Supporting Information

I_2-catalyzed tandem sp^3 C-H oxidation and annulation of aryl methyl ketones with amidoximes for the synthesis of 5-aroyl-1, 2, 4-oxadiazoles

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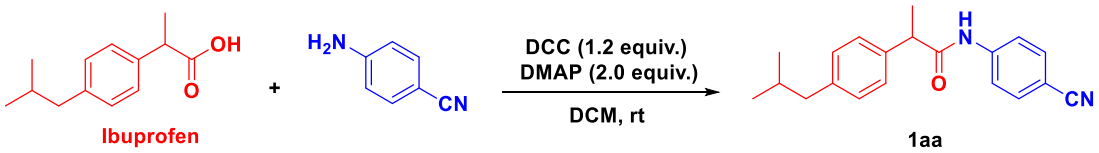
General Methods

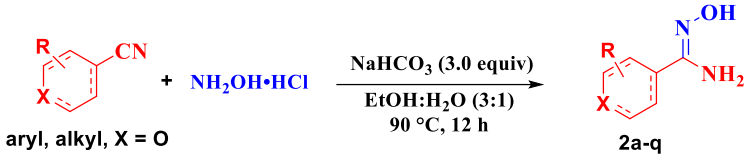
We purchased commercially available chemicals from Alfa Aesar, Sigma-Aldrich, TCI, and Combi-Block and used them as received. We synthesized starting materials following the reported procedures. For reaction monitoring, thin-layer chromatography (TLC) was performed using Merck silica gel 60 F254 precoated plates (0.25 mm) and visualized with a UV lamp. Silica gel for column chromatography (particle size 100–200 mesh) was obtained from Finar. We recorded ^{1}H and ^{13}C NMR (nuclear magnetic resonance) spectra on a Bruker 400 MHz instrument, with chemical shifts reported in parts per million (ppm) relative to tetramethylsilane (δ 0.00), chloroform (7.26 ppm), or DMSO-d_6 (2.50 ppm). ^{1}H NMR splitting patterns were designated as s (singlet), br s (broad singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), m (multiplet), etc. ^{13}C NMR spectral values were reported relative to $CDCl_3$ (77.16 ppm) or DMSO-d_6 (39.70 ppm). FT-IR spectra were recorded on a Perkin Elmer spectrometer and reported in the absorption frequency (cm^{-1}). High-resolution mass spectrometry (HRMS) analysis was conducted using an Agilent Q-TOF 6230 instrument. Crystal data was collected using a Bruker Kappa APEX II CCD diffractometer.

Procedure for synthesis of *N*-(4-acetylphenyl)-2-(4-isobutylphenyl)propenamide (1aa)[1]



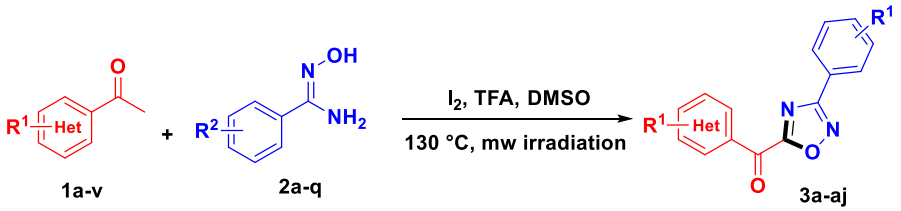
To the oven-dried round bottom flask equipped with a magnetic stir bar was added 4-aminoacetophenone (200 mg, 1.48 mmol, and 1.0 equiv.), ibuprofen (397 mg, 1.92 mmol, 1.3 equiv.), DMAP (362 mg, 2.96 mmol, 2.0 equiv.), DCC (366 mg, 1.78 mmol, 1.2 equiv.) and 10 mL of DCM. The resulting reaction mixture was stirred at room temperature, and the progress of the reaction was monitored by TLC. After the completion of the reaction (6 h), the reaction mixture was washed with water and extracted with EtOAc (3 x 20 mL). The combined organic layers were washed with brine, dried with anhydrous Na_2SO_4, and concentrated under a vacuum. The crude product was purified by silica gel column chromatography (eluent: petroleum ether/EtOAc = 9.5:0.5, v/v) to afford *N*-(4-acetylphenyl)-2-(4-isobutylphenyl)propenamide **1aa** as a white solid in 393 mg, 82% yield.

General procedure for the synthesis of amidoximes (2a-q)[2]



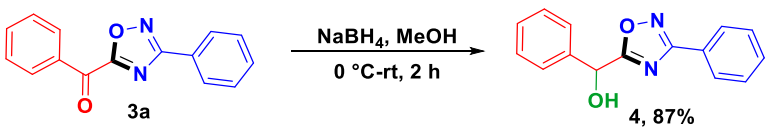
A round bottom flask containing the solution of tetrahydro-2*H*-pyran-4-carbonitrile (200 mg, 1.80 mmol, 1.0 equiv.), hydroxylamine hydrochloride (250 mg, 3.60 mmol, 2.0 equiv.) and $NaHCO_3$ (454 mg, 5.40 mmol, 3.0 equiv.) in 3:1 ratio of EtOH: H_2O was heated with stirring in an oil bath at 90 ºC. The progress of the reaction was monitored by TLC. After completion of the reaction (8 h), the reaction mixture was diluted with water (10 mL) and extracted with DCM (15 mL × 3). The organic phase was dried over Na_2SO_4 and concentrated in a vacuum to afford *N*′-hydroxytetrahydro-2*H*-pyran-4-carboximidamide **2m** as an off-white solid in 231 mg, 89% yield. All other compounds **2a-q** were synthesized by following the same procedure.

General procedure for the synthesis of 5-aroyl-1, 2, 4-oxadiazoles (3a-aj)



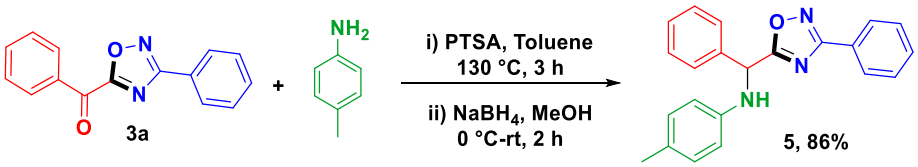
An oven dried 20 mL microwave vial was charged with acetophenone (100 mg, 0.83 mmol, 1.0 equiv.), *N*′-hydroxybenzimidamide (113 mg, 0.83 mmol, 1.0 equiv.), TFA (0.16 mL, 2.50 mmol), iodine (42.2 mg, 0.166 mmol, 0.2 equiv.) and 2 mL of DMSO. The resulting reaction mixture was subject to microwave irradiation at 130 °C. The progress of the reaction was monitored by TLC. After completion of the reaction (1 h), the reaction mixture was allowed to cool to room temperature, then washed with sodium thiosulphate to quench iodine and extracted with EtOAc (20 mL × 3). The combined organic layers were washed with brine, dried with Na_2SO_4, and the solvent was evaporated under a vacuum. The crude product was purified by column chromatography on silica gel (eluent: petroleum ether/EtOAc = 19:1, v/v) to afford pure product **3a** in 149 mg, 72% yield. All other compounds **3b-aj** were synthesized by following the same procedure.

Procedure for the synthesis of phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanol[1]



An oven-dried round bottom was charged with phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (**3a**) (50 mg, 0.199 mmol, 1.0 equiv.), and 2 mL of MeOH. To this solution, sodium borohydride (11.3 mg, 0.299 mmol, 1.50 equiv.) was added. The resulting reaction mixture was stirred at room temperature, and the reaction progress was monitored by TLC. After completion of the reaction, the reaction mixture was quenched with H_2O (8 mL) and extracted with ethyl acetate (3 × 10 mL). The combined organic layers were washed with brine (8 mL), dried with Na_2SO_4, and the solvent was evaporated under vacuum to afford crude compound. The crude product was purified by column chromatography on silica gel (Hexane/EtOAc) to afford pure product phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanol **4** in 44 mg, 87% yield.

Procedure for synthesis of 4-methoxy-*N*-(phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methyl)aniline[3]



Step-1:

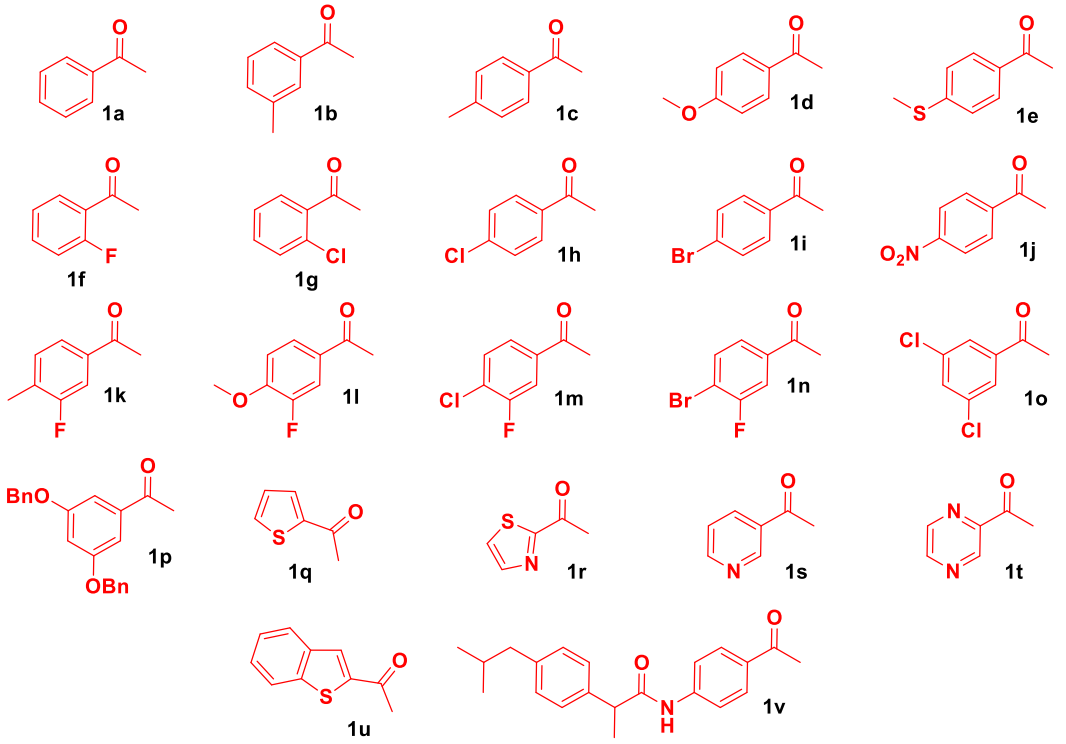
An oven-dried 25 mL of two nech round bottom flask equipped with Dean–Stark condenser and argon balloon was charged with phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanone **3a** (100 mg, 0.399 mmol, 1.0 equiv.), *p*-methoxyaniline (69 mg, 0.399 mmol 1.0 equiv.) and PTSA (5 mg, 0.039 mmol, 0.1 equiv.) and 5 mL of toluene. The resulting reaction mixture was kept in an oil bath and stirred at 130 °C. After completion of the reaction, the mixture was allowed to cool to room temperature. The reaction mixture was quenched with H_2O (10 mL), extracted with ethyl acetate (3 × 15 mL). The combined organic layers were washed with brine (10 mL), dried with Na_2SO_4, and the solvent was evaporated under vacuum to afford *N*-(4-methoxyphenyl)-1-phenyl-1-(3-phenyl-1,2,4-oxadiazol-5-yl)methanimine. The crude product was taken to next step without further purification.

Step-2:

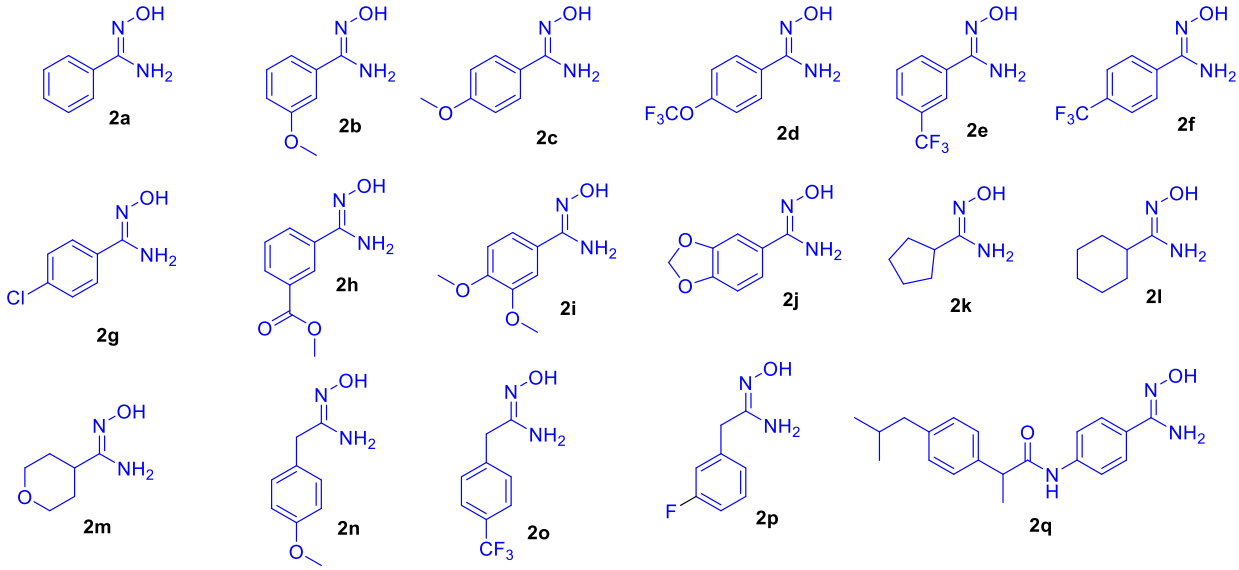
An oven-dried 25 mL of two neck round bottom flask was charged with *N*-(4-methoxyphenyl)-1-phenyl-1-(3-phenyl-1,2,4-oxadiazol-5-yl)methanimine (142 mg, 0.399 mmol, 1.0 equiv.), sodium borohydride (23 mg, 0.599 mmol, 1.5 equiv.) and 5 mL of MeOH. The resulting reaction mixture was stirred at room temperature. After completion of the reaction, the reaction mixture was quenched with H_2O (10 mL), extracted with ethyl acetate (3 × 15 mL). The combined organic layers were washed with brine (10 mL), dried with Na_2SO_4, and the solvent

was evaporated under vacuum. The crude product was purified by column chromatography on silica gel (Hexane/EtOAc) to afford pure product 4-methoxy-*N*-(phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methyl)aniline **5** in 122 mg, 86% yield.

Aryl methyl ketones used in this work:

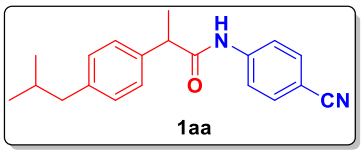


Amidoximes used in this work:



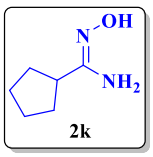
Physical and spectroscopic characterization of compounds

***N*-(4-Cyanophenyl)-2-(4-isobutylphenyl)propenamide (1aa)**



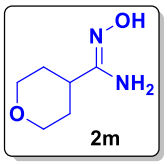
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off white solid; Yield: 354 mg, 68%; m.p: 119-120 ºC; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.52 (m, 4H), 7.47 (s, 1H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 3.74 (q, *J* = 7.1 Hz, 1H), 2.49 (d, *J* = 7.2 Hz, 2H), 1.93 – 1.83 (m, 1H), 1.60 (d, *J* = 7.1 Hz, 3H), 0.93 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.2, 142.2, 141.5, 137.5, 133.3, 130.1, 127.5, 119.5, 119.0, 106.9, 47.9, 45.1, 30.3, 22.5, 18.5; FT-IR (KBr) ν (cm^{-1}) 3319, 3194, 3113, 2951, 2222, 1675, 1597, 1460; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{20}H_{23}N_2O$: 307.1810; found: 307.1810.

***N′*-Hydroxycyclopentanecarboximidamide (2k):**



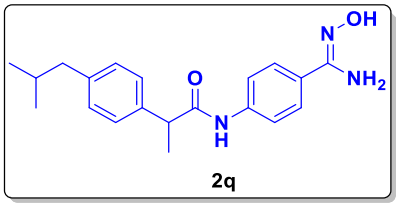
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 7:3 (v/v); Grey solid; Yield: 238 mg, 88%; m.p: 77-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.89 (br s, 1H), 4.54 (br s, 2H), 2.64 – 2.52 (m, 1H), 1.95 – 1.83 (m, 2H), 1.74 – 1.54 (m, 6H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 156.8, 41.5, 30.1, 25.5; FT-IR (KBr) ν (cm^{-1}) 3464, 3361, 3185, 1661; HRMS (ESI) (m/z) [M + H]$^+$ calcd. for $C_6H_{13}N_2O$: 129.1028; found: 129.1025.

***N′*-Hydroxytetrahydro-2*H*-pyran-4-carboximidamide (2m):**



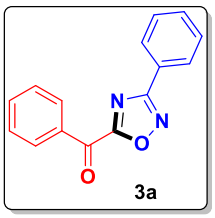
Purified by column chromatography eluting with DCM/MeOH = 9:1 (v/v); Off-white solid; Yield: 231 mg, 89%; m.p: 134-135 °C; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.81 (s, 1H), 5.29 (s, 2H), 3.84 (dt, *J* = 11.4, 3.3 Hz, 2H), 3.33 – 3.21 (m, 2H), 2.28 – 2.15 (m, 1H), 1.61– 1.57 (m, 4H); ^{13}C{^{1}H} (100 MHz, DMSO-d_6) δ 155.3, 67.0, 37.4, 30.0; FT-IR (KBr) ν (cm^{-1}) 3454, 3408, 3353, 3196, 1388, 1268, 1240, 1120; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_6H_{13}N_2O_2$: 145.0977; found: 145.0966.

***N*-(4-(*N′*-Hydroxycarbamimidoyl)phenyl)-2-(4-isobutylphenyl)propenamide (2q):**



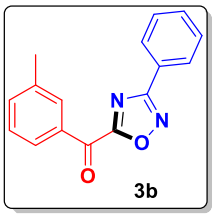
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 7:3 (v/v); Off-white solid; Yield: 259 mg, 79%; m.p: 119-120 ℃; ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.12 (s, 1H), 9.50 (s, 1H), 7.58 (s, 4H), 7.29 (d, J = 8.1 Hz, 2H), 7.10 (d, J = 8.2 Hz, 2H), 5.71 (s, 2H), 3.80 (q, J = 6.9 Hz, 1H), 2.40 (d, J = 7.1 Hz, 2H), 1.84 – 1.74(m, 1H), 1.39 (d, J = 7.0 Hz, 3H), 0.84 (d, J = 6.6 Hz, 6H); ^{13}C{^{1}H} (100 MHz, DMSO-d_6) δ 172.5, 150.5, 139.8, 139.6, 139.1, 129.0, 128.1, 127.0, 125.8, 118.6, 45.6, 44.3, 29.7, 22.2, 18.7; FT-IR (KBr) ν (cm^{-1}) 3446, 3334, 3320, 3150, 3072, 2954, 2923, 1655, 1591, 1405; HRMS (ESI) (m/z) [M + H]$^{+}$ calcd. for $C_{20}H_{26}N_3O_2$: 340.2025; found: 340.2015.

Phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3a):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); off-white solid; yield: 159 mg, 76%; m.p: 58-60 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (dd, J = 8.5, 1.3 Hz, 2H), 8.18 (dd, J = 8.0, 1.7 Hz, 2H), 7.77 – 7.68 (m, 1H), 7.62 – 7.47 (m, 5H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.4, 170.1, 169.0, 135.4, 134.1, 131.9, 131.0, 129.1, 129.0, 127.8, 126.0; FT-IR (KBr) ν (cm^{-1}) 3071, 2926, 1671, 1594, 1555, 1468, 1447, 1316, 1298; HRMS (ESI) (m/z) [M + H]$^{+}$ calcd. for $C_{15}H_{11}N_2O_2$: 251.0821; found: 251.0827.

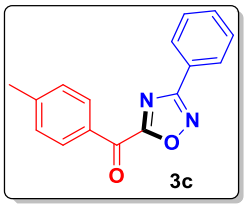
(3-Phenyl-1,2,4-oxadiazol-5-yl)(*m*-tolyl)methanone (3b):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 128 mg, 65%; m.p: 51-52 ℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 7.6 Hz, 1H), 8.20 – 8.17 (m, 3H), 7.58 – 7.49 (m, 4H), 7.46 (t, J = 7.7 Hz, 1H), 2.47 (s, 3H);

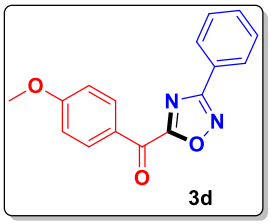
$^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 178.7, 170.3, 169.0, 139.0, 136.3, 134.2, 131.9, 131.1, 129.1, 128.9, 128.4, 127.8, 126.1, 21.5; FT-IR (KBr) ν (cm^{-1}) 3126, 3062, 2921, 1670, 1601, 1550, 1445, 1316, 1298; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{13}N_2O_2$: 265.0977; found: 265.0978.

(3-Phenyl-1,2,4-oxadiazol-5-yl)(*p*-tolyl)methanone (3c):



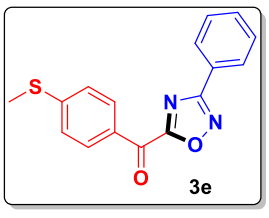
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 130 mg, 66%; m.p: 74-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.2 Hz, 2H), 8.21 – 8.14 (m, 2H), 7.56 – 7.48 (m, 3H), 7.35 (d, *J* = 7.8 Hz, 2H), 2.45 (s, 3H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 178.0, 170.3, 168.9, 146.8, 131.8, 131.7, 131.1, 129.7, 129.1, 127.7, 126.1, 22.0; FT-IR (KBr) ν (cm^{-1}) 3124, 3039, 2917, 1665, 1605, 1551, 1443, 1316, 1298; HRMS (ESI) (m/z) [M + H]$^+$ calcd. for $C_{16}H_{13}N_2O_2$: 265.0977; found: 265.0979.

(4-Methoxyphenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3d):



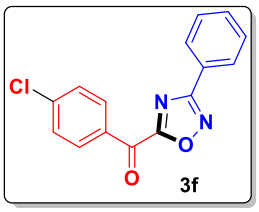
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); off-white solid; yield: 142 mg, 76%; m.p: 85-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, *J* = 9.0 Hz, 2H), 8.19 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.58 – 7.50 (m, 3H), 7.04 (d, *J* = 9.0 Hz, 2H), 3.93 (s, 3H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 176.8, 170.6, 168.9, 165.6, 133.7, 131.8, 129.1, 127.8, 127.2, 126.2, 114.5, 55.8; FT-IR (KBr) ν (cm^{-1}) 3133, 3090, 2935, 2843, 1658, 1595, 1550, 1448, 1320, 1266; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{13}N_2O_3$: 281.0926; found: 281.0931.

(4-(Methylthio)phenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3e):



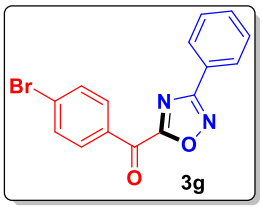
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Yellow solid; Yield: 137 mg, 77%; m.p: 57-59 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.7 Hz, 2H), 8.18 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.57 – 7.49 (m, 3H), 7.35 (d, *J* = 8.7 Hz, 2H), 2.56 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 177.1, 170.3, 168.9, 149.8, 131.8, 131.2, 130.2, 129.1, 127.7, 126.1, 124.9, 14.6; FT-IR (KBr) ν (cm^{-1}) 3135, 3090, 2991, 2921, 1650, 1581, 1437, 1358, 966; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{13}N_2O_2S$: 297.0698; found: 297.0696.

(4-Chlorophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3f):



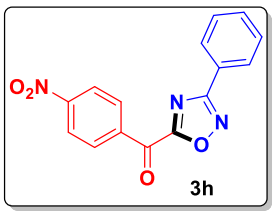
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 116 mg, 63%; m.p: 92-94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.7 Hz, 2H), 8.16 (d, *J* = 6.8 Hz, 2H), 7.59 – 7.48 (m, 5H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 177.1, 169.8, 169.1, 142.3, 132.5, 132.4, 132.0, 129.5, 129.2, 127.8, 125.9; FT-IR (KBr) ν (cm^{-1}) 3088, 2962, 1664, 1586, 1553, 1462, 1403, 1314, 1298, 715, 695; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_{10}ClN_2O_2$: 285.0431; found: 285.0433.

(4-Bromophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3g):



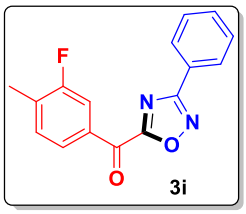
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 113 mg, 68%; m.p: 97-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (d, *J* = 8.7 Hz, 2H), 8.20 – 8.14 (m, 2H), 7.73 (d, *J* = 8.7 Hz, 2H), 7.58 – 7.50 (m, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 177.3, 169.8, 169.1, 132.9, 132.5, 132.4, 132.0, 131.3, 129.2, 127.8, 125.9; FT-IR (KBr) ν (cm^{-1}) 3062, 2921, 1670, 1601, 1550, 1467, 1316, 1227, 684; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_{10}BrN_2O_2$: 328.9926; found: 328.9917.

(4-Nitrophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3h):



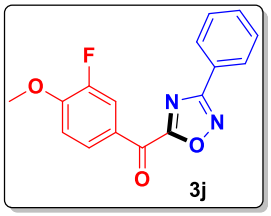
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 109 mg, 61%; m.p: 102-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 9.1 Hz, 2H), 8.44 (d, *J* = 9.1 Hz, 2H), 8.19 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.61 – 7.53 (m, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.7, 169.4, 169.2, 151.5, 138.5, 132.3, 132.2, 129.3, 127.8, 125.7, 124.1; FT-IR (KBr) ν (cm^{-1}) 3055, 2956, 1672, 1603, 1524, 1447, 1339, 1317; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_{10}N_3O_4$: 296.0671; found: 296.0677.

(3-Fluoro-4-methylphenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3i)



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 123 mg, 66%; m.p: 109-111 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 – 8.12(m, 4H), 7.60 – 7.48 (m, 3H), 7.39 (t, *J* = 7.1 Hz, 1H), 2.40 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.8, 169.8, 169.0, 161.2 (d, *J* = 250.0 Hz), 133.9 (d, *J* = 10.0 Hz), 133.6 (d, *J* = 7.7 Hz), 132.1 (d, *J* = 10.0 Hz), 132.0, 129.2, 127.8, 126.7 (d, *J* = 20.0 Hz), 126.0, 117.2 (d, *J* = 20.0 Hz), 15.3 (d, *J* = 3.7 Hz); FT-IR (KBr) ν (cm^{-1}) 3103, 3034, 2954, 1646, 1615, 1572, 1553, 1465, 1320, 1300, 1277, 1028; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{12}FN_2O_2$: 283.0883; found: 285.0888.

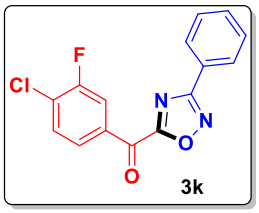
(3-Fluoro-4-methoxyphenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3j):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 121 mg, 68%; m.p: 102-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (ddd, *J* = 8.7, 2.2, 1.2 Hz, 1H), 8.26 (dd, *J* = 11.8, 2.2 Hz, 1H), 8.20 – 8.14 (m, 2H), 7.59 – 7.49 (m, 3H), 7.11 (t, *J* = 8.4 Hz, 1H), 4.02 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 175.7 (d, *J* = 2.6 Hz),

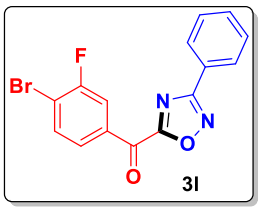
170.0, 169.0, 154.0 (d, J = 10.0 Hz), 152.0 (d, J = 250 Hz), 131.9, 129.4 (d, J = 3.5 Hz), 129.1, 127.7, 127.1 (d, J = 10.0 Hz), 126.0, 118.3 (d, J = 20.0 Hz), 112.7 (d, J = 1.9 Hz), 56.6; FT-IR (KBr) ν (cm^{-1}) 3166, 3026, 2977, 1662, 1608, 1555, 1516, 1466, 1320, 1285, 1013; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{12}FN_2O_3$: 299.0832; found: 299.0838.

(4-Chloro-3-fluorophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3k):



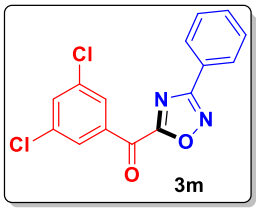
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); off-white solid; yield: 120 mg, 68%; m.p: 79-81 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.35 (dd, J = 9.5, 1.9 Hz, 1H), 8.31 (ddd, J = 8.4, 2.0, 0.8 Hz, 1H), 8.19 – 8.14 (m, 2H), 7.63 (dd, J = 8.4, 7.1 Hz, 1H), 7.59 – 7.50 (m, 3H); $^{13}C\{^1H\}$ (100 MHz, $CDCl_3$) 175.9 (d, J = 2.3 Hz), 169.4, 169.2, 158.2 (d, J = 250 Hz), 134.0 (d, J = 6.2 Hz), 132.1, 131.5, 129.4 (d, J = 20.0 Hz), 129.2, 127.8, 127.5 (d, J = 4.1 Hz), 125.8, 118.8 (d, J = 20.0 Hz); FT-IR (KBr) ν (cm^{-1}) 3091, 3041, 1681, 1595, 1573, 1549, 1486, 1444, 1419, 1353, 1277, 1257, 714, 689; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_9ClFN_2O_2$: 303.0337; found: 303.0339.

(4-Bromo-3-fluorophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3l):



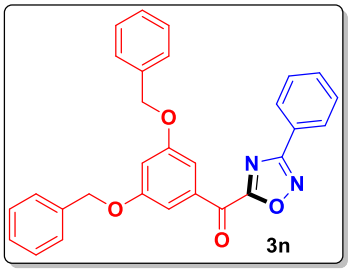
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); off-white solid; yield: 104 mg, 65%; m.p: 89-91 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, J = 9.1, 1.7 Hz, 1H), 8.25 – 8.20 (m, 1H), 8.20 – 8.14 (m, 2H), 7.81 (ddd, J = 8.3, 6.8, 1.6 Hz, 1H), 7.61 – 7.50 (m, 3H); $^{13}C\{^1H\}$ (100 MHz, $CDCl_3$) δ 176.1, 169.4, 169.2, 159.4 (d, J = 250 Hz), 134.8 (d, J = 5.3 Hz), 134.5, 132.1, 129.2, 127.8, 127.6 (d, J = 3.9 Hz), 125.8, 118.5 (d, J = 20.0 Hz), 118.2 (d, J = 20.0 Hz); FT-IR (KBr) ν (cm^{-1}) 3073, 3049, 1677, 1593, 1554, 1476, 1445, 1319, 1235, 1043, 821, 691, 548; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_9BrFN_2O_2$: 346.9831; found: 346.9831.

(3,5-Dichlorophenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3m):



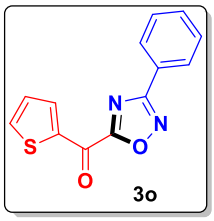
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 132 mg, 78%; m.p: 96-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 1.9 Hz, 2H), 8.19 – 8.16 (m, 2H), 7.70 (t, *J* = 1.9 Hz, 1H), 7.59 – 7.52 (m, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 175.8, 169.3, 169.1, 136.3, 136.1, 134.9, 132.2, 129.3 (2C), 127.8, 125.7; FT-IR (KBr) ν (cm^{-1}) 3077, 3071, 1689, 1558, 1466, 1391, 1317, 1286, 715, 688; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_9Cl_2N_2O_2$: 319.0041; found: 319.0040.

(3,5-Bis(benzyloxy)phenyl)(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3n):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Yellow solid; Yield: 106 mg, 76%; m.p: 97-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.69 (d, *J* = 2.3 Hz, 2H), 7.57 – 7.50 (m, 3H), 7.46 – 7.42 (m, 4H), 7.39 (ddd, *J* = 7.9, 6.8, 1.1 Hz, 4H), 7.36 – 7.31 (m, 2H), 6.96 (t, *J* = 2.3 Hz, 1H), 5.13 (s, 4H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.2, 170.2, 169.0, 160.3, 136.3, 135.8, 131.9, 129.2, 128.8, 128.4, 127.9, 127.8, 127.7, 126.1, 109.8, 70.6; FT-IR (KBr) ν (cm^{-1}) 3103, 3058, 3034, 2963, 1671, 1591, 1554, 1468, 1380, 1317, 1300, 1273, 1178; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{29}H_{23}N_2O_4$: 463.1658; found: 463.1658.

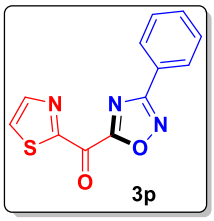
(3-Phenyl-1,2,4-oxadiazol-5-yl)(thiophen-2-yl)methanone (3o):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Yellow solid; Yield: 173 mg, 85%; m.p: 87-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 – 8.63 (m, 1H), 8.18 (dt, *J* = 8.2, 1.8 Hz, 2H), 7.92 (dt, *J* = 4.9, 1.2 Hz, 1H), 7.59 – 7.49 (m, 3H), 7.29

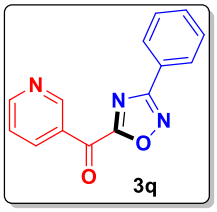
(ddd, J = 5.0, 3.9, 1.3 Hz, 1H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 169.7, 169.6, 169.1, 140.3, 138.4, 138.3, 131.9, 129.1, 129.0, 127.7, 125.9; FT-IR (KBr) ν (cm^{-1}) 3085, 2922, 1645, 1551, 1516, 1439, 1348, 1290, 1047, 922; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{13}H_9N_2O_2S$: 257.0385; found: 257.0370.

(3-Phenyl-1,2,4-oxadiazol-5-yl)(thiazol-2-yl)methanone (3p):



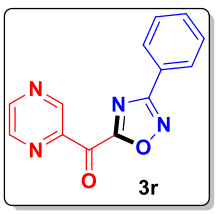
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Yellow solid; Yield: 166 mg, 82%; m.p: 67-68 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (d, J = 2.9 Hz, 1H), 8.22 – 8.19 (m, 2H), 7.97 (d, J = 2.9 Hz, 1H), 7.57 – 7.51 (m, 3H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 170.1, 169.4, 169.3, 162.2, 146.8, 132.0, 129.2, 129.1, 127.9, 125.8; FT-IR (KBr) ν (cm^{-1}) 3098, 2924, 1664, 1550, 1443, 1352, 1286; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{12}H_8N_3O_2S$: 258.0337; found: 258.0340.

(3-Phenyl-1,2,4-oxadiazol-5-yl)(pyridin-3-yl)methanone (3q):



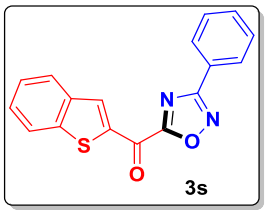
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Yellow solid; Yield: 79 mg, 38%; m.p: 52-54 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (d, J = 2.2 Hz, 1H), 8.94 (dd, J = 4.8, 1.7 Hz, 1H), 8.77 (dt, J = 8.1, 2.0 Hz, 1H), 8.19 (dt, J = 8.1, 1.2 Hz, 2H), 7.60 – 7.51 (m, 4H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 177.1, 169.3, 155.2, 152.2, 138.1, 132.1, 130.0, 129.2 (2C), 127.8, 125.8, 123.9; FT-IR (KBr) ν (cm^{-1}) 3044, 2921, 1679, 1583, 1446, 1320, 1204; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{14}H_{10}N_3O_2$: 252.0773; found: 252.0763.

(3-Phenyl-1,2,4-oxadiazol-5-yl)(pyrazin-2-yl)methanone (3r):



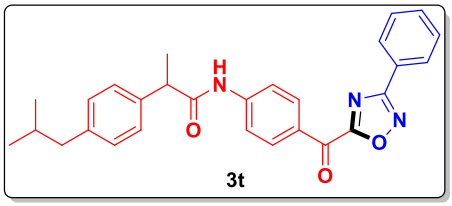
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 7:3 (v/v); Yellow solid; Yield: 75 mg, 36%; m.p: 127-129 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.57 (d, *J* = 1.5 Hz, 1H), 8.92 (d, *J* = 2.4 Hz, 1H), 8.84 (dd, *J* = 2.4, 1.5 Hz, 1H), 8.22 – 8.13 (m, 2H), 7.59 – 7.49 (m, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.6, 169.9, 169.2, 149.0, 146.6, 146.3, 144.6, 132.0, 129.2, 127.9, 125.8; FT-IR (KBr) ν (cm^{-1}) 3014, 2968, 1689, 1562, 1519, 1440, 1316, 1216; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{13}H_9N_4O_2$: 253.0726; found: 253.0729.

Benzo[*b*]thiophen-2-yl(3-phenyl-1,2,4-oxadiazol-5-yl)methanone (3s):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Off-white solid; Yield: 125 mg, 72%; m.p: 135-137 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 0.8 Hz, 1H), 8.26 – 8.20 (m, 2H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.93 (dq, *J* = 8.2, 0.9 Hz, 1H), 7.60 – 7.53 (m, 4H), 7.48 (ddd, *J* = 8.1, 7.1, 1.1 Hz, 1H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 171.4, 169.5, 169.3, 144.3, 140.0, 139.2, 136.3, 132.1, 129.2, 129.1, 127.9, 127.4, 126.0, 125.7, 123.1; FT-IR (KBr) ν (cm^{-1}) 3090, 2923, 1647, 1556, 1495, 1443, 1333, 1292, 1074, 919; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{11}N_2O_2S$: 307.0541; found: 307.0539.

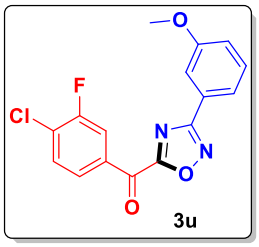
2-(4-Isobutylphenyl)-*N*-(4-(3-phenyl-1,2,4-oxadiazole-5-carbonyl)phenyl)propenamide (3t):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Yellow solid; Yield: 44 mg, 31%; m.p: 140-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 – 8.40 (m, 2H), 8.10 (d, *J* = 8.8 Hz, 2H), 7.76 – 7.70 (m, 1H), 7.61 – 7.57 (m, 4H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.22 (s, 1H), 7.18 (d, *J* = 8.1 Hz, 2H), 3.73 (q, *J* = 7.2 Hz, 1H), 2.49 (d, *J* = 7.2 Hz, 2H), 1.93 – 1.83 (m, 1H), 1.62 (d, *J* = 7.2 Hz, 3H), 0.92 (d, *J* = 6.6 Hz, 6H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.6, 172.9, 170.1, 168.5, 141.5, 141.2, 137.8, 135.4, 134.2, 131.0, 130.2, 129.1, 128.8, 127.6, 121.5, 119.6, 48.1, 45.2, 30.3, 22.5, 18.6; FT-IR (KBr) ν (cm^{-1}) 3356, 3156,

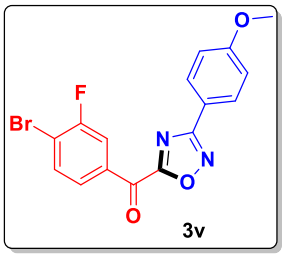
3050, 2955, 1648, 1579, 1513, 1467, 1320, 1261, 1156; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{28}H_{28}N_3O_3$: 454.2131; found: 454.2117.

(4-Chloro-3-fluorophenyl)(3-(3-methoxyphenyl)-1,2,4-oxadiazol-5-yl)methanone (3u):



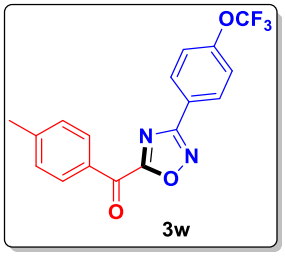
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 122 mg, 63%; m.p: 52-54 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.27 (m, 2H), 7.77 (td, *J* = 8.0, 1.2 Hz, 1H), 7.68 (dd, *J* = 2.7, 1.5 Hz, 1H), 7.64 (dd, *J* = 8.4, 7.0 Hz, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.11 (ddd, *J* = 8.3, 2.7, 1.0 Hz, 1H), 3.90 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.0 (d, *J* = 1.9 Hz), 169.4, 169.2, 160.2, 158.3 (d, *J* = 250 Hz), 134.0 (d, *J* = 10.0 Hz), 131.5, 130.4, 129.4 (d, *J* = 20.0 Hz), 127.5 (d, *J* = 10.0 Hz), 127.0, 120.3, 118.8 (d, *J* = 20.0 Hz), 118.3, 112.6, 55.7; FT-IR (KBr) ν (cm^{-1}) 3102, 3046, 3013, 2996, 1674, 1601, 1574, 1518, 1469, 1309, 1239, 1031, 904, 798, 683; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{11}ClFN_2O_3$: 333.0442; found: 333.0467.

(4-Bromo-3-fluorophenyl)(3-(4-methoxyphenyl)-1,2,4-oxadiazol-5-yl)methanone (3v):



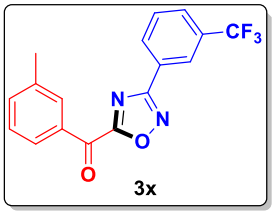
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 125 mg, 72%; m.p: 88-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, *J* = 9.0, 2.0 Hz, 1H), 8.22 (ddd, *J* = 8.3, 2.0, 0.7 Hz, 1H), 8.11 (d, *J* = 8.9 Hz, 2H), 7.80 (dd, *J* = 8.4, 6.7 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 3.90 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.2 (d, *J* = 1.9 Hz), 169.2, 168.9, 162.7, 159.3 (d, *J* = 250 Hz), 134.9 (d, *J* = 6.2 Hz), 134.5, 129.5, 127.6 (d, *J* = 10.0 Hz), 118.6 (d, *J* = 30.0 Hz), 118.2, 118.1 (d, *J* = 30.0 Hz), 114.7, 55.6; FT-IR (KBr) ν (cm^{-1}) 3148, 3095, 3018, 2985, 1666, 1615, 1468, 1417, 1311, 1253, 1049, 622; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{11}BrFN_2O_3$: 376.9937; found: 376.9959.

***p*-Tolyl(3-(4-(trifluoromethoxy)phenyl)-1,2,4-oxadiazol-5-yl)methanone (3w):**



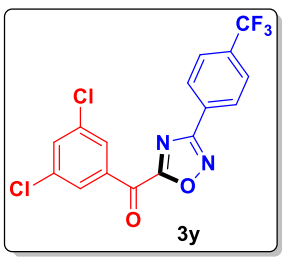
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); off-white solid; Yield: 180 mg, 69%; m.p: 56-58 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (d, *J* = 8.3 Hz, 2H), 8.25 (d, *J* = 8.9 Hz, 2H), 7.42 – 7.35 (m, 4H), 2.49 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.0, 170.7, 168.0, 151.8, 147.1, 131.7, 131.2, 129.9, 129.6, 124.7, 121.4, 120.4 (q, *J* = 257.0 Hz), 22.1; FT-IR (KBr) ν (cm^{-1}) 3156, 3088, 2926, 1661, 1604, 1555, 1474, 1421, 1312, 1266, 1216, 1025; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{12}F_3N_2O_3$: 349.0800; found: 349.0807.

***m*-Tolyl(3-(3-(trifluoromethyl)phenyl)-1,2,4-oxadiazol-5-yl)methanone (3x):**



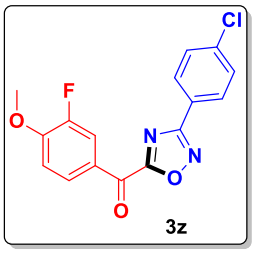
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); off-white solid; Yield: 159 mg, 64%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 8.39 (d, *J* = 7.8 Hz, 1H), 8.26 (d, *J* = 7.8 Hz, 1H), 8.17 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 2.48 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 178.6, 170.8, 168.0, 139.2, 136.5, 134.1, 131.8 (q, *J* = 30.0 Hz), 131.1, 131.0, 129.8, 129.0, 128.5, 128.4, 127.0, 124.8 (q, *J* = 10.0 Hz), 123.7 (q, *J* = 270.0 Hz), 21.5; FT-IR (KBr) ν (cm^{-1}) 3163, 3065, 2931, 1677, 1603, 1559, 1418, 1325, 1300, 1270, 1072; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{12}F_3N_2O_2$: 333.0851; found: 333.0856.

(3,5-Dichlorophenyl)(3-(4-(trifluoromethyl)phenyl)-1,2,4-oxadiazol-5-yl)methanone (3y):



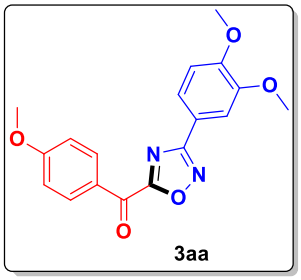
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 19:1 (v/v); Off-white solid; Yield: 149 mg, 73%; m.p: 81-83 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 1.9 Hz, 2H), 8.32 (dd, *J* = 8.8, 0.9 Hz, 2H), 7.82 (d, *J* = 8.2 Hz, 2H), 7.72 (t, *J* = 1.9 Hz, 1H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 175.6, 169.5, 168.3, 136.3, 136.1, 135.1, 133.9 (q, *J* = 33 Hz), 129.2, 129.1, 128.3, 126.3 (q, *J* = 4.0 Hz), 123.8 (q, *J* = 271 Hz); FT-IR (KBr) ν (cm^{-1}) 3083, 2962, 1681, 1567, 1536, 1417, 1320, 1190, 1168, 1127, 1104, 714, 670; HRMS (ESI) (m/z) [M + H]$^{+}$ calcd. for $C_{16}H_8Cl_2F_3N_2O_2$: 386.9915; found: 386.9906.

(3-(4-Chlorophenyl)-1,2,4-oxadiazol-5-yl)(3-fluoro-4-methoxyphenyl)methanone (3z):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Pale green solid; Yield: 129 mg, 65%; m.p: 95-97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (ddd, *J* = 8.7, 2.2, 1.2 Hz, 1H), 8.26 (dd, *J* = 11.8, 2.2 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 2H), 7.52 (d, *J* = 8.6 Hz, 2H), 7.12 (t, *J* = 8.4 Hz, 1H), 4.03 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 175.7 (d, *J* = 2.4 Hz), 170.2, 168.2, 154.2 (d, *J* = 10.0 Hz), 152.1 (d, *J* = 248 Hz), 138.3, 129.6, 129.4 (d, *J* = 3.2 Hz), 129.1, 127.1 (d, *J* = 10.0 Hz), 124.6, 118.3 (d, *J* = 20.0 Hz), 112.8, 56.6; FT-IR (KBr) ν (cm^{-1}) 3118, 3080, 2982, 1665, 1606, 1580, 1516, 1440, 1314, 1286, 1134, 1091, 766, 658; HRMS (ESI) (m/z) [M + H]$^{+}$ calcd. for $C_{16}H_{11}ClFN_2O_3$: 333.0442; found: 333.0455.

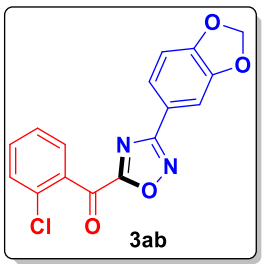
(3-(3,4-Dimethoxyphenyl)-1,2,4-oxadiazol-5-yl)(4-methoxyphenyl)methanone (3aa):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 1:1 (v/v); Pale yellow solid; Yield: 134 mg, 59%; m.p: 97-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 9.1 Hz, 2H), 7.80 (dd, *J* = 8.4, 1.9 Hz, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.04 (d, *J* = 9.0 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 1H), 3.99 (s, 3H), 3.96 (s, 3H), 3.94 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 177.0, 170.5, 168.6, 165.5, 152.1, 149.4, 133.6, 127.3, 121.5, 118.7, 114.4, 111.2, 110.1, 56.2,

56.1, 55.8; FT-IR (KBr) ν (cm^{-1}) 3156, 3120, 3076, 3008, 1651, 1603, 1571, 1511, 1439, 1303, 1265, 1240, 1171, 1025; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{18}H_{17}N_2O_5$: 341.1137; found: 341.1143.

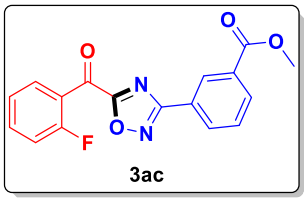
(3-(Benzo[*d*][1,3]dioxol-5-yl)-1,2,4-oxadiazol-5-yl)(2-chlorophenyl)methanone (3ab)



3ab

Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Pale green solid; Yield: 119 mg, 56%; m.p: 61-63 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.70 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.62 – 7.55 (m, 2H), 7.53 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.47 (td, *J* = 7.5, 1.3 Hz, 1H), 6.91 (d, *J* = 8.1 Hz, 1H), 6.05 (s, 2H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 179.8, 170.2, 169.0, 150.8, 148.4, 134.8, 134.2, 133.7, 131.5, 131.1, 127.2, 123.0, 119.7, 108.9, 107.8, 101.9; FT-IR (KBr) ν (cm^{-1}) 3126, 3096, 2961, 1697, 1683, 1588, 1564, 1463, 1256, 1114, 1041, 737, 667; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{16}H_{10}ClN_2O_4$: 329.0329; found: 329.0336.

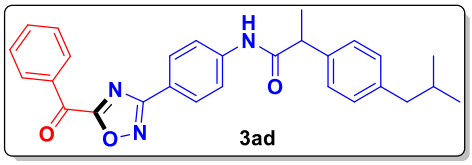
Methyl 3-(5-(2-fluorobenzoyl)-1,2,4-oxadiazol-3-yl)benzoate (3ac):



3ac

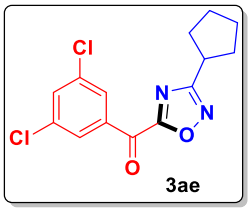
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); White solid; Yield: 146 mg, 62%; m.p: 88-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (t, *J* = 1.8 Hz, 1H), 8.35 (dt, *J* = 7.8, 1.5 Hz, 1H), 8.23 (dt, *J* = 7.9, 1.5 Hz, 1H), 8.09 – 8.00 (m, 1H), 7.77 – 7.68 (m, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.38 (td, *J* = 7.6, 1.1 Hz, 1H), 7.26 – 7.21 (m, 1H), 3.97 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 177.5, 170.9, 168.5, 166.3, 162.2 (d, *J* = 259 Hz), 136.8 (d, *J* = 10 Hz), 132.9, 132.0, 131.9, 131.4, 129.4, 129.0, 126.5, 124.8 (d, *J* = 10.0 Hz), 123.8 (d, *J* = 10.0 Hz), 117.2 (d, *J* = 20.0 Hz), 52.6; FT-IR (KBr) ν (cm^{-1}) 3126, 3095, 3010, 2958, 1732, 1680, 1609, 1455, 1318, 1291, 1256, 1122, 1026; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{12}FN_2O_4$: 327.0781; found: 327.0775.

***N*-(4-(5-benzoyl-1,2,4-oxadiazol-3-yl)phenyl)-2-(4-isobutylphenyl)propenamide (3ad):**



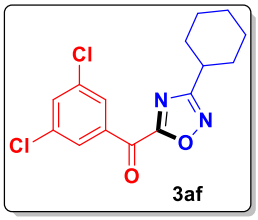
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); White solid; Yield: 105 mg, 28%; m.p: 160-161 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.9 Hz, 2H), 8.17 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.65 (d, *J* = 8.9 Hz, 2H), 7.57 – 7.50 (m, 3H), 7.38 (s, 1H), 7.27 (d, *J* = 6.4 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 3.75 (q, *J* = 7.1 Hz, 1H), 2.48 (d, *J* = 7.2 Hz, 2H), 1.92 – 1.85 (m, 1H), 1.61 (d, *J* = 7.1 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.9, 173.1, 170.4, 169.0, 144.4, 141.7, 137.5, 132.8, 131.9, 130.3, 129.6, 129.2, 127.8, 127.6, 126.1, 118.9, 48.2, 45.1, 30.3, 22.5, 18.6; FT-IR (KBr) ν (cm^{-1}) 3396, 3162, 3085, 2958, 1696, 1655, 1602, 1558, 1512, 1459, 1303, 1250, 1172, 1013; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{28}H_{28}N_3O_3$: 454.2131; found: 454.2134.

(3-Cyclopentyl-1,2,4-oxadiazol-5-yl)(3,5-dichlorophenyl)methanone (3ae):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 53 mg, 32%; m.p: 72-73 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 2.0 Hz, 2H), 7.69 (t, *J* = 1.9 Hz, 1H), 3.40 (quint, *J* = 8.0 Hz, 1H), 2.20 – 2.12 (m, 2H), 1.97 – 1.85 (m, 4H), 1.79 – 1.71 (m, 2H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.1, 175.2, 168.9, 136.4, 136.1, 134.8, 129.2, 36.8, 31.8, 25.7; FT-IR (KBr) ν (cm^{-1}) 3123, 3115, 3091, 1811, 1684, 1567, 1503, 1421, 1397, 1193, 1038, 749, 666; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{14}H_{13}Cl_2N_2O_2$: 311.0354; found: 311.0352.

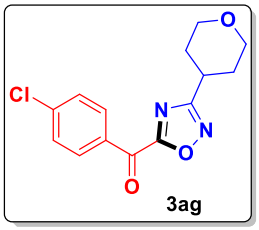
(3-Cyclohexyl-1,2,4-oxadiazol-5-yl)(3,5-dichlorophenyl)methanone (3af):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Off-white solid; Yield: 60 mg, 35%; m.p: 90-91 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 1.9 Hz, 2H), 7.69 (t, *J* = 1.9 Hz, 1H), 2.98 (tt, *J* = 11.4, 3.6 Hz, 1H), 2.14 – 2.08 (m, 2H), 1.88 (dt,

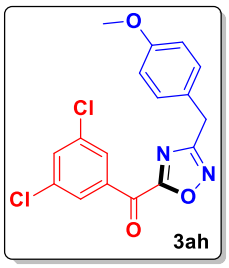
J = 13.4, 3.8 Hz, 2H), 1.79 – 1.73 (m, 1H), 1.71 – 1.60 (m, 2H), 1.50 – 1.40 (m, 2H), 1.39 – 1.30 (m, 1H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 176.0, 175.2, 168.8, 136.4, 136.1, 134.8, 129.2, 36.1, 30.7, 25.7 (2C); FT-IR (KBr) ν (cm^{-1}) 3135, 3115, 3063, 3088, 1800, 1681, 1566, 1500, 1454, 1303, 1265, 1119, 1038, 764, 668; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_{15}Cl_2N_2O_2$: 325.0511; found: 325.0501.

(4-Chlorophenyl)(3-(tetrahydro-2H-pyran-4-yl)-1,2,4-oxadiazol-5-yl)methanone (3ag):



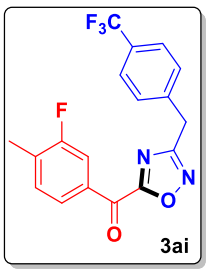
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 1:9 (v/v); green solid; Yield: 72 mg, 38%; m.p: 60-62 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.7 Hz, 2H), 7.55 (d, *J* = 8.7 Hz, 2H), 4.10 (t, *J* = 3.5 Hz, 1H), 4.07 (t, *J* = 3.5 Hz, 1H), 3.64 – 3.54 (m, 2H), 3.29 – 3.18 (m, 1H), 2.08 – 2.00 (m, 4H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 177.1, 173.6, 169.7, 142.3, 132.4, 132.3, 129.5, 67.2, 33.4, 30.2; FT-IR (KBr) ν (cm^{-1}) 3162, 3126, 3050, 2991, 1682, 1587, 1562, 1402, 1308, 1243, 1024, 741, 642; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{14}H_{14}ClN_2O_3$: 293.0693; found: 293.0700.

(3,5-Dichlorophenyl)(3-(4-methoxybenzyl)-1,2,4-oxadiazol-5-yl)methanone (3ah):



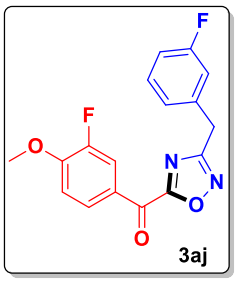
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Pale yellow solid; Yield: 95 mg, 49%; m.p: 57-59 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 1.9 Hz, 2H), 7.67 (t, *J* = 1.9 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 2H), 6.89 (d, *J* = 8.7 Hz, 2H), 4.18 (s, 2H), 3.79 (s, 3H); $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) δ 175.8, 170.8, 169.1, 159.1, 136.2, 136.1, 134.9, 130.2, 129.2, 126.7, 114.4, 55.4, 31.7; FT-IR (KBr) ν (cm^{-1}) 3123, 3087, 2969, 1681, 1612, 1566, 1513, 1404, 1304, 1249, 1036, 779, 673; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{13}Cl_2N_2O_3$: 363.0303; found: 363.0295

(3-Fluoro-4-methylphenyl)(3-(4-(trifluoromethyl)benzyl)-1,2,4-oxadiazol-5-yl)methanone (3ai):



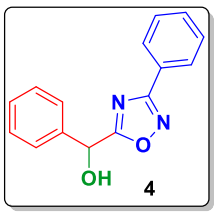
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Pale yellow solid; Yield: 108 mg, 45%; m.p: 81-83 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.9, 1.8 Hz, 1H), 8.03 (dd, *J* = 10.1, 1.8 Hz, 1H), 7.62 (d, *J* = 8.1 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 1H), 4.30 (s, 2H), 2.39 (d, *J* = 2.0 Hz, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 176.7 (d, *J* = 1.8 Hz), 170.2, 169.6, 161.3 (d, *J* = 246 Hz), 138.9, 134.1 (d, *J* = 20.0 Hz), 133.5 (d, *J* = 7.6 Hz), 132.1 (d, *J* = 10.0 Hz), 130.0 (q, *J* = 30.0 Hz), 129.6, 126.7 (d, *J* = 10.0 Hz), 126.0 (q, *J* = 10.0 Hz), 124.2 (q, *J* = 270.0 Hz), 117.1 (d, *J* = 30.0 Hz), 32.4, 15.3 (d, *J* = 3.5 Hz); FT-IR (KBr) ν (cm^{-1}) 3106, 3086, 2999, 1679, 1618, 1574, 1504, 1421, 1327, 1243, 1118, 1020; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{18}H_{13}F_4N_2O_2$: 365.0913; found: 365.0915.

(3-Fluoro-4-methoxyphenyl)(3-(3-fluorobenzyl)-1,2,4-oxadiazol-5-yl)methanone (3aj):



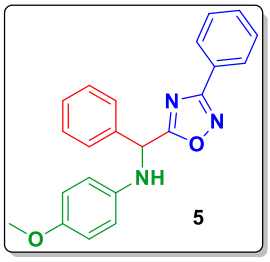
Purified by column chromatography eluting with petroleum ether/ethyl acetate = 9:1 (v/v); Grey solid; Yield: 89 mg, 45%; m.p: 73-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (ddd, *J* = 8.7, 2.2, 1.2 Hz, 1H), 8.15 (dd, *J* = 11.8, 2.2 Hz, 1H), 7.32 (td, *J* = 8.0, 5.9 Hz, 1H), 7.15 (dd, *J* = 7.7, 0.7 Hz, 1H), 7.13 – 7.03 (m, 2H), 6.98 (tdd, *J* = 8.5, 2.6, 1.0 Hz, 1H), 4.23 (s, 2H), 4.00 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 175.7 (d, *J* = 2.0 Hz), 170.2, 169.7, 163.0 (d, *J* = 245 Hz), 154.1 (d, *J* = 10.0 Hz), 152.1 (d, *J* = 250 Hz), 137.2 (d, *J* = 10.0 Hz), 130.4 (d, *J* = 10.0 Hz), 129.3 (d, *J* = 3.3 Hz), 127.0 (d, *J* = 10.0 Hz), 124.8 (d, *J* = 3.0 Hz), 118.2 (d, *J* = 20.0 Hz), 116.2 (d, *J* = 20.0 Hz), 114.6 (d, *J* = 20.0 Hz), 112.7, 56.6, 32.2; FT-IR (KBr) ν (cm^{-1}) 3156, 3070, 2984, 1666, 1614, 1520, 1492, 1446, 1325, 1290, 1227, 1144, 1019; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{17}H_{13}F_2N_2O_3$: 331.0894; found: 331.0899.

Phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methanol (4):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Pale pink solid; Yield: 44 mg, 87%; m.p: 102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (dd, *J* = 8.1, 1.7 Hz, 2H), 7.53 – 7.44 (m, 5H), 7.42 – 7.34 (m, 3H), 6.07 (s, 1H), 3.67 (s, 1H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 179.6, 168.3, 137.9, 131.6, 129.4, 129.2, 129.0, 127.7, 126.8, 126.4, 69.7; FT-IR (KBr) ν (cm^{-1}) 3267, 3063, 3032, 2912, 1595, 1568, 1478, 1361, 1213, 1099, 1023; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{15}H_{13}N_2O_2$: 253.0977; found: 253.0973.

4-Methoxy-*N*-(phenyl(3-phenyl-1,2,4-oxadiazol-5-yl)methyl)aniline (5):



Purified by column chromatography eluting with petroleum ether/ethyl acetate = 8:2 (v/v); Pale yellow solid; Yield: 122 mg, 86%; m.p: 113-114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.57 – 7.52 (m, 2H), 7.50 – 7.43 (m, 3H), 7.42 – 7.31 (m, 3H), 6.75 (d, *J* = 9.0 Hz, 2H), 6.66 (d, *J* = 9.0 Hz, 2H), 5.85 (d, *J* = 4.4 Hz, 1H), 4.62 (s, 1H), 3.71 (s, 3H); ^{13}C{^{1}H} (100 MHz, $CDCl_3$) δ 179.5, 168.5, 153.3, 139.9, 137.4, 131.5, 129.3, 129.0 (2C), 127.7, 127.4, 126.6, 115.5, 115.0, 56.9, 55.8; FT-IR (KBr) ν (cm^{-1}) 3383, 3123, 3074, 2993, 1595, 1573, 1515, 1447, 1356, 1242, 1185, 1028; HRMS (ESI) (m/z) $[M + H]^+$ calcd. for $C_{22}H_{20}N_3O_2$: 358.1556; found: 358.1545.

References:

1. M. Arockiaraj and V. Rajeshkumar, Adv. *Synth. Catal.*, **2024**, *366*, 2557– 2564.
2. (a) M. A. Khanfar, D. Reiner, S. Hagenow and H. Stark, *Bioorg. Med. Chem.*, **2018**, *26*, 4034–4046; (b) L. G. Maciel, A. D. S. Barbosa, E. B. de Alencar-Filho, T. A. Soares and J. V. D. Anjos, *RSC Med. Chem.*, **2021**, *12*, 222–236.
3. A. F. Abdel-Magid, K. G. Carson, B. D. Harris, C. A. Maryanoff and R. D. Shah, *J. Org. Chem.*, **1996**, *61*, 3849−3862.

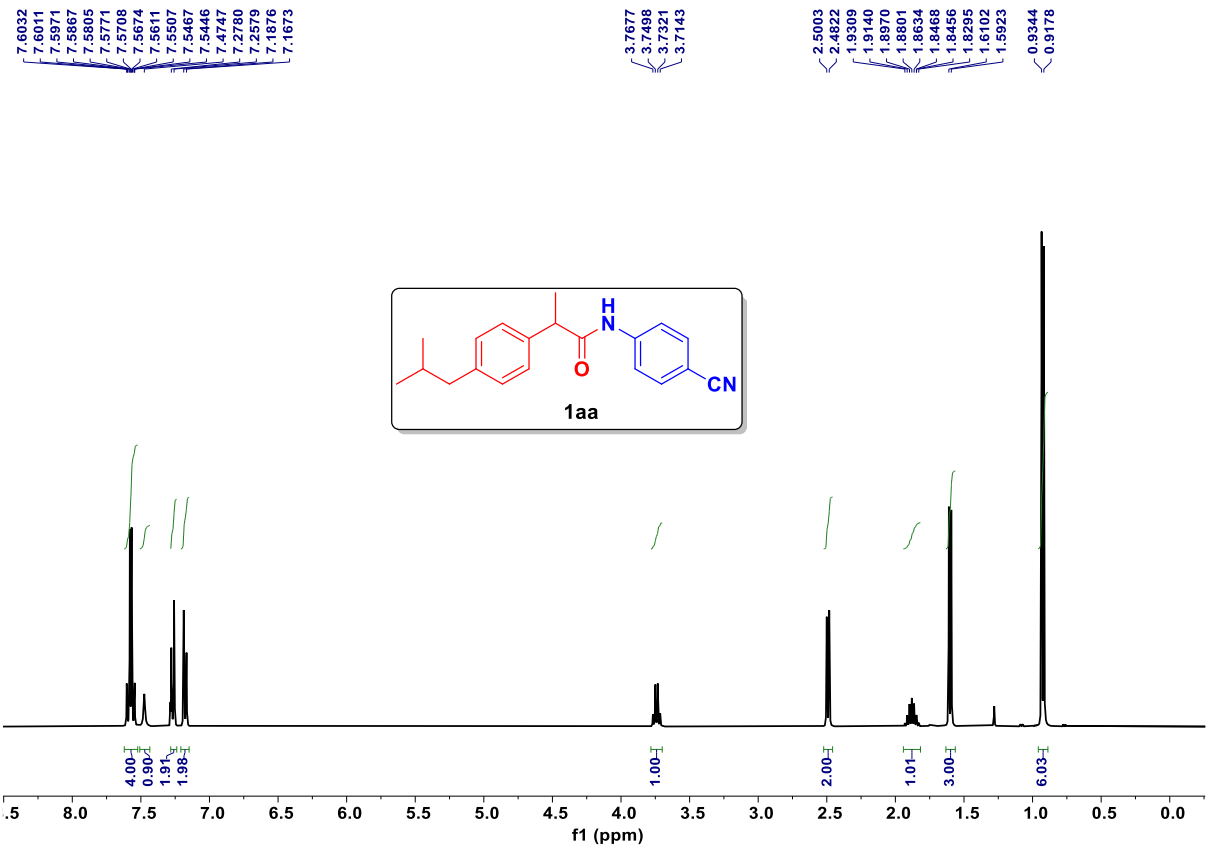


Figure 1. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1aa**

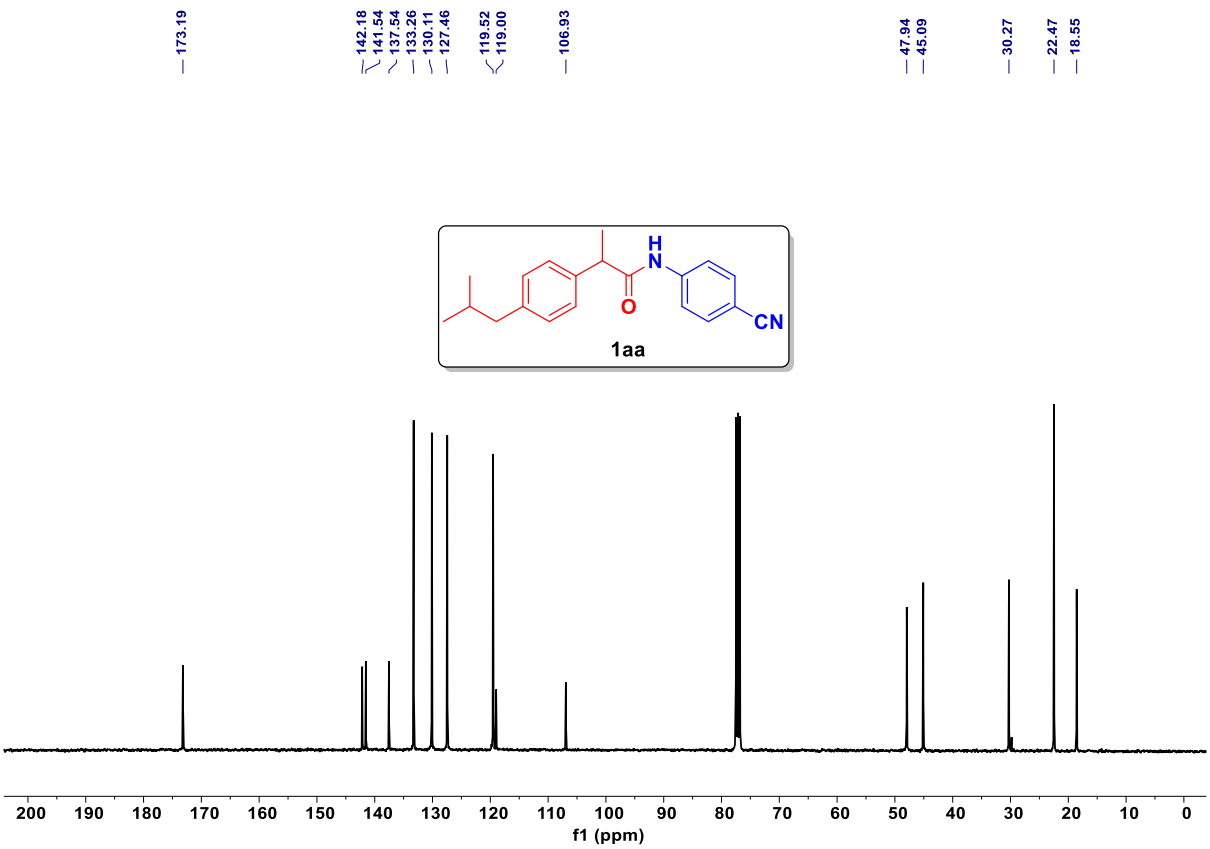


Figure 2. $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) of compound **1aa**

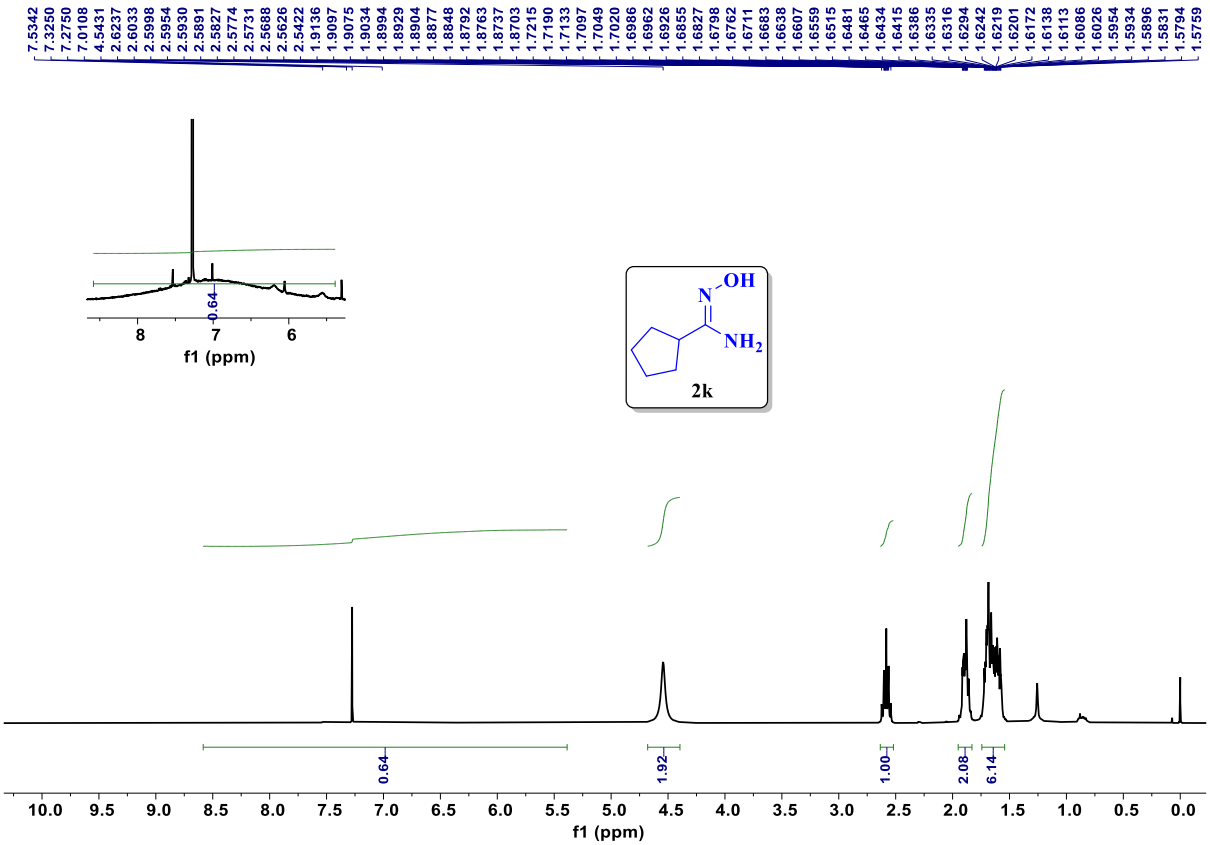


Figure 3. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2k**

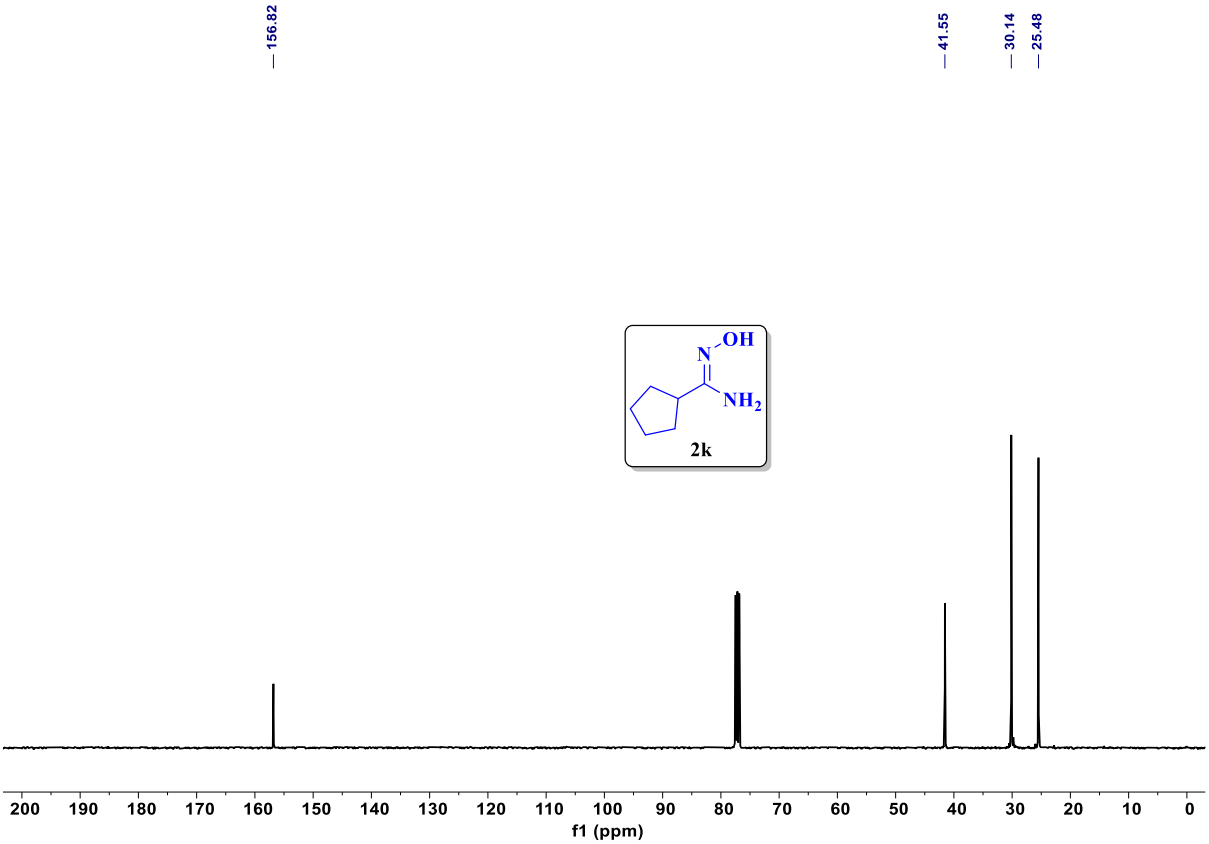


Figure 4. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **2k**

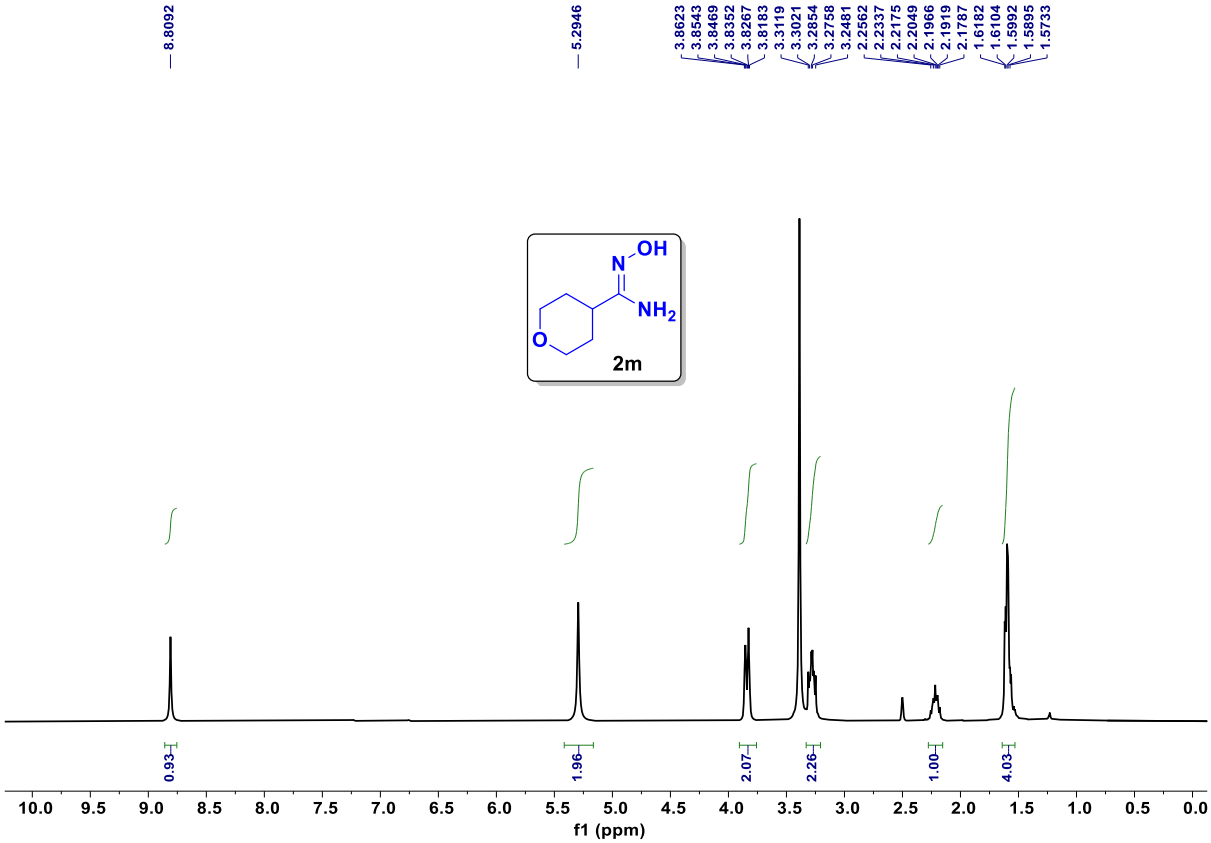


Figure 5. ^{1}H NMR (400 MHz, DMSO-d_6) of compound **2m**

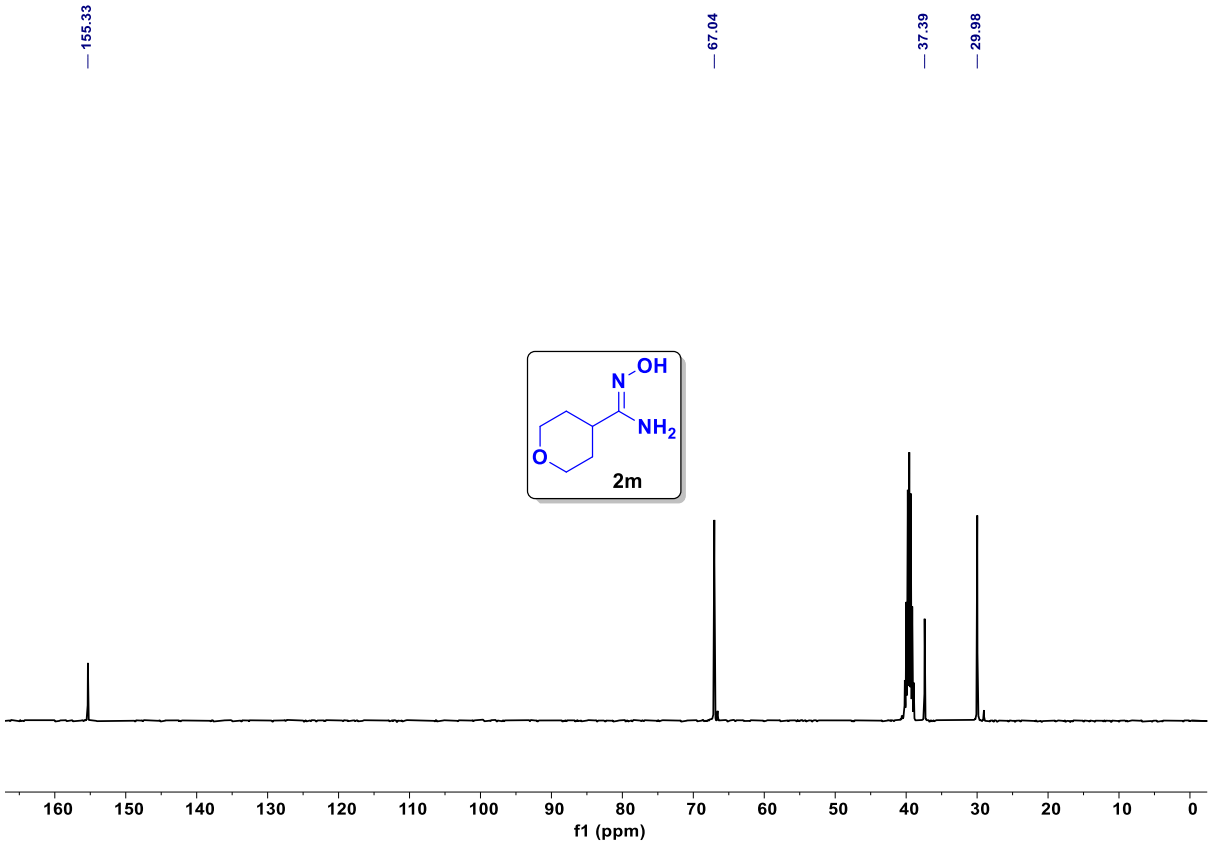


Figure 6. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) of compound **2m**

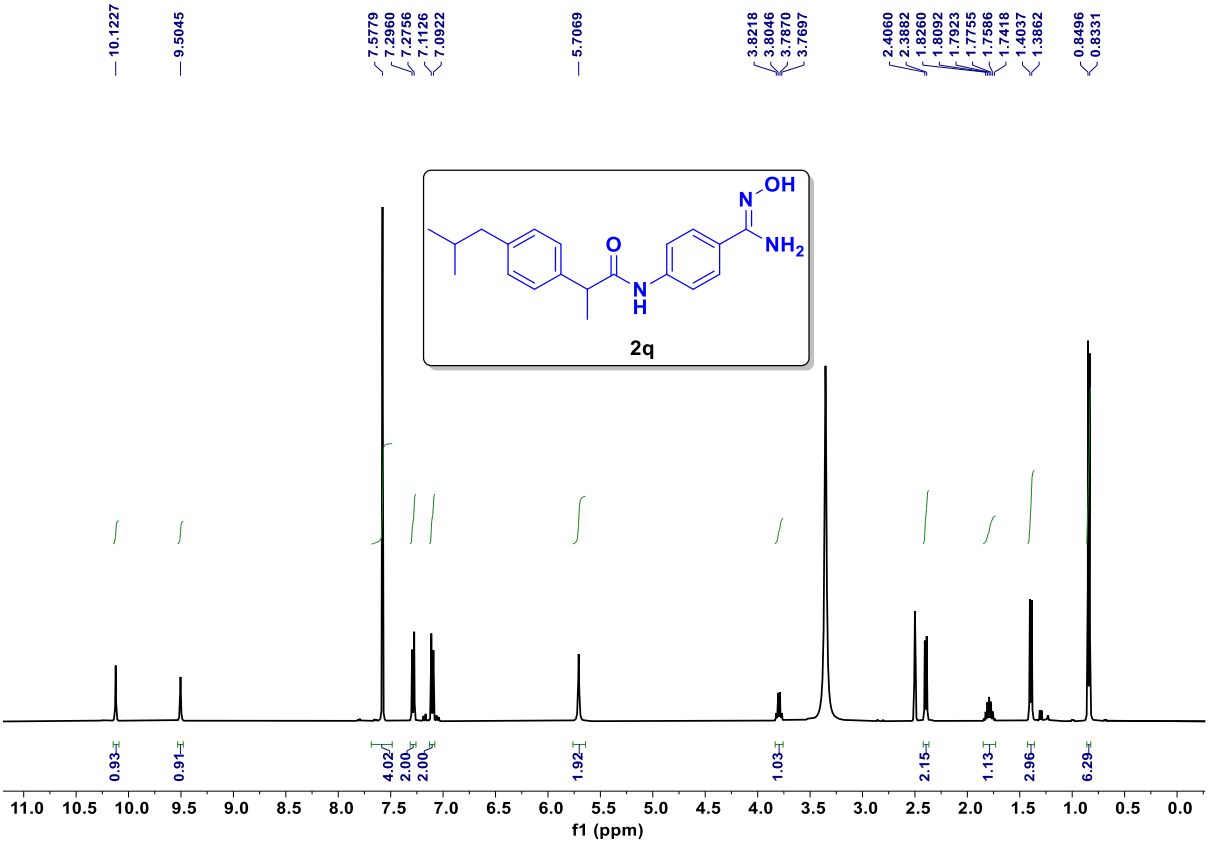


Figure 7. ^{1}H NMR (400 MHz, DMSO-d_6) of compound **2q**

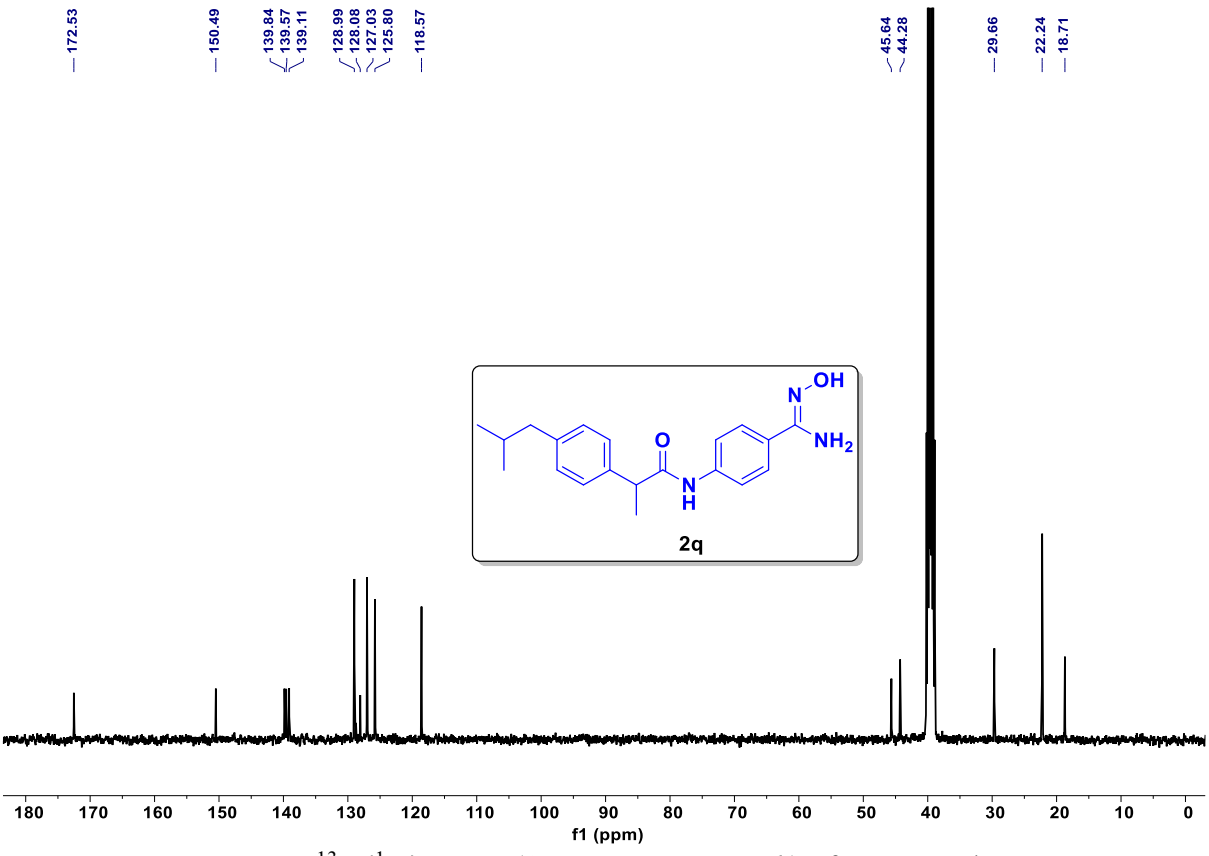


Figure 8. ^{13}C{^{1}H} NMR (100 MHz, DMSO-d_6) of compound **2q**

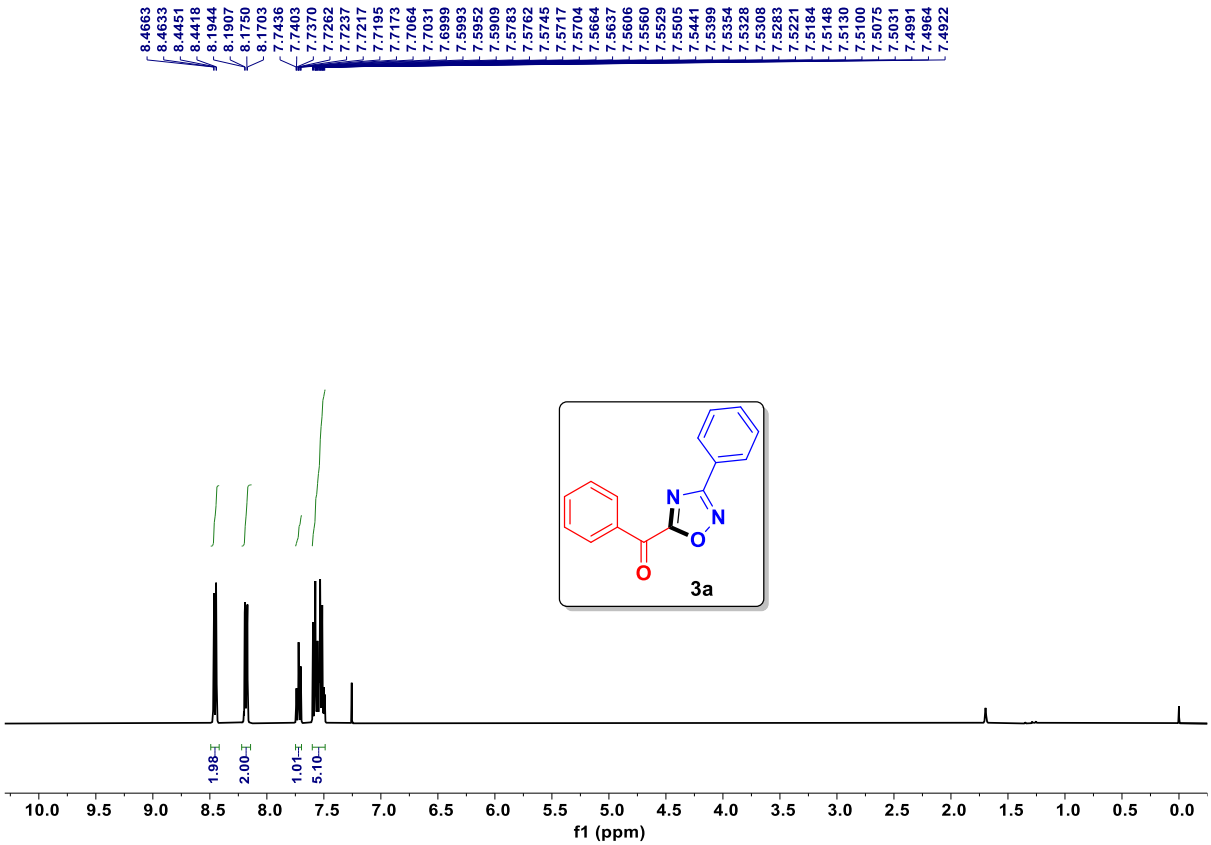


Figure 9. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3a**

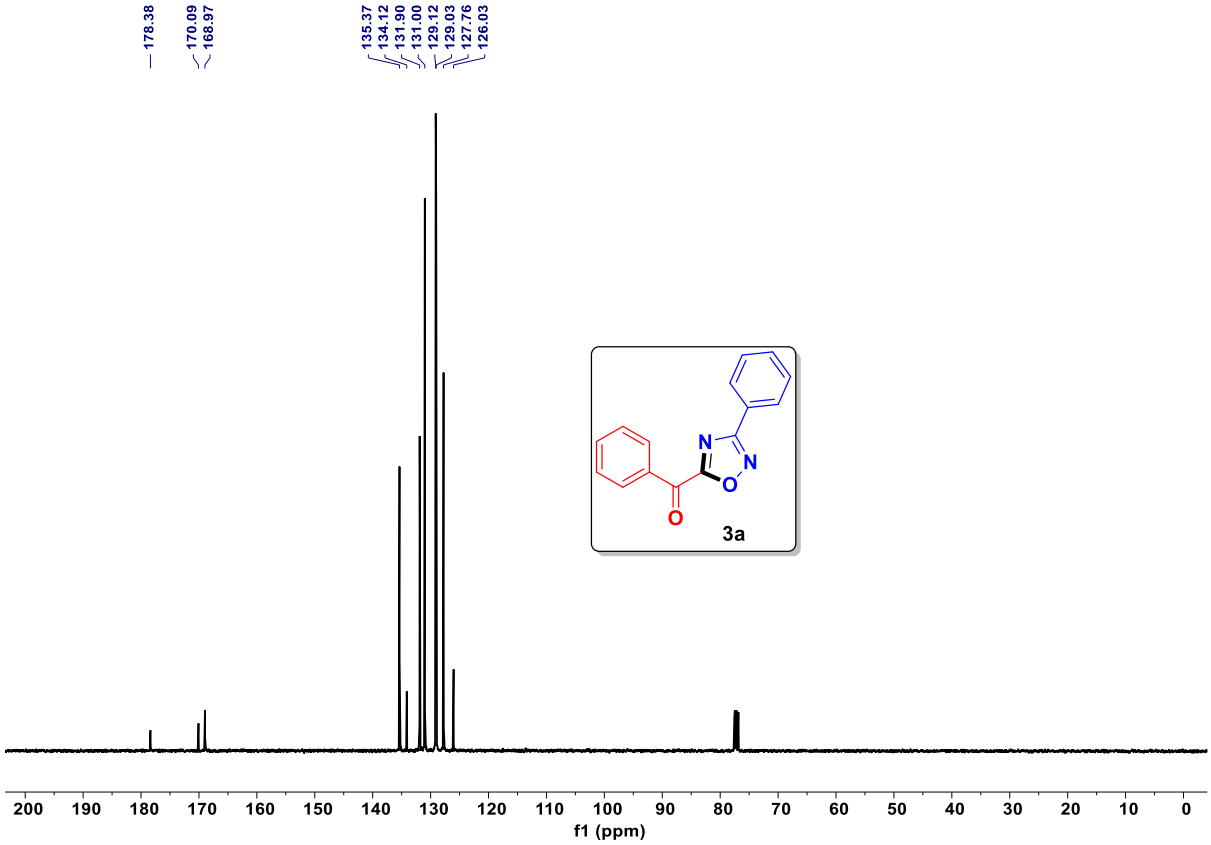


Figure 10. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3a**

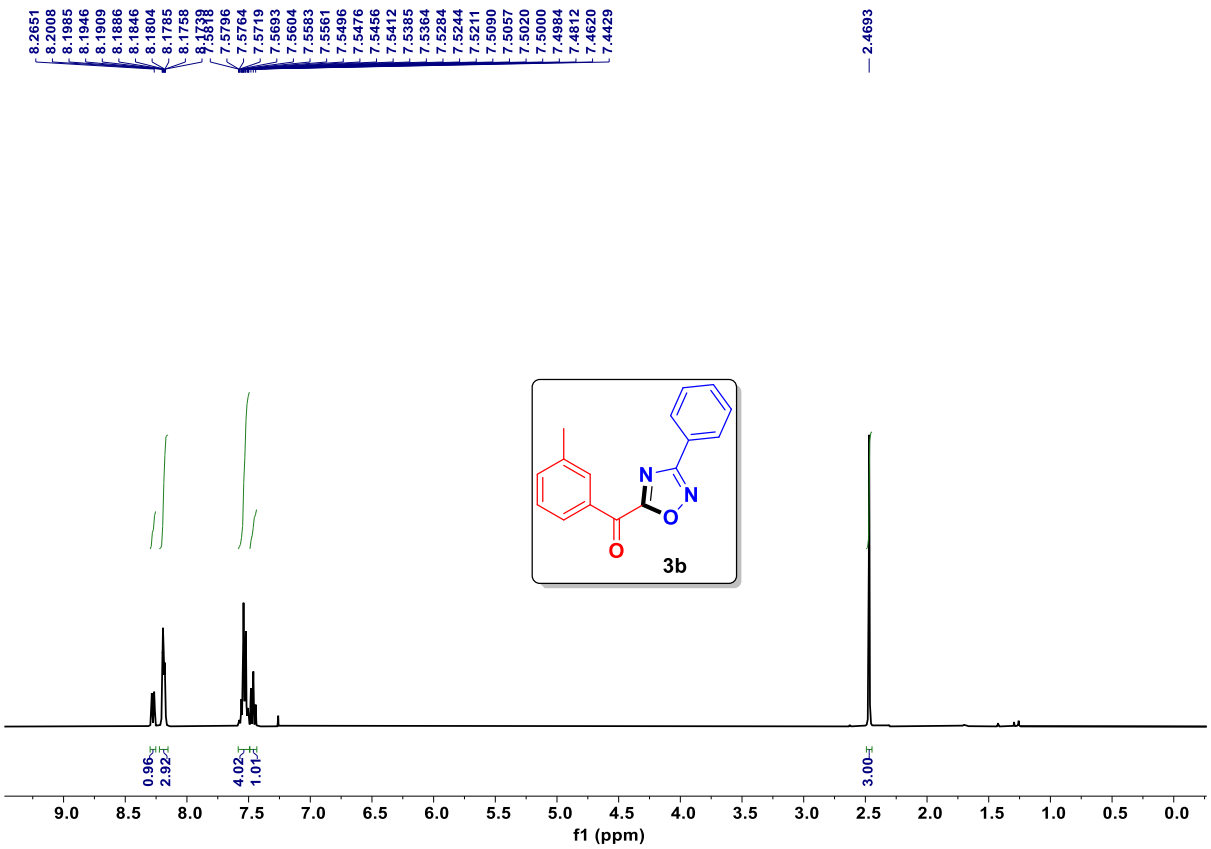


Figure 11. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3b**

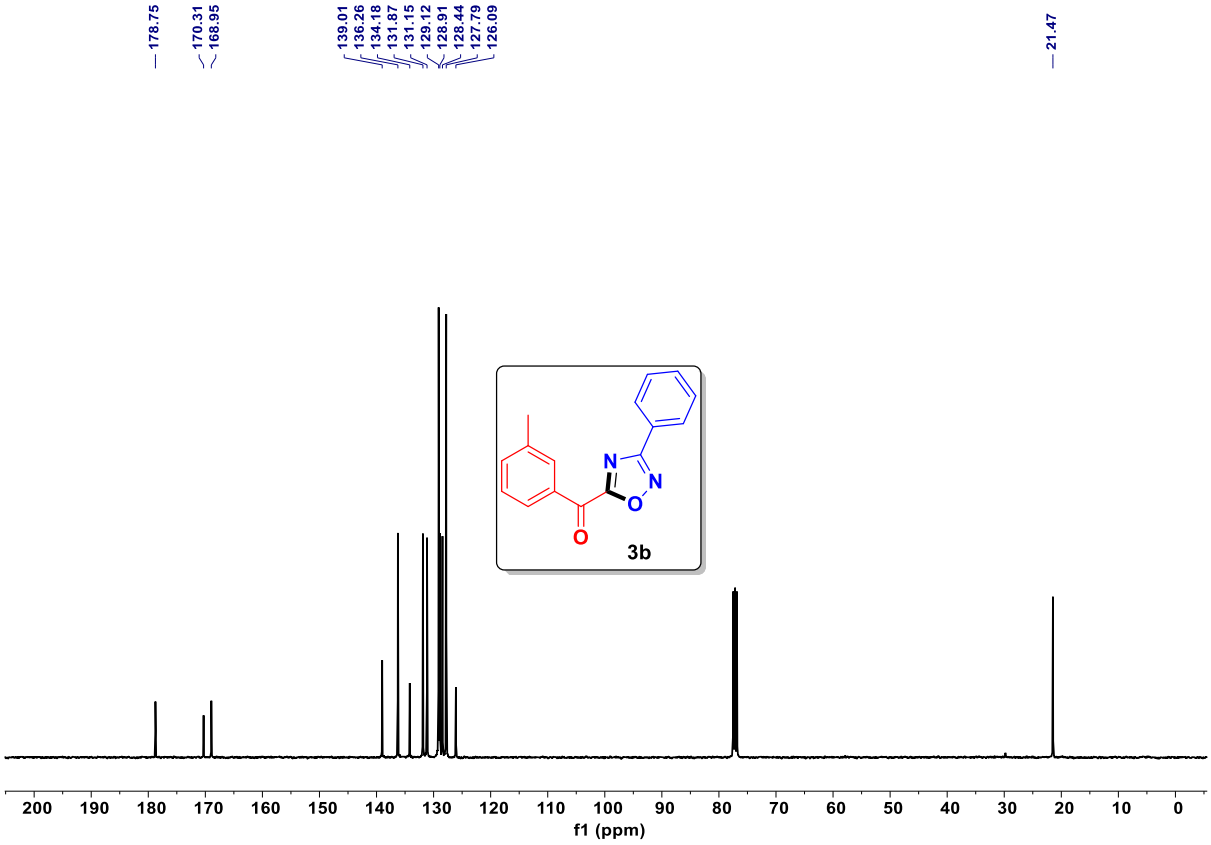


Figure 12. $^{13}C\{^{1}H\}$ (100 MHz, $CDCl_3$) of compound **3b**

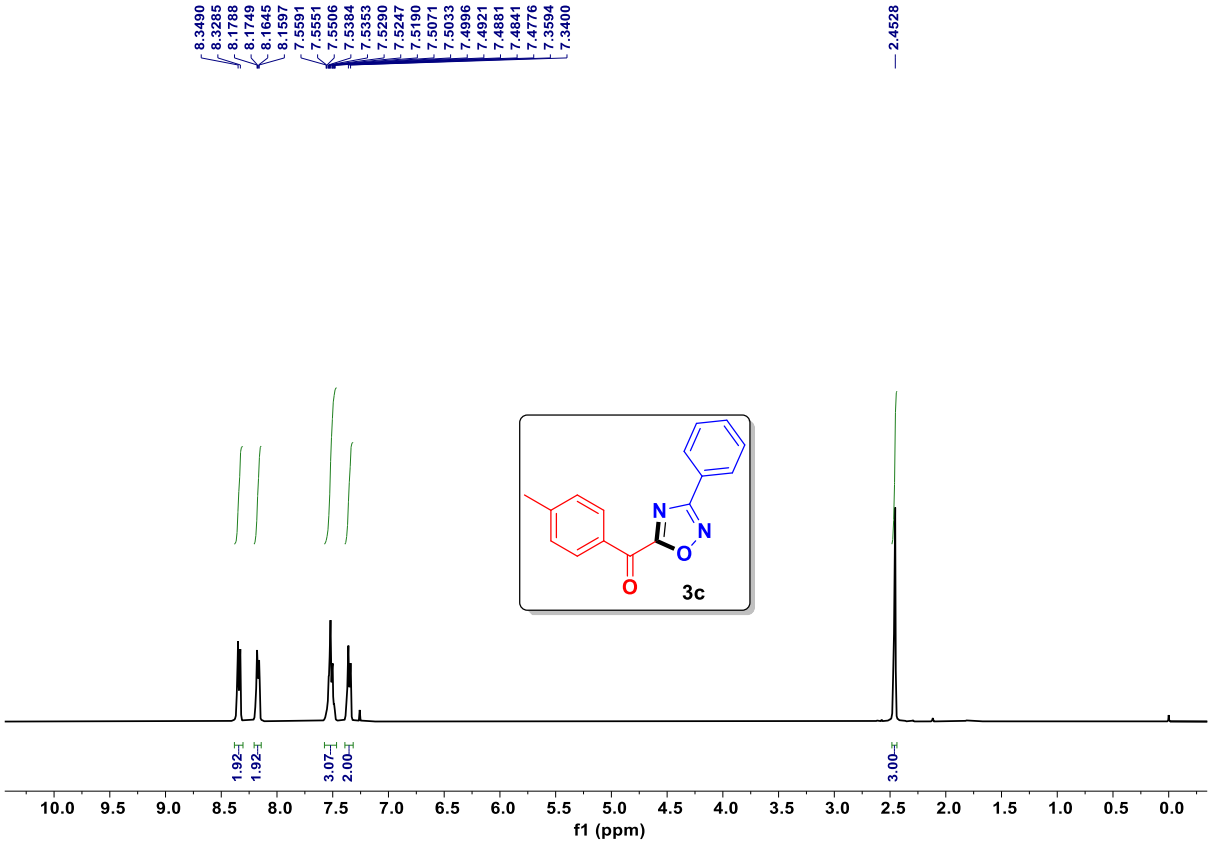


Figure 13. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3c**

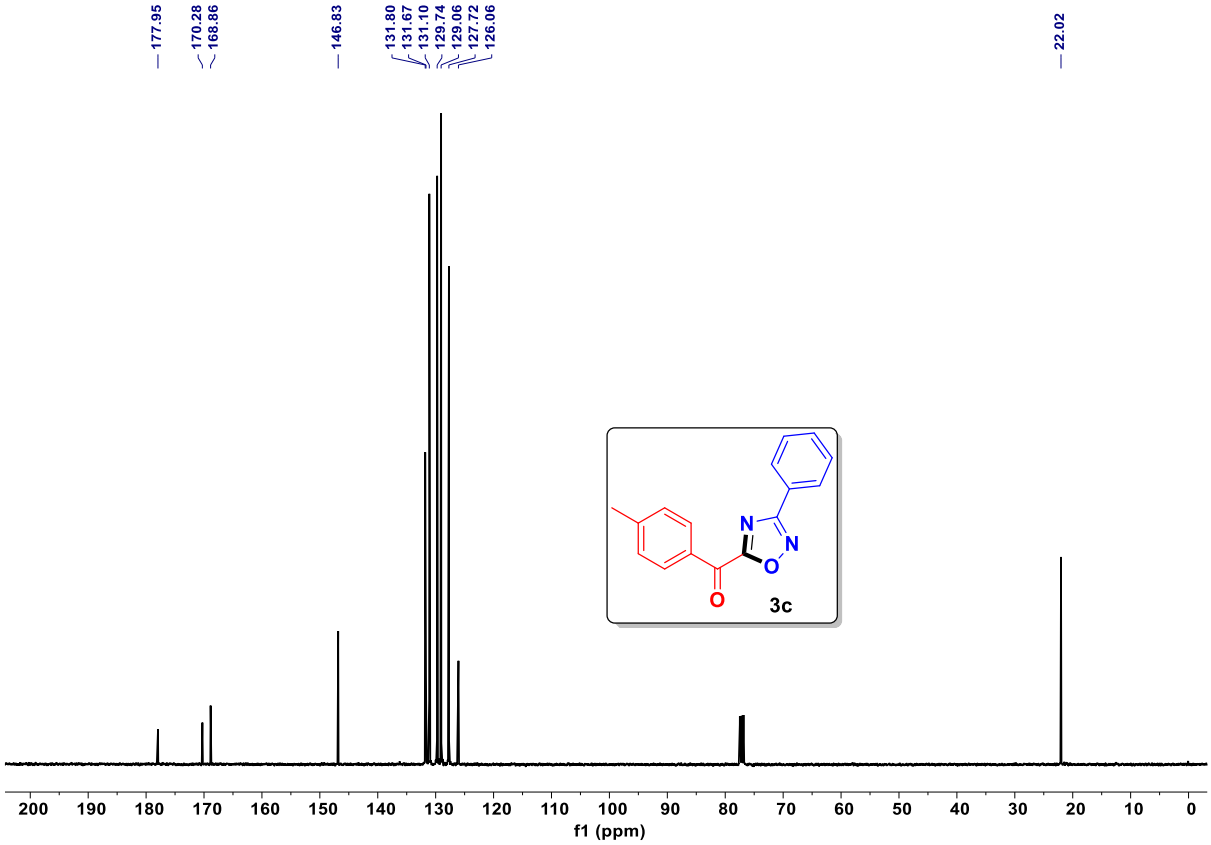


Figure 14. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3c**

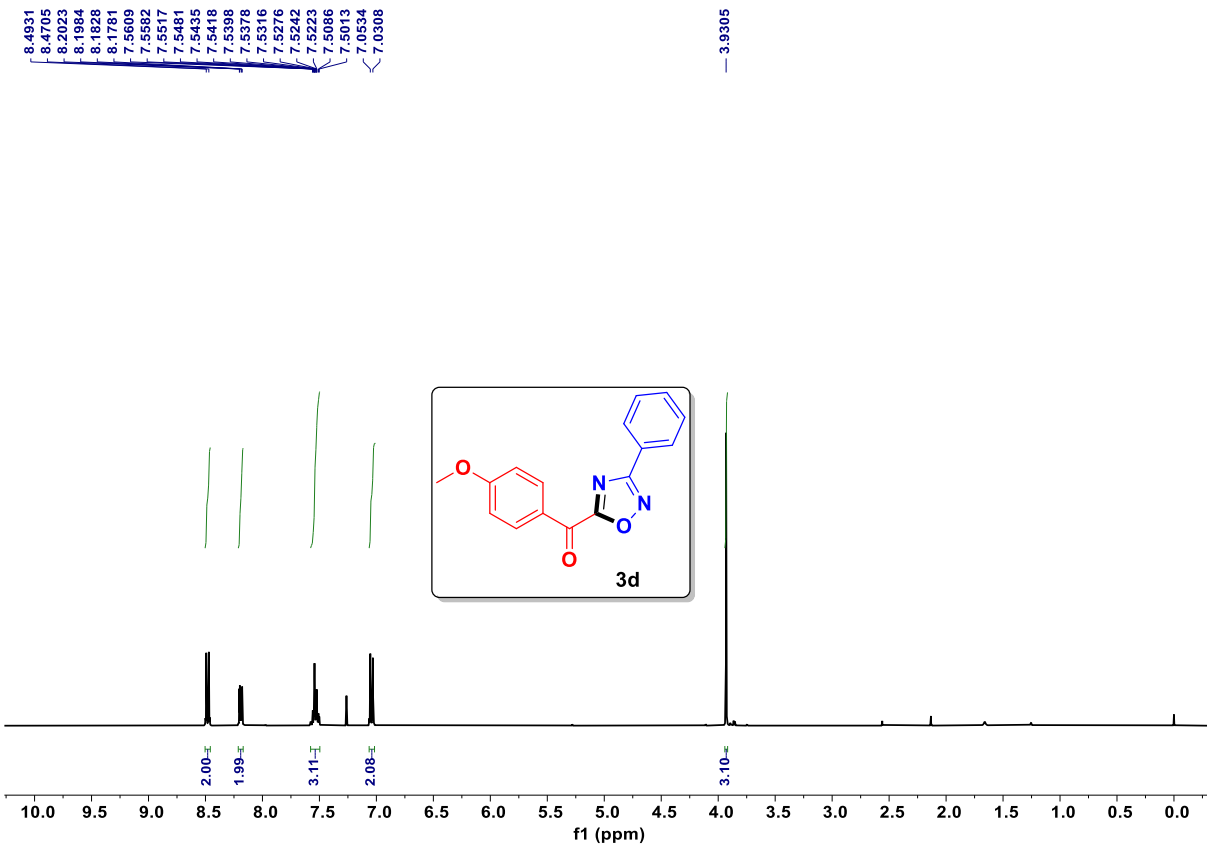


Figure 15. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3d**

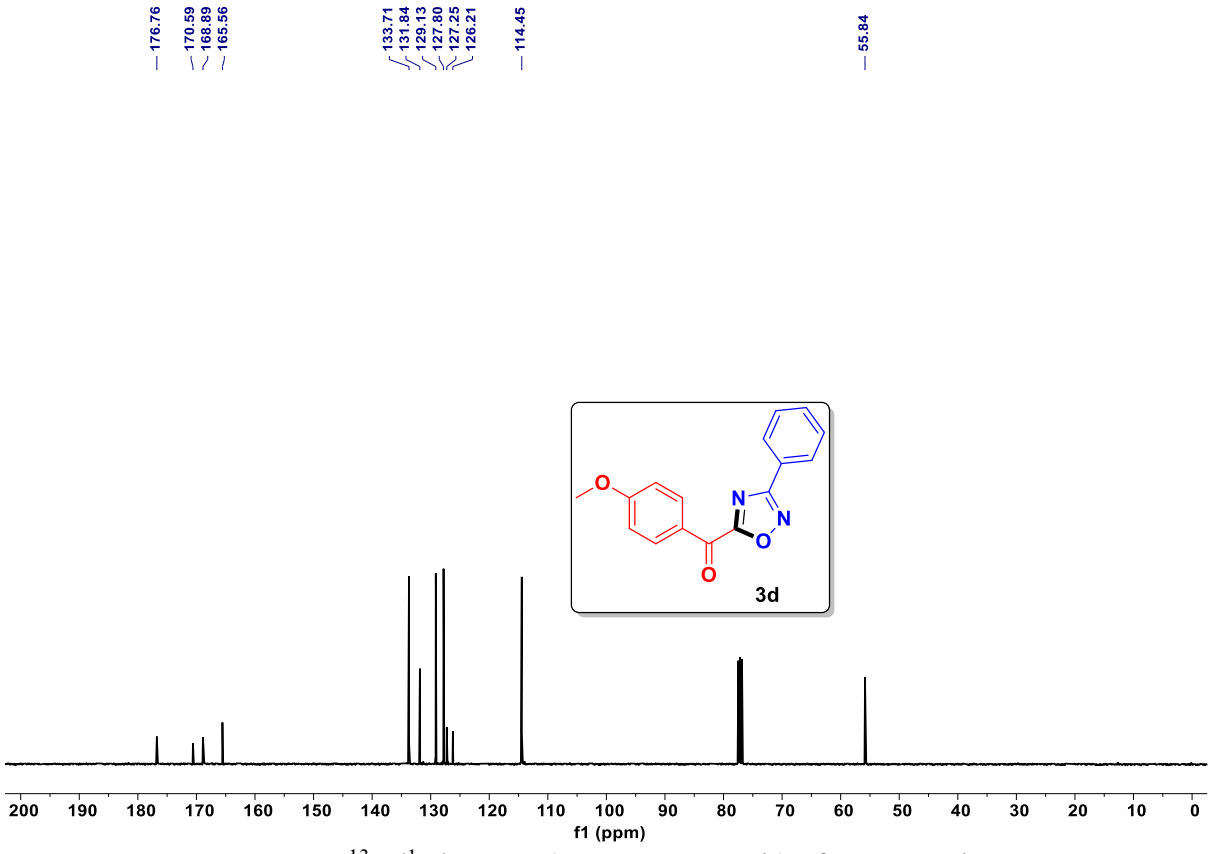


Figure 16. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3d**

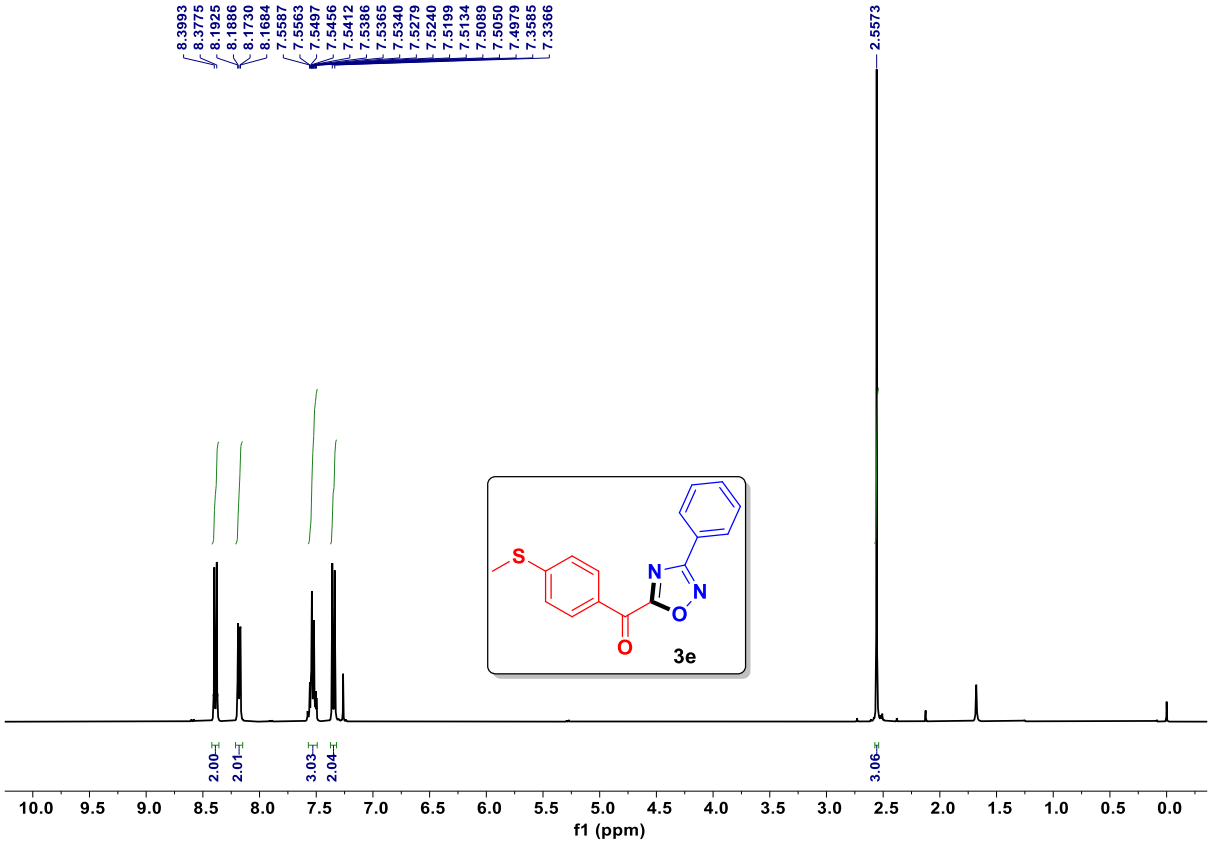


Figure 17. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3e**

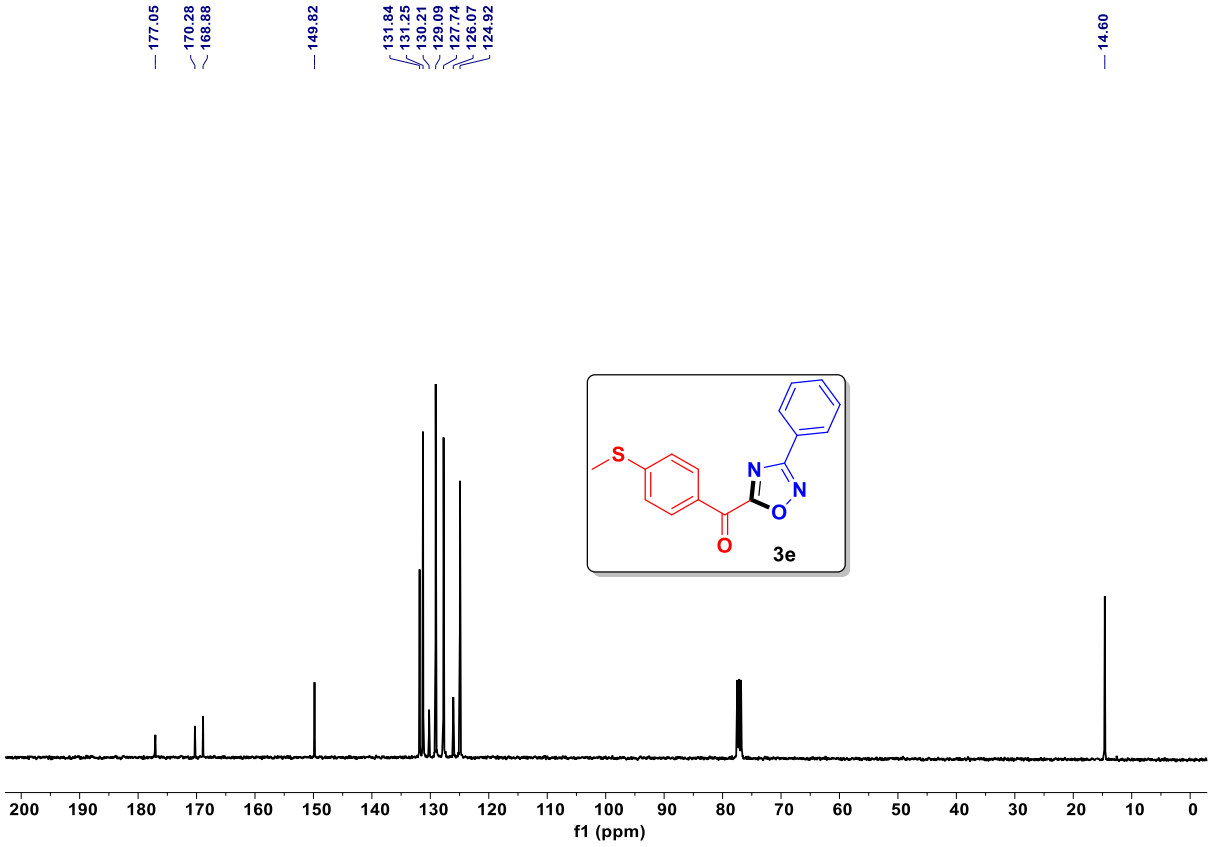


Figure 18. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3e**

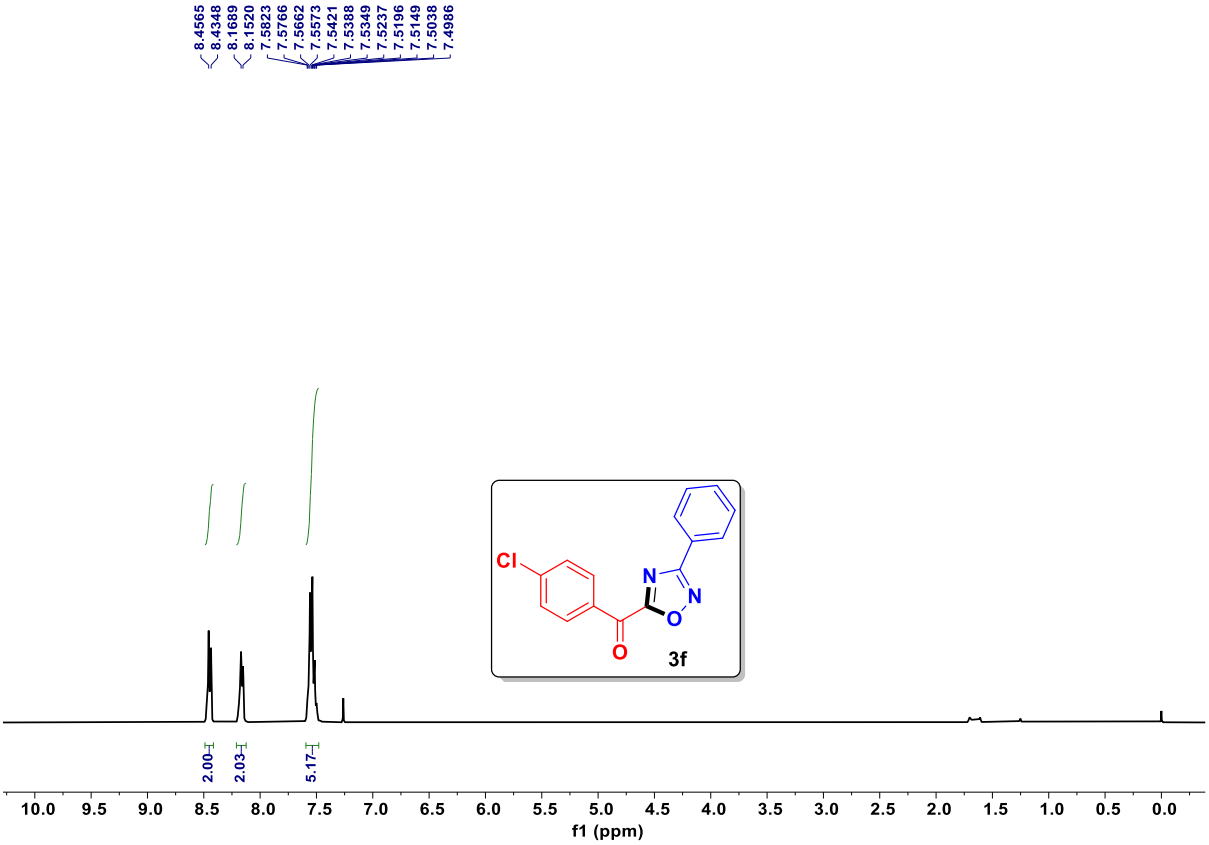


Figure 19. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3f**

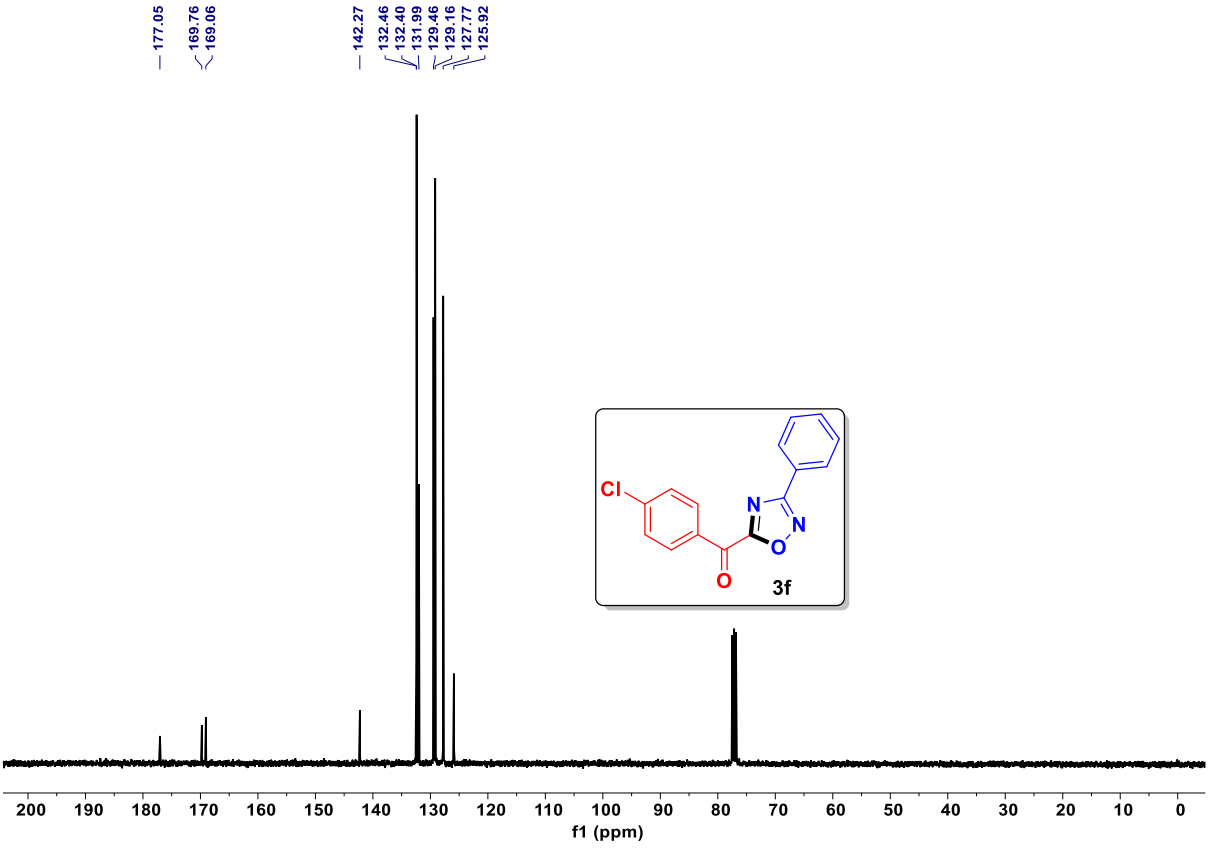


Figure 20. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3f**

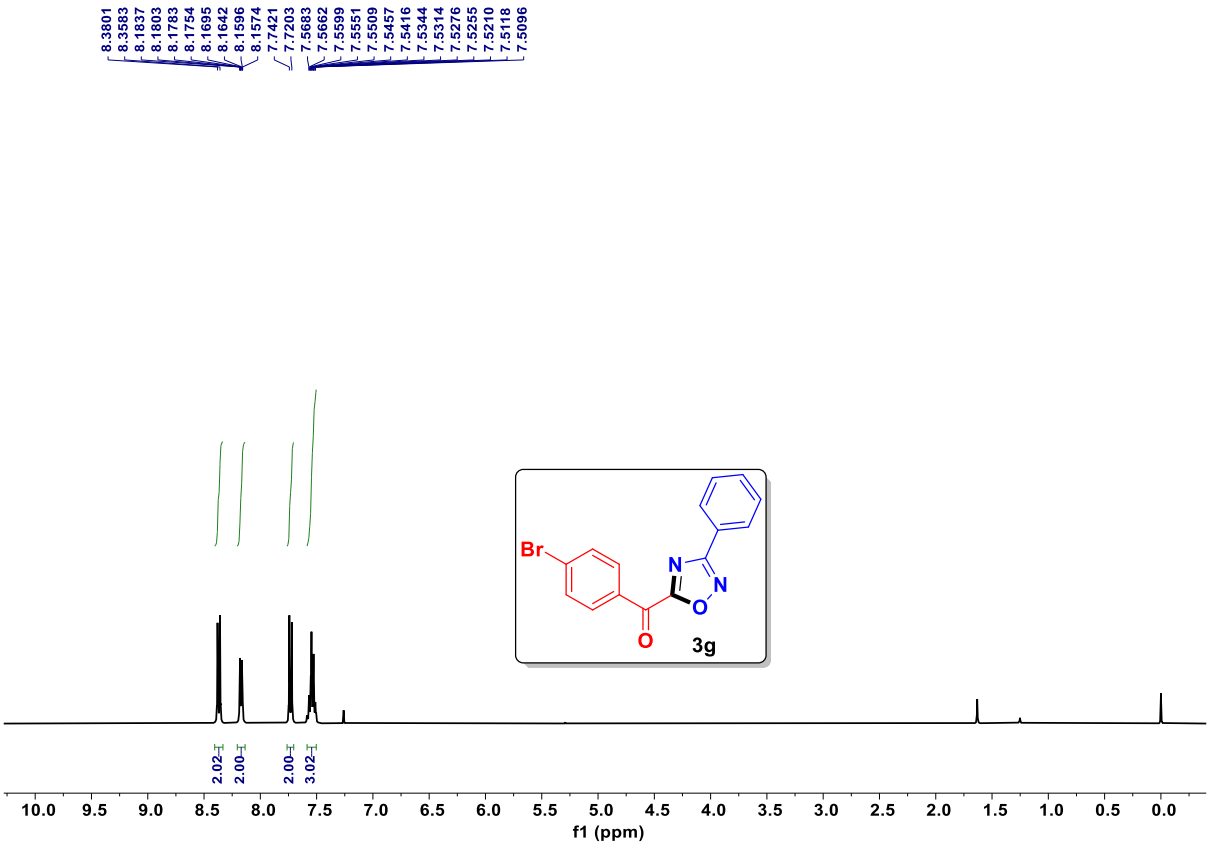


Figure 21. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3g**

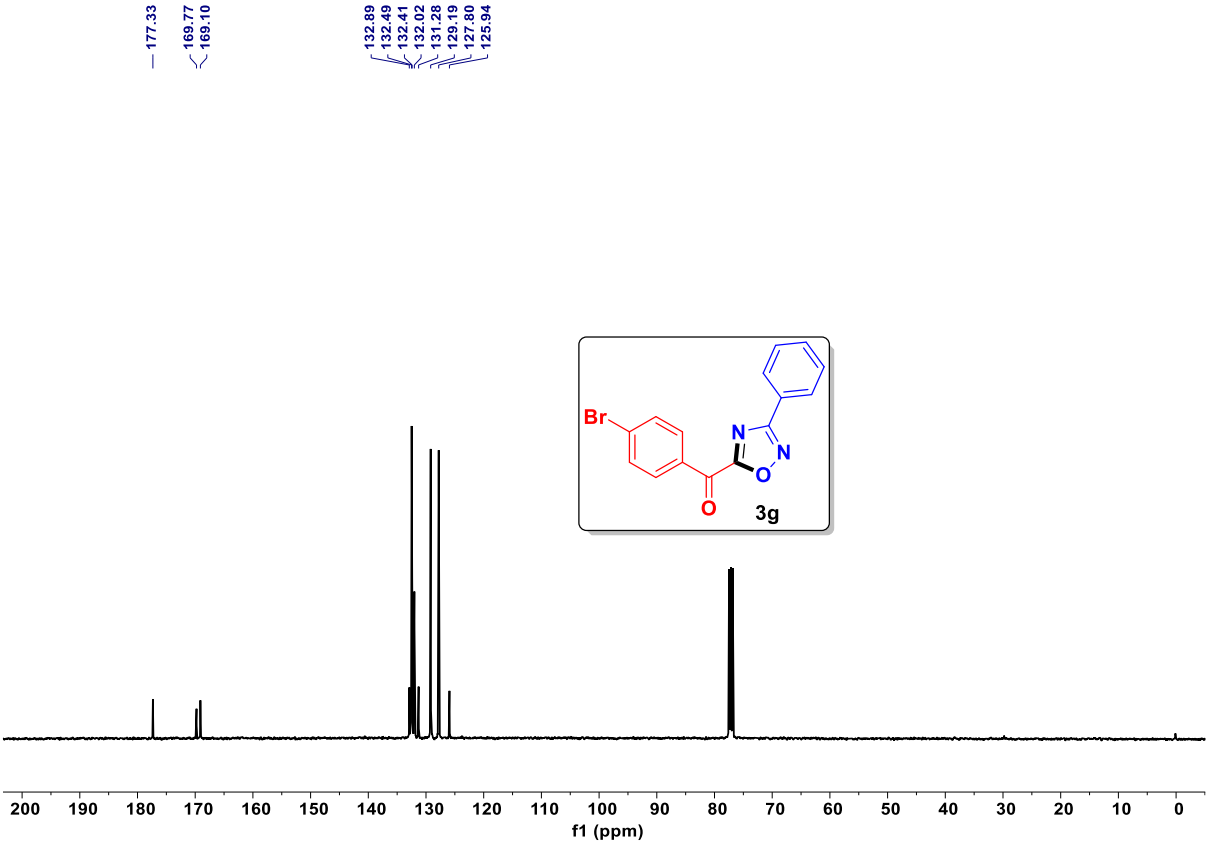


Figure 22. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of compound **3g**

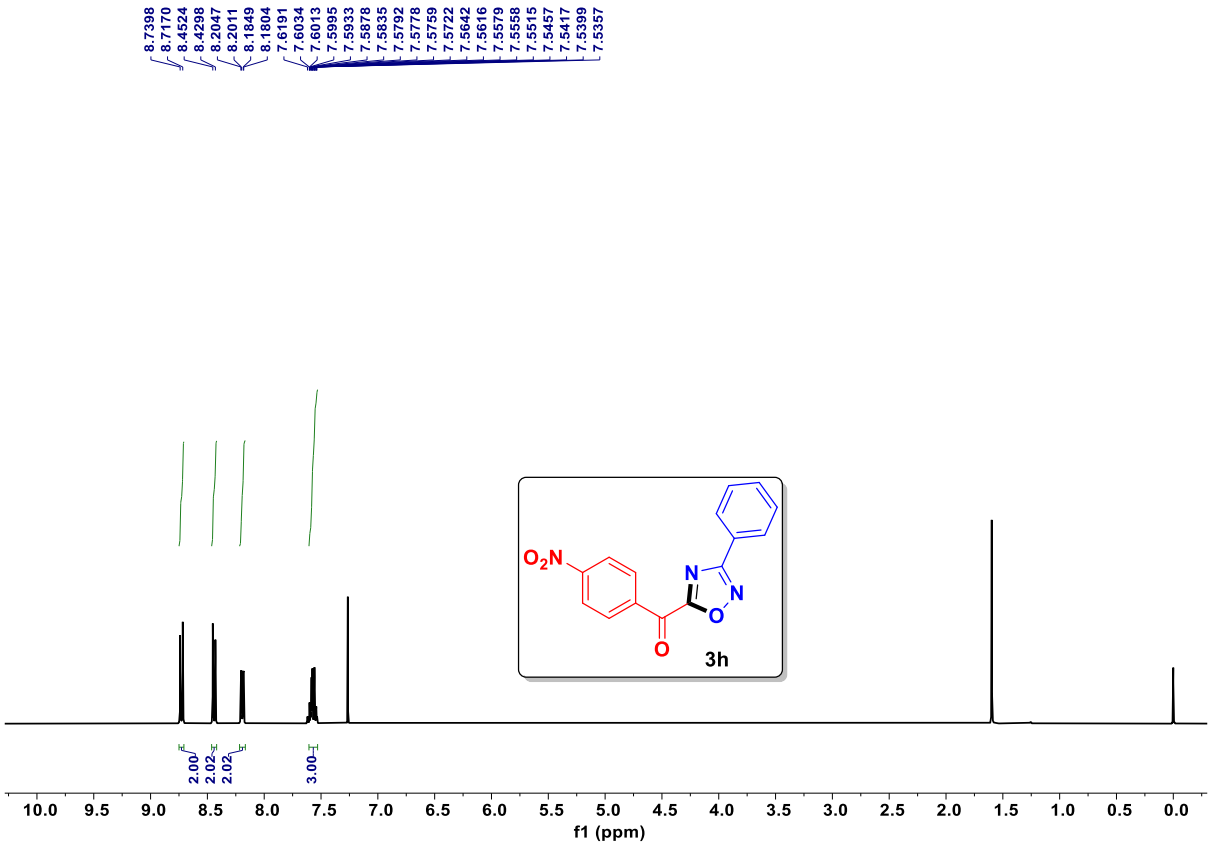


Figure 23. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3h**

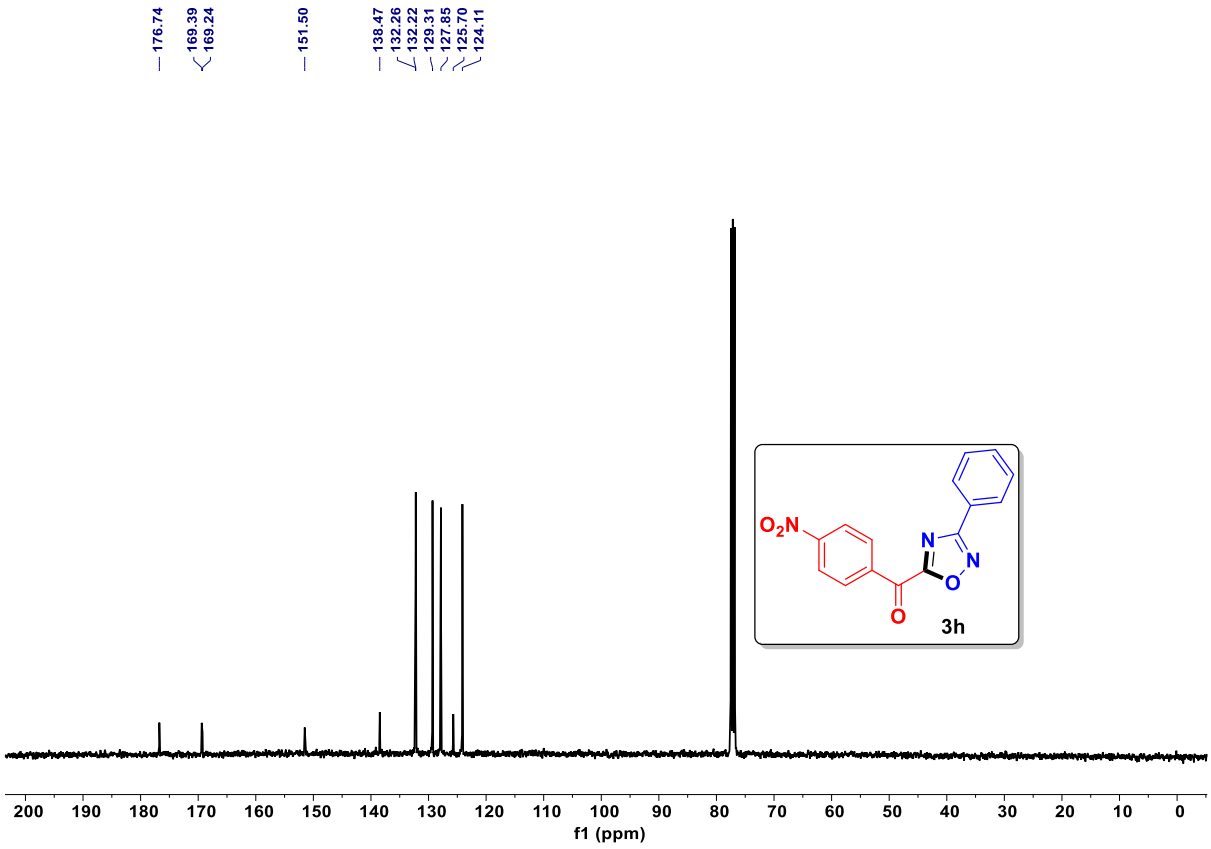


Figure 24. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3h**

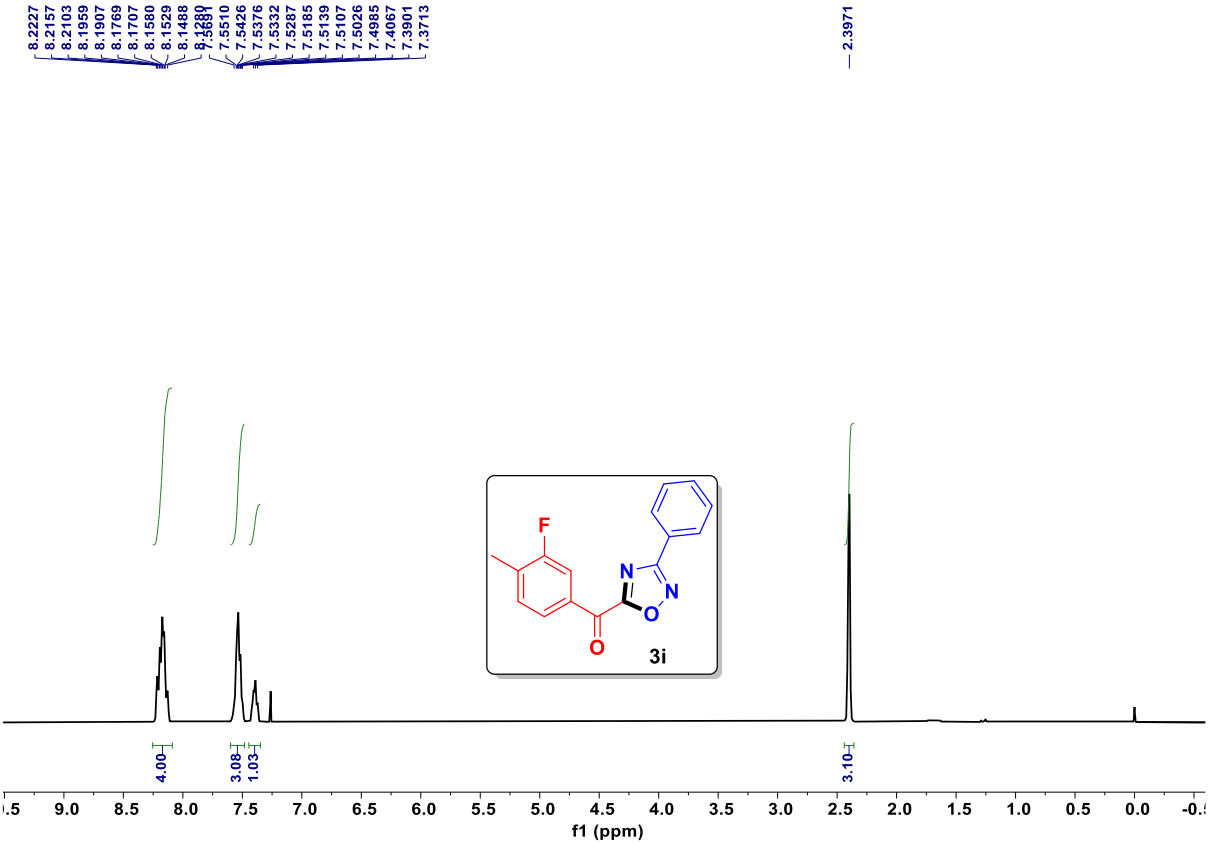


Figure 25. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3i**

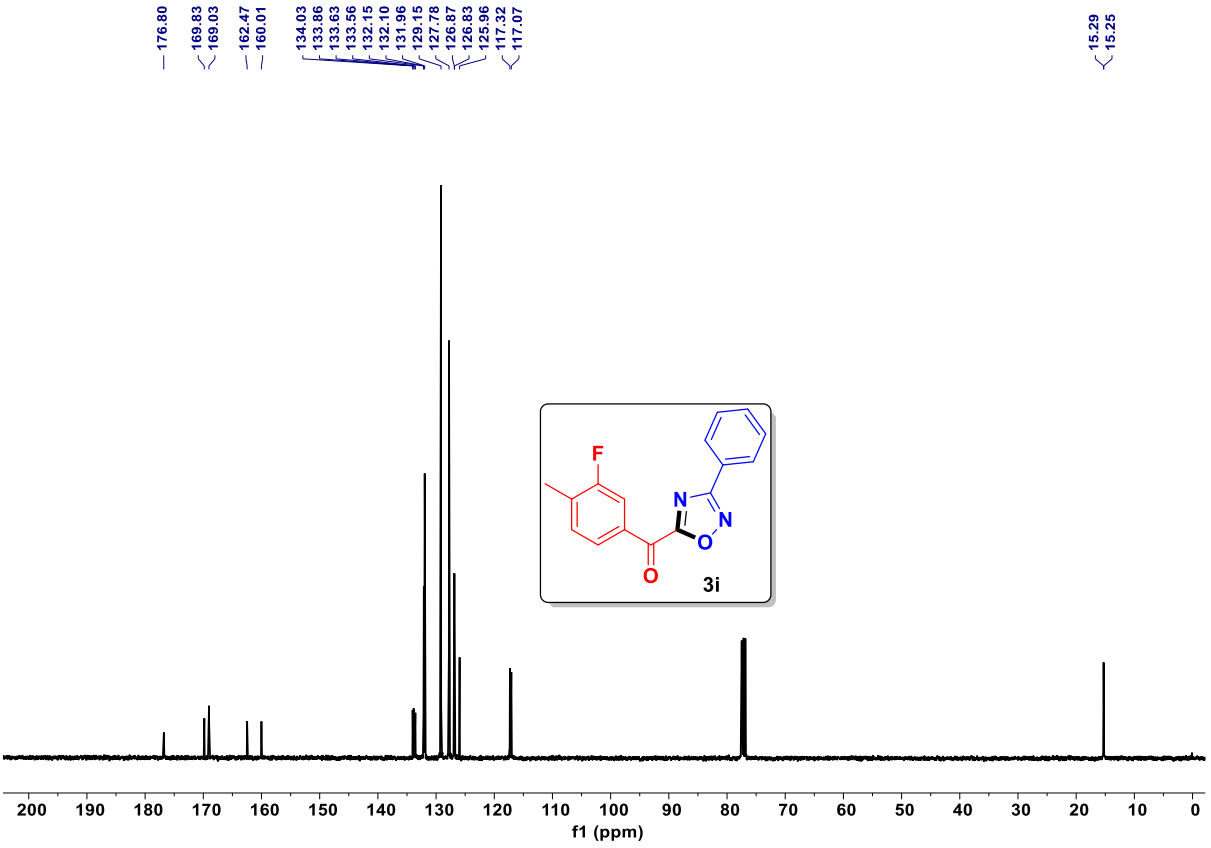


Figure 26. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3i**

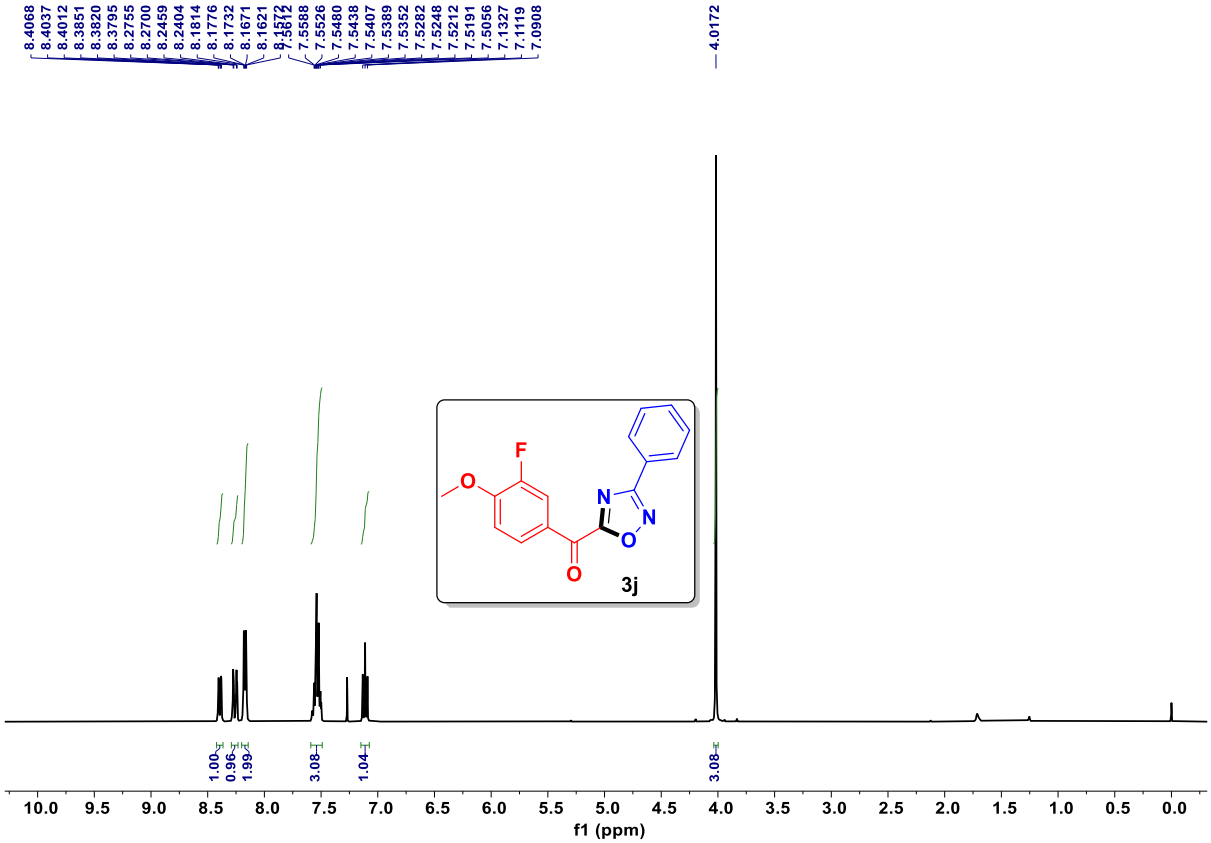


Figure 27. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3j**

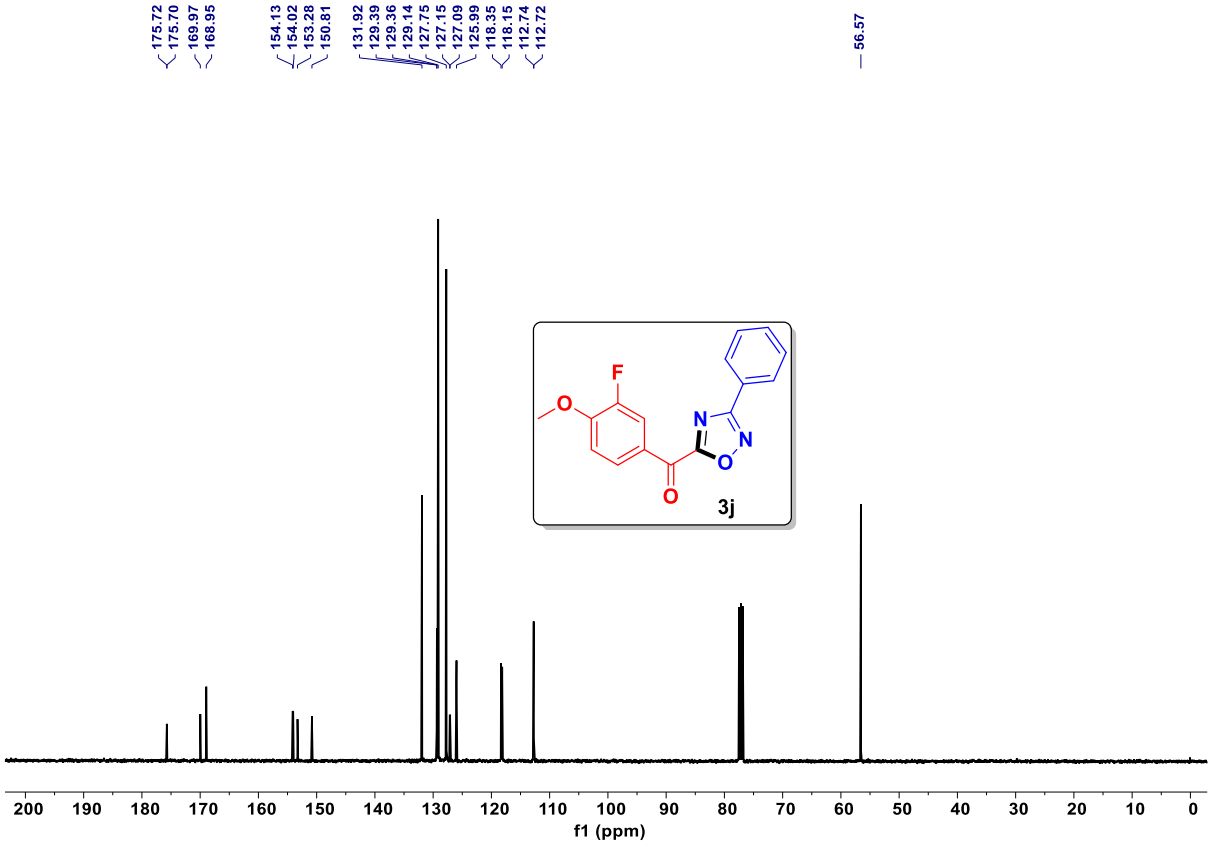


Figure 28. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3j**

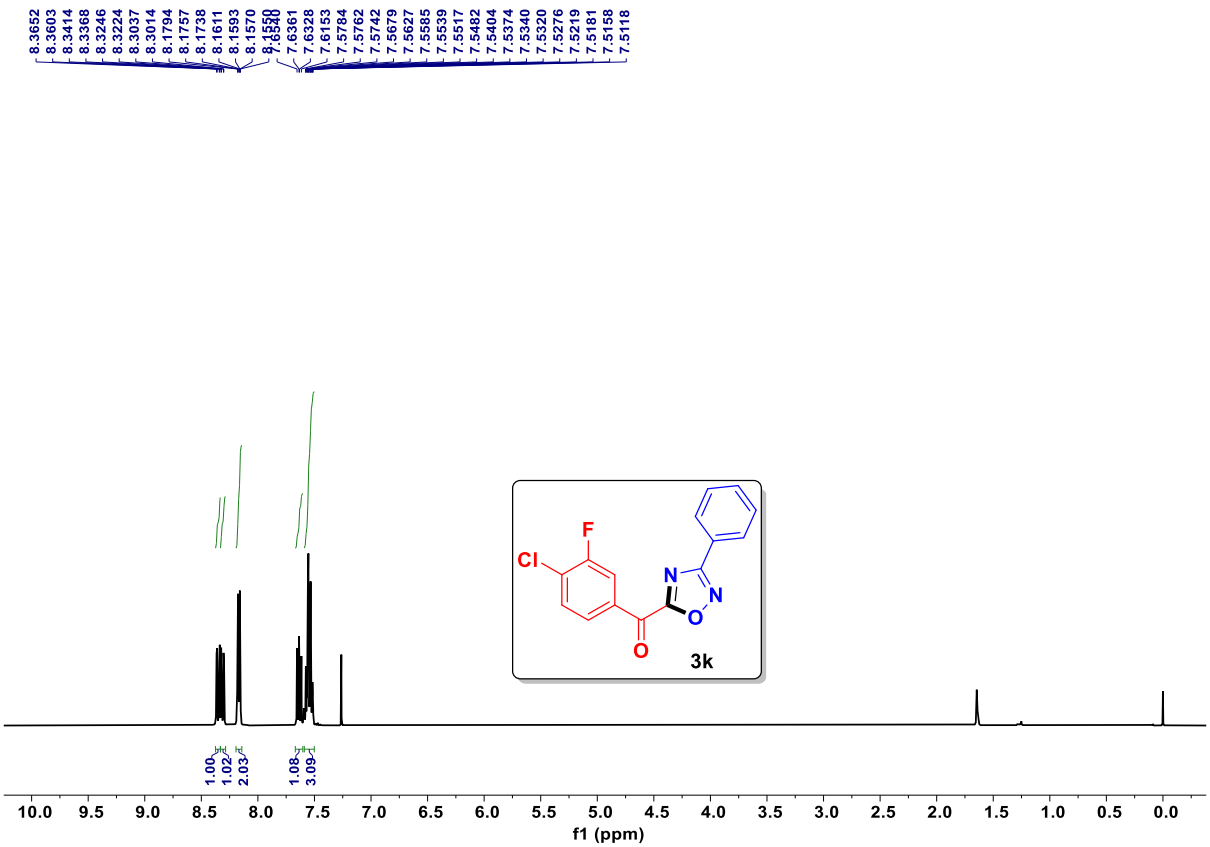


Figure 29. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3k**

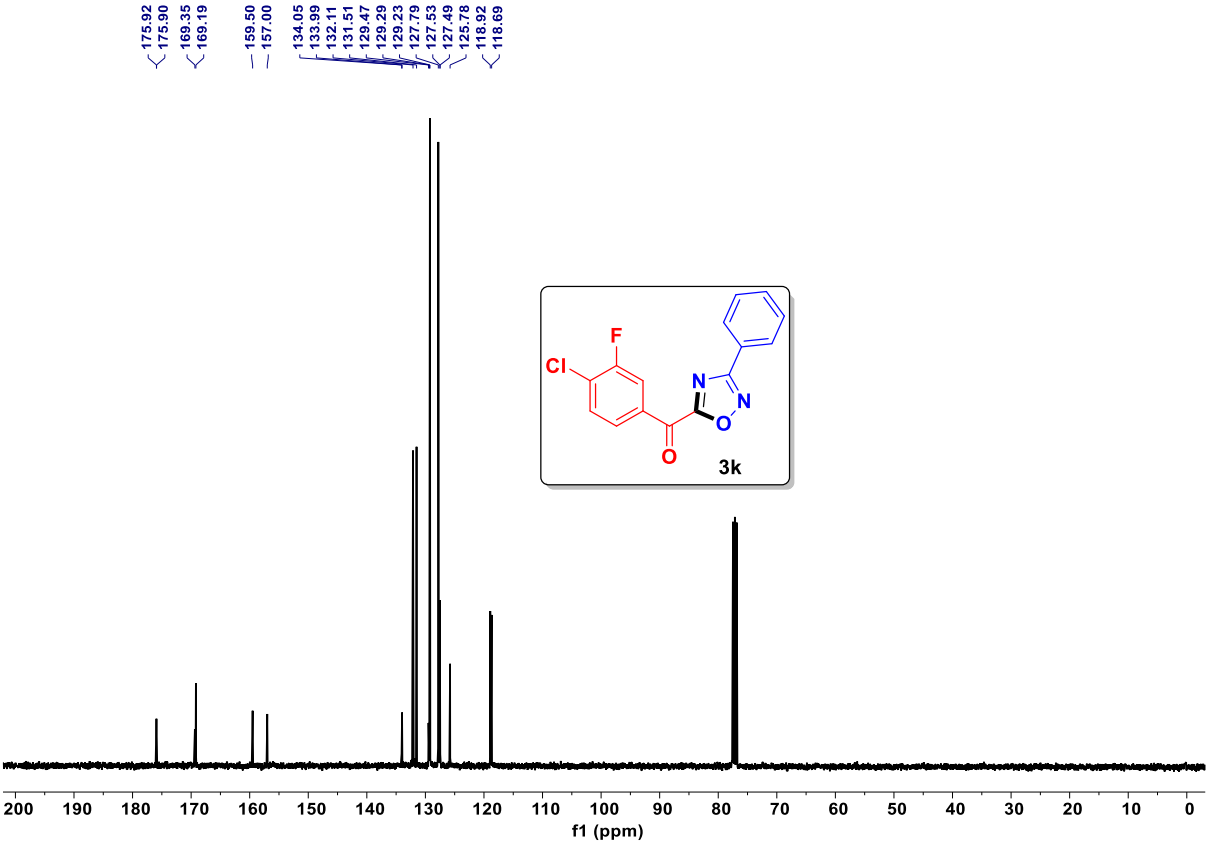


Figure 30. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3k**

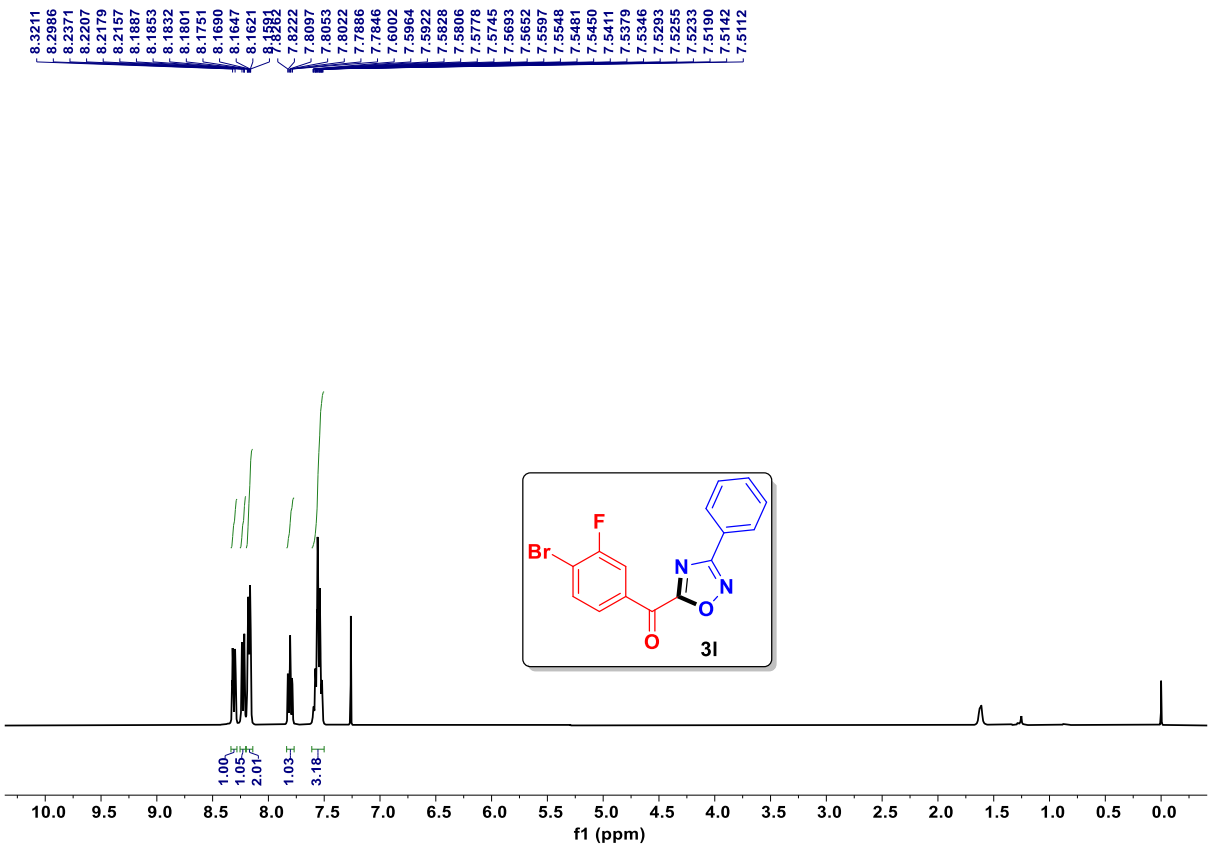


Figure 31. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3l**

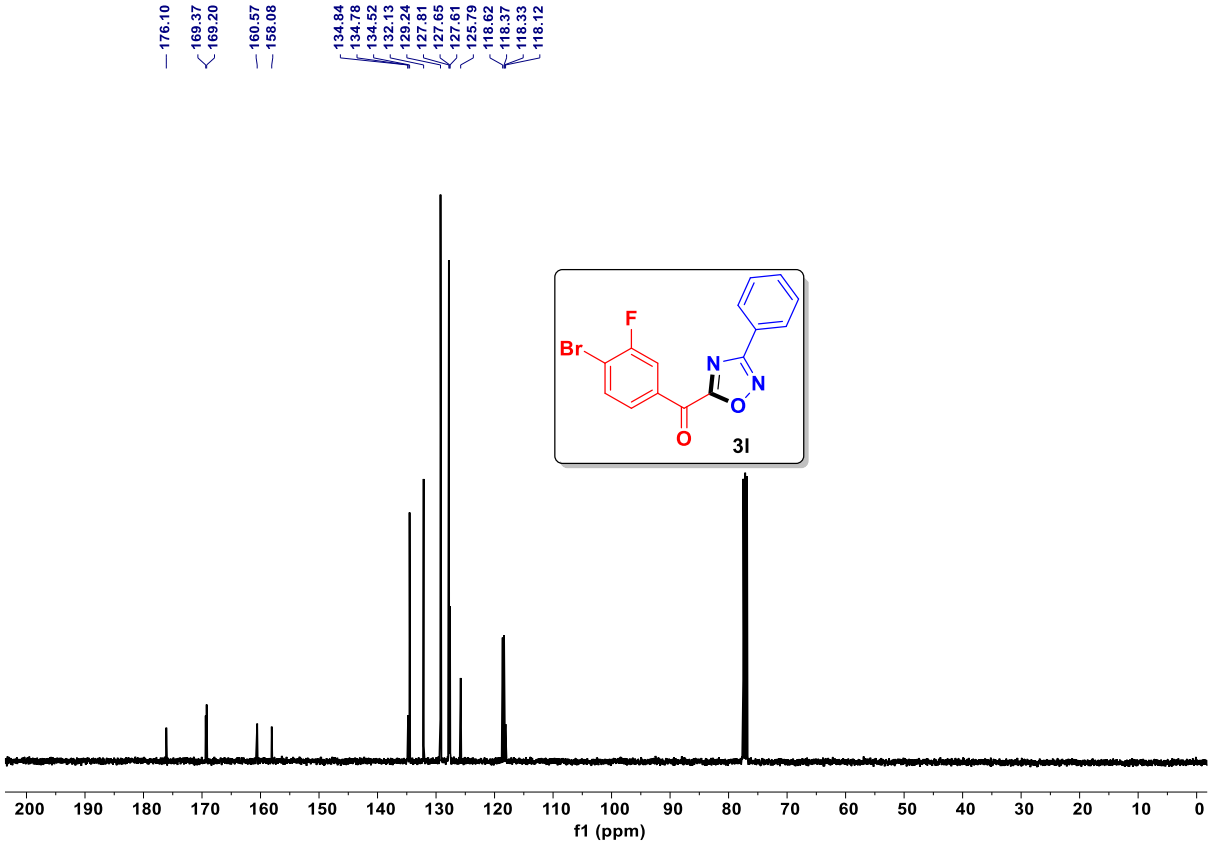


Figure 32. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3l**

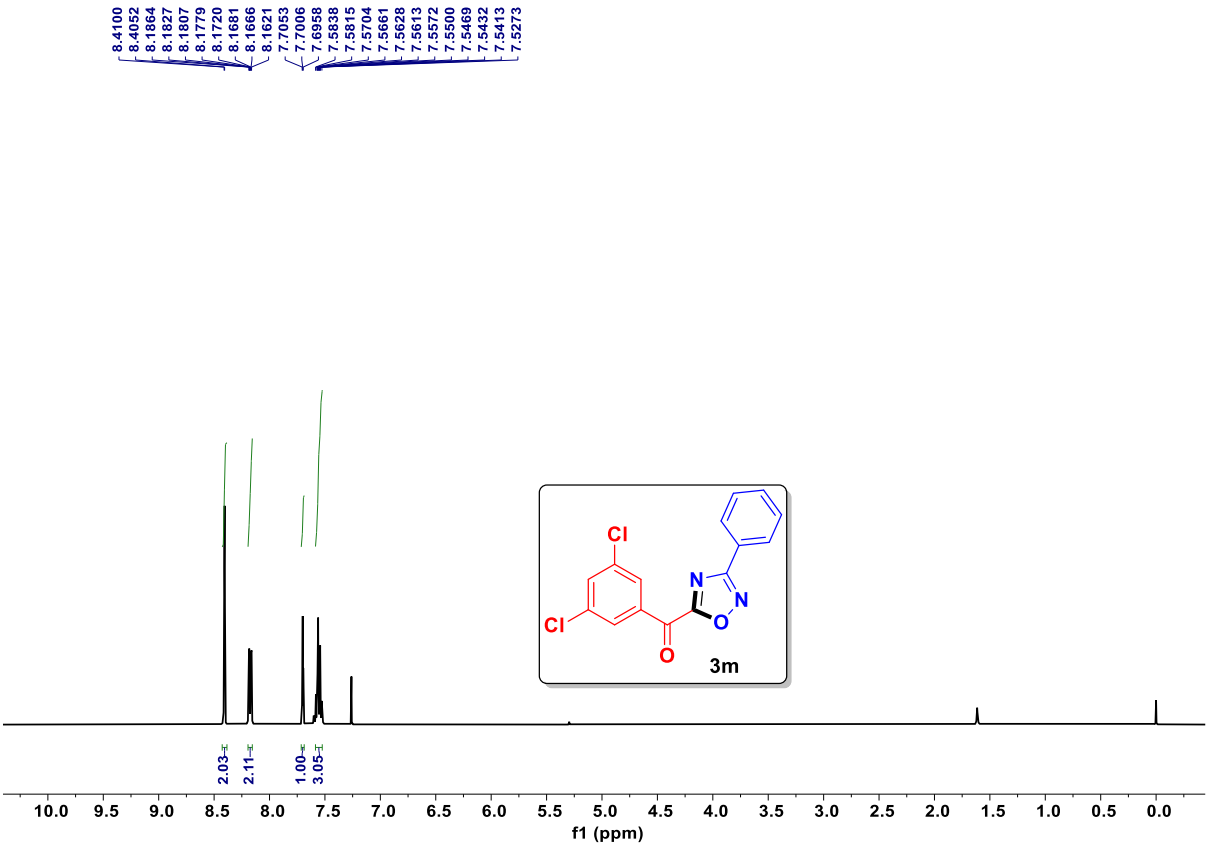


Figure 33. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3m**

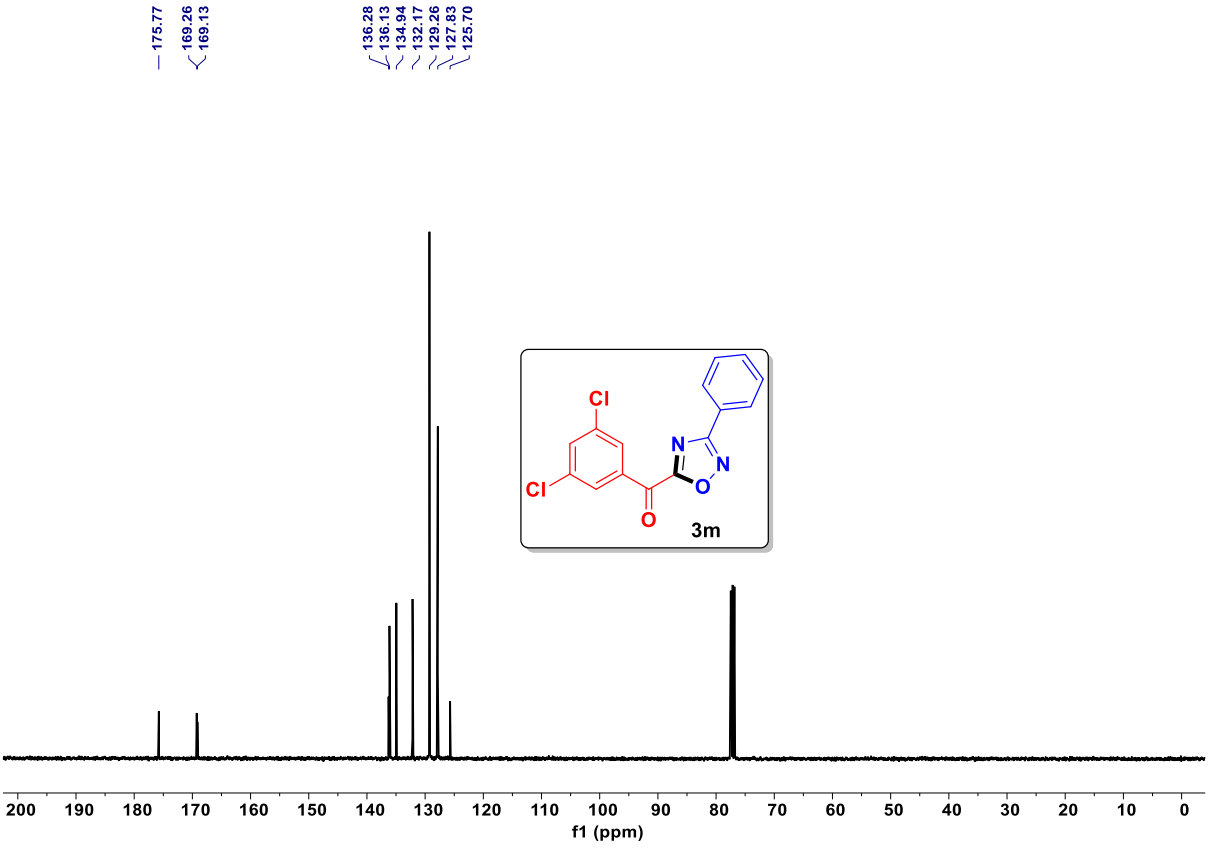


Figure 34. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3m**

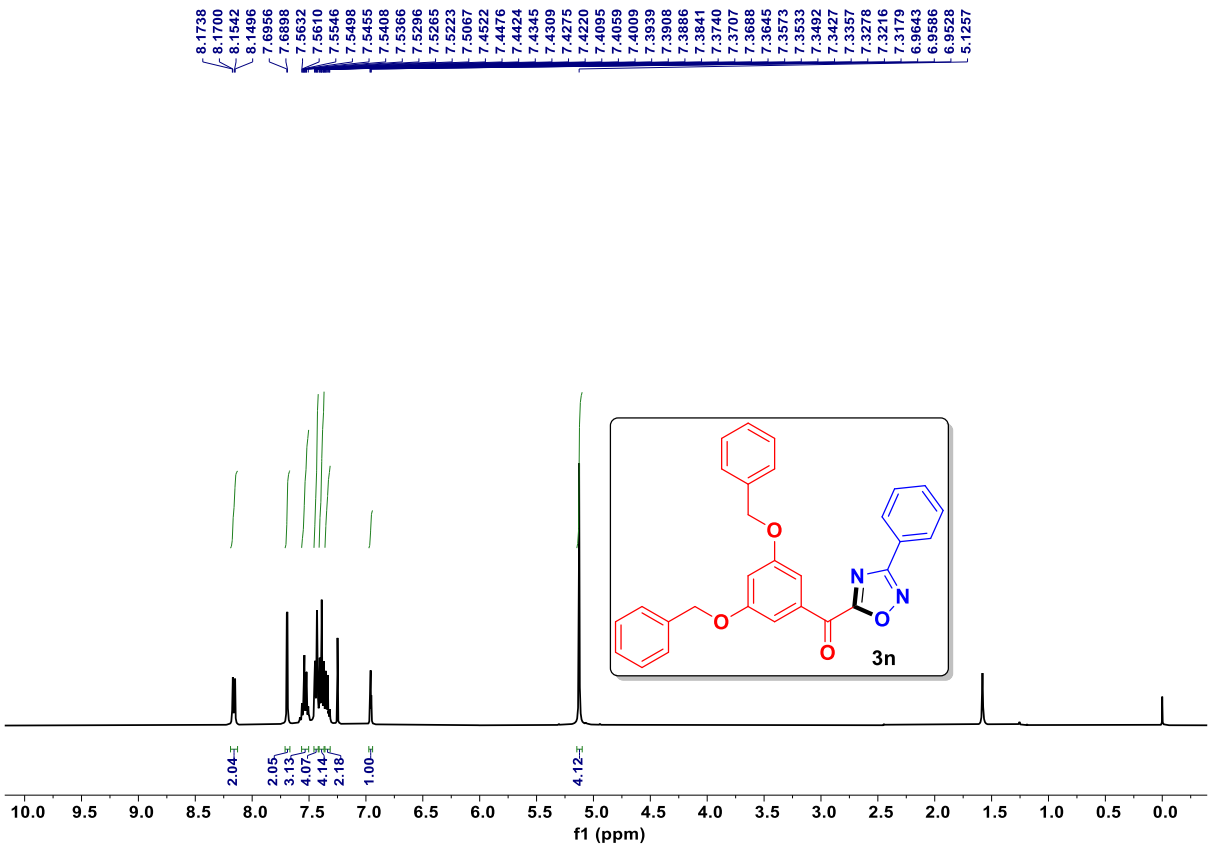


Figure 35. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3n**

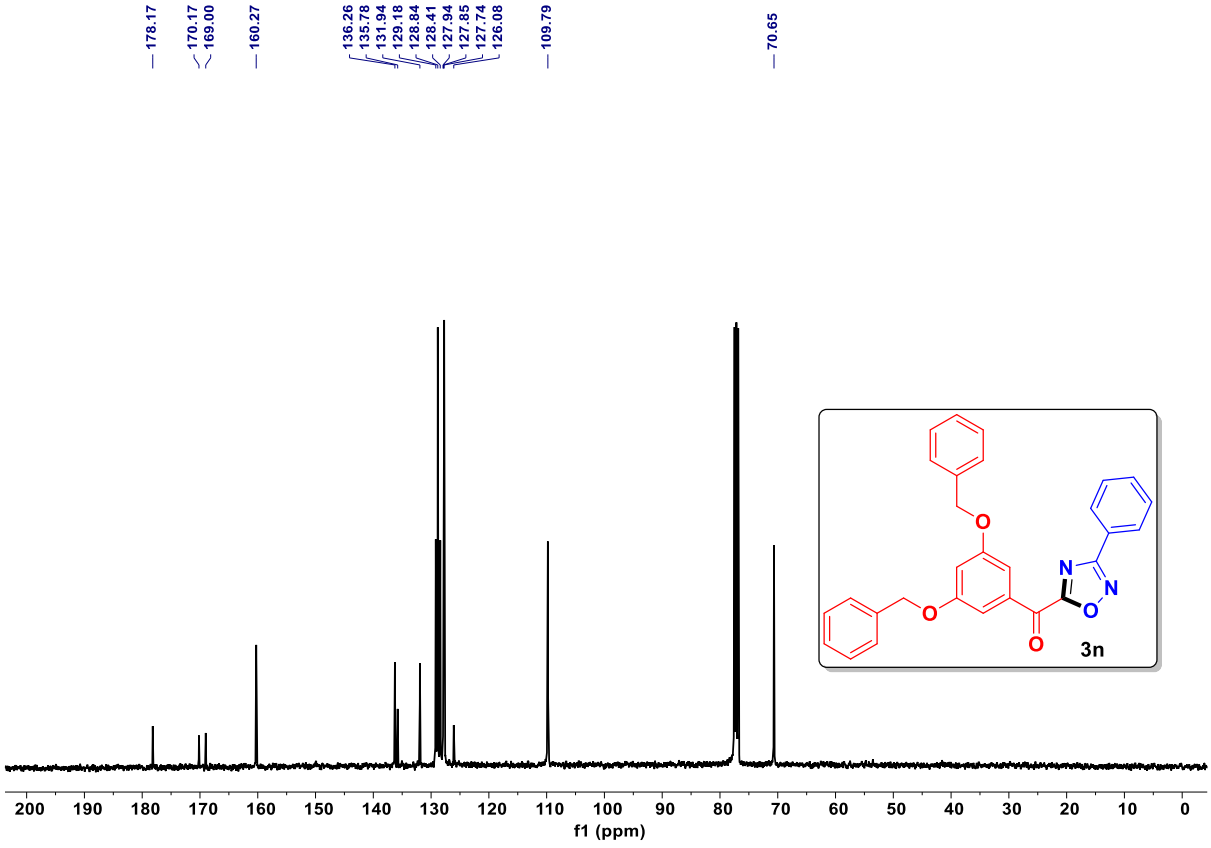


Figure 36. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3n**

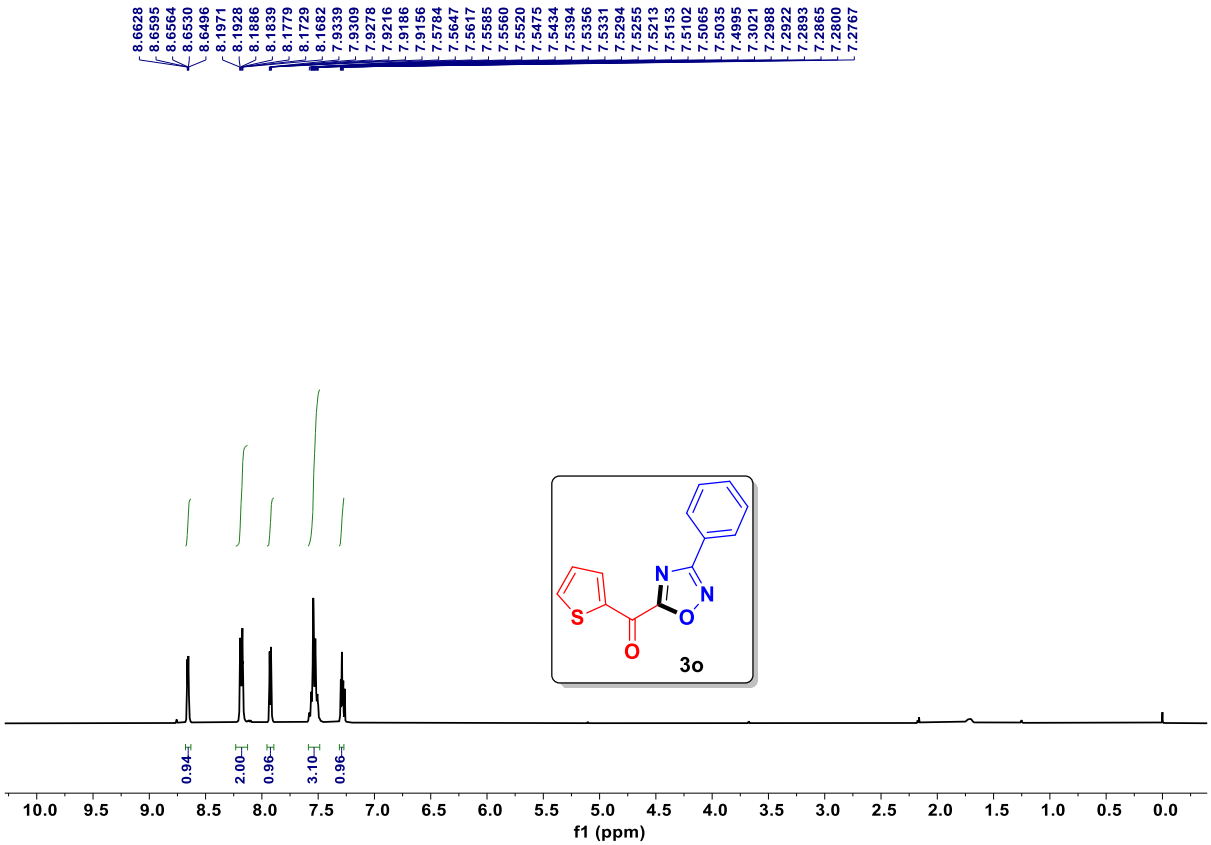


Figure 37. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3o**

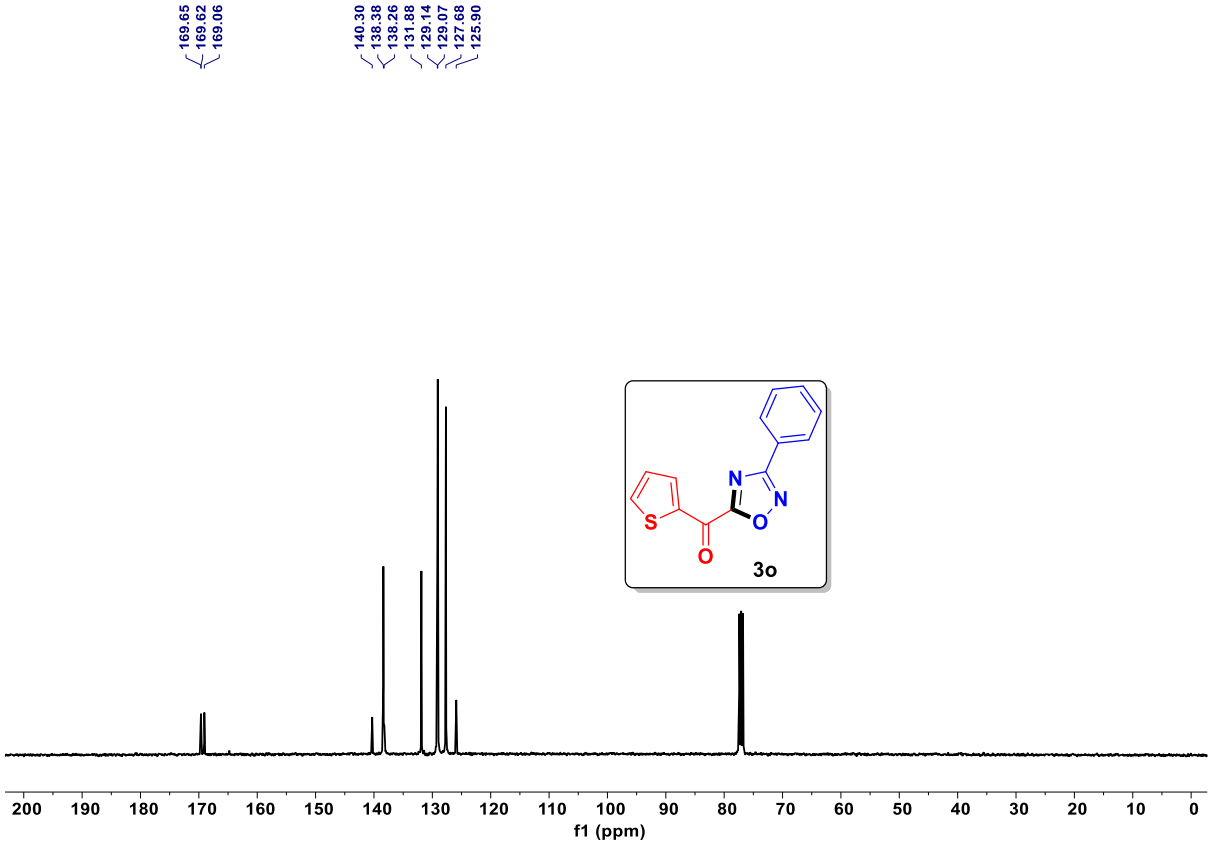


Figure 38. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3o**

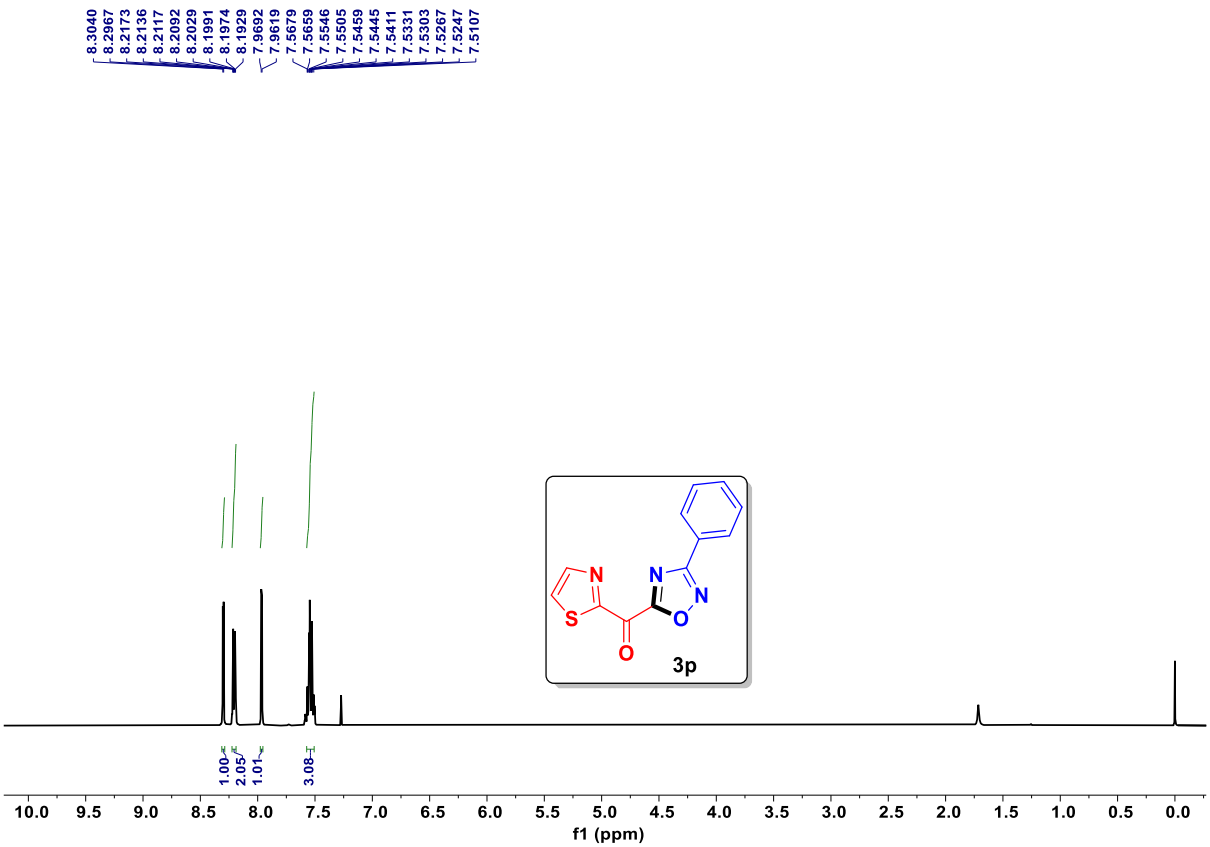


Figure 39. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3p**

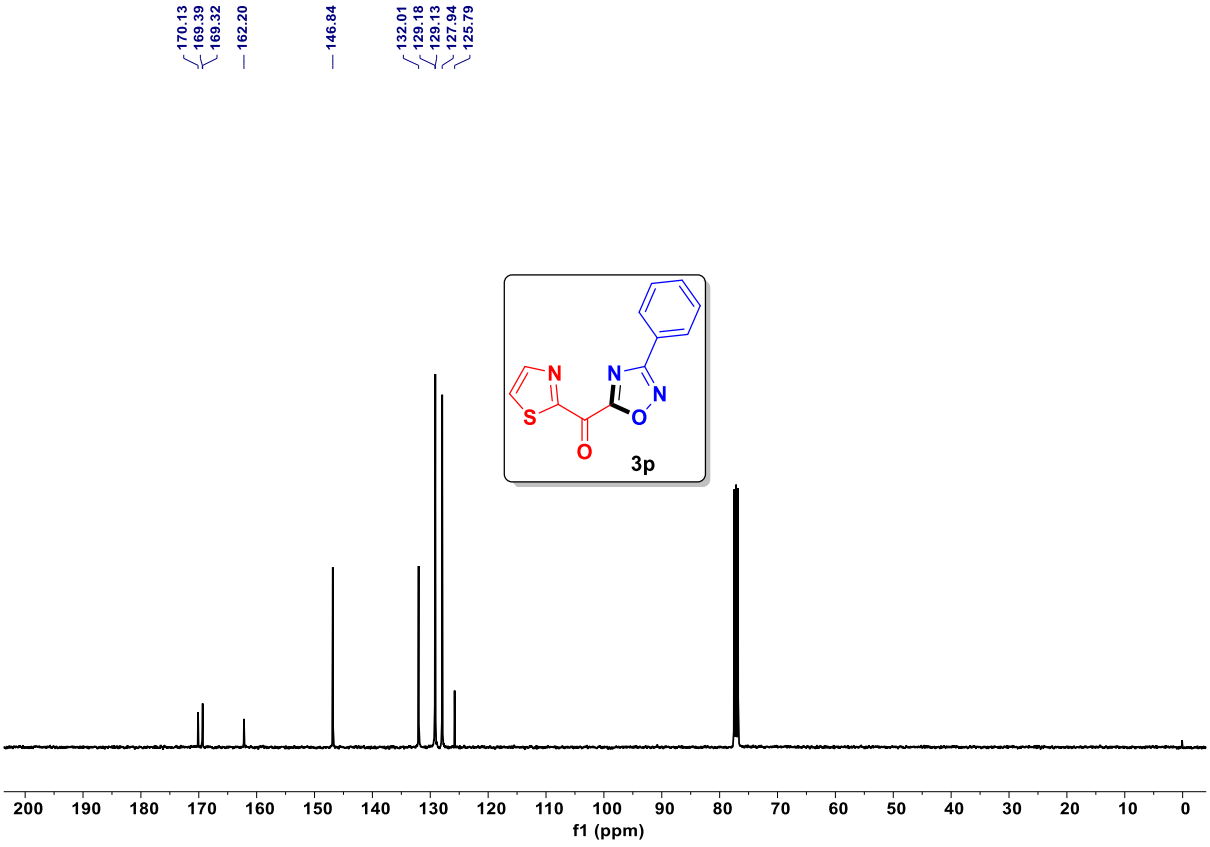


Figure 40. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3p**

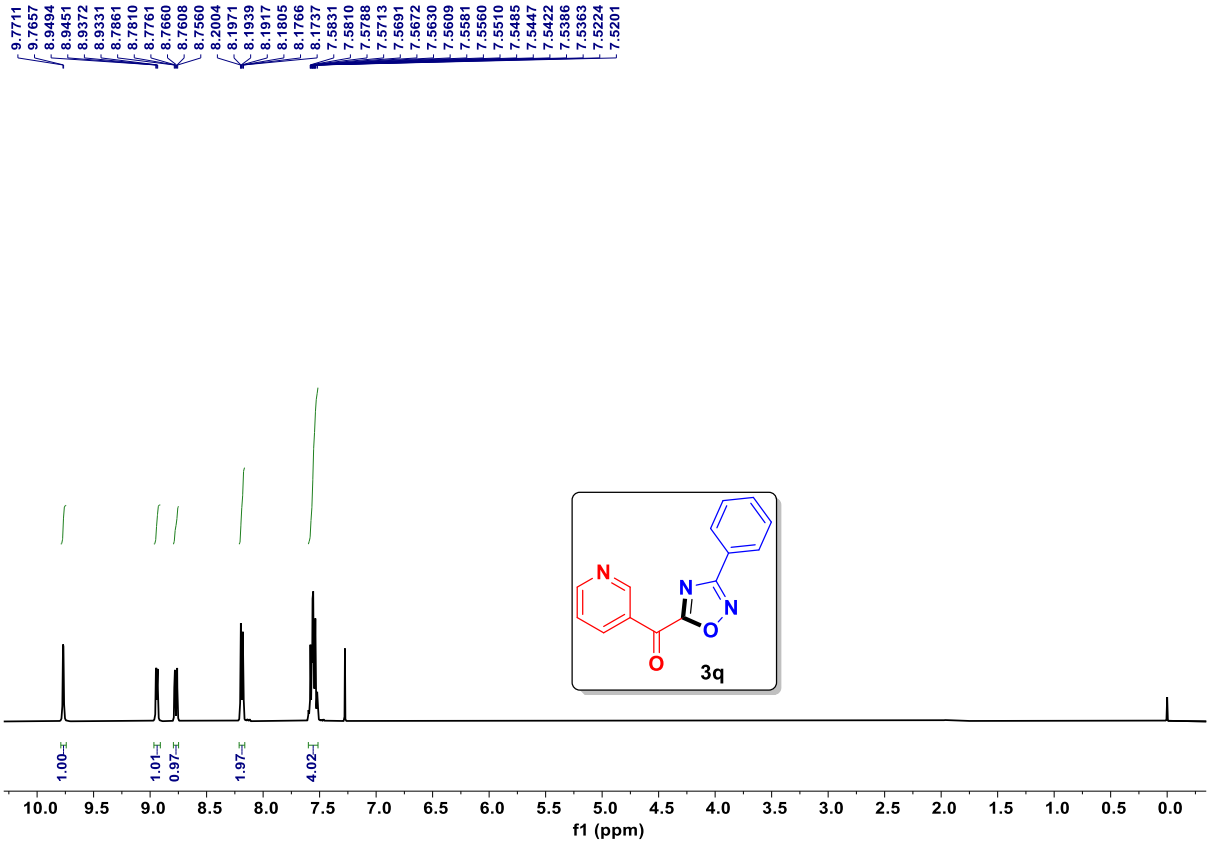


Figure 41. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3q**

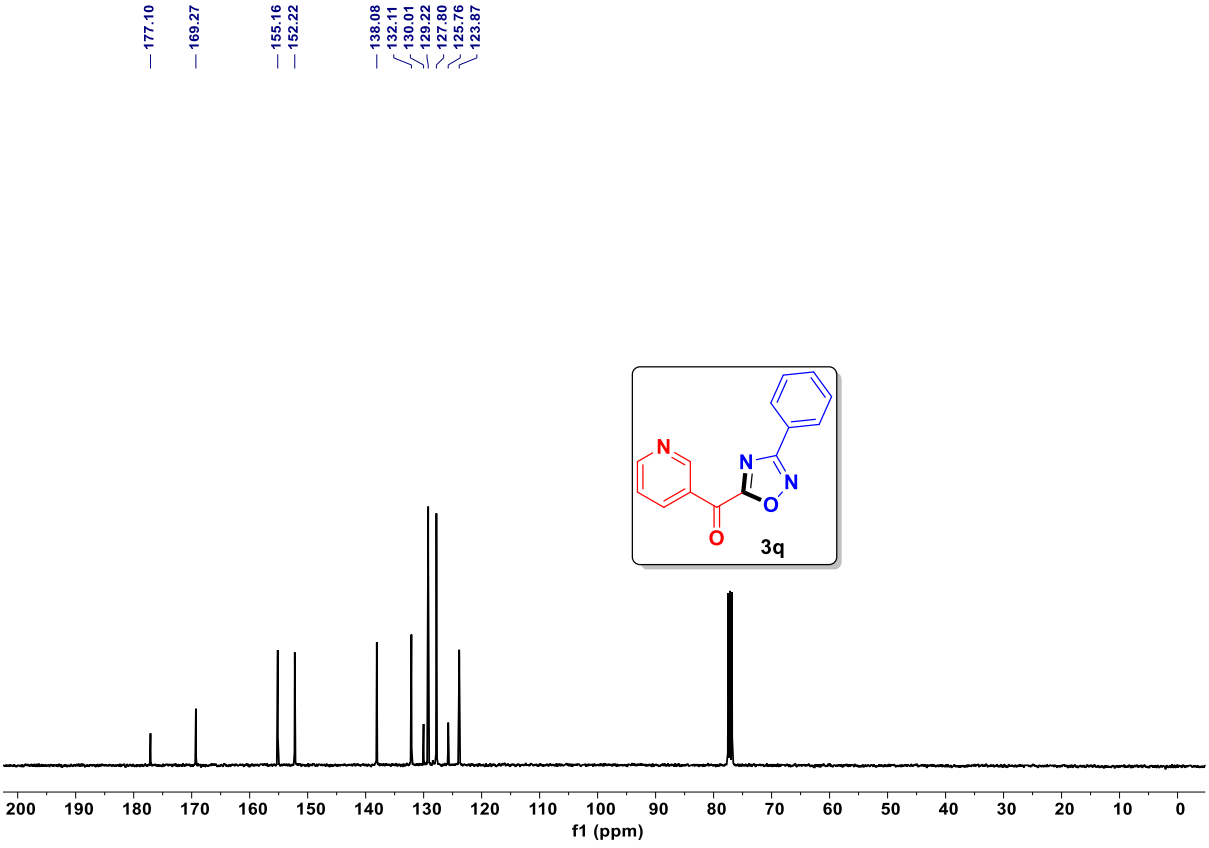


Figure 42. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3q**

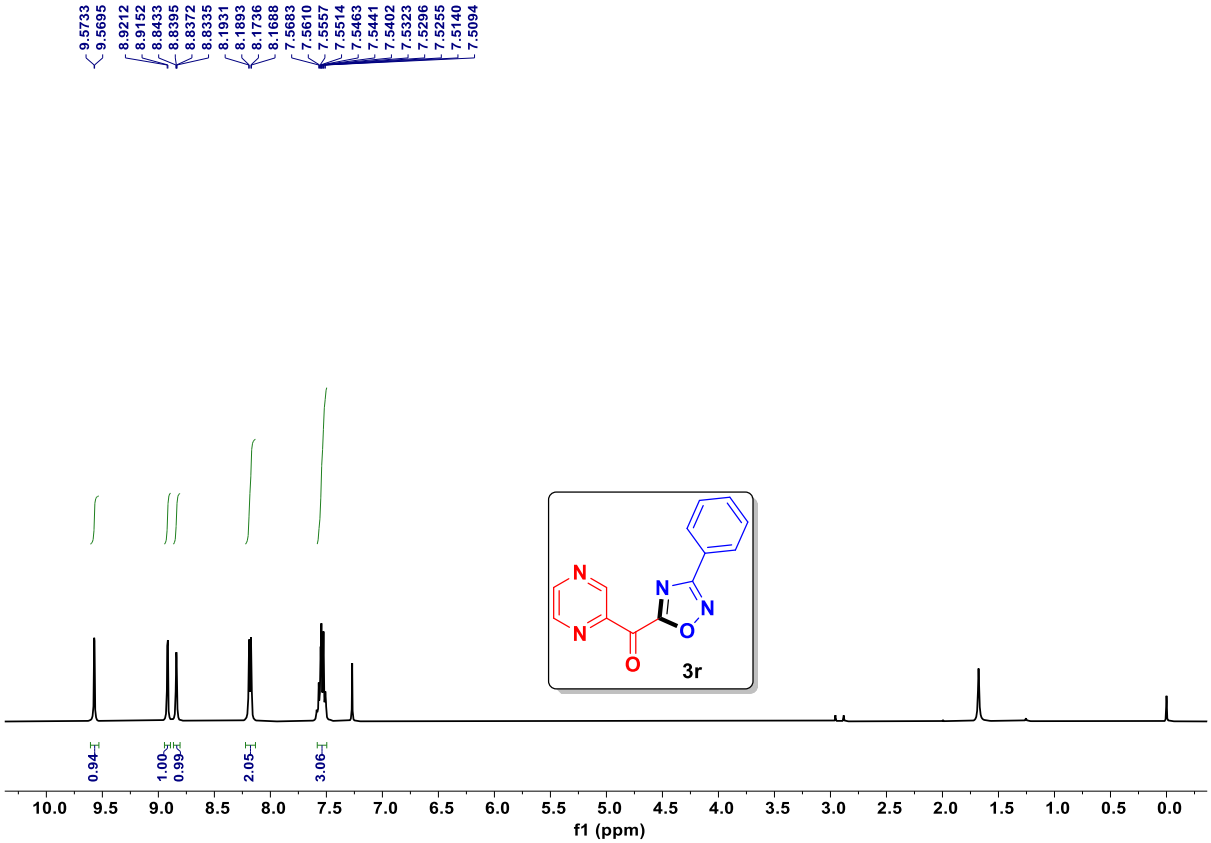


Figure 43. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3r**

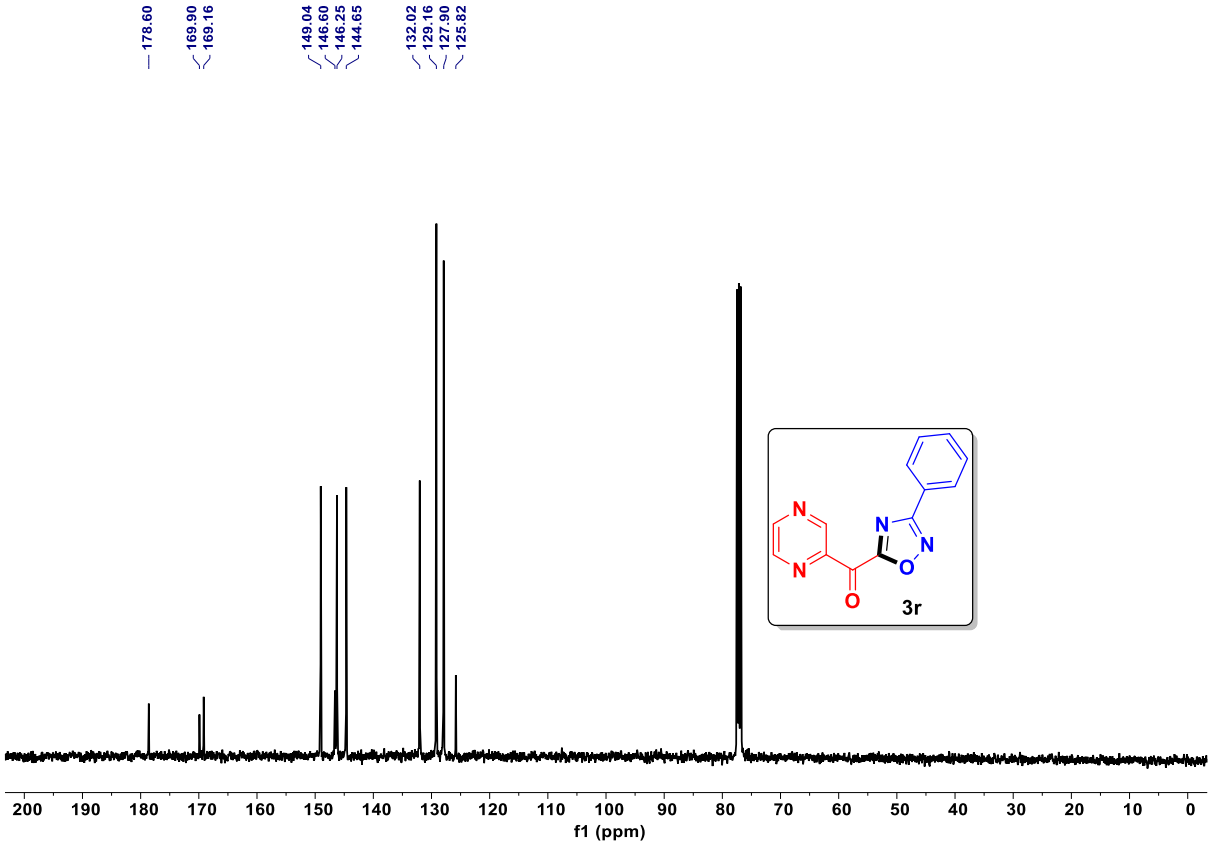


Figure 44. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3r**

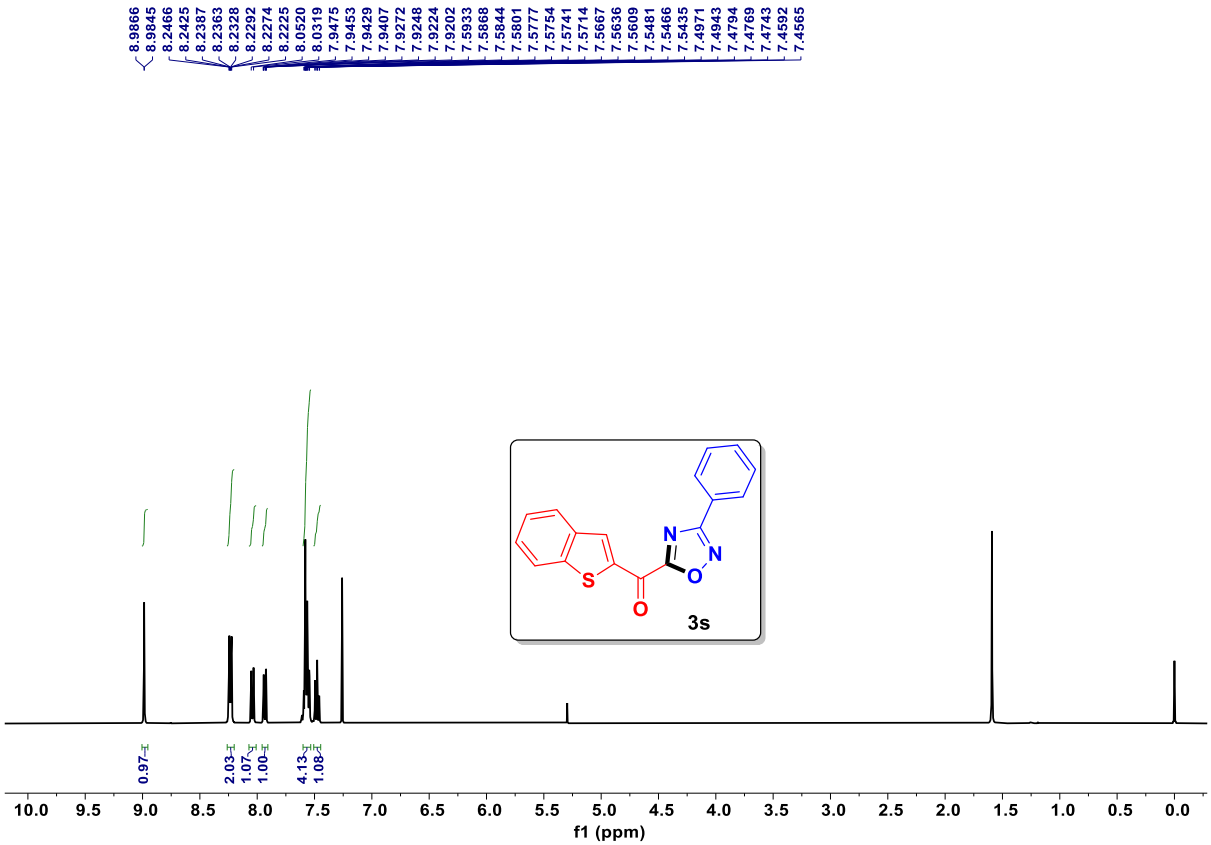


Figure 45. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3s**

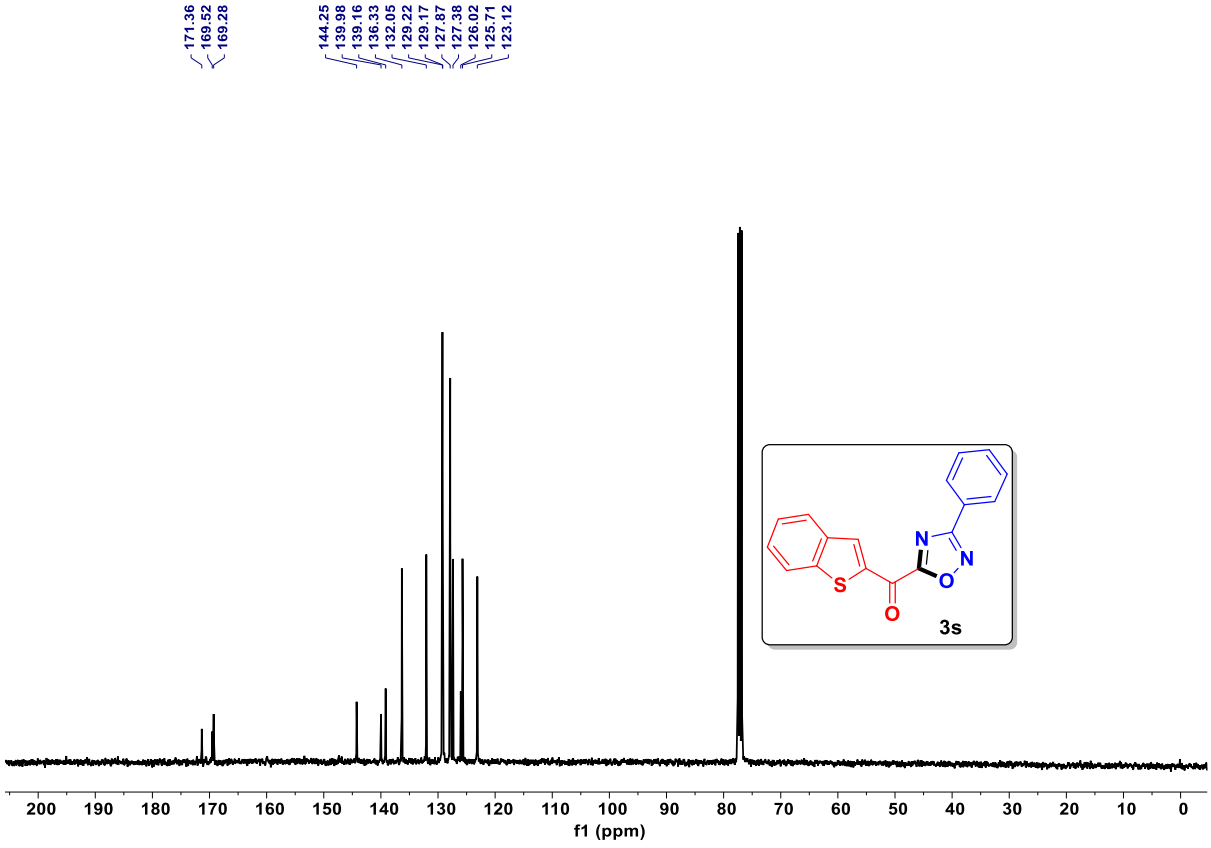


Figure 46. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3s**

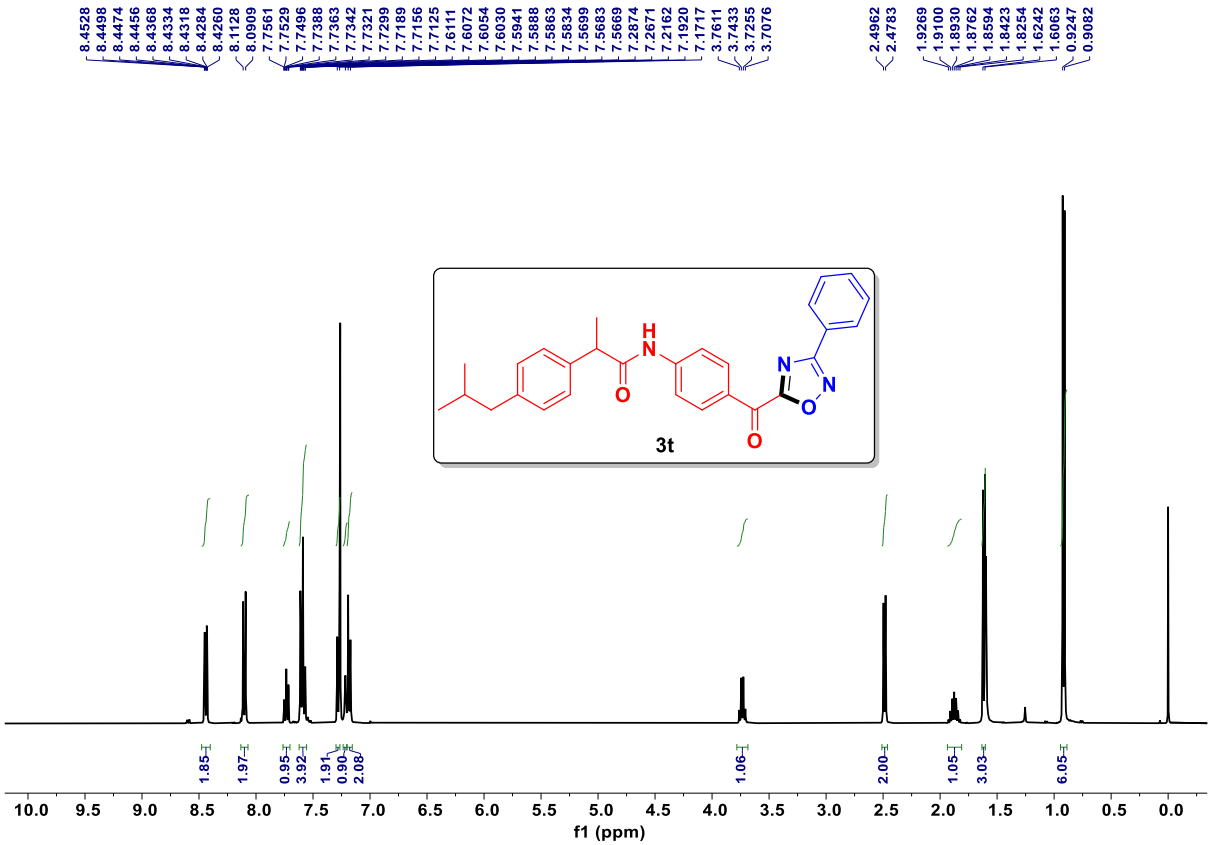


Figure 47. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3t**

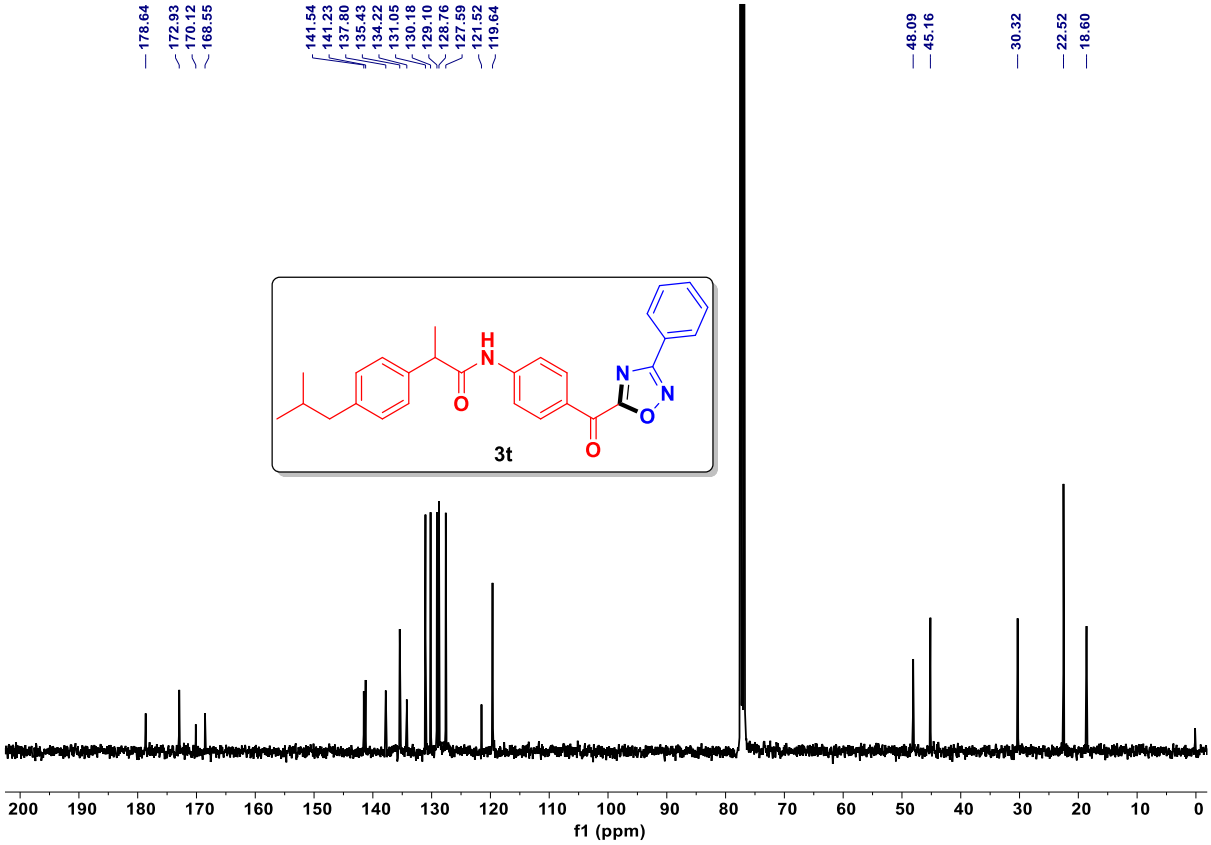


Figure 48. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of compound **3t**

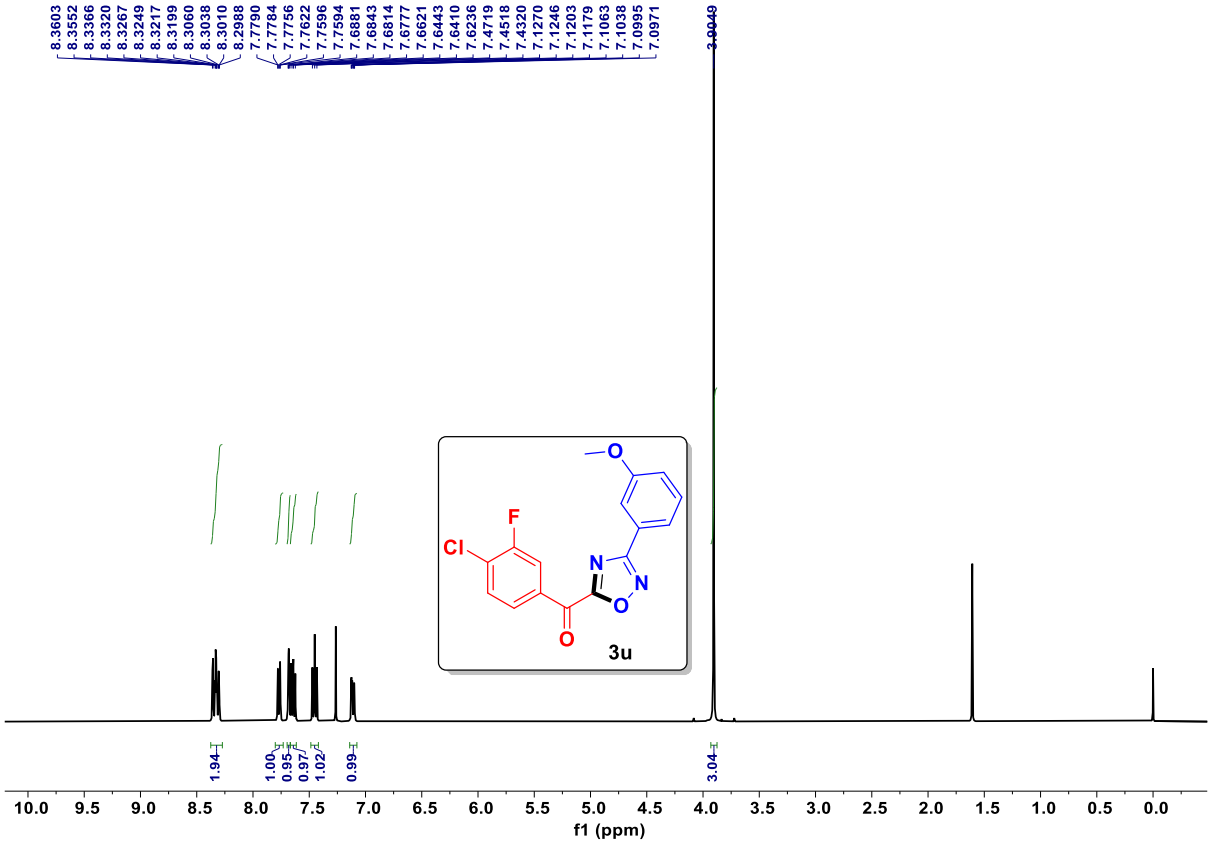


Figure 49. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3u**

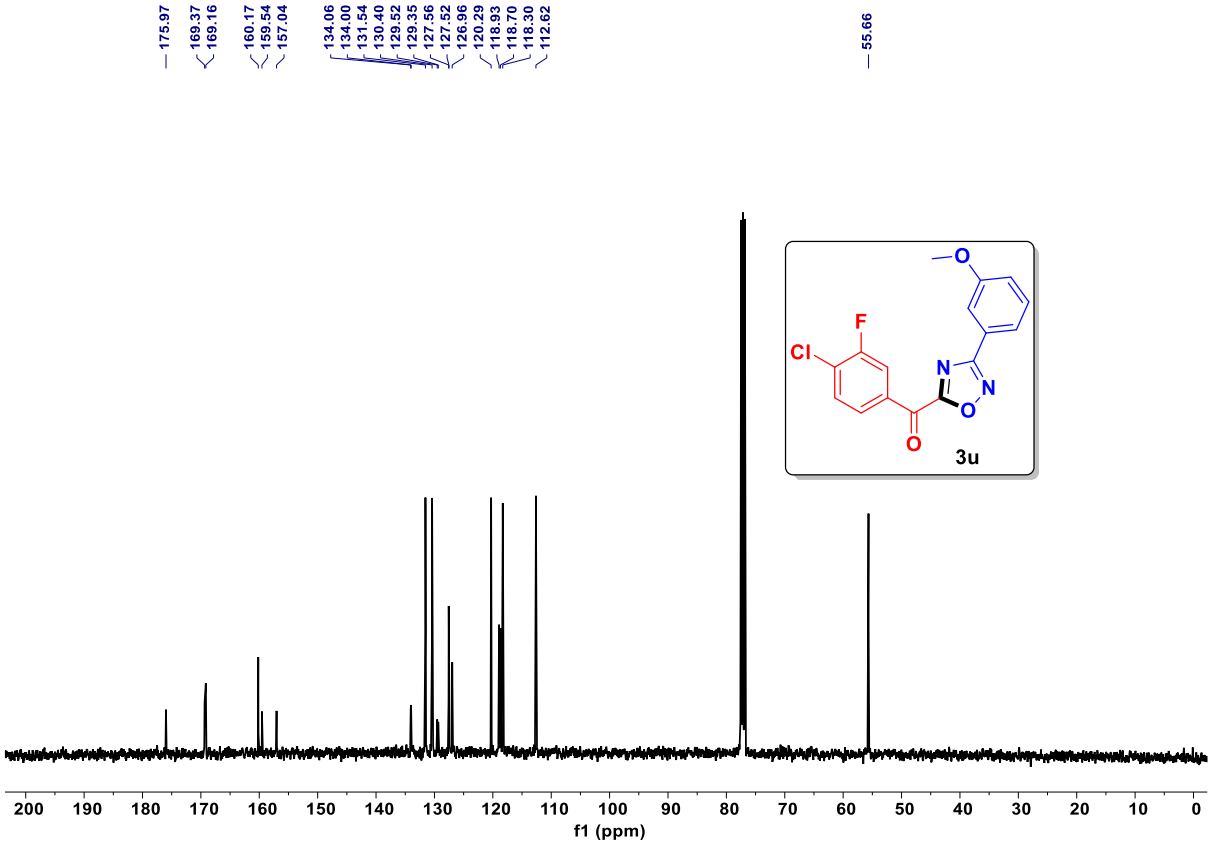


Figure 50. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3u**

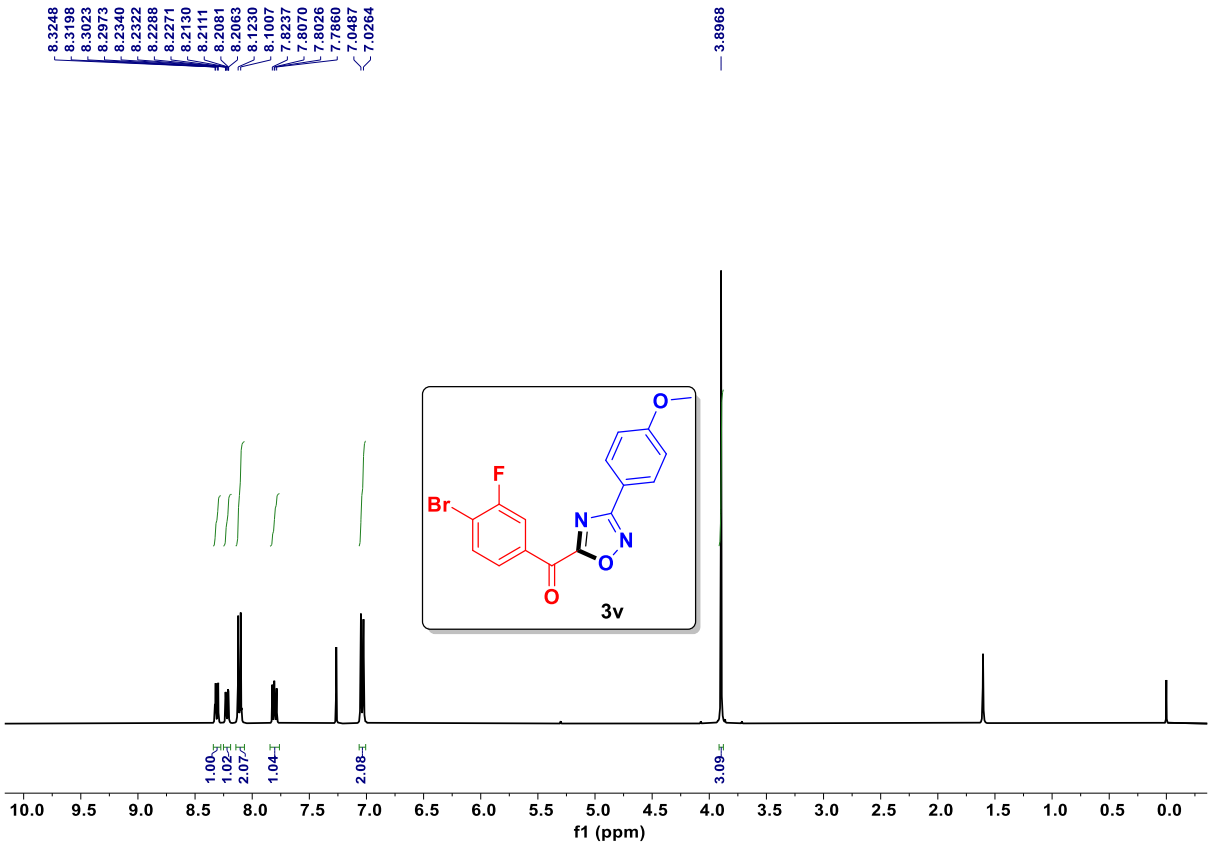


Figure 51. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3v**

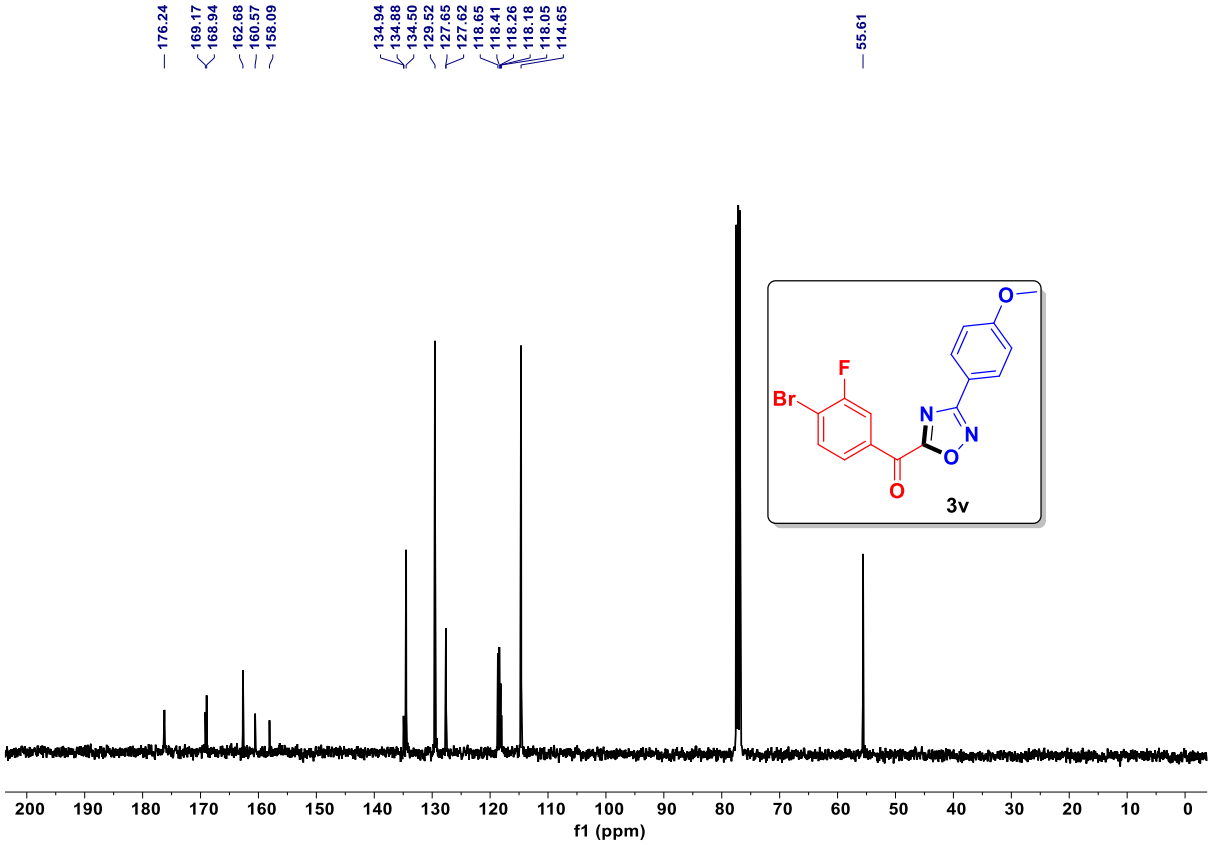


Figure 52. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3v**

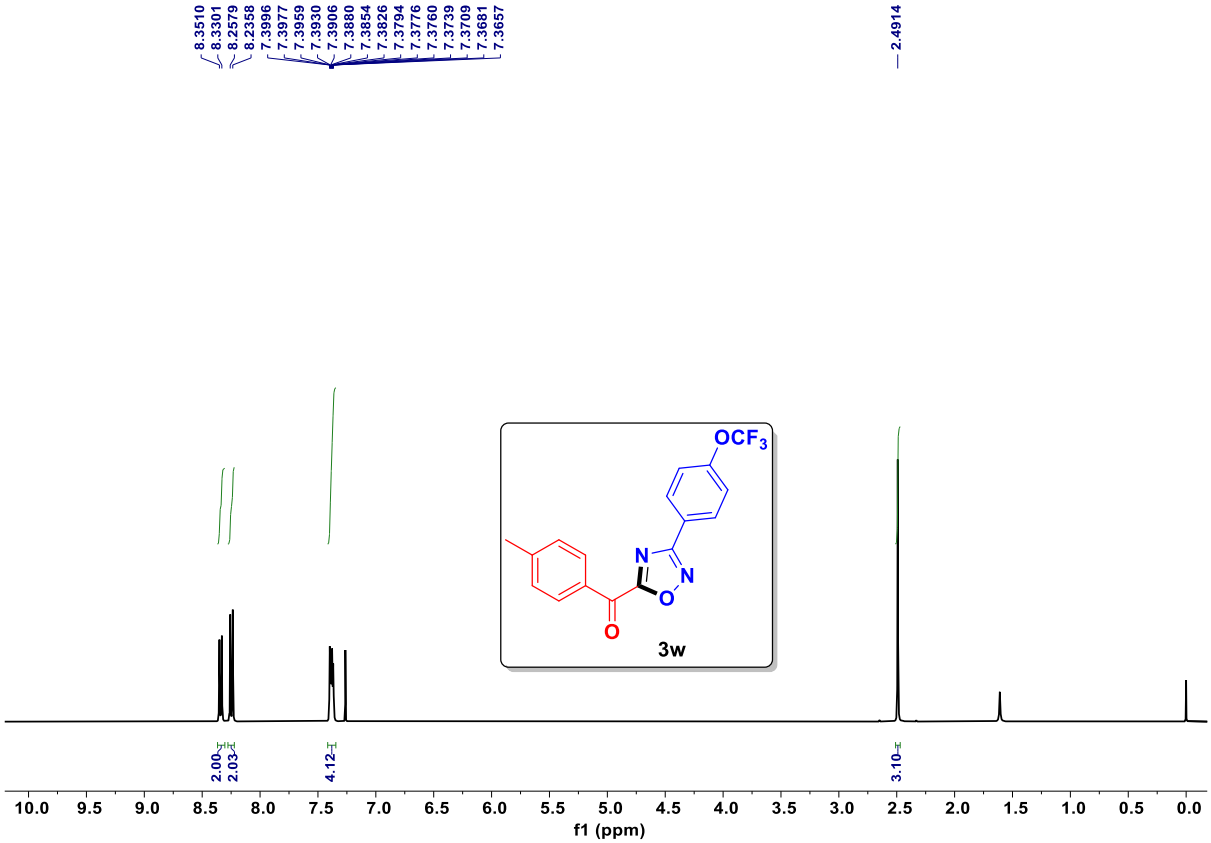


Figure 53. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3w**

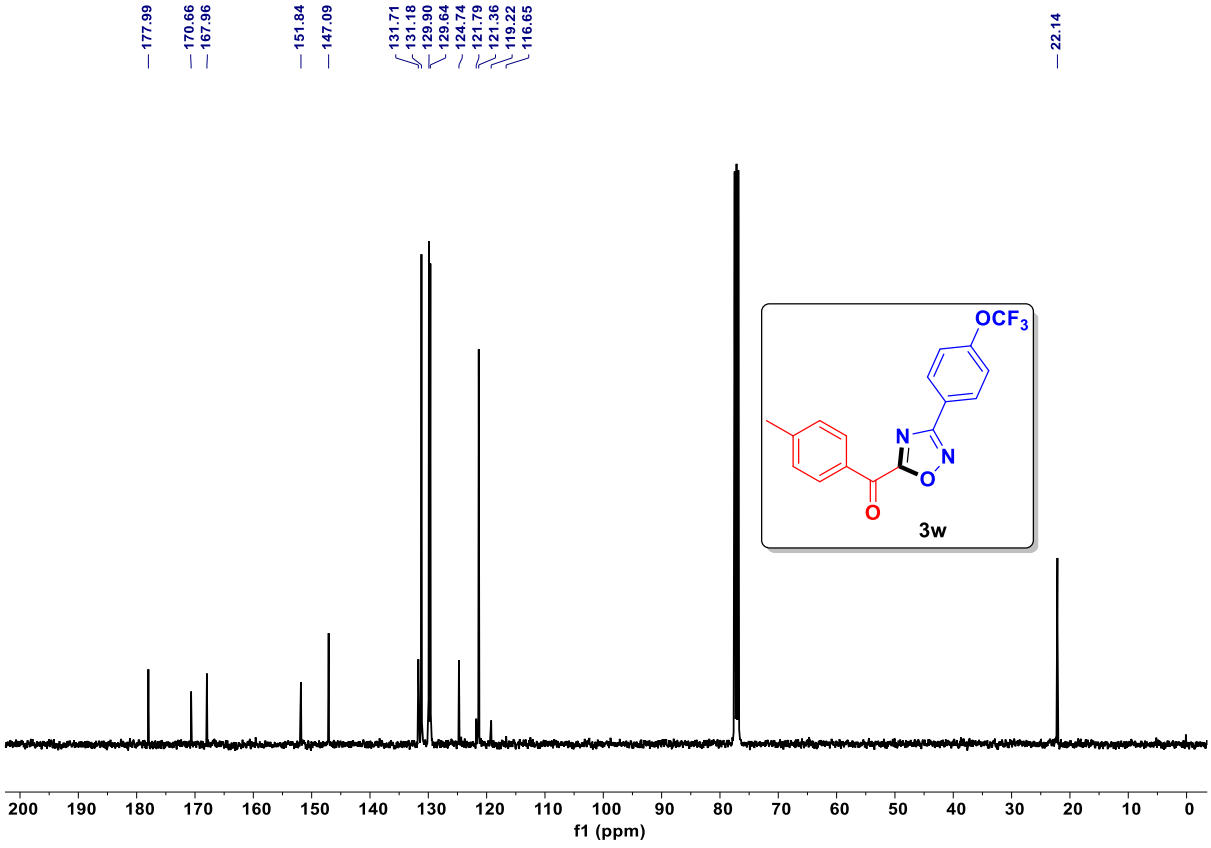


Figure 54. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3w**

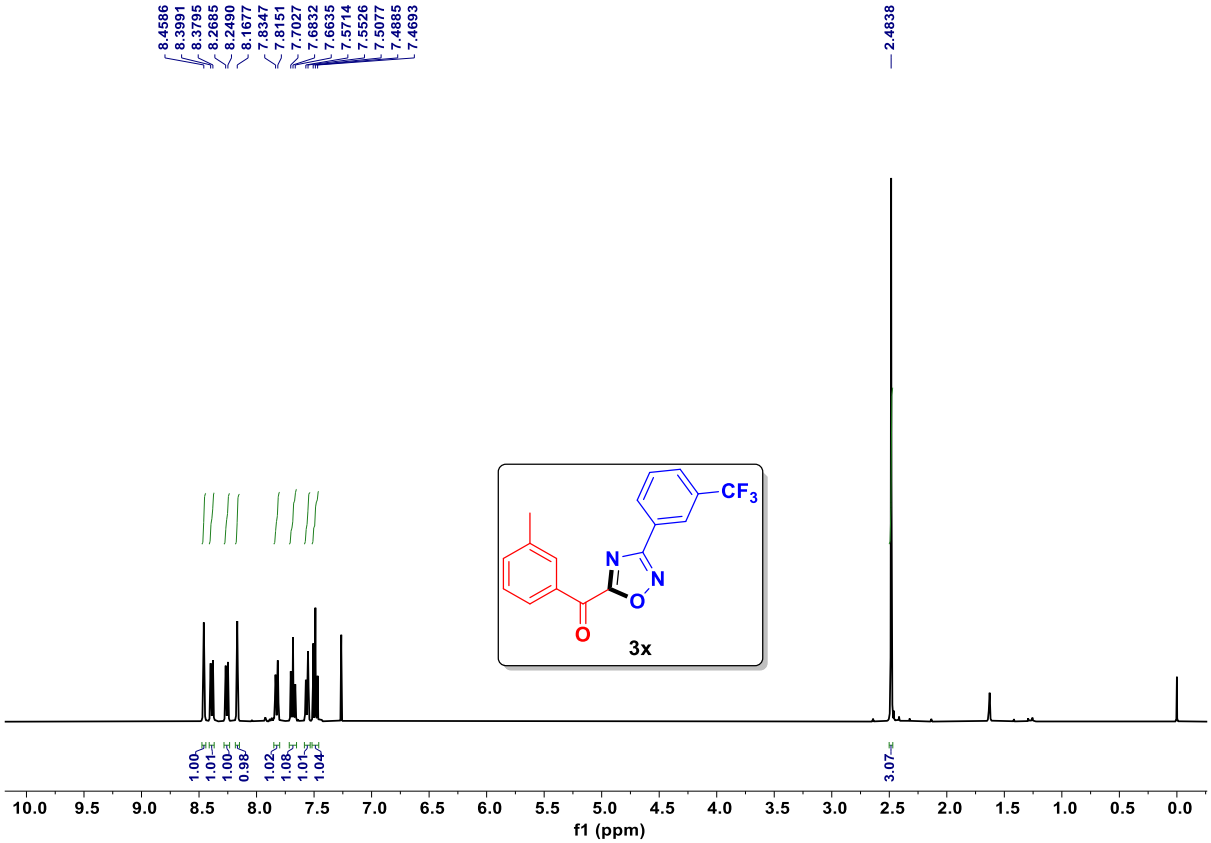


Figure 55. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3x**

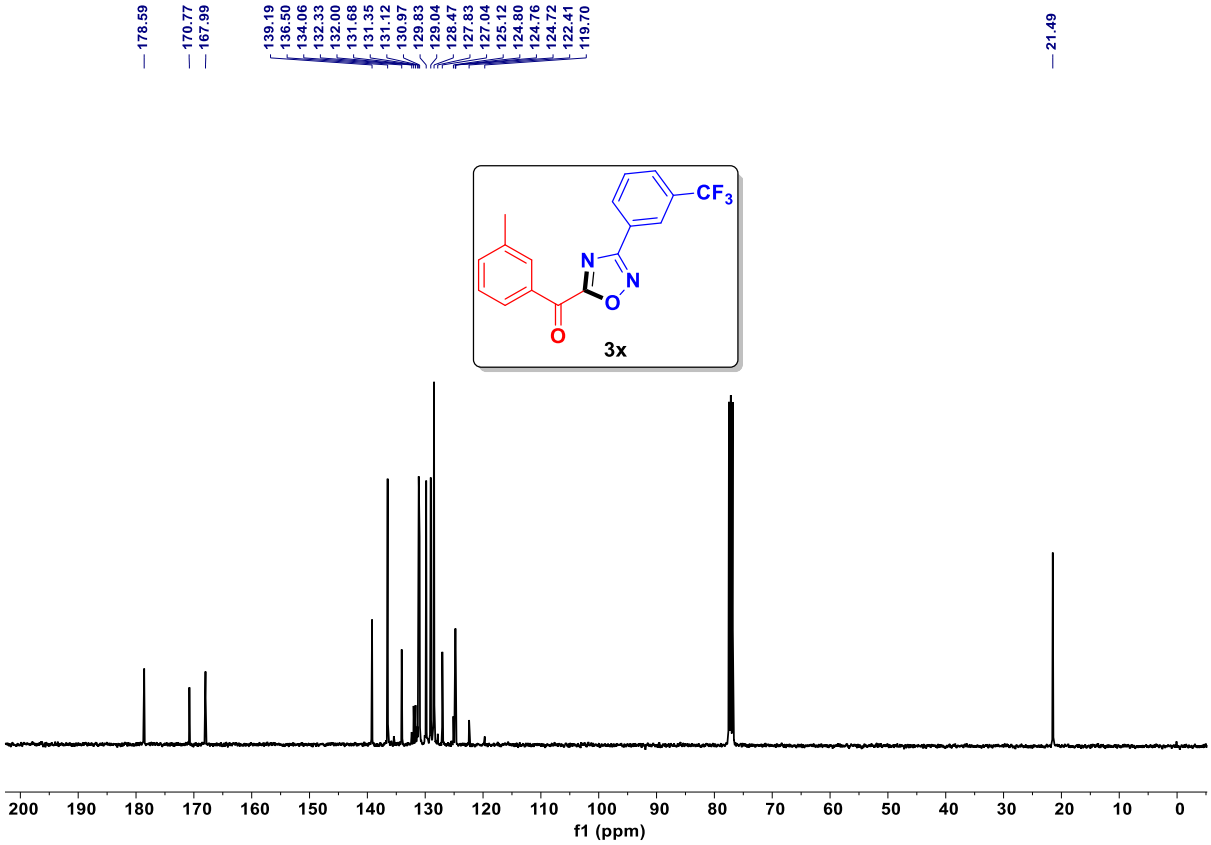


Figure 56. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3x**

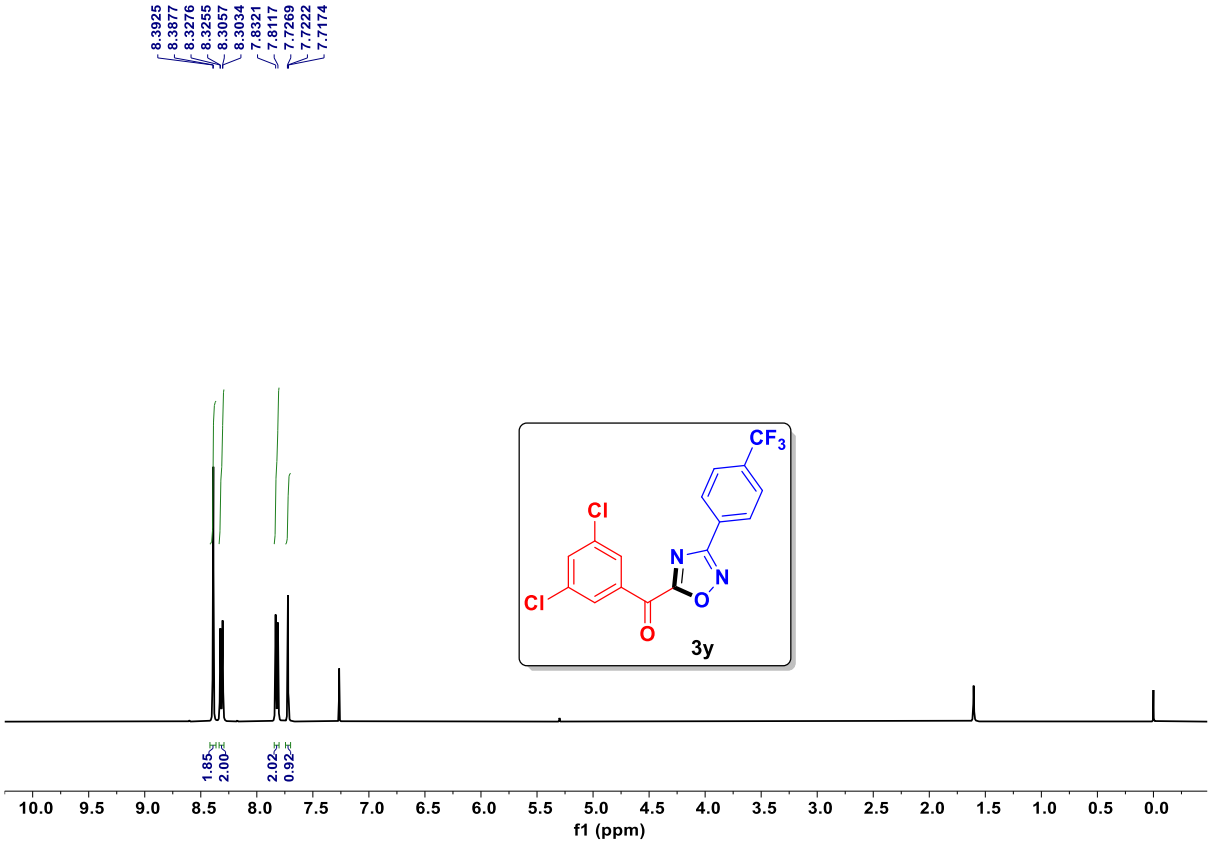


Figure 57. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3y**

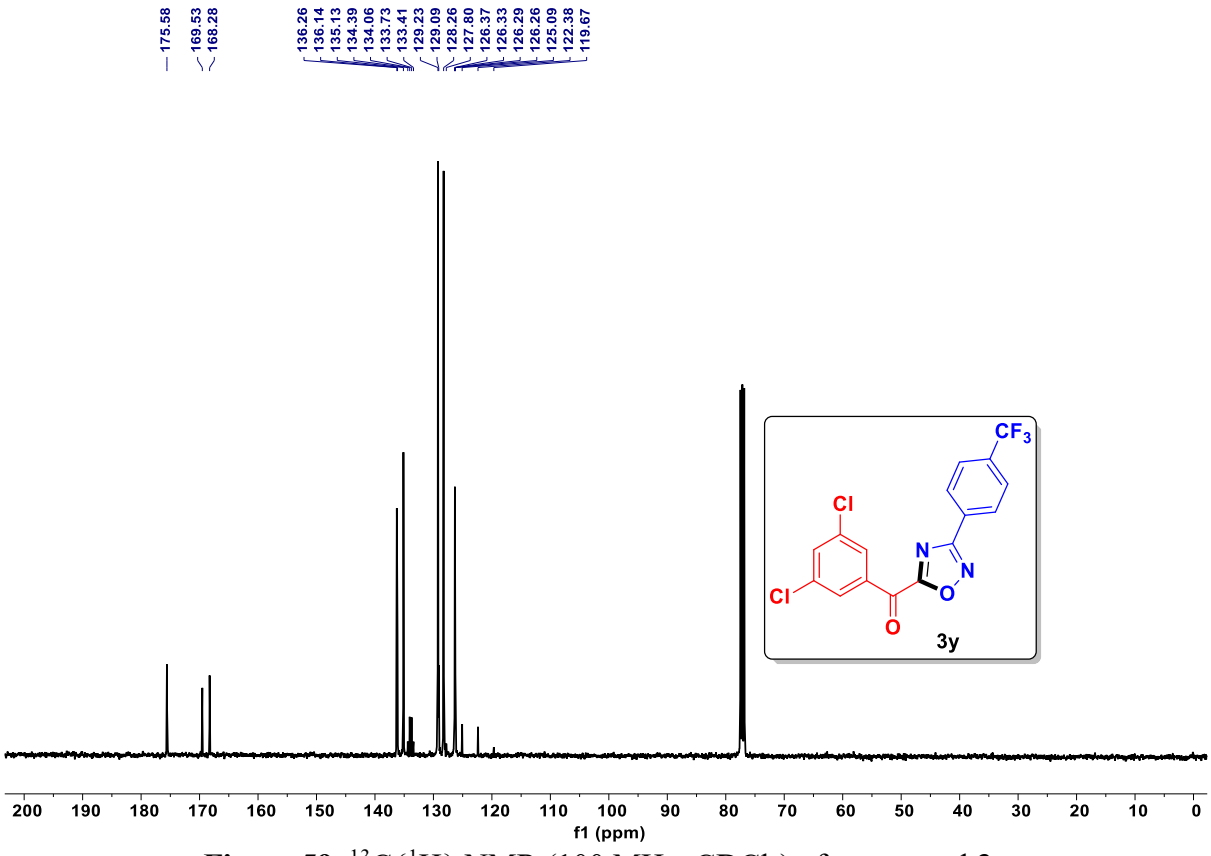


Figure 59. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of compound **3y**

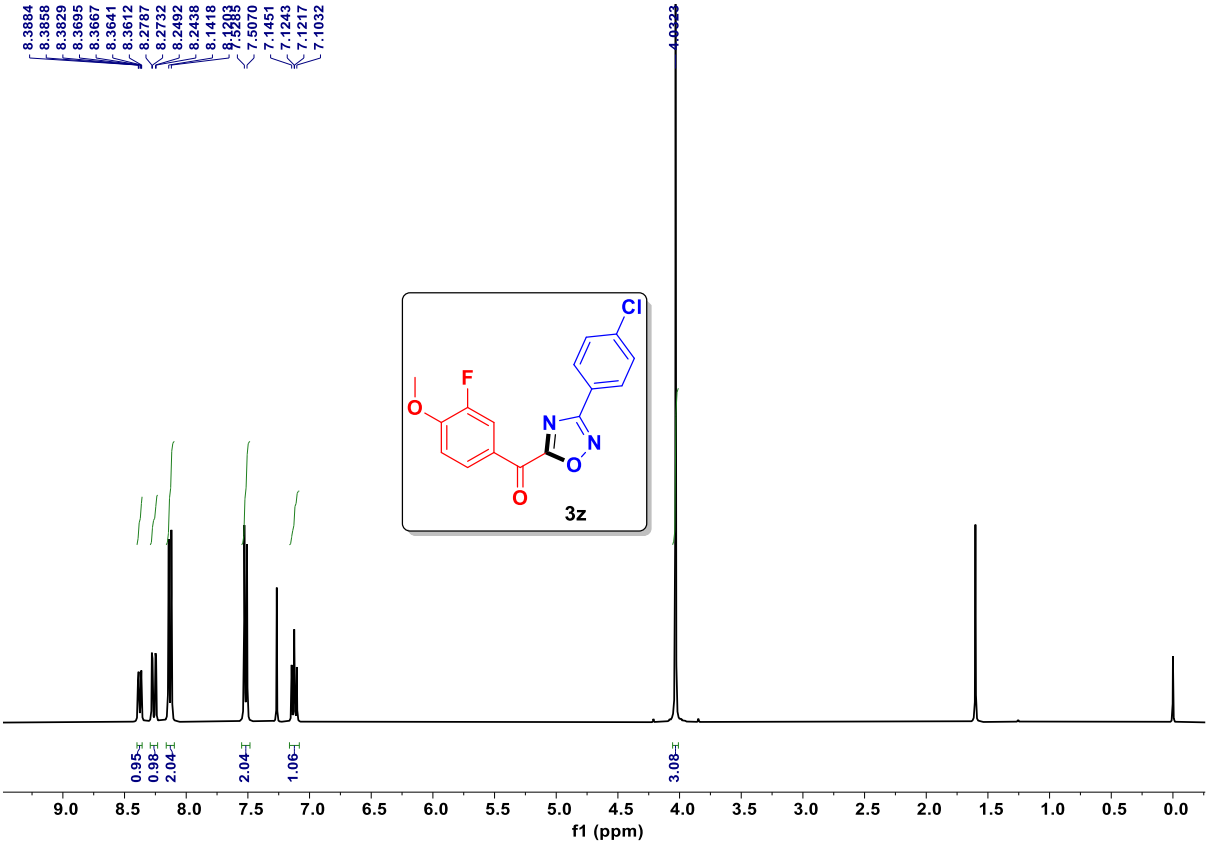


Figure 59. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3z**

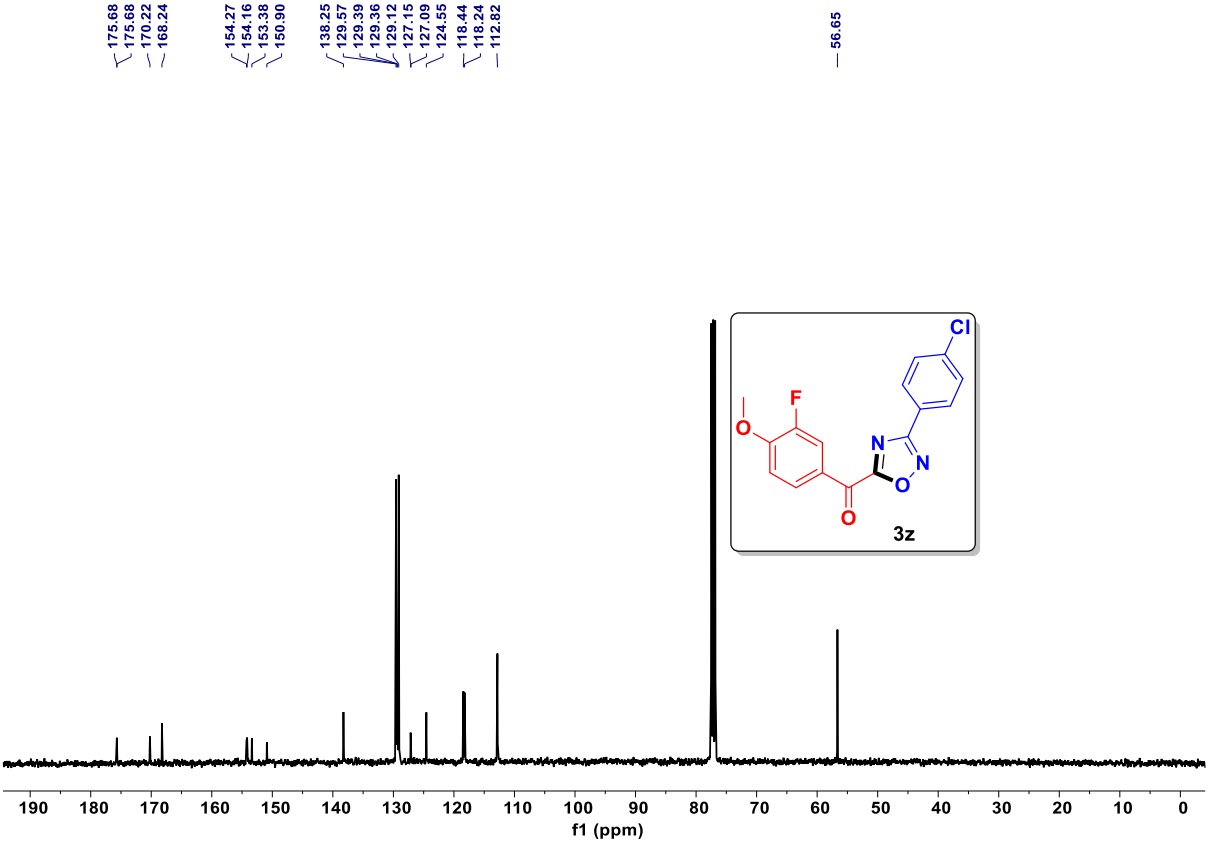


Figure 60. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3z**

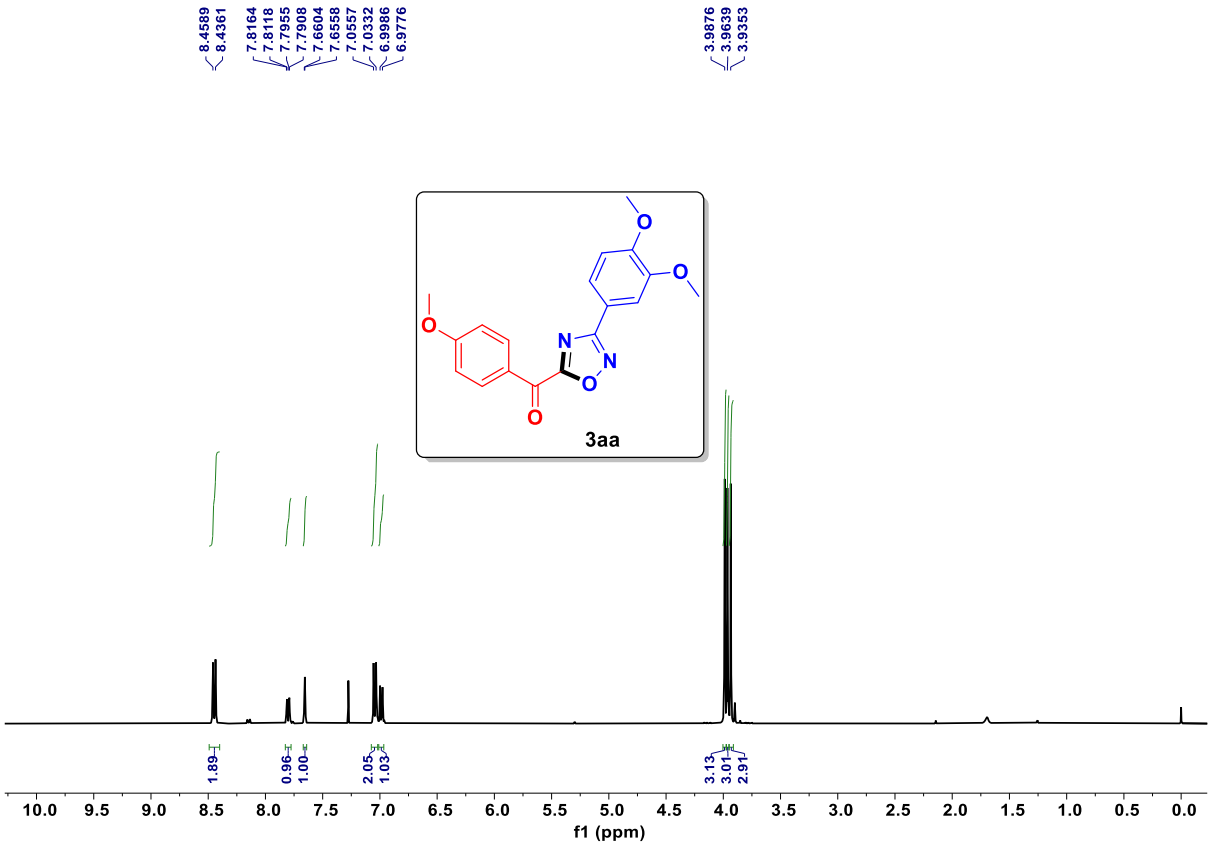


Figure 61. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa**

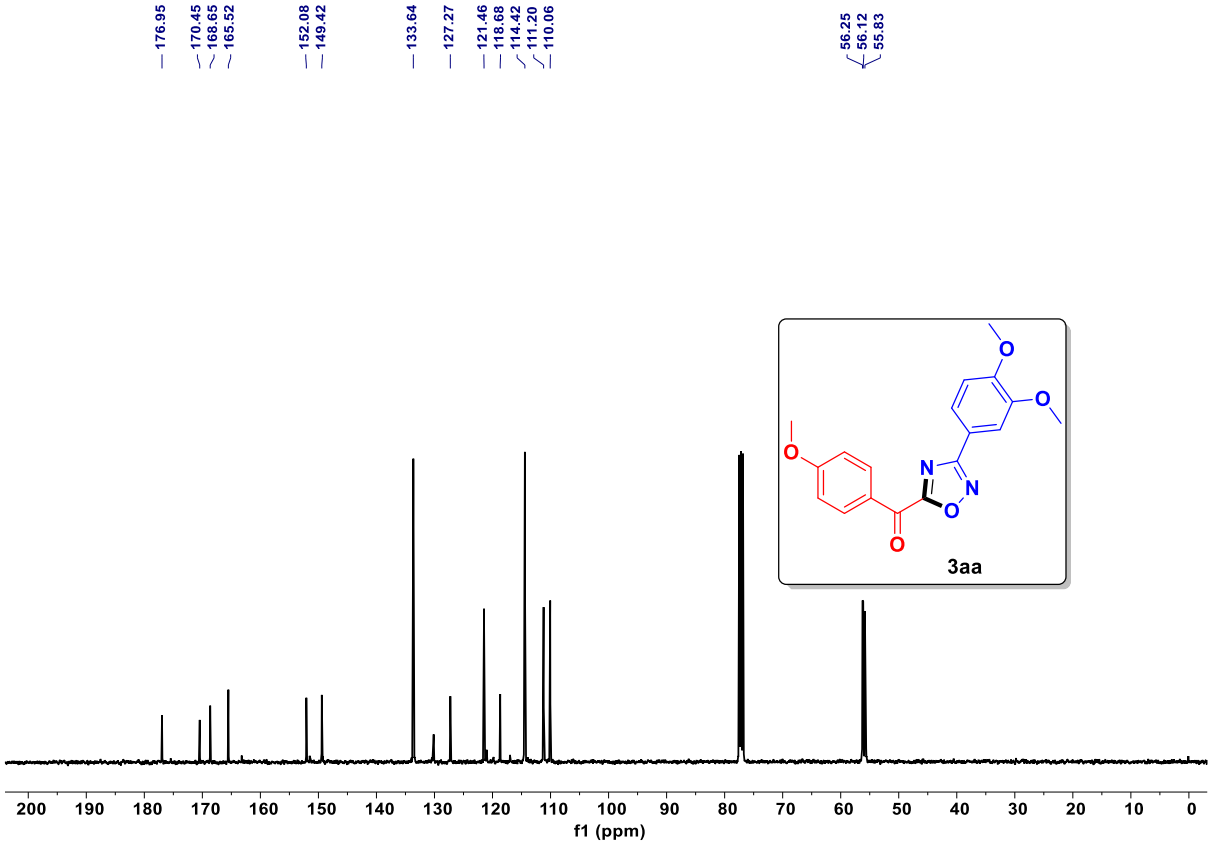


Figure 61. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3aa**

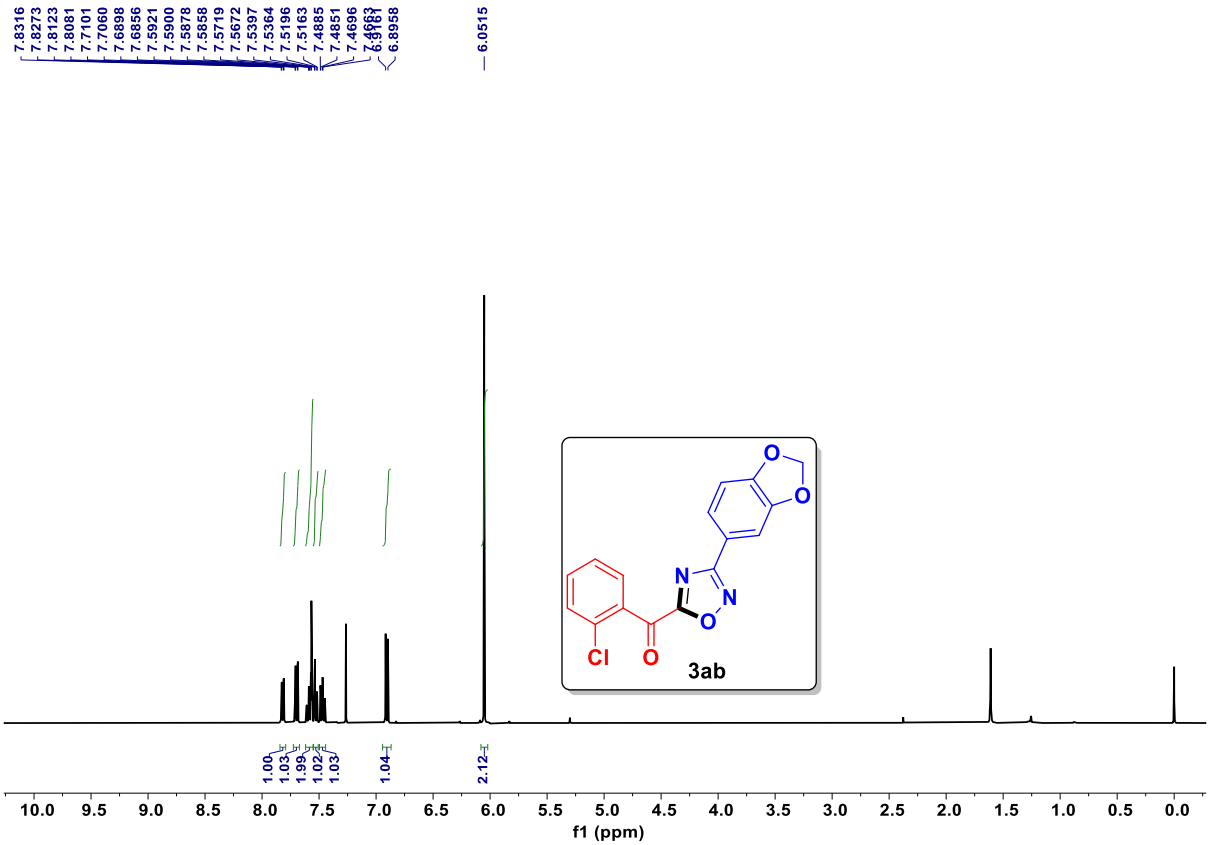


Figure 63. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab**

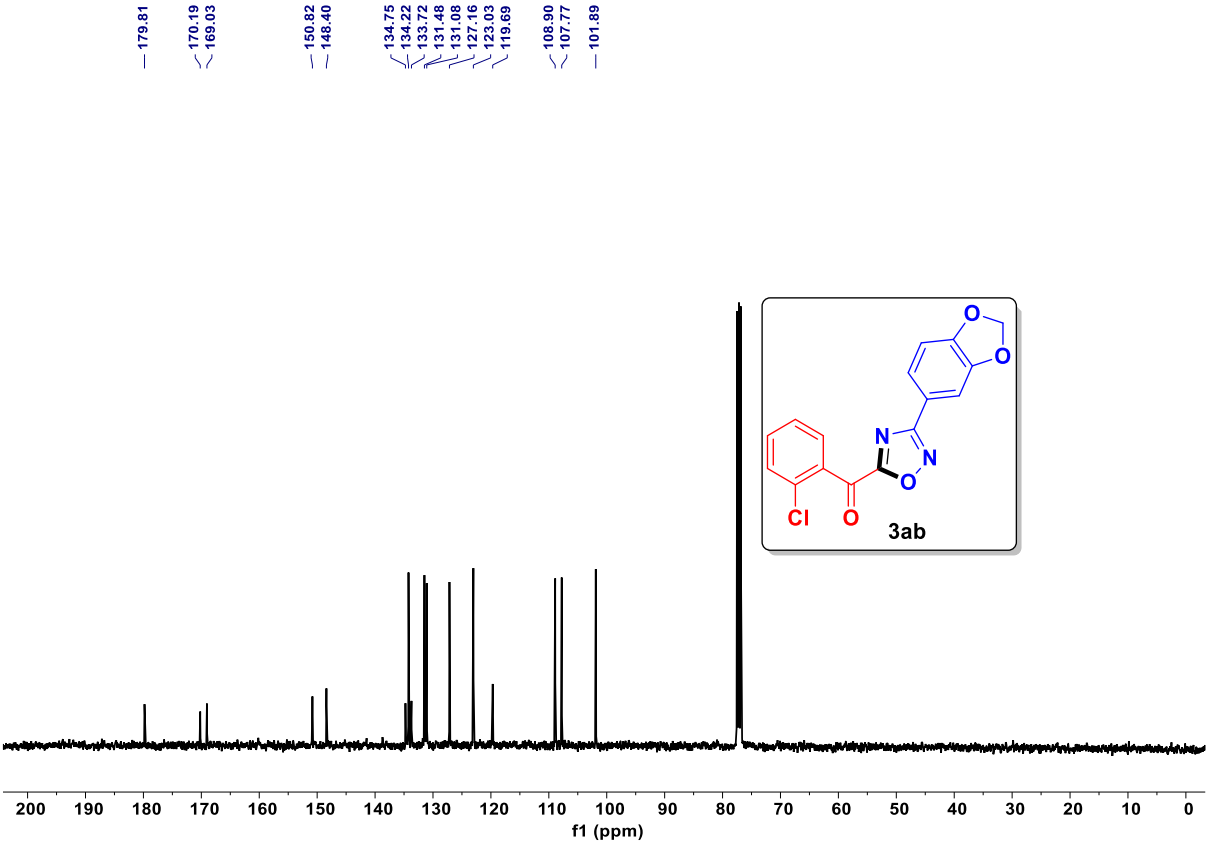


Figure 64. ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) of compound **3ab**

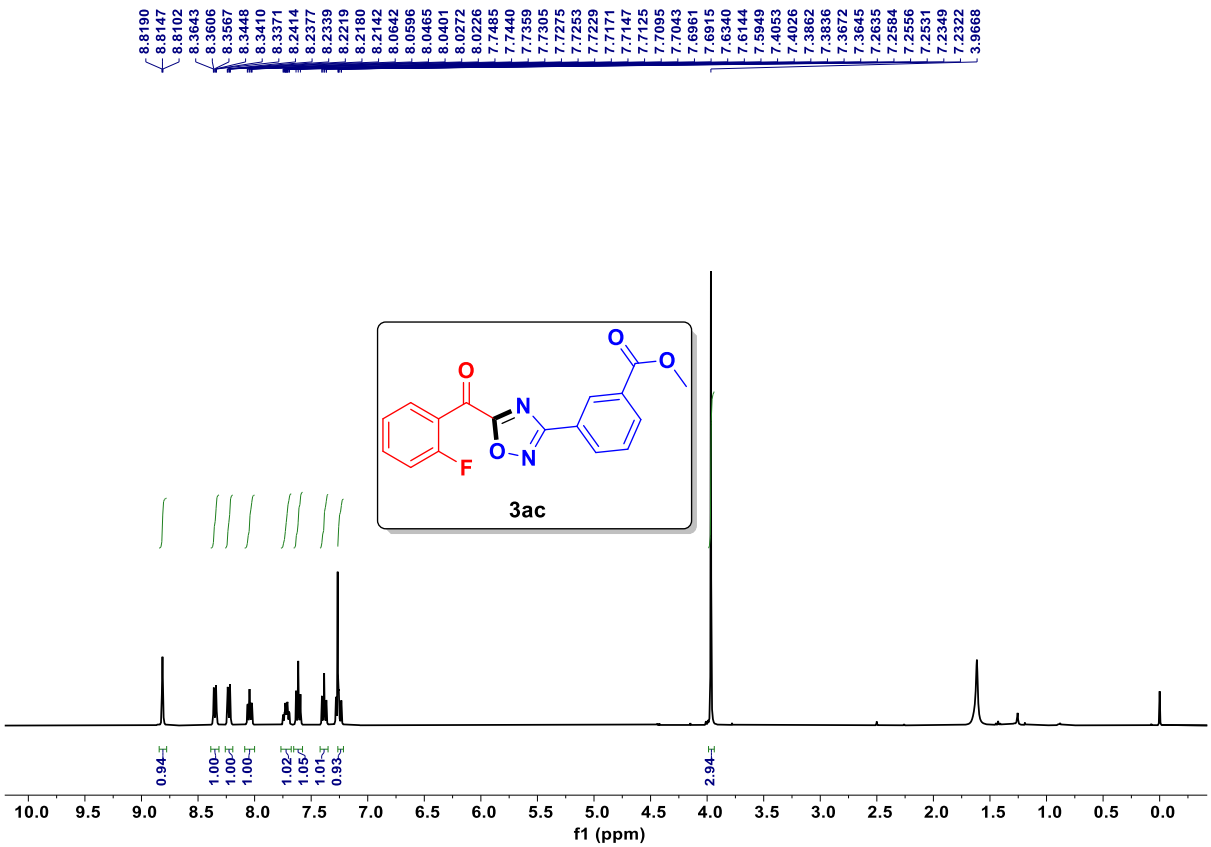


Figure 85. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ac**

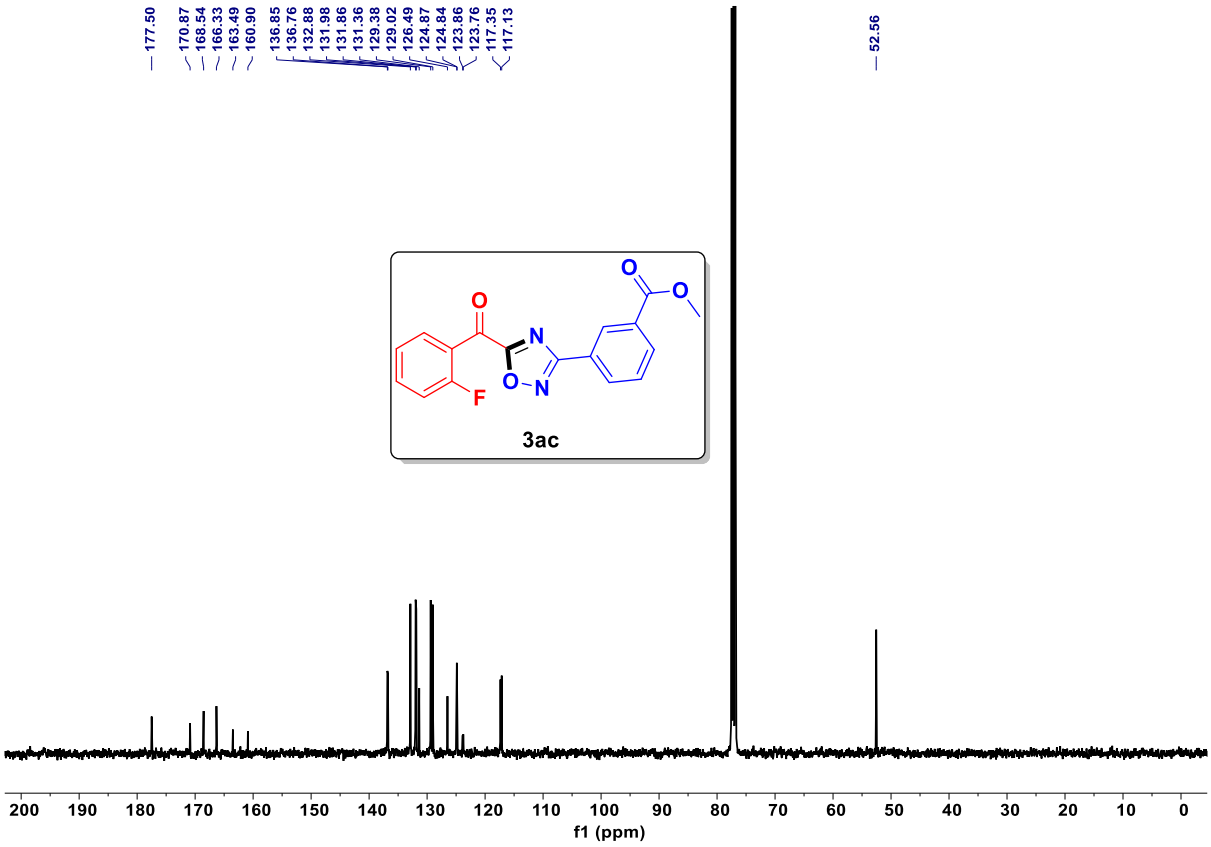


Figure 86. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ac**

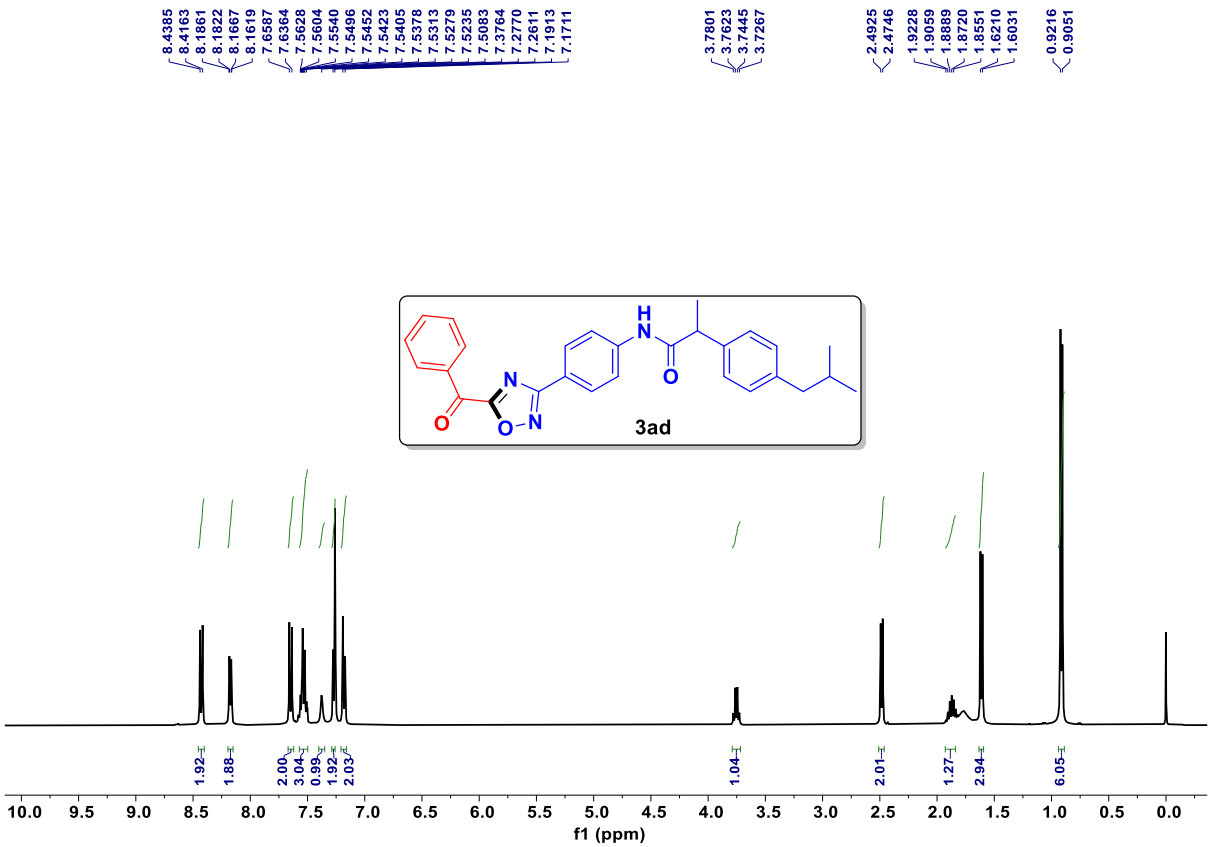


Figure 67. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ad**

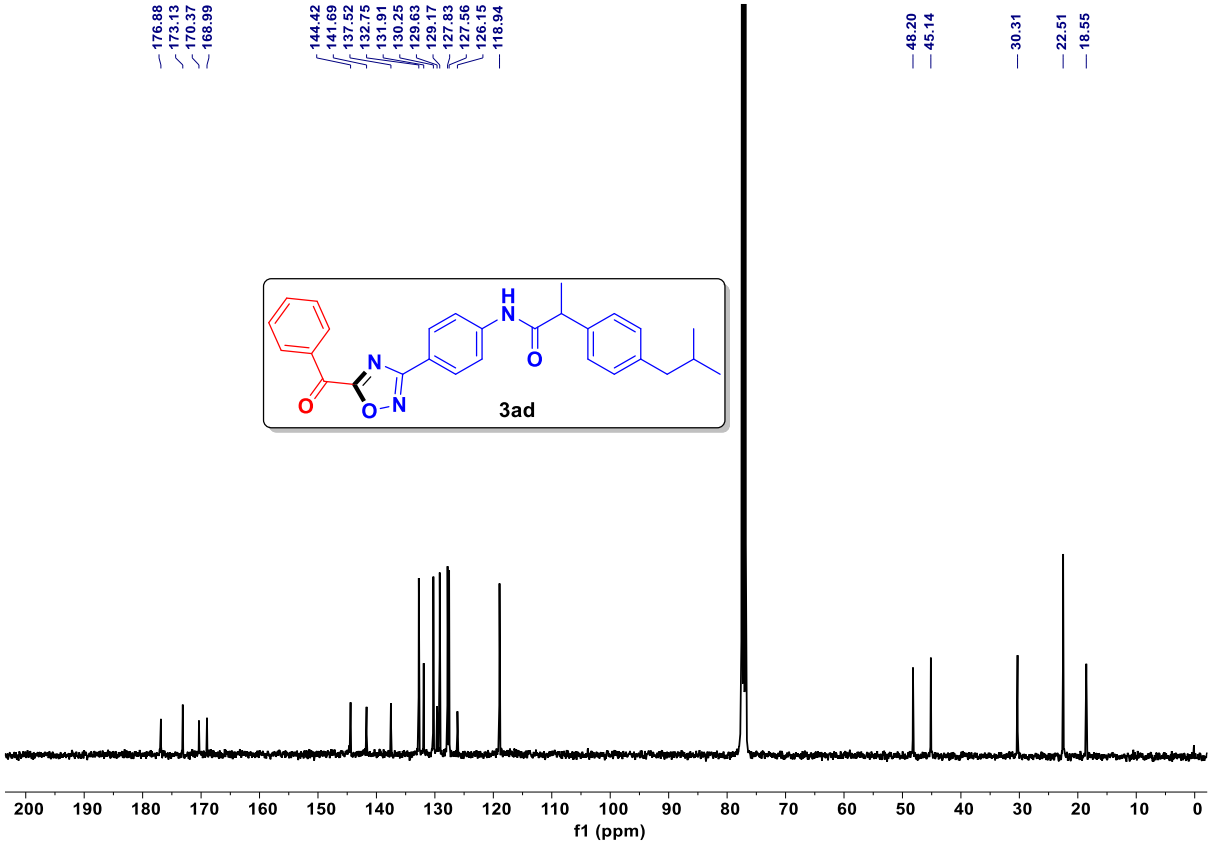


Figure 68. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ad**

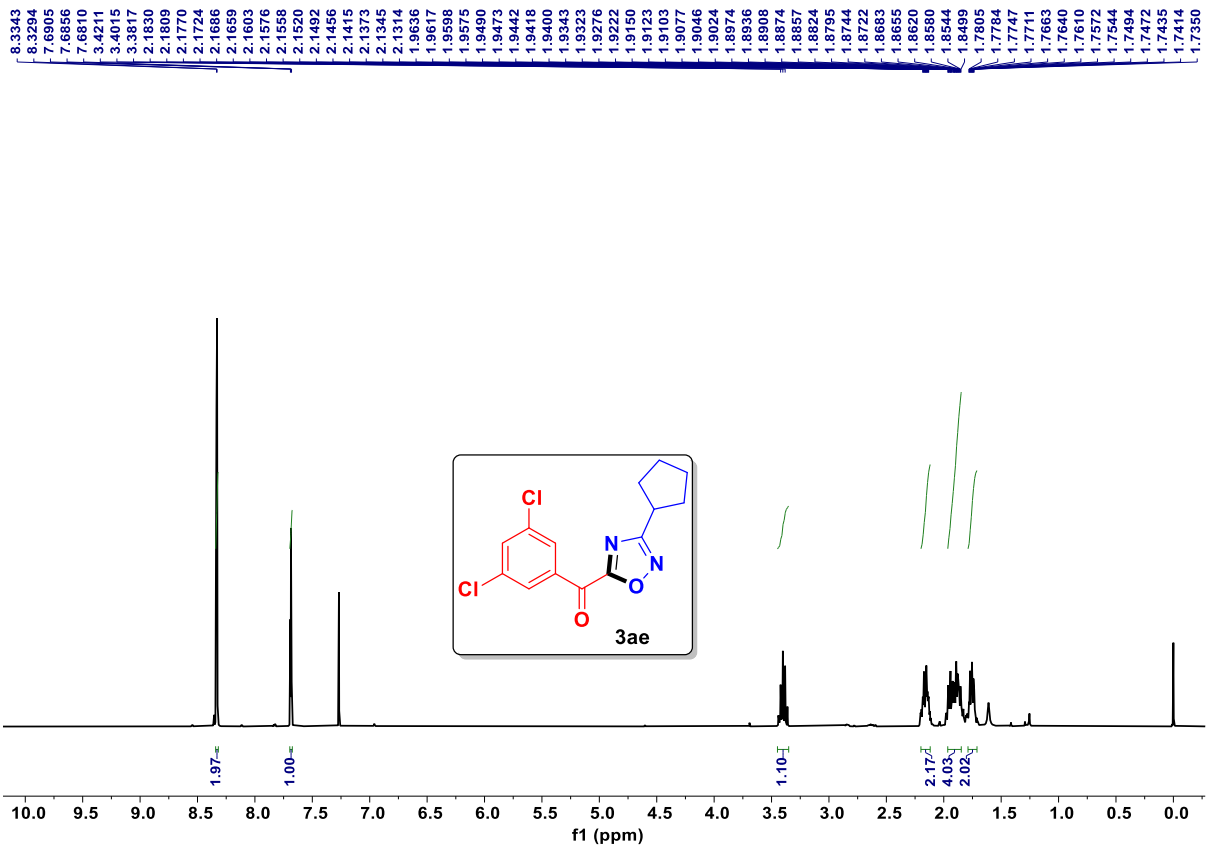


Figure 69. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ae**

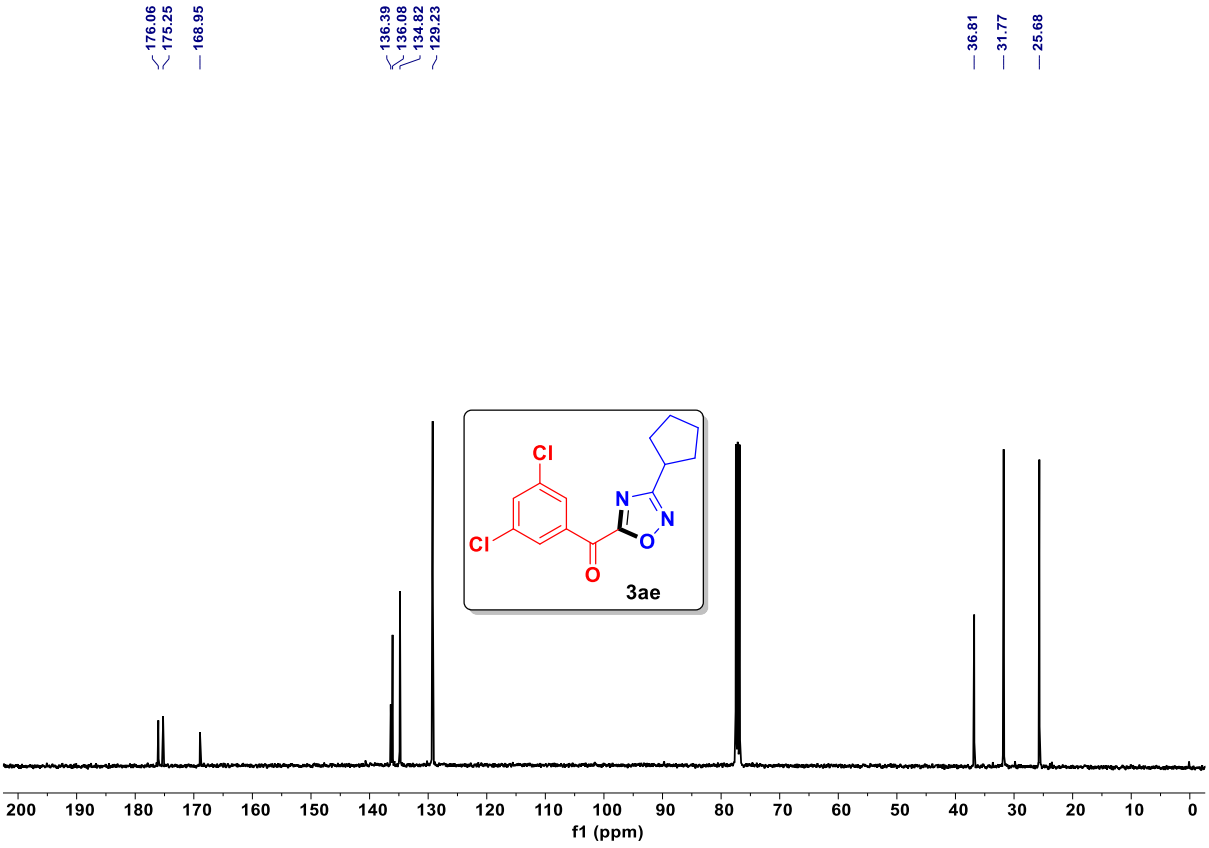


Figure 70. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ae**

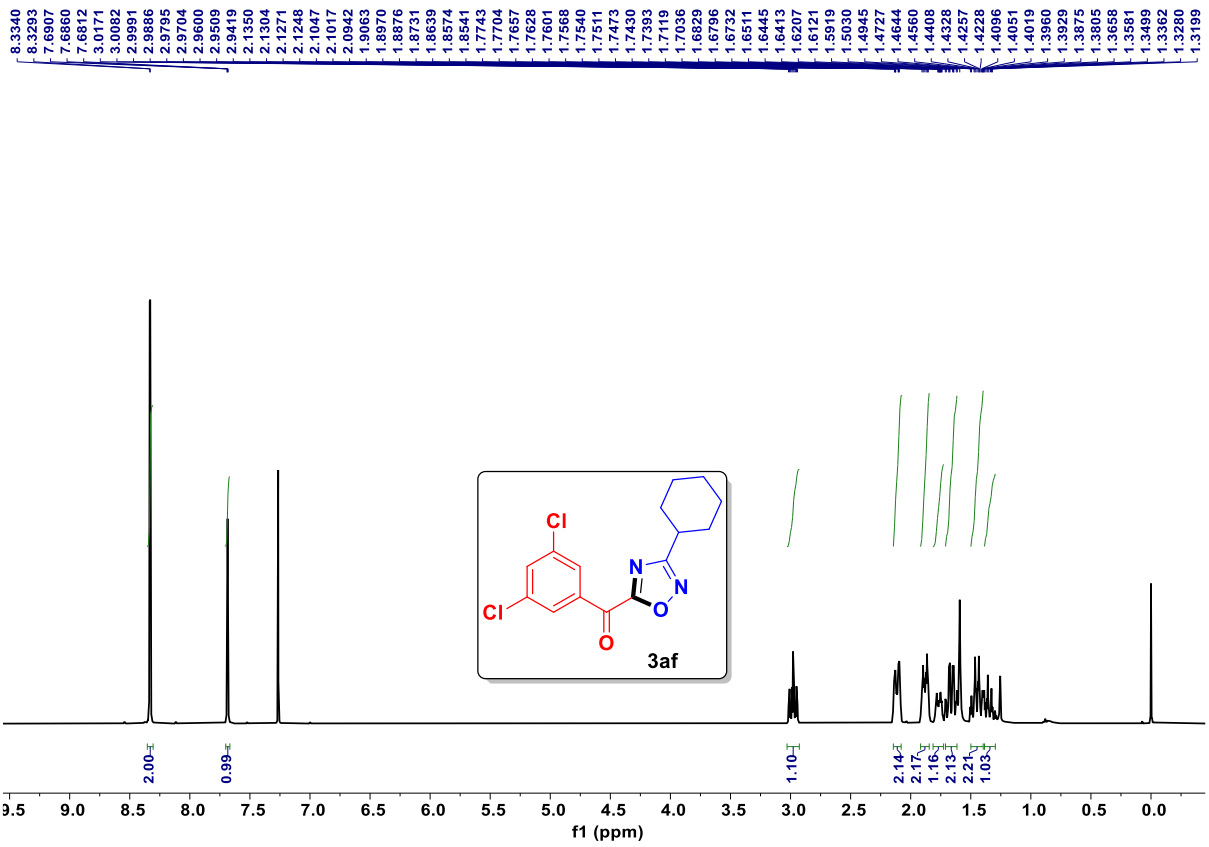


Figure 71. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3af**

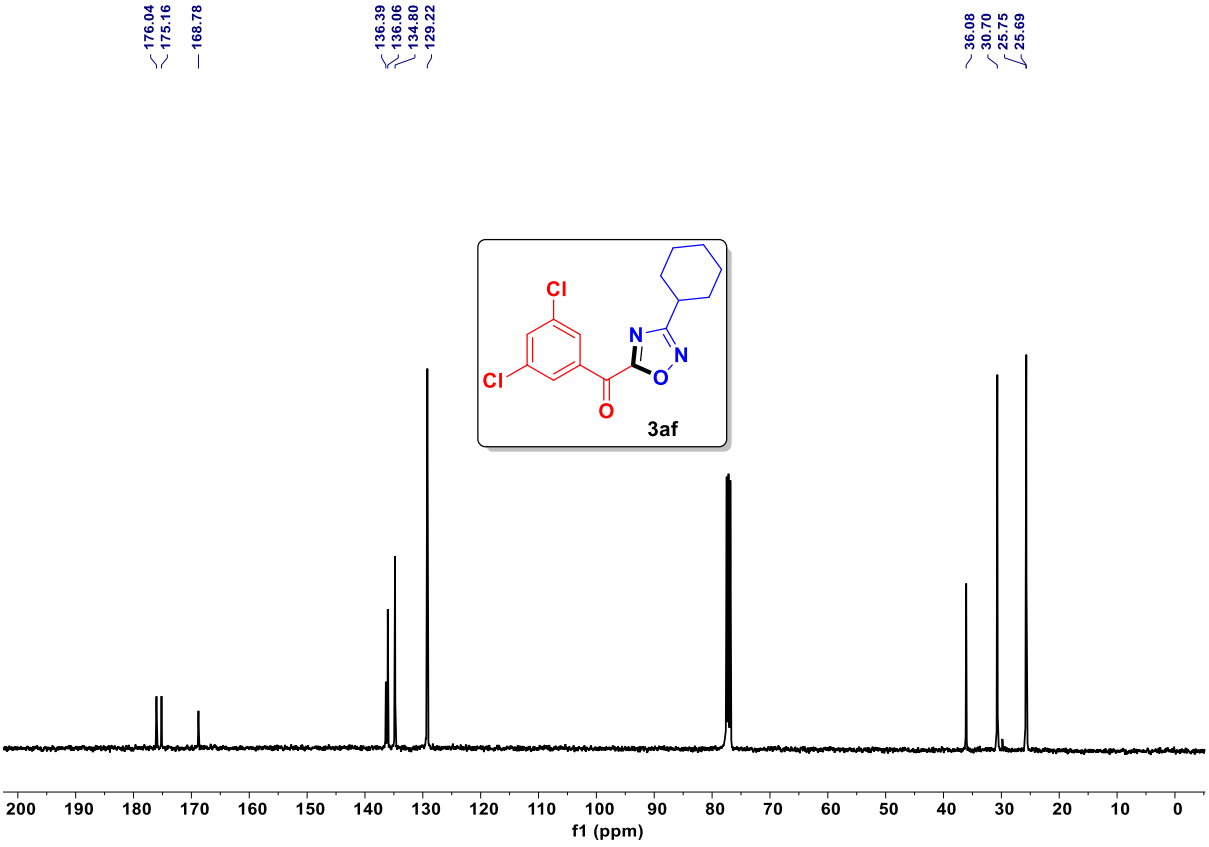


Figure 72. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3af**

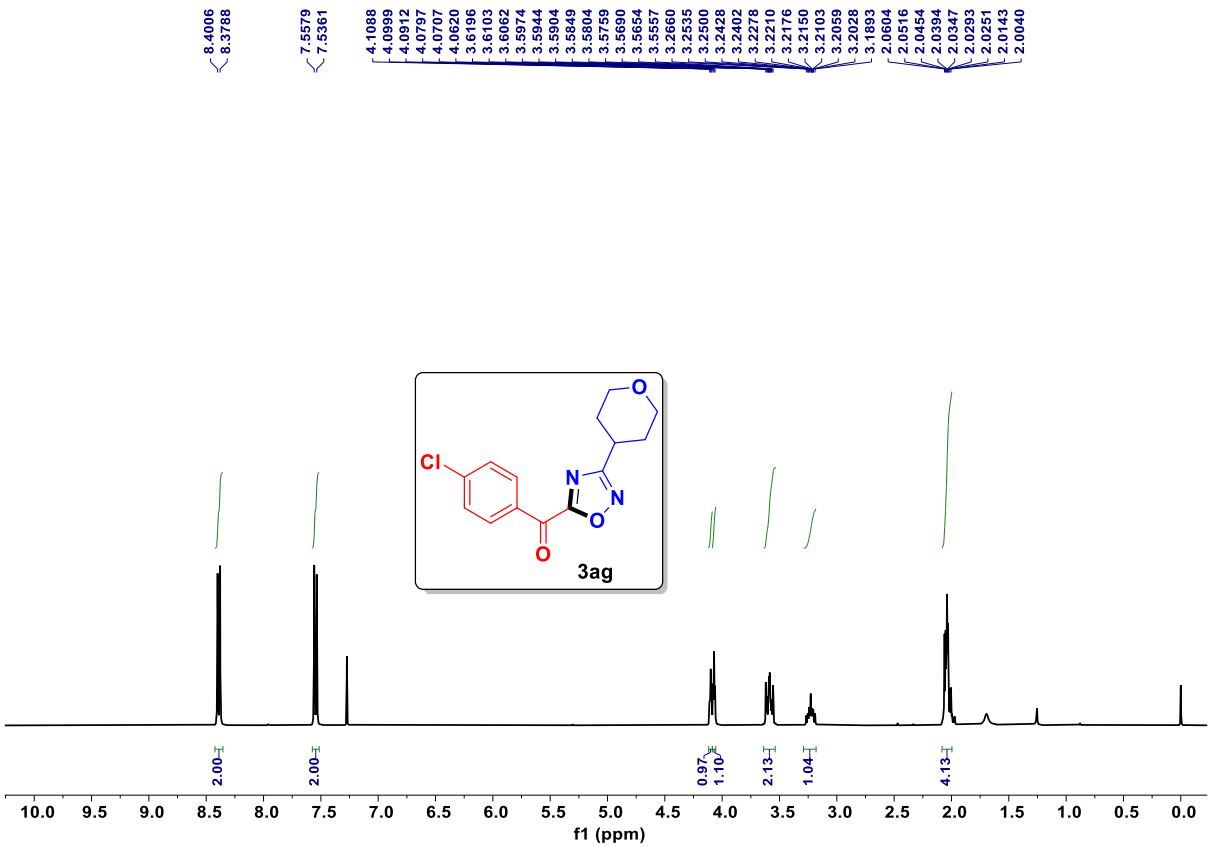


Figure 73. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ag**

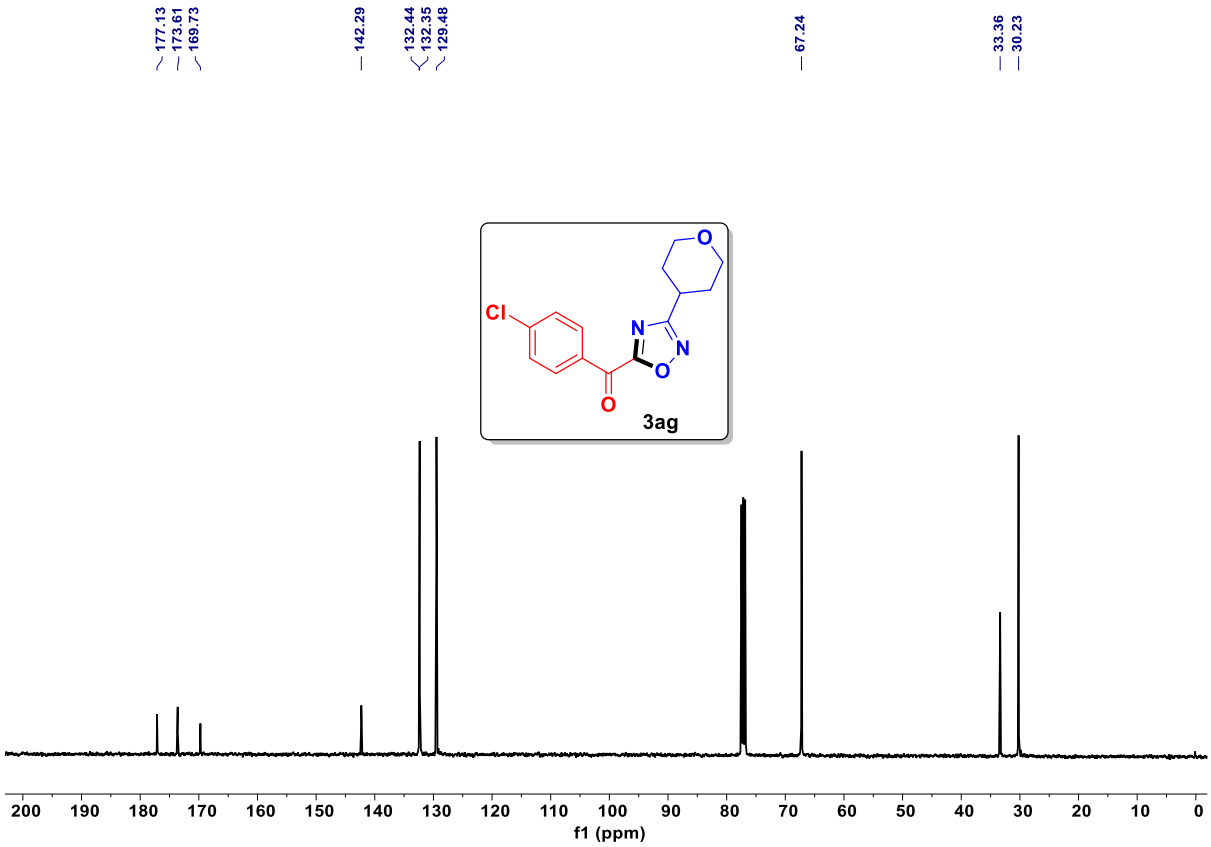


Figure 74. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ag**

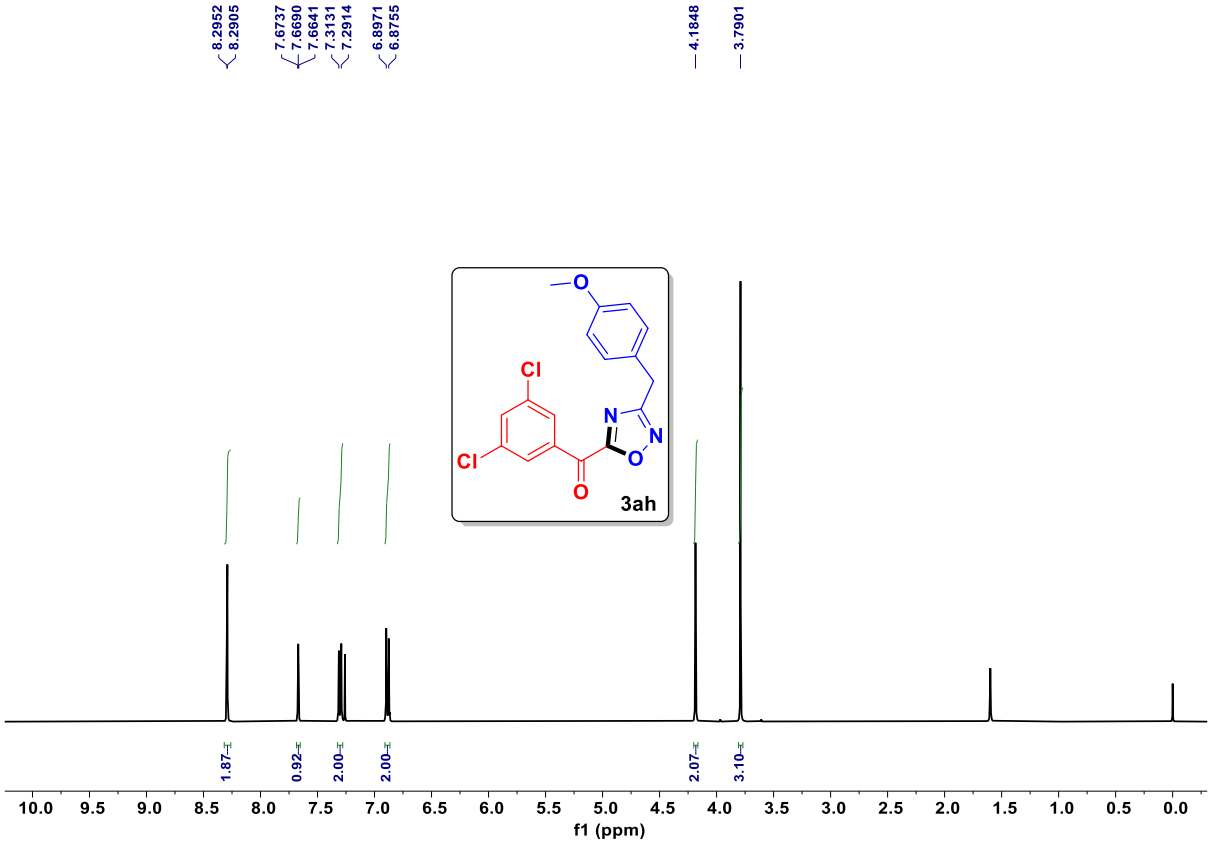


Figure 75. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ah**

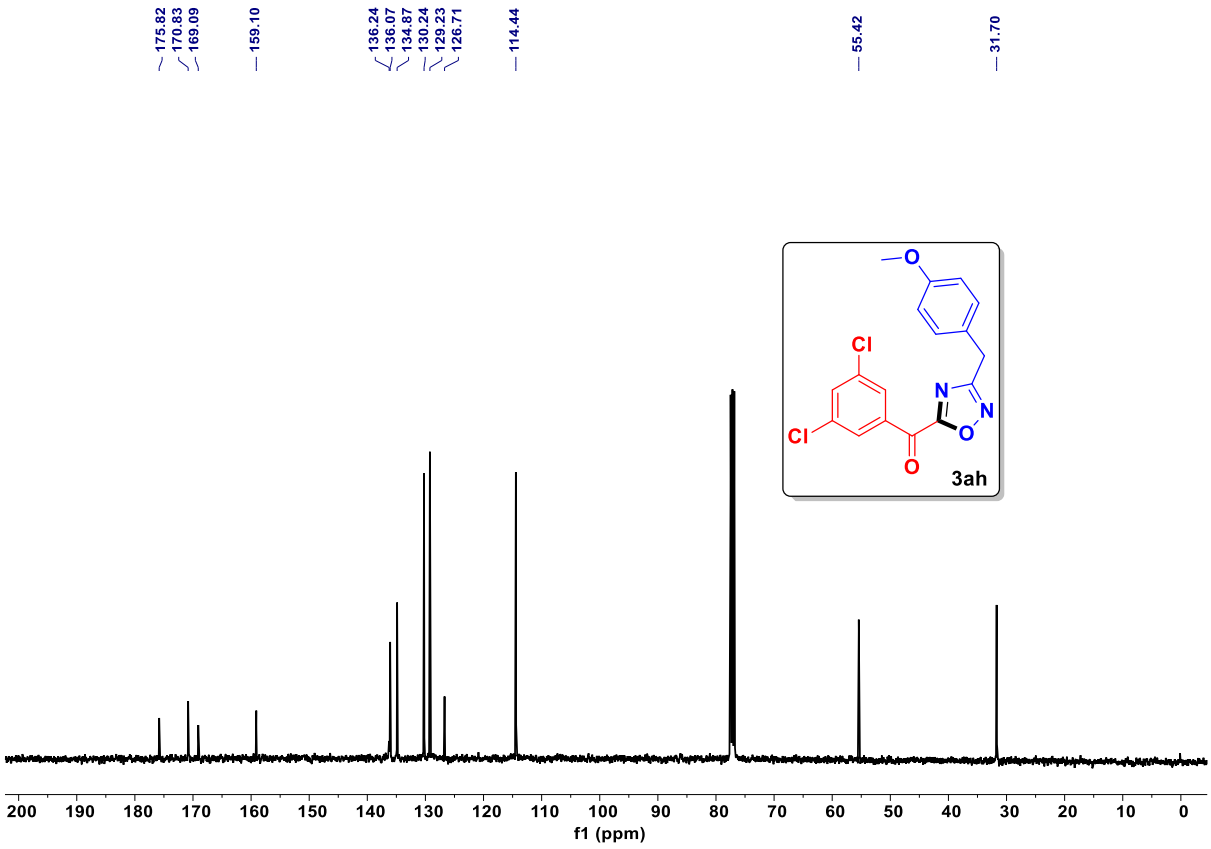


Figure 76. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ah**

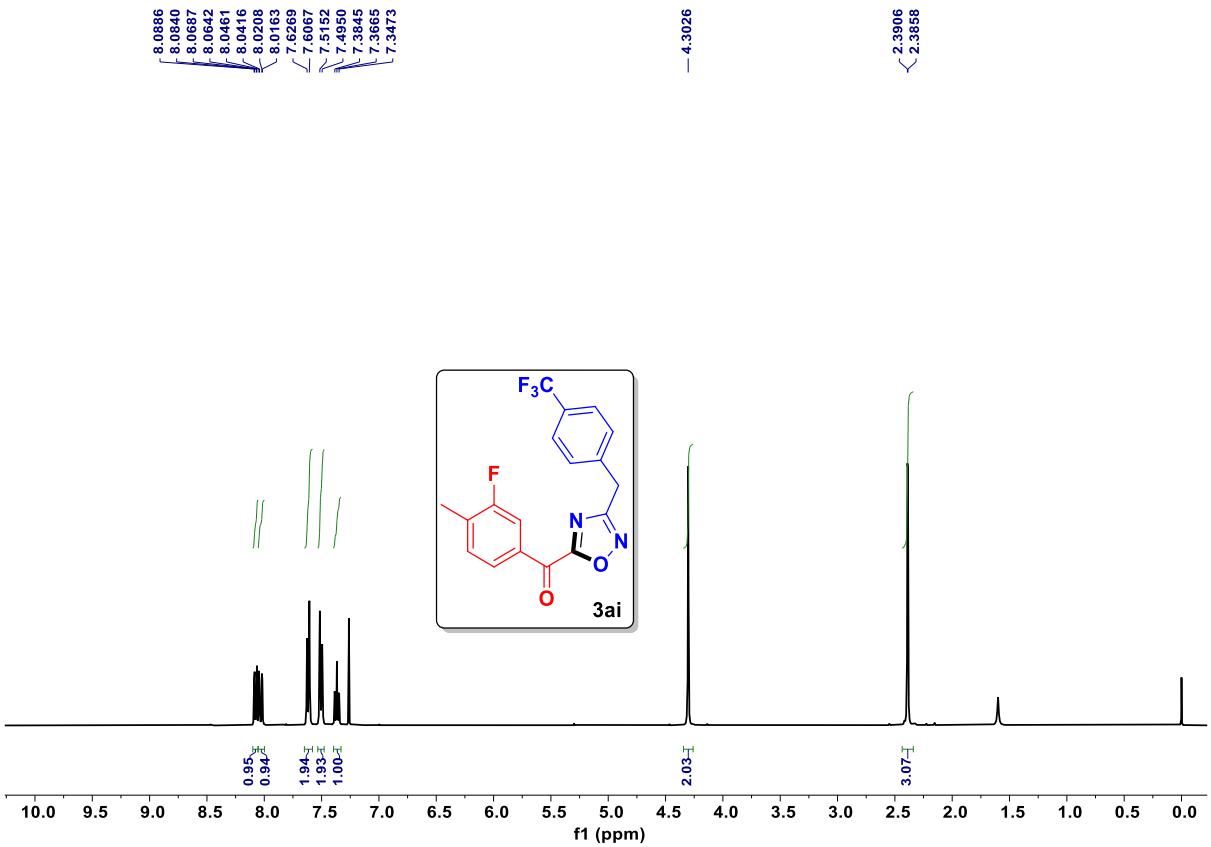


Figure 77. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ai**

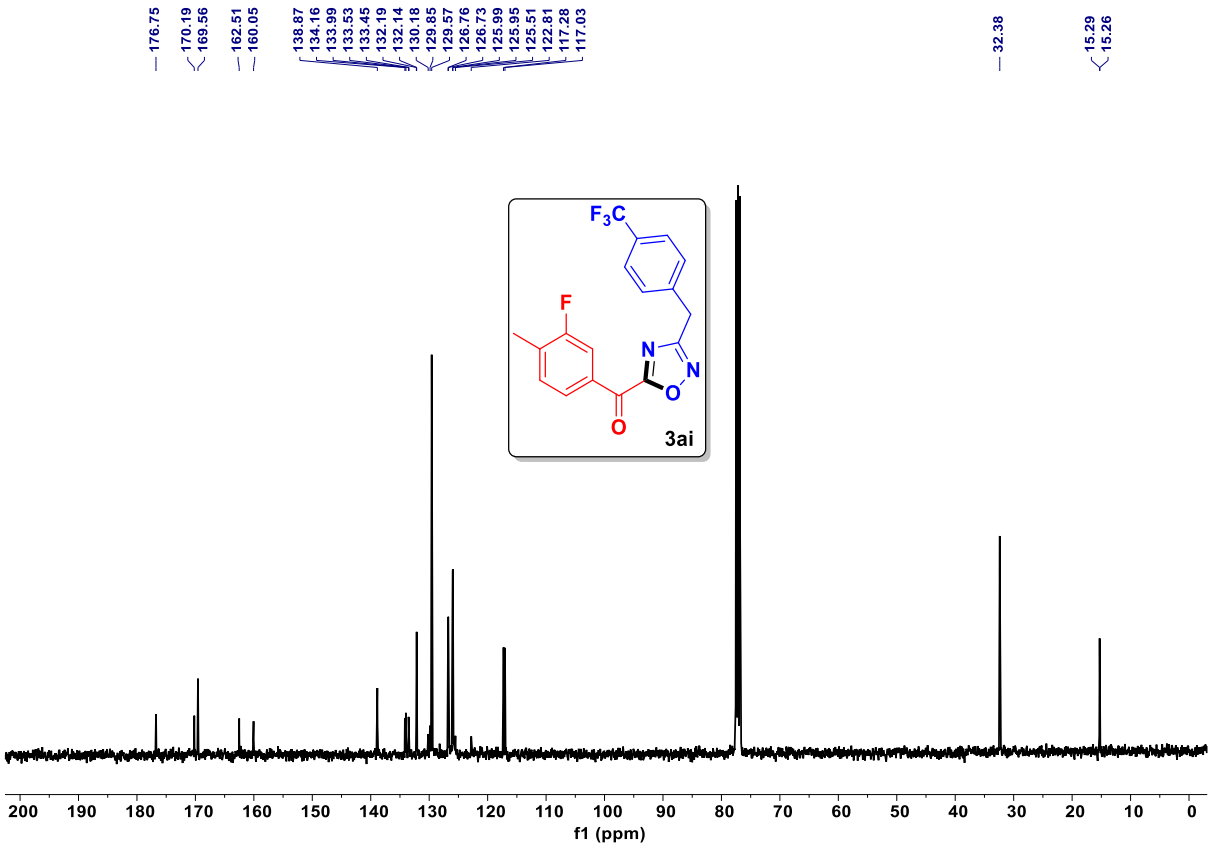


Figure 78. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3ai**

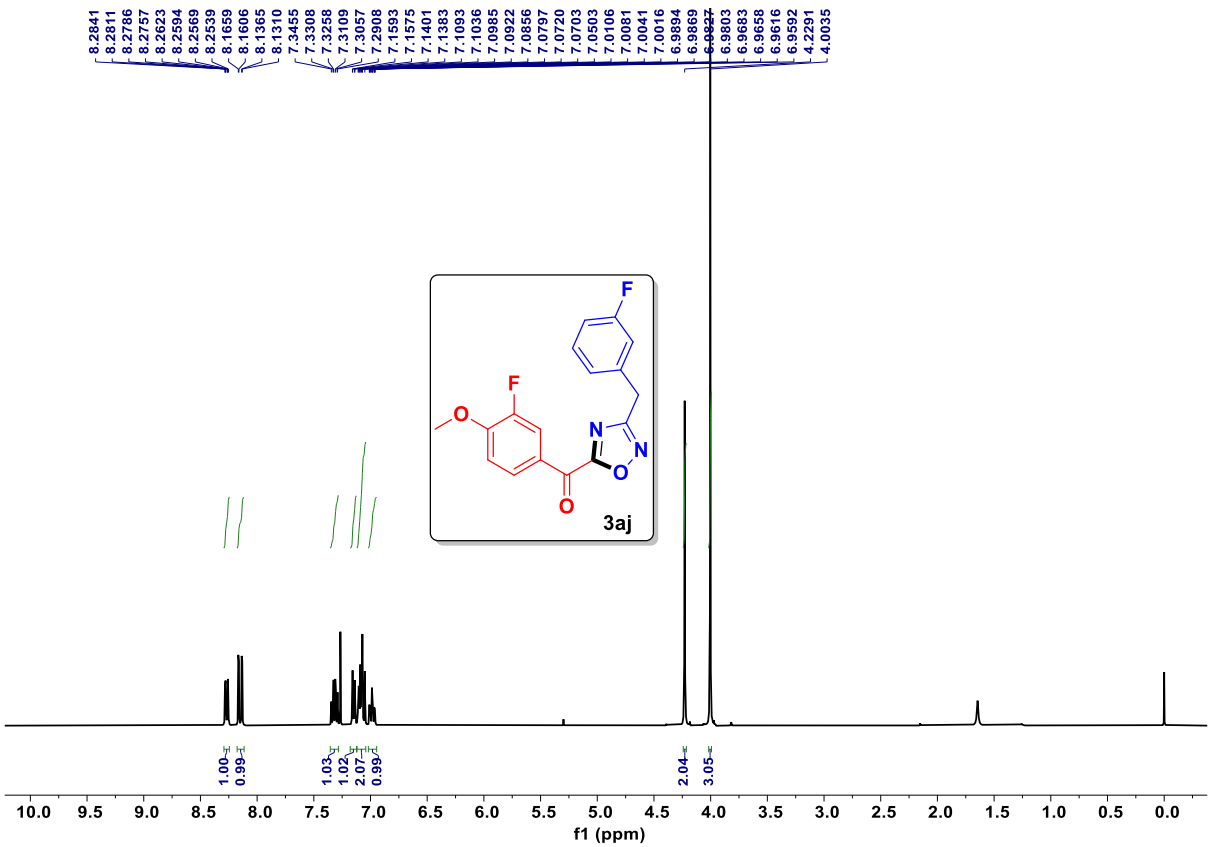


Figure 79. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aj**

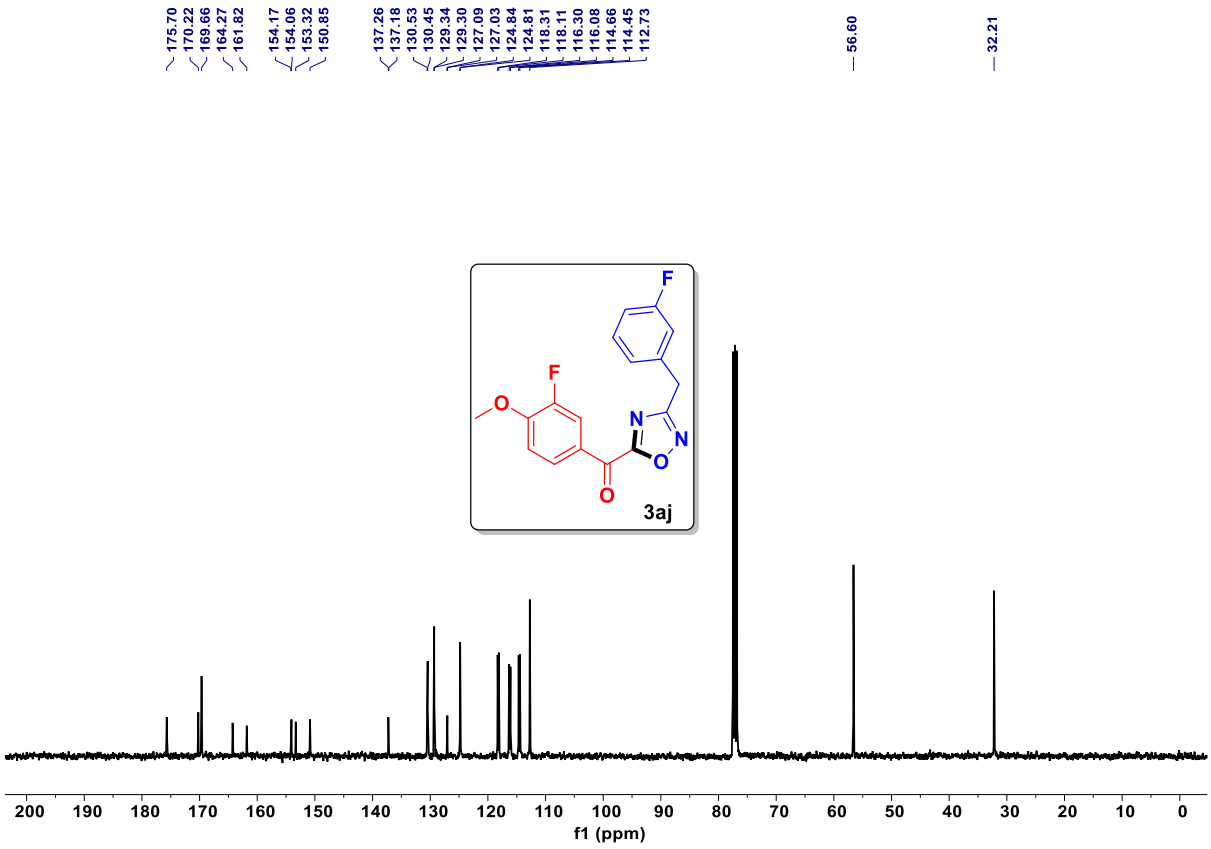


Figure 80. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **3aj**

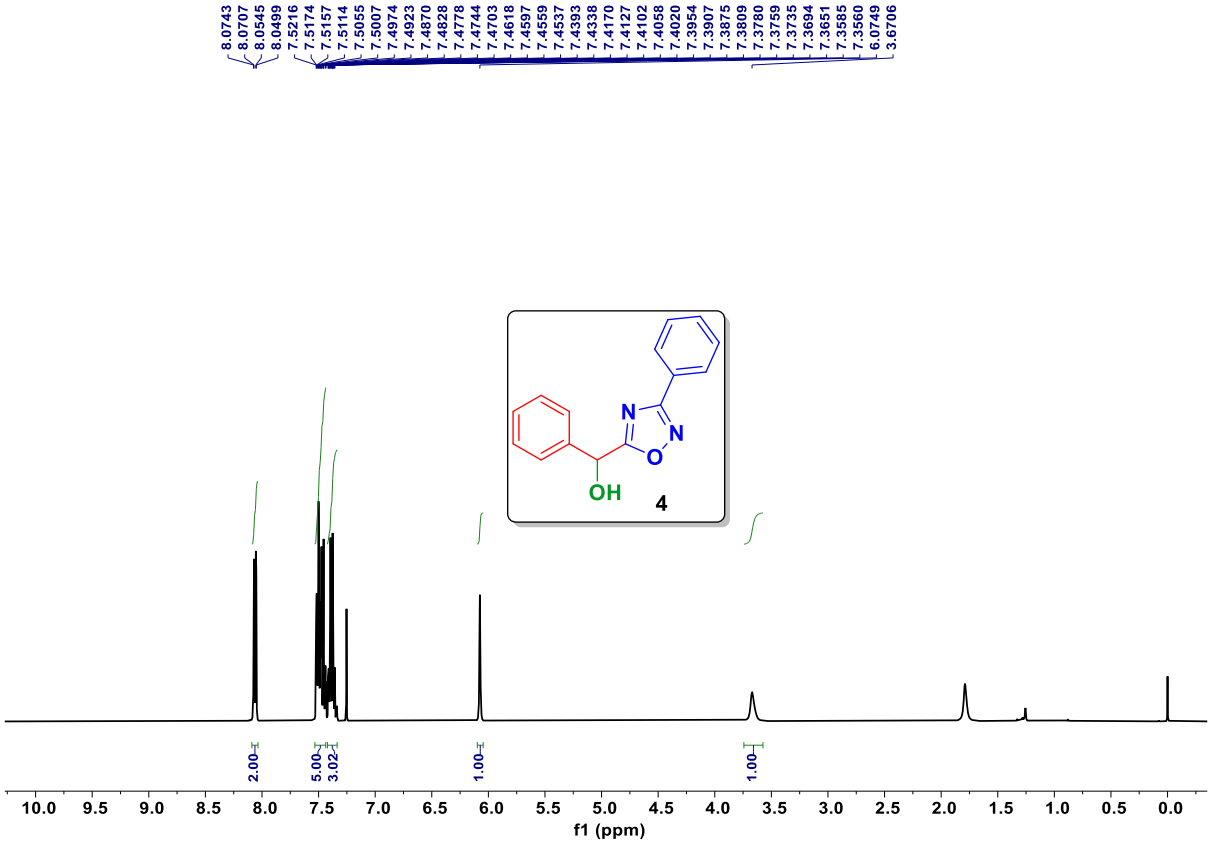


Figure 81. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **4**

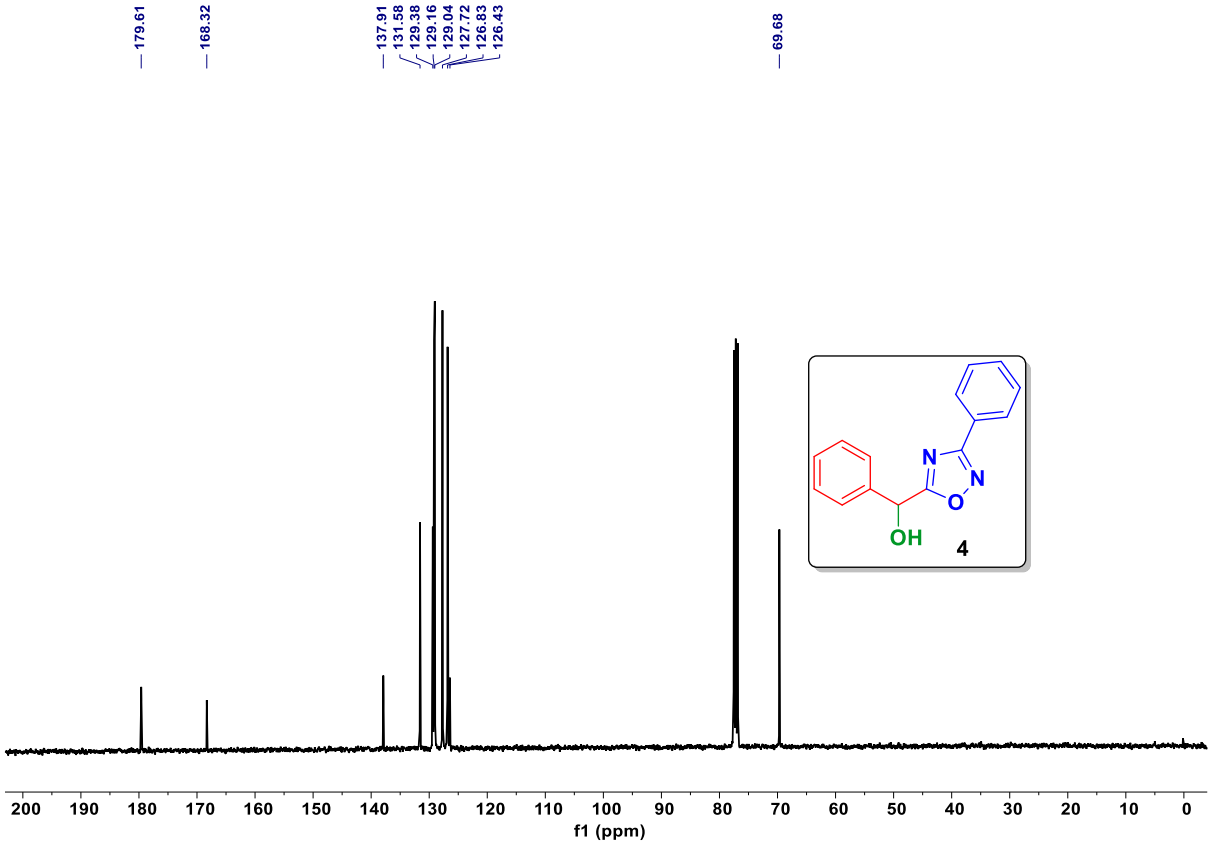


Figure 82. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **4**

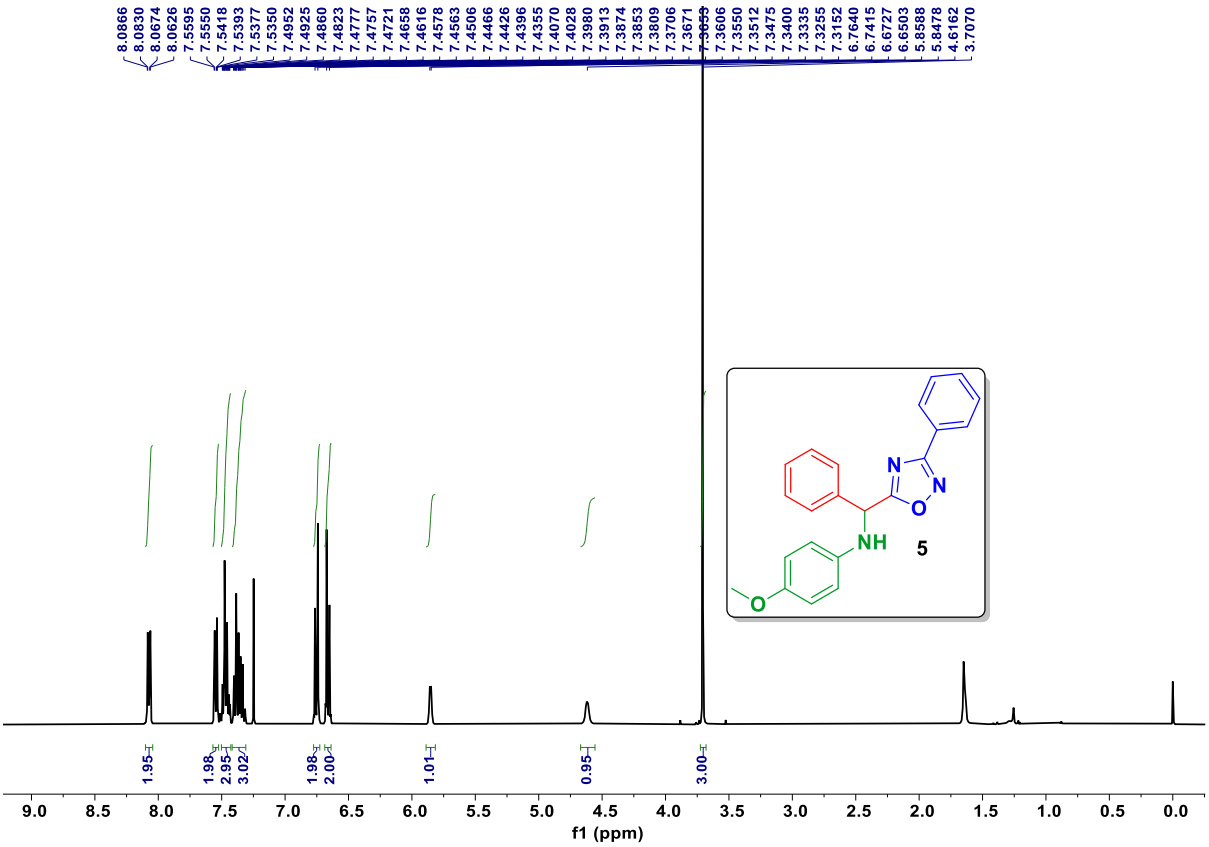


Figure 83. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **5**

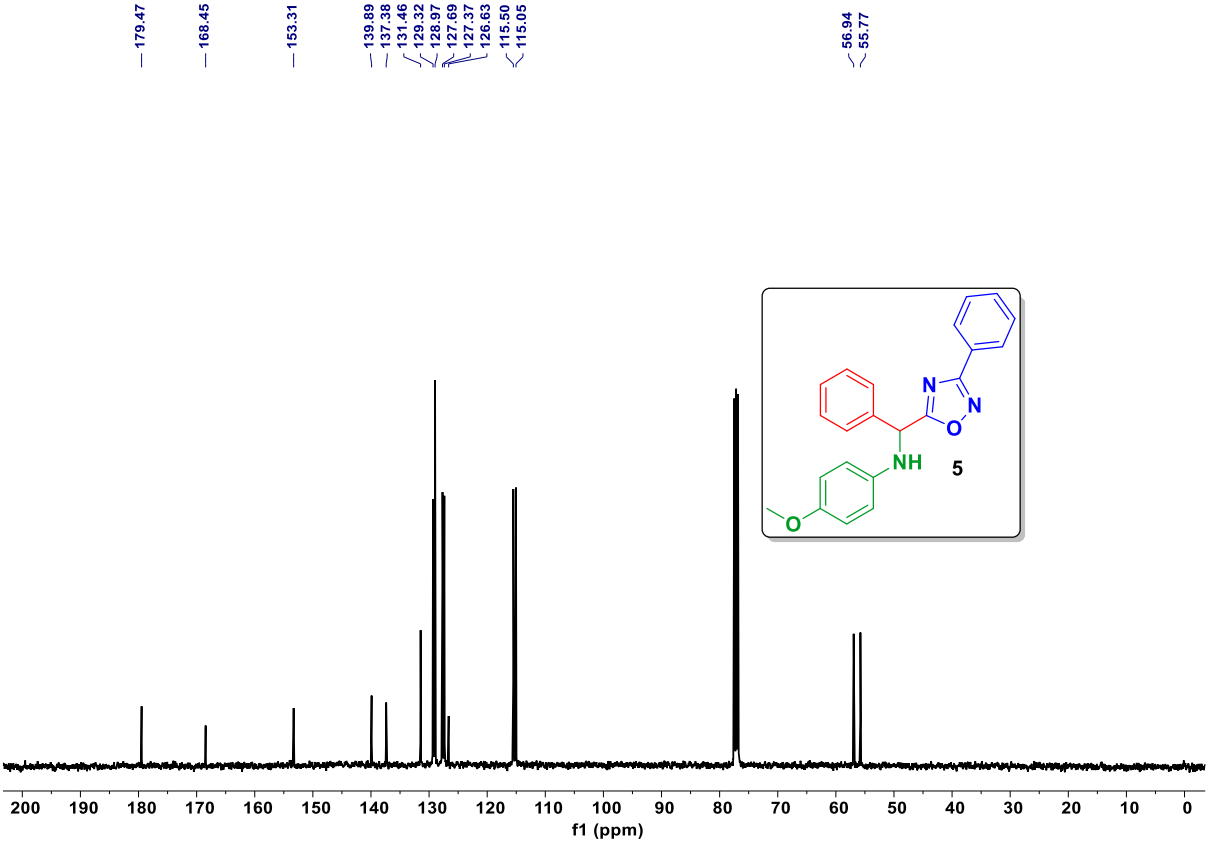


Figure 84. $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$) of compound **5**

X-Ray crystal structure of compound 3y

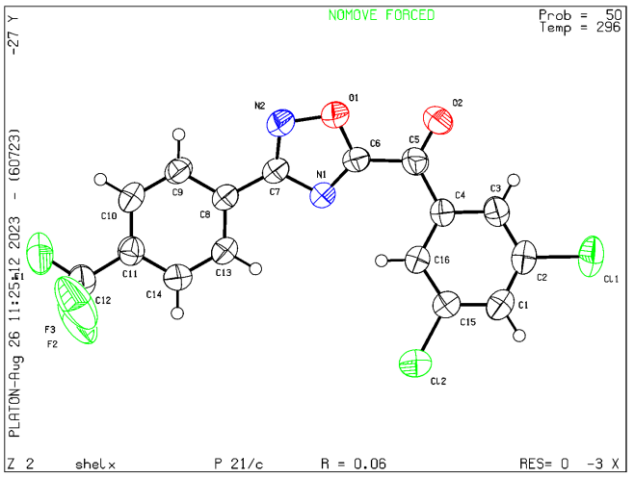


Figure 85. X-Ray crystal structure of compound **3y**

Table 1. Crystal data and structure refinement for 3y

Identification code	shelx
Empirical formula	C16 H7 Cl2 F3 N2 O2
Formula weight	387.14
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 7.6950(5) A alpha = 90 deg. b = 13.3275(11) A beta = 93.638(4) deg. c = 15.5682(14) A gamma = 90 deg.
Volume	1593.4(2) A^3
Z, Calculated density	4, 1.614 Mg/m^3
Absorption coefficient	0.453 mm^-1
F(000)	776
Crystal size	0.500 x 0.400 x 0.300 mm
Theta range for data collection	2.622 to 28.405 deg.
Limiting indices	-10<=h<=9, -16<=k<=17, -20<=l<=19
Reflections collected / unique	17321 / 3971 [R(int) = 0.0347]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.876 and 0.805
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3971 / 0 / 226
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0592, wR2 = 0.1628
R indices (all data)	R1 = 0.1071, wR2 = 0.1949
Extinction coefficient	n/a
Largest diff. peak and hole	0.683 and -0.406 e.A^-3

X-Ray crystal structure of compound 3ag

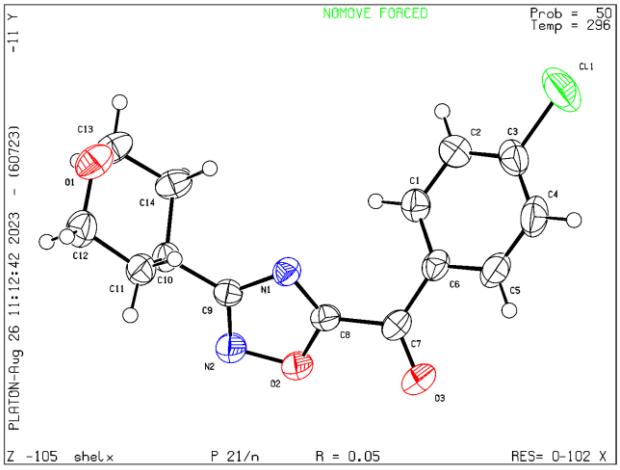


Figure 86. X-Ray crystal structure of compound **3ag**

Table 1. Crystal data and structure refinement for 3ag

Identification code	shelx
Empirical formula	C14 H13 Cl N2 O3
Formula weight	292.71
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 6.9833(6) A alpha = 90 deg. b = 7.9155(7) A beta = 91.509(5) deg. c = 24.658(2) A gamma = 90 deg.
Volume	1362.5(2) A^3
Z, Calculated density	4, 1.427 Mg/m^3
Absorption coefficient	0.289 mm^-1
F(000)	608
Crystal size	0.400 x 0.300 x 0.200 mm
Theta range for data collection	2.703 to 28.381 deg.
Limiting indices	-9<=h<=9, -10<=k<=8, -32<=l<=32
Reflections collected / unique	15969 / 3330 [R(int) = 0.0364]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.944 and 0.893
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3330 / 0 / 181
Goodness-of-fit on F^2	0.990
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.1193
R indices (all data)	R1 = 0.0732, wR2 = 0.1373
Extinction coefficient	n/a
Largest diff. peak and hole	0.232 and -0.401 e.A^-3