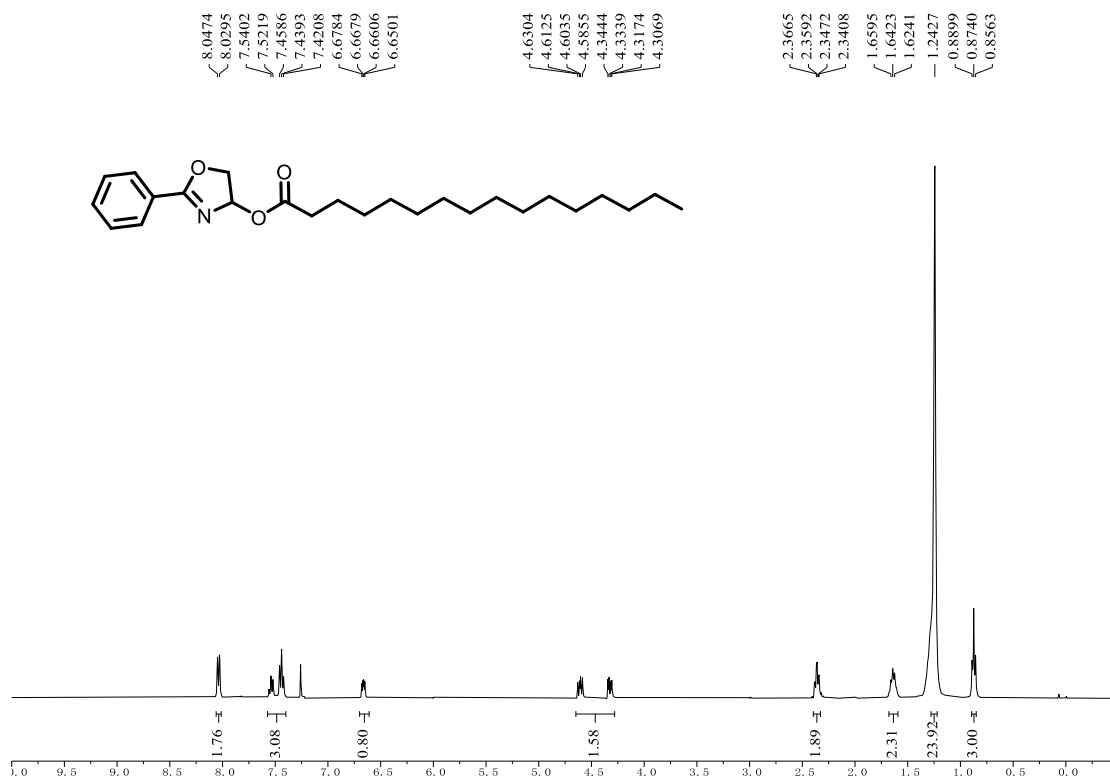
¹H NMR (400 MHz, CDCl₃) of compound **4n**



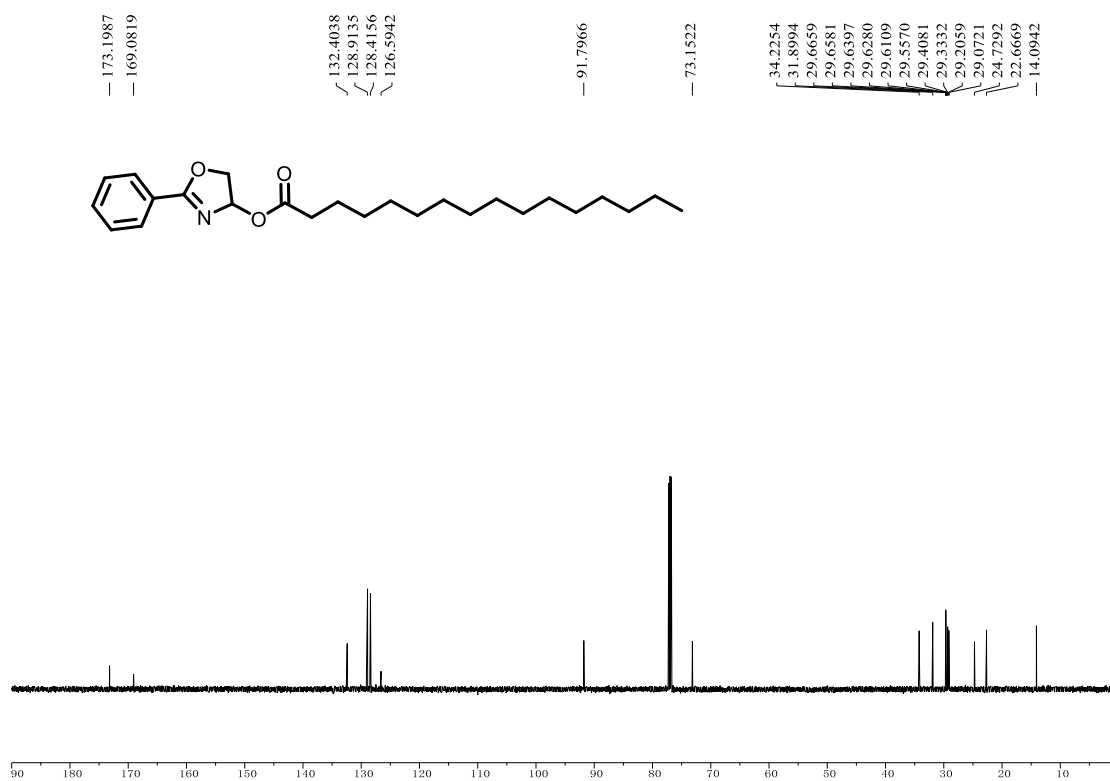
¹³C NMR (151 MHz, CDCl₃) of compound **4n**



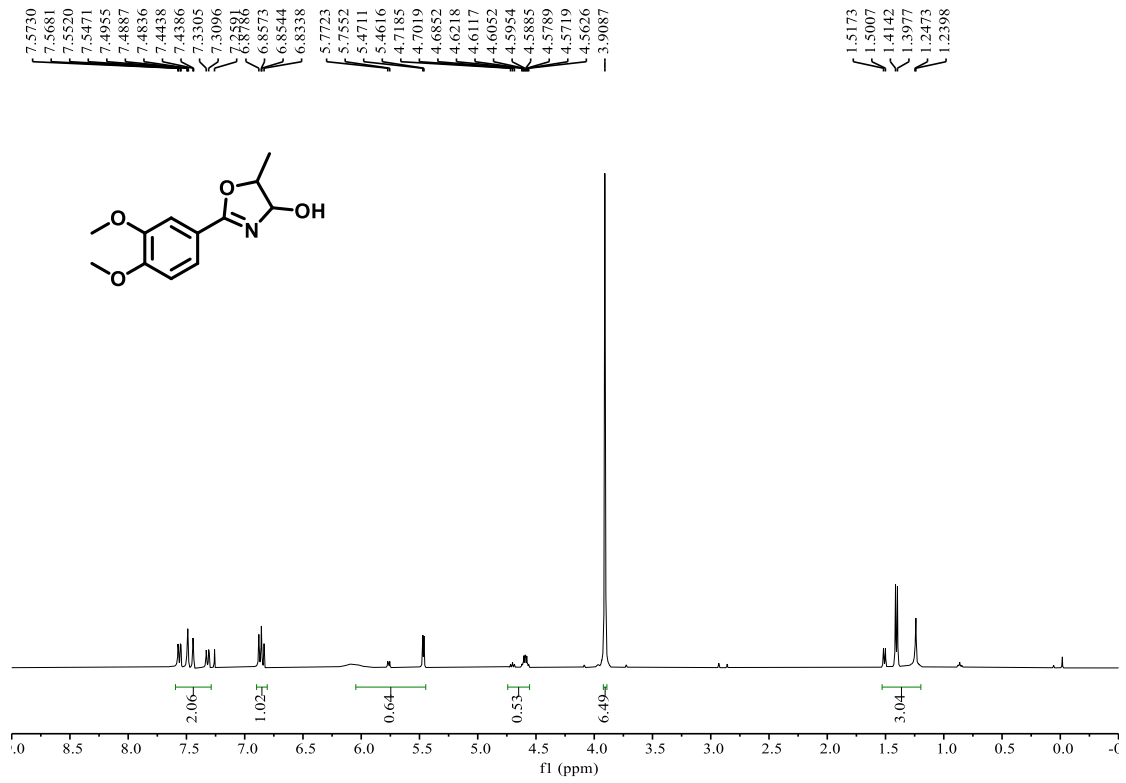
¹H NMR (400 MHz, CDCl₃) of compound **4o**



¹³C NMR (151 MHz, CDCl₃) of compound **4o**



¹H NMR (400 MHz, CDCl₃) of compound **2y**



¹³C NMR (151 MHz, CDCl₃) of compound **2y**

