Supporting Information

RHODIUM-CATALYZED OXIDATIVE OLEFINATION OF N-(2-(4,5-DIHYDROOXAZOL-2-YL)PHENYL)AMIDES WITH ARYLETHENES VIA EXTRAORDINARY N-ARYL C-H BOND FUNCTIONALIZATION

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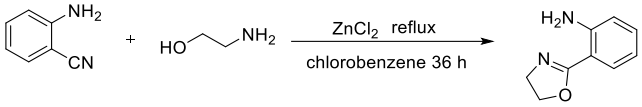
1. General Remarks

Products were purified by flash chromatography on 200-300 mesh silica gels. ^{1}H NMR and ^{13}C NMR spectra were recorded on Mercury 400 MHz in $CDCl_3$ using TMS as internal standard. All ^{1}H NMR and ^{13}C NMR chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All new compounds were further characterized by HRMS. Copies of their ^{1}H NMR and ^{13}CNMR spectra were provided. Commercially available reagents and solvents were used without further purification.

2. Experimental section

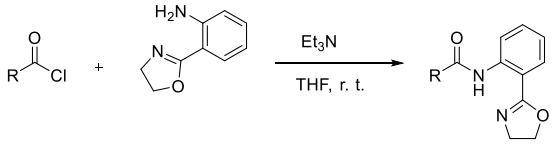
2.1 General procedure for the synthesis of starting materials

2.1.1 Synthesis of 2-(4, 5-dihydrooxazol-2-yl)aniline[1,2].



In a 500mL three-necked flask, 2-aminobenzonitrile (250 mmol) and $ZnCl_2$ (25 mmol) was added and suspended in chlorobenzene (350 mL) under nitrogen. 2-aminoethanol (45 mL, 750 mmol) was added to the suspension via a syringe. The mixture was slowly heated to reflux until no gas was produced. After refluxing for 36 h, the reaction mixture was cooled down to room temperature and the solvent was removed in a rotary evaporator. CH_2Cl_2 (250 mL) was added to the residue and washed with saturated $NaHCO_3$ (150 mL) and H_2O (150 mL). The aqueous fraction was extracted with CH_2Cl_2 (250 mL × 3). The combined organic phase was dried over Na_2SO_4, filtered and the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the compound 2-(4,5-dihydrooxazol-2-yl)aniline.

2.1.2 Preparation of substrates[2,3]



Acid chlorides (5 mmol) prepared from the corresponding carboxylic acid and oxalyl chloride and 2-(4,5-dihydrooxazol-2-yl)aniline (5 mmol) were added to a 50 mL flask and then dissolved with THF (10 mL). Et_3N (7.5 mmol) was taken to the vigorously stirred solution via a syringe. The reaction mixture was stirred at room temperature for 6 h and quenched with saturated $NaHCO_3 \cdot H_2O$ (100 mL) was added to the mixture and extracted with EtOAc (150 mL × 3). Combined organic phase was washed with saturated NaCl (aq) and dried over Na_2SO_4, and then filtered; the solvent was removed in a rotary evaporator. The crude product was recrystallized from EtOAc/Hexane to give colorless crystals of the product.

2.2 Typical procedure for N-aryl oxidative olefination of amide tethered aryl oxazoline

An oven-dried Schlenk tube was charged with N-(2-(4,5-dihydrooxazol-2-yl)phenyl)amides **1** (0.1 mmol), arylethenes **2** (2.0 equiv), $[RhCp^*Cl_2]_2$ (3 mol%), $Cu(OAc)_2$ (2.0 equiv), $AgBF_4$ (0.1 equiv) , then DCE (1 mL) was added to the reaction system. The reaction was stirred at 70 ^oC under air for 10 h (TLC monirored). Upon completion of the reaction, cooling to room temperature, the reaction mixture diluted with ethyl acetate and washed with saturated brine. The combined organic phase was dried over anhydrous Na_2SO_4. After the solvent was evaporated in vacuo, the residues were purified by column chromatography, eluting with PET (petroleum ether)/ EtOAc to afford the desired **3**.

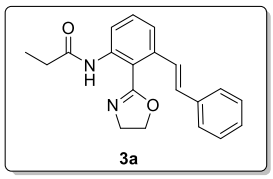
3. References

[1] M. Shang, S. Z. Sun, H.-X Dai, and J. Q. Yu, *J. Am. Chem. Soc.*, **2014**, 136, 3354-3357

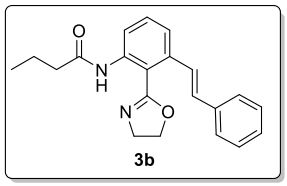
[2] R. Giri, N. L. Maugel, B. M. Foxman, and J. Q. Yu, *Organometallics*, **2008**, 27, 1667

[3] I. G. Dorota, C. Grzegorz, K. W. Agata, T. Piotr, and D. Krystyna, *Eur. J. Med. Chem*. **2013**, 69, 863.

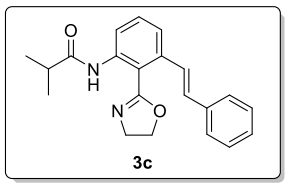
4. Characterization data of products



(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)propionamide (3a): White solid (Yield:78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.11 (s, 1H), 8.52 (d, J = 8.2 Hz, 1H), 7.53-7.44 (m, 3H), 7.41 (d, J = 8.2 Hz, 1H), 7.37-7.34 (m, 3H), 7.28-7.25 (m, 1H), 6.91 (d, J = 16.0 Hz, 1H), 4.44 (t, J = 9.6 Hz, 2H), 4.15 (t, J = 9.6 Hz, 2H), 2.43 (q, J = 7.6 Hz, 2H), 1.25 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.48, 164.75, 138.95, 137.42, 131.32, 130.50, 128.63, 127.70, 126.64, 121.90, 119.79, 111.77, 66.79, 54.24, 31.50, 9.63 ppm; HRMS (ESI) calcd for $C_{20}H_{21}N_2O_2$ $[M+H]^+$: 321.1603; found: 321.1608.

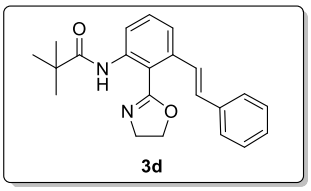


(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)butyramide(3b): White solid (Yield: 74%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.09 (s, 1H), 8.52 (d, J = 8.2 Hz, 1H), 7.53-7.47 (m, 3H), 7.41 (t, J = 8.0 Hz, 1H), 7.37-7.34 (m, 3H), 7.28-7.25 (m, 1H), 6.91 (d, J = 16.0 Hz, 1H), 4.44 (t, J = 9.6 Hz, 2H), 4.15 (t, J = 9.6 Hz, 2H), 2.37 (t, J = 7.6 Hz, 2H), 1.80-1.74 (m, 2H), 1.01 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 171.71, 164.75, 138.95, 137.43, 131.31, 130.50, 128.64, 127.70, 126.64, 121.92, 119.84, 66.79, 54.27, 40.42, 18.96, 13.73; HRMS (ESI) calcd for $C_{21}H_{23}N_2O_2$ $[M+H]^+$: 335.1760; found: 335.1763.



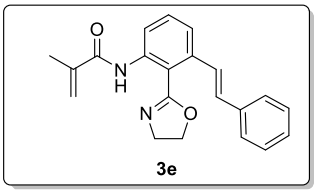
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)isobutyramide (3c): White solid (Yield: 62%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.60 (s, 1H), 8.52 (d, J = 8.4 Hz, 1H), 7.22 (t, J = 8.0 Hz, 1H), 7.14-7.12 (m, 3H), 7.09-7.07 (m, 2H), 6.88 (d, J = 8.0 Hz, 1H), 6.83 (d, J = 12.0 Hz, 1H), 6.52 (d, J = 12.0 Hz, 1H), 4.38 (t, J = 9.6 Hz, 2H), 4.08 (t, J = 9.6 Hz, 2H), 2.62-2.55 (m, 1H), 1.29 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ175.96, 165.19, 139.70, 139.24, 136.58, 131.35, 131.17, 129.19, 128.76,

128.04, 126.94, 125.32, 119.51, 113.73, 66.64, 54.04, 37.44, 19.61 ppm; HRMS (ESI) calcd for $C_{21}H_{23}N_2O_2$ $[M+H]^+$: 335.1760; found: 335.1768.



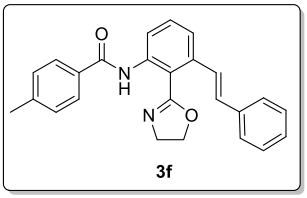
3d

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)pivalamide (3d): White solid (Yield: 72%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.17 (s, 1H), 8.54 (d, J = 8.2 Hz, 1H), 7.51-7.47 (m, 3H), 7.41 (t, J = 8.0 Hz, 1H), 7.37-7.33 (m, 3H), 7.28-7.24 (m, 1H), 6.91 (d, J = 16.0 Hz, 1H), 4.44 (t, J = 9.6 Hz, 2H), 4.14 (t, J = 9.6 Hz, 2H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 177.43, 164.66, 139.15, 138.81, 137.40, 131.24, 130.45, 128.62, 128.46, 127.69, 126.62, 121.70, 119.88, 114.05, 66.81, 54.22, 40.25, 27.61 ppm; HRMS (ESI) calcd for $C_{22}H_{25}N_2O_2$ $[M+H]^+$: 349.1916; found: 349.1910.



3e

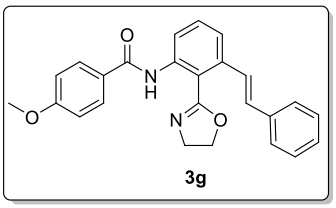
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)methacrylamide (3e): White solid (Yield: 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.59 (s, 1H), 8.61 (dd, J = 8.2, 1.0 Hz, 1H), 7.55-7.42 (m, 4H), 7.38-7.34 (m, 3H), 7.29-7.25 (m, 1H), 6.92 (d, J = 16.0 Hz, 1H), 5.95 (s, 1H), 5.50-5.49 (m, 1H), 4.45 (t, J = 14.4, 2H), 4.15 (t, J = 14.4, 2H), 2.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.53, 164.90, 144.48, 140.90, 139.07, 137.45, 132.00, 131.41, 130.59, 128.67, 127.74, 126.68, 122.13, 120.81, 119.81, 113.90, 104.89, 66.87, 54.23, 18.73 ppm; HRMS (ESI) calcd for $C_{21}H_{21}N_2O_2$ $[M+H]^+$: 333.1603; found: 333.1604.



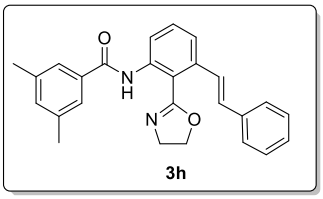
3f

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-4-methylbenzamide (3f): White solid (Yield: 84%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.10 (s, 1H), 8.72 (dd, J = 8.4, 0.8 Hz, 1H), 7.91 (d, J = 8.2 Hz, 2H), 7.57 (d, J = 16.0 Hz, 1H), 7.51-7.48 (m, 3H), 7.40-7.35 (m, 3H), 7.31-7.25 (m, 3H), 6.93 (d, J = 16.0 Hz, 1H), 4.46 (t, J = 9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.54, 165.17, 142.17, 139.42, 139.18, 137.50, 132.46, 131.50, 130.59, 129.33, 128.80,

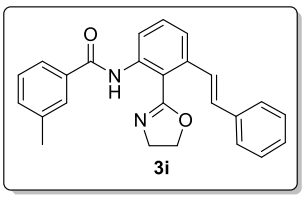
128.68, 127.74, 127.47, 126.70, 122.17, 119.95, 113.87. 66.89, 54.23, 21.49; HRMS (ESI) calcd for $C_{25}H_{23}N_2O_2$ $[M+H]^+$: 383.1760; found: 383.1763.



(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-4-methoxybenzamide (3g): White solid (Yield: 68%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.08 (s, 1H), 8.71 (dd, J = 8.2, 0.8 Hz, 1H), 8.00-7.97 (m, 2H), 7.57 (d, J = 16.0 Hz, 1H), 7.51-7.45 (m, 3H), 7.38-7.35 (m, 3H), 7.27-7.25 (m, 1H), 7.00-6.98 (m, 2H), 6.93 (d, J = 16.0 Hz, 1H), 4.48 (t, J = 9.6 Hz, 2H), 4.20 (t, J = 9.6 Hz, 2H), 3.87 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.21, 162.38, 139.50, 139.16, 137.48, 131.49, 130.52, 129.31, 128.83, 128.67, 127.72, 127.54, 126.68, 122.06, 119.89, 113.83, 113.75, 66.87, 55.41, 54.21 ppm; HRMS (ESI) calcd for $C_{25}H_{23}N_2O_3$ $[M+H]^+$: 399.1709; found: 399.1714.

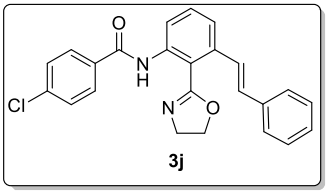


(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-3,5-dimethylbenzamide (3h): White solid (Yield: 81%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.06 (s, 1H), 8.73 (dd, J = 8.3, 0.8 Hz, 1H), 7.63 (s, 2H), 7.57 (d, J = 16.0 Hz, 1H), 7.51-7.46 (m, 3H), 7.40-7.35 (m, 3H), 7.29-7.25 (m, 1H), 7.17 (s, 1H), 6.93 (d, J = 16.0 Hz, 1H), 4.47 (t, J = 9.6 Hz, 2H), 4.21 (t, J = 9.6 Hz, 2H), 2.40 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.88, 165.14, 139.40，139.17, 138.22, 137.49, 135.22, 133.27, 131.52, 130.62, 128.75, 128.68, 127.74, 126.70, 125.33, 122.15, 119.89, 113.88, 66.90, 54.15, 21.35 ppm; HRMS (ESI) calcd for $C_{26}H_{25}N_2O_2$ $[M+H]^+$: 397.1916; found: 397.1914.



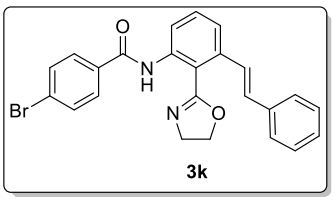
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-3-methylbenzamide (3i): White solid (Yield: 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.13 (s, 1H), 8.74 (d, J = 8.0 Hz, 1H), 7.84-7.79 (m, 2H), 7.57 (d, J = 16.0 Hz, 1H), 7.50-7.46 (m, 3H), 7.40-7.38 (m, 2H), 7.36-7.33 (m, 3H), 7.29-7.25 (m, 1H), 6.92 (d, J = 16.0 Hz, 1H), 4.46 (t, J = 9.6, 2H), 4.19 (t, J = 9.6 Hz, 2H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.69,

165.14, 139.36, 139.20, 138.38, 137.47, 135.21, 132.41, 131.50, 130.61, 128.76, 128.67, 128.49, 128.31, 127.74, 126.68, 124.38, 122.22, 119.90, 113.86, 66.89, 54.16, 21.45 ppm; HRMS (ESI) calcd for $C_{25}H_{23}N_2O_2$ $[M+H]^+$: 383.1760; found: 383.1768.



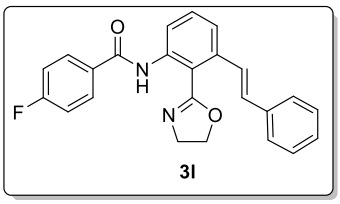
3j

(*E*)-4-chloro-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)benzamide (3j): White solid (Yield: 63%). ^{1}H NMR (400 MHz,) δ 12.35 (s, 1H), 8.71 (dd, J = 8.2, 0.8 Hz, 1H), 7.97-7.95 (m, 2H), 7.59 (d, J = 16.0 Hz, 1H), 7.51-7.48 (m, 3H), 7.47-7.46 (m, 1H), 7.41-7.35 (m, 3H), 7.30-7.25 (m, 1H), 6.92 (d, J = 16.0 Hz, 1H), 4.47 (t, J = 9.6 Hz, 2H), 4.18 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.49, 139.44, 139.28, 137.97, 137.46, 133.73, 131.62, 130.75, 128.90, 128.70, 127.80, 126.71, 122.61, 119.84, 113.66, 66.93, 54.10; HRMS (ESI) calcd for $C_{24}H_{20}ClN_2O_2$ $[M+H]^+$: 403.1213; found: 403.1212.



3k

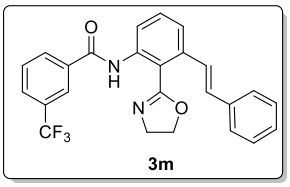
(*E*)-4-bromo-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)benzamide (3k): White solid (Yield: 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.37 (s, 1H), 8.71 (dd, J = 8.2, 0.8 Hz, 1H), 7.90-7.88 (m, 2H), 7.85-7.57 (m, 3H), 7.51-7.47 (m, 3H), 7.41-7.35 (m, 3H), 7.30-7.26 (m, 1H), 6.92 (d, J = 16.0 Hz, 1H), 4.47 (t, J = 9.6 Hz, 2H), 4.18 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.59, 139.42, 139.25, 137.43, 134.17, 131.87, 131.63, 130.73, 129.08, 128.84, 128.70, 127.80, 126.71, 126.48, 122.62, 119.82, 113.63, 102.75, 66.93, 54.09 ppm; HRMS (ESI) calcd for $C_{24}H_{20}BrN_2O_2$ $[M+H]^+$: 447.0708; found: 447.0709.



3l

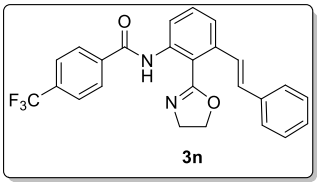
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-4-fluorobenzamide (3l): White solid (Yield: 65%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.29 (s, 1H), 8.71 (d, J = 8.0 Hz, 1H), 8.05-8.02 (m, 2H), 7.59 (d, J = 16.0 Hz, 1H), 7.51-7.47 (m, 3H), 7.41-7.35 (m, 3H), 7.30-7.28 (m, 1H), 7.18 (t, J = 8.0 Hz, 2H), 6.93 (d, J = 16.0 Hz, 1H), 4.48 (t, J =

9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.39, 164.47, 139.39, 137.47, 131.61, 130.71, 129.88, 129.79, 128.86, 128.70, 127.79, 126.71, 122.50, 119.85, 115.78, 115.56, 113.68, 66.91, 54.14 ppm; HRMS (ESI) calcd for $C_{24}H_{20}FN_2O_2$ $[M+H]^+$: 387.1509; found: 387.1506.



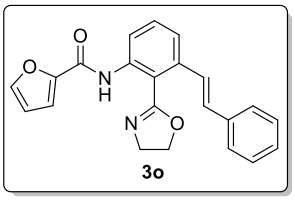
3m

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-3-(trifluoromethyl)benzamide (3m): White solid (Yield: 61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, J = 8.0 Hz, 1H), 8.33 (s, 1H), 8.25 (d, J = 8.0 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.64-7.60 (m, 2H), 7.51-7.48 (m, 3H), 7.41-7.35 (m, 3H), 7.30-7.25 (m, 1H), 6.91 (d, J = 16.0 Hz, 1H), 4.49 (t, J = 9.6 Hz, 2H), 4.21 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.54, 163.93, 139.59, 139.32, 137.41, 136.05, 131.73, 131.16, 130.76, 129.34, 128.96, 128.69, 128.17, 127.80, 126.70, 124.22, 122.85, 119.58, 113.35, 66.97, 53.76 ppm; HRMS (ESI) calcd for $C_{25}H_{20}F_3N_2O_2$ $[M+H]^+$: 437.1477; found: 437.1472.



3n

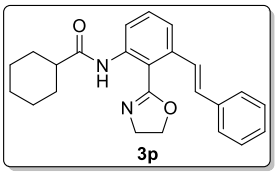
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)-4-(trifluoromethyl)benzamide (3n): White solid (Yield: 65%).^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (dd, J = 8.4, 1.0 Hz, 1H), 8.14 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H), 7.61 (d, J = 16.0 Hz, 1H), 7.52-7.49 (m, 3H), 7.43-7.36 (m, 3H), 7.30-7.25 (m, 1H), 6.92 (d, J = 16.0 Hz, 1H), 4.48 (t, J = 9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.48, 164.18, 139.57, 139.18, 138.61, 137.43, 131.69, 130.85, 128.86, 128.71, 127.93, 127.84, 126.72, 125.66, 122.90, 119.83, 113.64, 66.95, 54.06 (s) ppm; HRMS (ESI) calcd for $C_{25}H_{20}F_3N_2O_2$ $[M+H]^+$: 437.1477; found: 437.1478.



3o

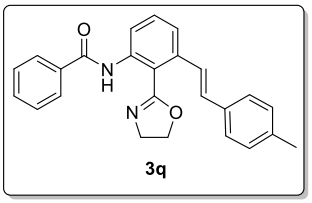
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)furan-2-carboxamide (3o): White solid (Yield: 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.85 (s, 1H), 8.62 (dd, J = 8.0, 1.0 Hz, 1H), 7.55-7.54 (m, 1H), 7.51-7.49 (m, 3H), 7.45 (d, J = 8.0 Hz, 1H), 7.41 -7.34 (m, 3H), 7.29-7.25 (m, 1H), 7.21 (dd, J = 3.6, 0.8 Hz, 1H), 6.95 (d, J = 16.0 Hz, 1H), 6.54 (dd, J = 3.6, 1.8 Hz, 1H), 4.48 (t, J = 9.6 Hz, 2H), 4.23 (t, J = 9.6 Hz, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.50, 156.49, 148.54, 144.49, 138.97, 138.42, 137.41, 131.36, 130.77, 128.67, 128.30, 127.78, 126.71, 122.17, 119.99, 114.87, 114.44, 112.24, 67.01, 54.38; HRMS (ESI) calcd for $C_{22}H_{19}N_2O_3$ $[M+H]^+$: 359.1396; found: 359.1393.



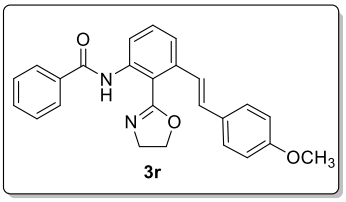
3p

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-styrylphenyl)cyclohexanecarboxamide (3p): White solid (Yield: 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 11.03 (s, 1H), 8.52 (d, J = 8.0 Hz, 1H), 7.52-7.47 (m, 3H), 7.40 (t, J = 8.0 Hz, 1H), 7.37-7.33 (m, 3H), 7.28-7.24 (m, 1H), 6.91 (d, J = 16.0 Hz, 1H), 4.44 (t, J = 9.6 Hz, 2H), 4.16 (t, J = 9.6 Hz, 2H), 2.31-2.25 (m, 1H), 2.02-1.98 (m, 2H), 1.86-1.81 (m, 2H), 1.73-1.69 (m, 1H), 1.55-1.52 (m, 2H), 1.39-1.24 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) : δ 174.84, 164.70, 139.04, 138.87, 137.43, 131.26, 130.47, 128.62, 128.55, 127.68, 126.63, 121.78, 119.95, 113.87, 66.79, 54.29, 47.04, 29.62, 25.81, 25.73; HRMS (ESI) calcd for $C_{24}H_{27}N_2O_2$ $[M+H]^+$: 375.2073; found: 375.2069.



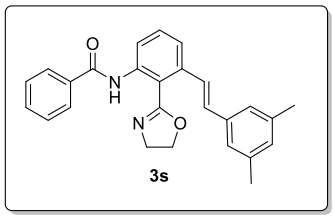
3q

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-(4-methylstyryl)phenyl)benzamide (3q): White solid (Yield: 70%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.16 (s, 1H), 8.71 (d, J = 8.0 Hz, 1H), 8.03-8.01 (m, 2H), 7.54-7.52 (m, 2H), 7.50-7.46 (m, 3H), 7.41-7.39 (m, 3H), 7.17 (d, J = 8.0 Hz, 2H), 6.91 (d, J = 16.0 Hz, 1H), 4.45 (t, J = 9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.50, 165.21, 139.39, 139.26, 137.70, 135.26, 134.70, 131.68, 131.48, 130.60, 129.39, 128.63, 127.73, 127.44, 126.62, 122.25, 119.76, 113.86, 66.88, 54.20, 21.25; HRMS (ESI) calcd for $C_{25}H_{23}N_2O_2$ $[M+H]^+$: 383.1760; found: 383.1764..



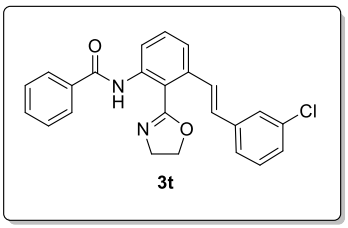
3r

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-(4-methoxystyryl)phenyl)benzamide (3r): White solid (Yield: 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.12 (s, 1H), 8.70 (d, J = 7.8 Hz, 1H), 8.03-8.01 (m, 2H), 7.55-7.52 (m, 2H), 7.50-7.48 (m, 2H), 7.46-7.42 (m, 3H), 7.39 (d, J = 7.8 Hz, 1H), 6.92-6.88 (m, 3H), 4.47 (t, J = 9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.50, 165.25, 159.44, 139.49, 139.24, 135.29, 131.68, 131.47, 130.24, 128.64, 127.94, 127.45, 126.57, 122.12, 119.63, 114.15, 113.84, 66.90, 55.33, 54.22 ppm; HRMS (ESI) calcd for $C_{25}H_{23}N_2O_3$ $[M+H]^+$: 399.1709; found: 399.1705.



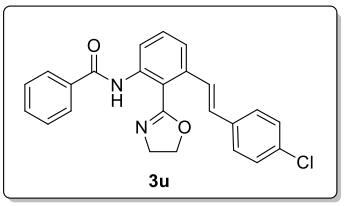
3s

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-(3,5-dimethylstyryl)phenyl)benzamide (3s): White solid (Yield: 59%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.19 (s, 1H), 8.74 (dd, J = 8.4, 1.0 Hz, 1H), 8.04-8.01 (m, 2H), 7.56-7.51 (m, 2H), 7.50-7.47 (m, 2H), 7.46-7.37 (m, 3H), 7.12-7.07 (m, 2H), 7.02 -7.00 (m, 1H), 4.45 (t, J = 9.8 Hz, 2H), 4.19 (t, J = 9.8 Hz, 2H), 2.39 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.51, 165.23, 139.72, 139.29, 136.28, 135.43, 135.26, 132.96, 131.68, 131.49, 130.35, 129.79, 128.73, 128.62, 128.45, 127.44, 126.33, 122.57, 119.83, 113.90, 66.89, 54.18, 21.12, 19.45 ppm; HRMS (ESI) calcd for $C_{26}H_{25}N_2O_2$ $[M+H]^+$: 397.1916; found: 397.1910.



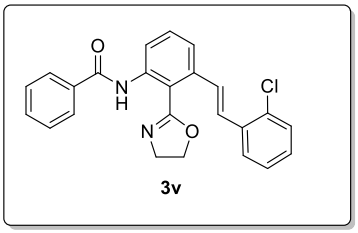
3t

(*E*)-N-(3-(3-chlorostyryl)-2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide （3t）: White solid (Yield: 86%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.25 (s, 1H), 8.76 (d, J = 8.4 Hz, 1H), 8.03-8.01 (m, 2H), 7.60-7.51 (m, 3H), 7.50-7.47 (m, 3H), 7.37-7.34 (m, 2H), 7.29 (t, J = 7.6 Hz, 1H), 7.25-7.23 (m, 1H), 6.84 (d, J = 16.0 Hz, 1H), 4.47 (t, J = 9.6 Hz, 2H), 4.20 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 165.57, 165.02, 139.48, 139.38, 138.75, 135.20, 134.62, 131.73, 131.59, 130.36, 129.88, 129.13, 128.64, 127.62, 127.46, 126.43, 125.00, 122.38, 120.28, 113.86, 66.96, 54.20 ppm; HRMS (ESI) calcd for $C_{24}H_{20}ClN_2O_2$ $[M+H]^+$: 403.1213; found: 403.1218.



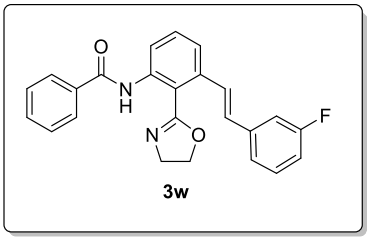
3u

(*E*)-N-(3-(4-chlorostyryl)-2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (3u): White solid (Yield: 67%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.21 (s, 1H), 8.75 (d, J = 8.2 Hz, 1H), 8.03-8.01 (m, 2H), 7.57-7.51 (m, 3H), 7.50-7.47 (m, 2H), 7.43-7.40 (m, 2H), 7.38-7.32 (m, 3H), 6.87 (d, J = 16.0 Hz, 1H), 4.46 (t, J = 9.6 Hz, 2H), 4.20 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.55, 165.09, 139.44, 138.99, 135.55, 135.23, 133.54, 131.71, 131.61, 131.39, 129.85, 128.64, 127.46, 126.89, 126.73, 122.78, 120.27, 113.87, 66.91, 54.21 ppm; HRMS (ESI) calcd for $C_{24}H_{20}ClN_2O_2$ $[M+H]^+$: 403.1213; found: 403.1215.



3v

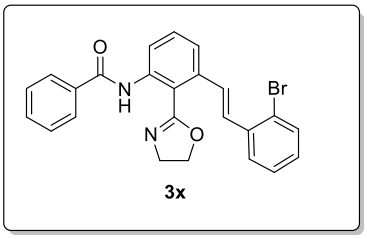
(*E*)-N-(3-(2-chlorostyryl)-2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (3v): White solid (Yield: 75%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.24 (s, 1H), 8.77 (dd, J = 8.4, 1.0 Hz, 1H), 8.03-8.01 (m, 2H), 7.66-7.63 (m, 1H), 7.59-7.51 (m, 2H), 7.50-7.48 (m, 3H), 7.43-7.38 (m, 2H), 7.32-7.25 (m, 2H), 7.23-7.20 (m, 1H), 4.46 (t, J = 9.8 Hz, 2H), 4.19 (t, J = 9.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.55, 165.09, 139.44, 138.99, 135.55, 135.23, 133.54, 131.71, 131.61, 131.39, 129.85, 128.64, 127.46, 126.89, 126.73, 122.78, 120.27, 113.87, 66.91, 54.21 ppm; HRMS (ESI) calcd for $C_{24}H_{20}ClN_2O_2$ $[M+H]^+$: 403.1213; found: 403.1211.



3w

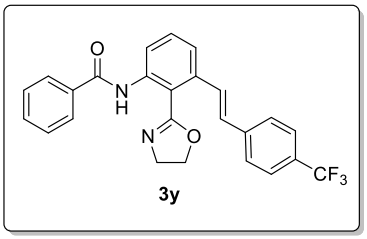
(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-(3-fluorostyryl)phenyl)benzamide (3w): White solid (Yield: 85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.24 (s, 1H), 8.76 (dd, J = 8.4, 1.0 Hz, 1H), 8.03-8.01 (m, 2H), 7.61-7.57 (m, 1H), 7.55-7.51 (m, 2H), 7.50-7.48 (m, 2H), 7.38-7.33 (m, 1H), 7.31-7.29 (m, 1H), 7.26-7.18 (m, 2H), 6.97 (td, J = 3.4, 1.0 Hz, 1H), 6.88 (d, J = 16.0 Hz, 1H), 4.48 (t, J = 9.6 Hz, 2H), 4.20 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.58, 165.05, 164.39, 161.95, 139.90, 139.48, ,

138.77, 135.22, 131.74, 131.60, 130.22, 130.17, 130.08, 129.40, 128.65, 127.47, 122.79, 122.37, 120.28, 114.64, 114.42, 113.90, 112.94, 112.73, 66.95, 54.21 ppm; HRMS (ESI) calcd for $C_{24}H_{20}FN_2O_2$ $[M+H]^+$: 387.1509; found: 387.1503.



3x

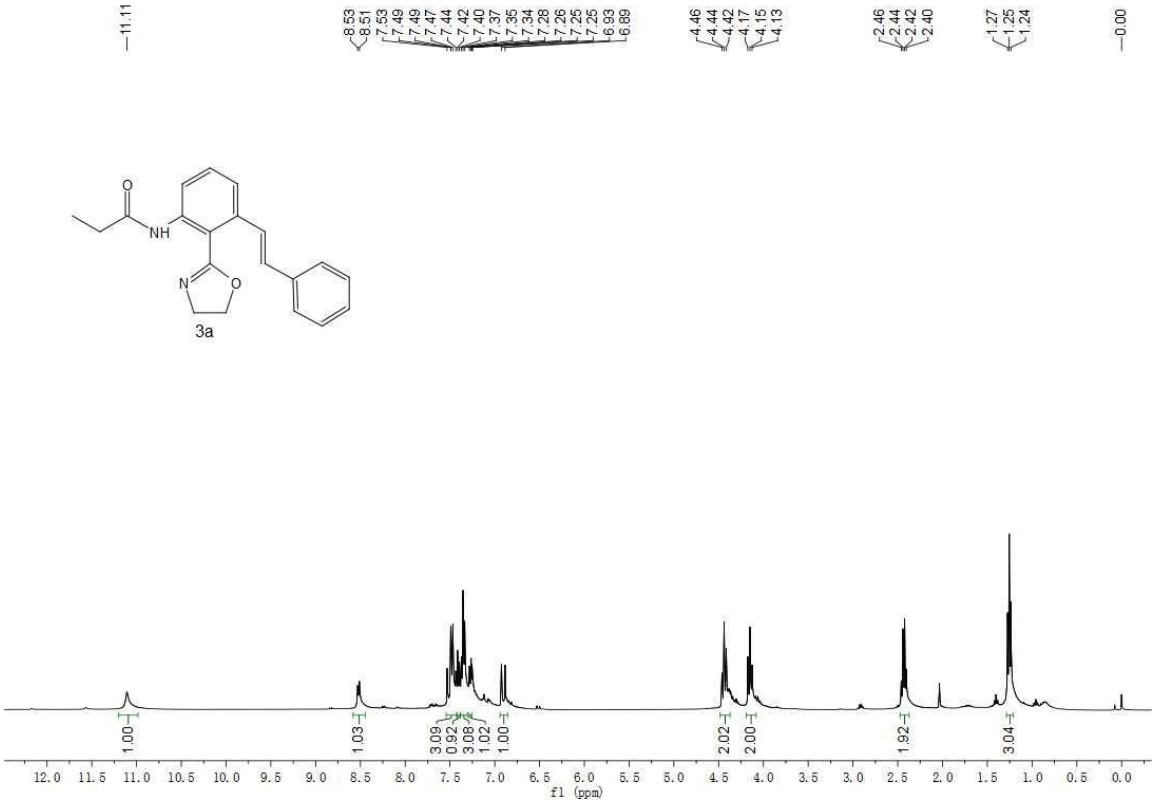
(*E*)-N-(3-(2-bromostyryl)-2-(4,5-dihydrooxazol-2-yl)phenyl)benzamide (3x): White solid (Yield: 89%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 12.24 (s, 1H), 8.77 (dd, J = 8.4, 1.0 Hz, 1H), 8.03-8.01 (m, 2H), 7.64-7.58 (m, 2H), 7.55-7.48 (m, 5H), 7.43 (d, J = 7.8 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.27-7.23 (m, 1H), 7.15-7.11 (m, 1H), 4.46 (t, J = 9.6 Hz, 2H), 4.19 (t, J = 9.6 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.56, 165.10, 139.47, 138.93, 137.29, 135.24, 133.10, 131.71, 131.63, 131.58, 129.38, 128.90, 128.64, 127.53, 127.47, 126.94, 124.18, 122.83, 120.29, 113.85, 66.91, 54.21 ppm; HRMS (ESI) calcd for $C_{24}H_{20}BrN_2O_2$ $[M+H]^+$: 447.0708; found: 447.0704.

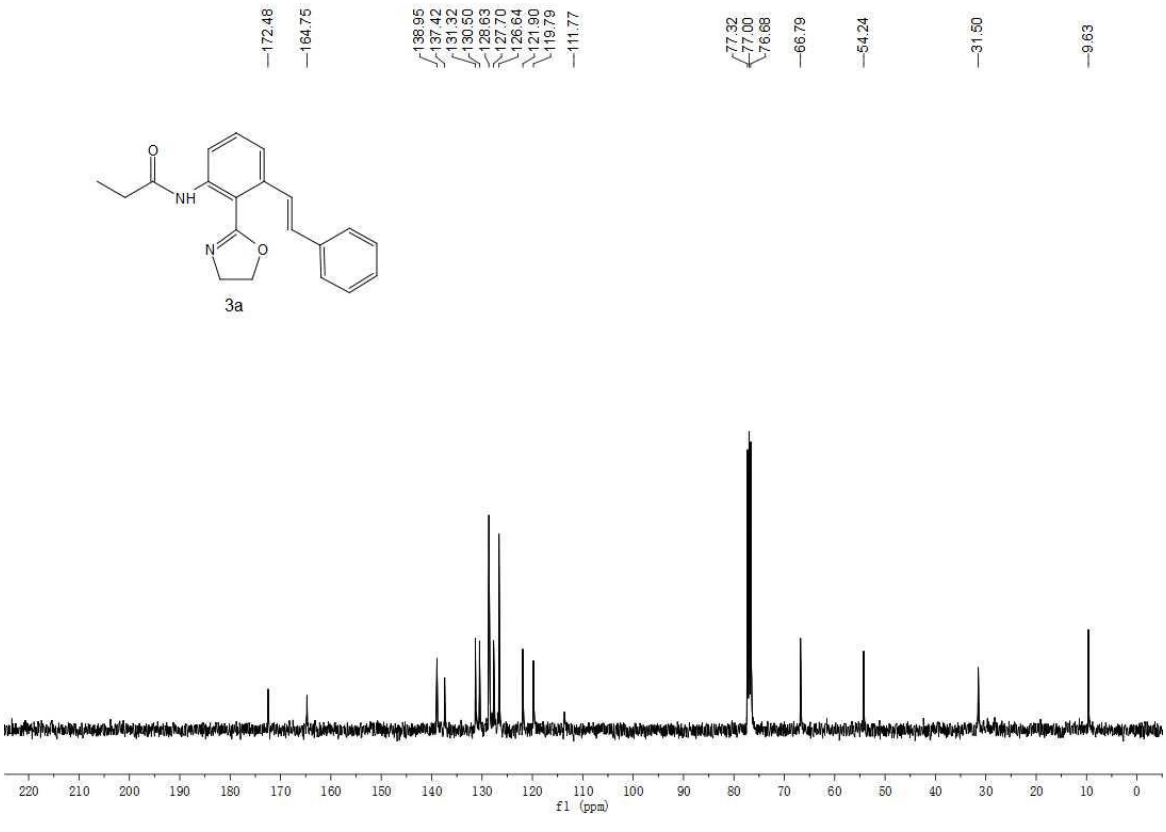


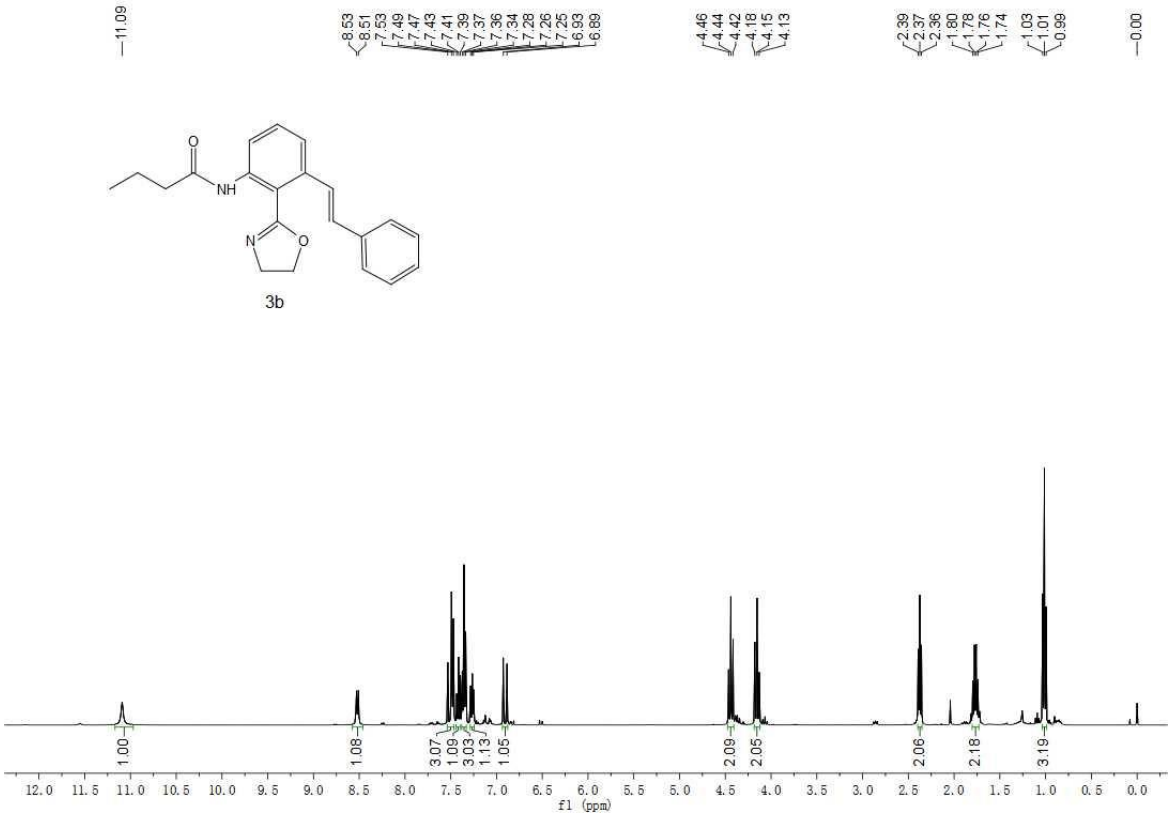
3y

(*E*)-N-(2-(4,5-dihydrooxazol-2-yl)-3-(4-(trifluoromethyl)styryl)phenyl)benzamide (3y): White solid (Yield: 91%). ^{1}H NMR (400 MHz, $CDCl_3$):δ 12.29 (s, 1H), 8.79 (dd, J = 8.4, 1.0 Hz, 1H), 8.03-8.01 (m, 2H), 7.67 (d, J = 16.0 Hz, 1H), 7.62-7.60 (m, 2H), 7.58-7.56 (m, 2H), 7.55-7.52 (m, 2H), 7.50-7.48 (m, 2H), 7.37 (d, J = 7.6 Hz, 1H), 6.92 (d, J = 16.0 Hz, 1H), 4.46 (t, J = 9.4 Hz, 2H), 4.20 (t, J = 9.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$):δ 165.59, 164.98, 140.95, 139.58, 138.61, 135.17, 131.76, 131.63, 131.51, 129.53, 129.32, 129.21, 129.00, 128.65, 127.46, 126.76, 125.64, 125.60, 122.42, 120.47, 113.86, 66.93, 54.19 ppm; HRMS (ESI) calcd for $C_{25}H_{20}F_3N_2O_2$ $[M+H]^+$: 437.1477; found: 437.1480.

5. ^{1}H NMR and ^{13}C NMR spectra



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4.18
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2.37
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1.74
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1.01
0.99
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N
O
3b
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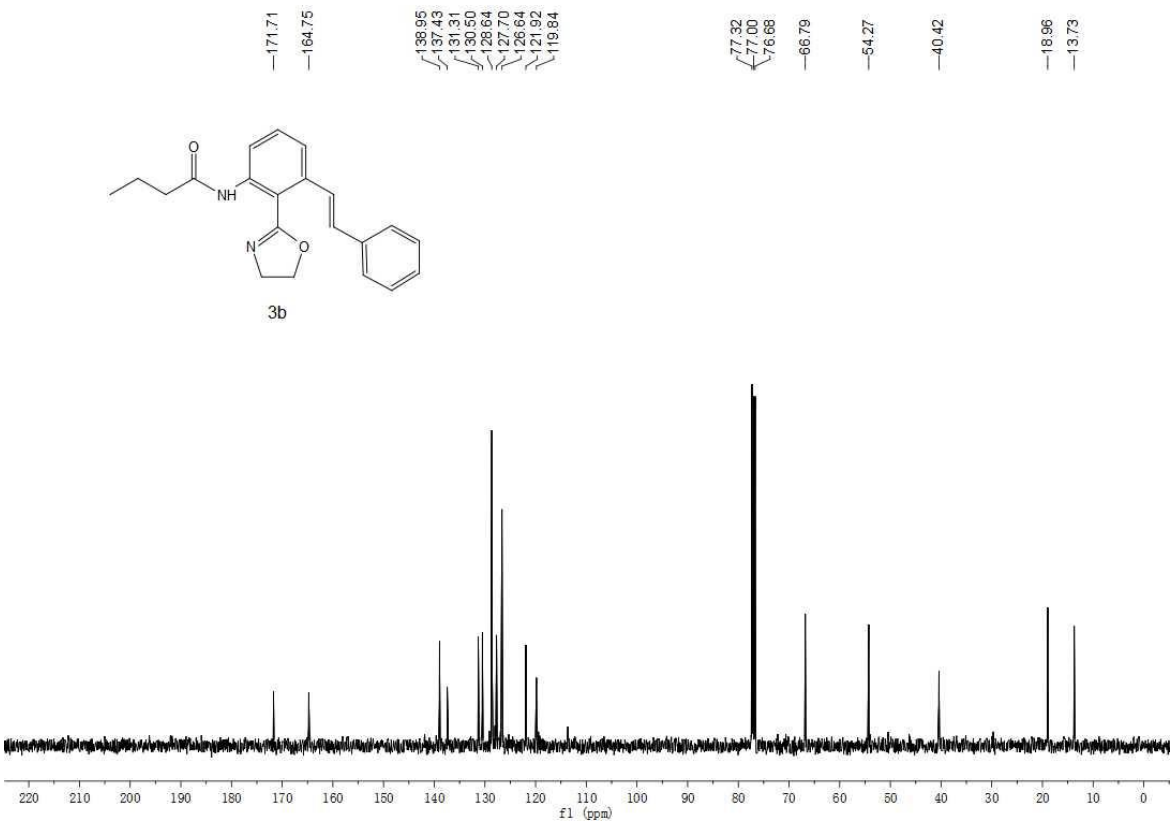
3.03
1.13
1.05
2.09
2.05
2.06
2.18
3.19
f1 (ppm)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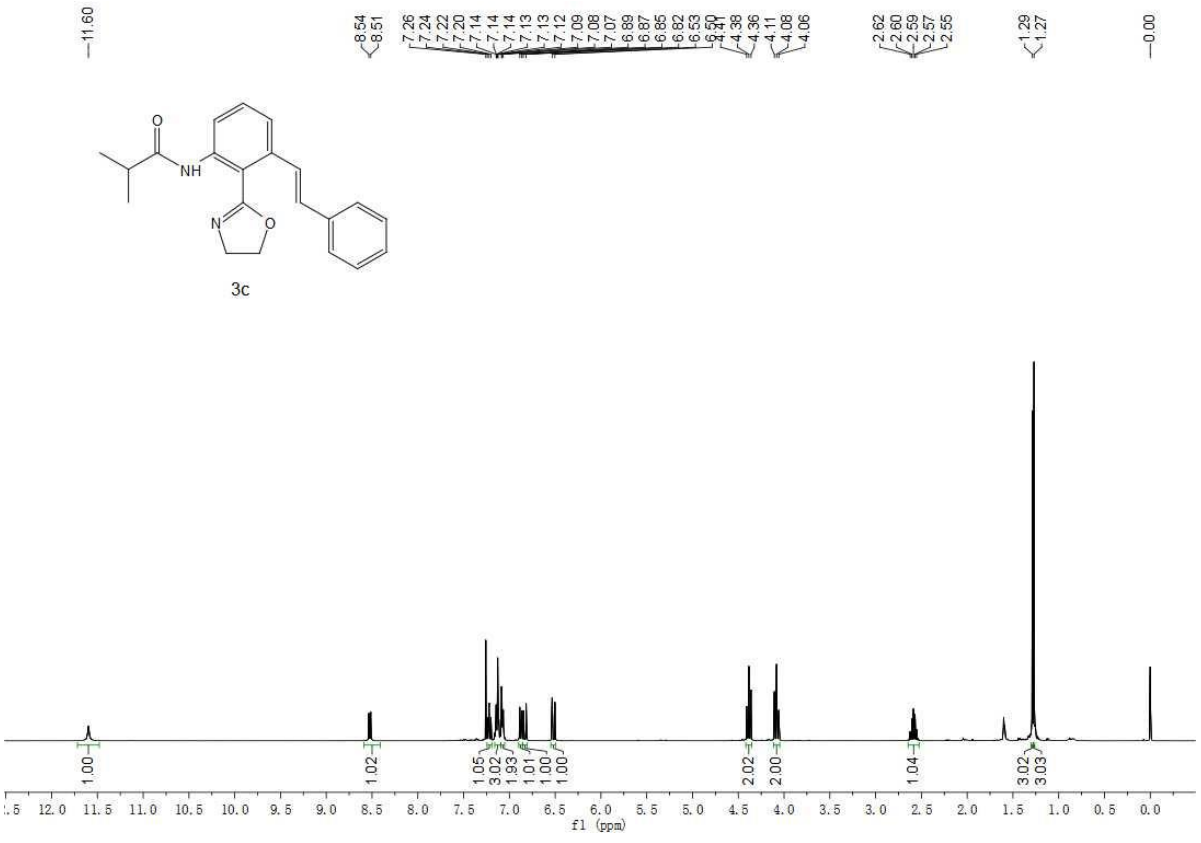
O
3b
f1 (ppm)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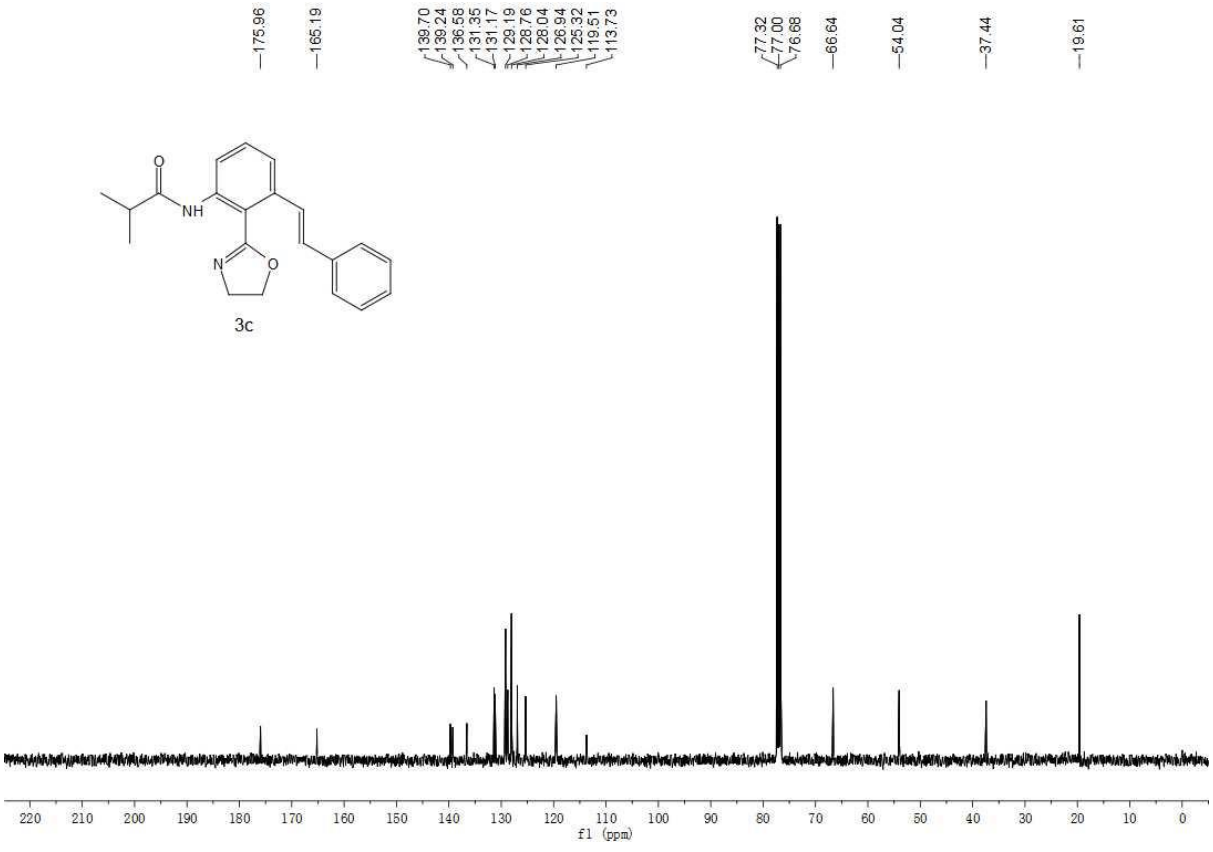
f1 (ppm)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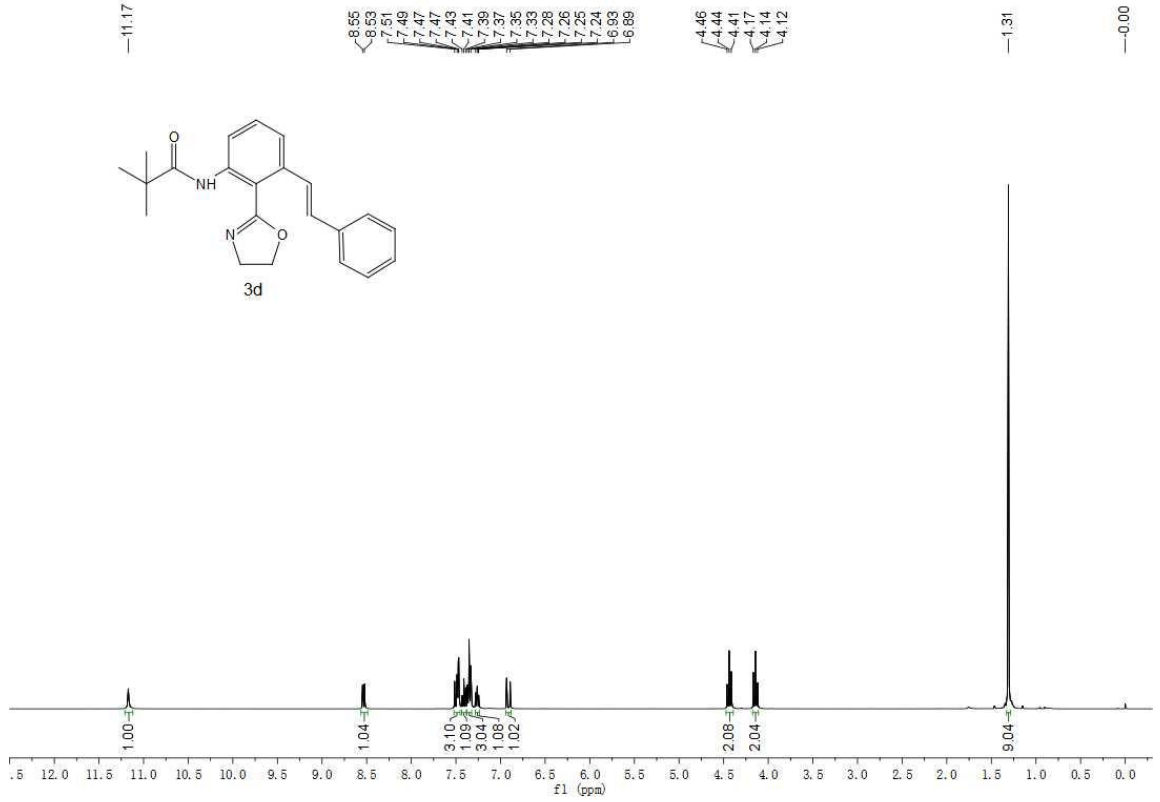
66.64
54.04
37.44
19.61
O
NH
N
O
3c
f1 (ppm)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7.47
7.43
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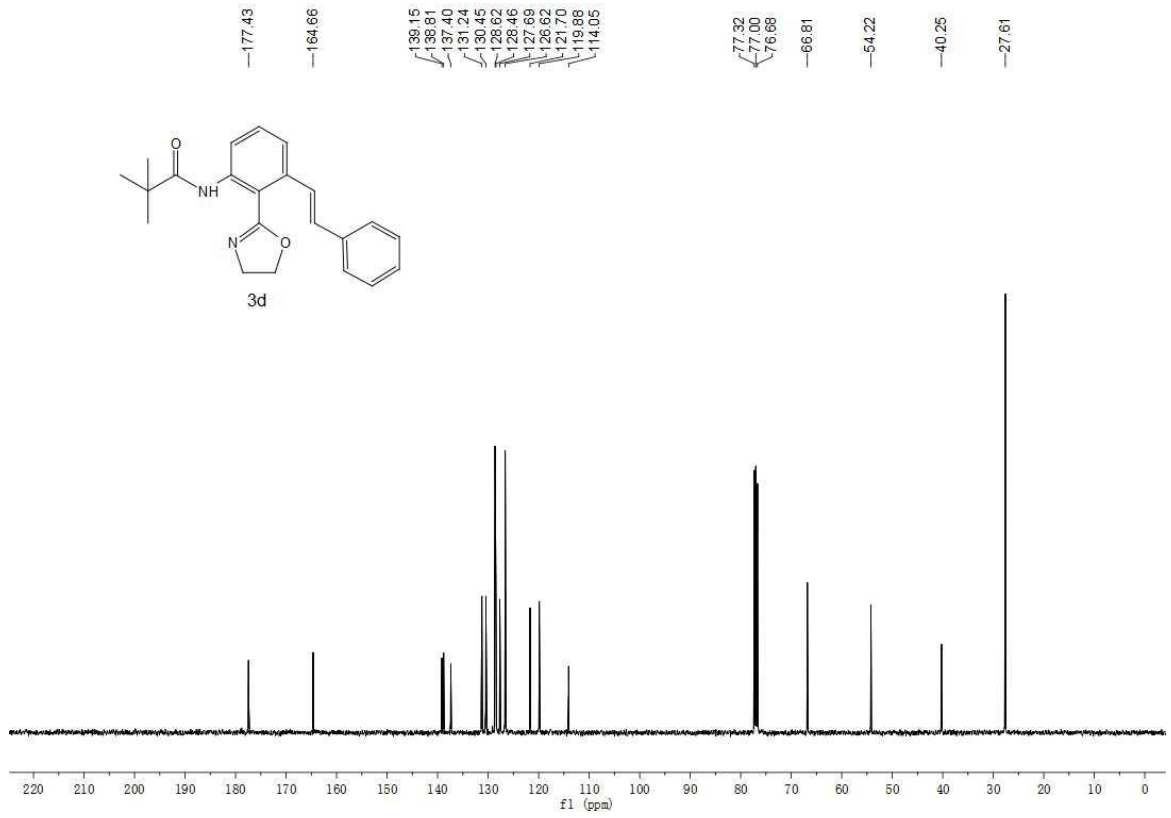
7.39
7.37
7.35
7.33
7.28
7.26
7.25
7.24
6.93
6.89
4.46
4.44
4.41
4.17
4.14
4.12
1.31
0.00
3d
1.00
1.04
3.10
1.09
3.04
1.08
1.02
2.08
2.04
9.04
f1 (ppm)


177.43
164.66
139.15
138.81
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131.24
130.45
128.62
128.46
127.69
126.62
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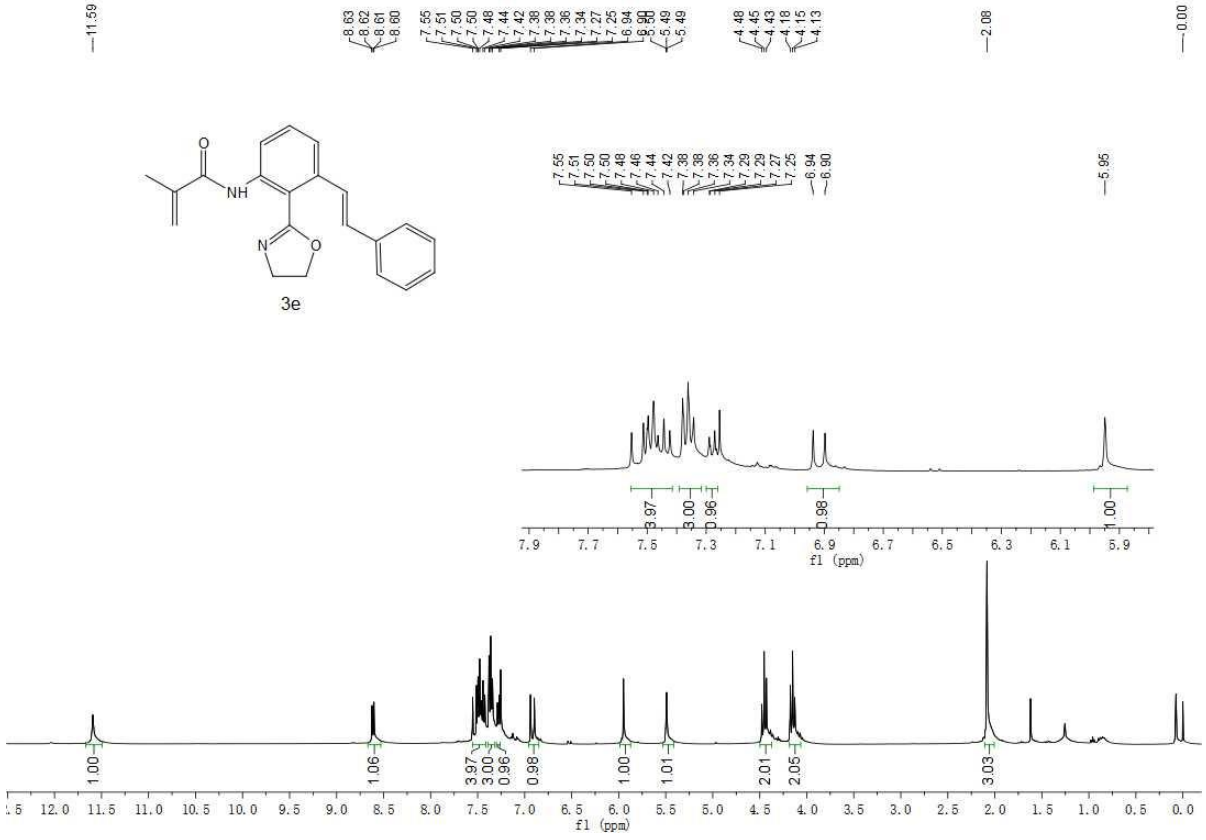
114.05
77.32
77.00
76.68
66.81
54.22
40.25
27.61
3d
f1 (ppm)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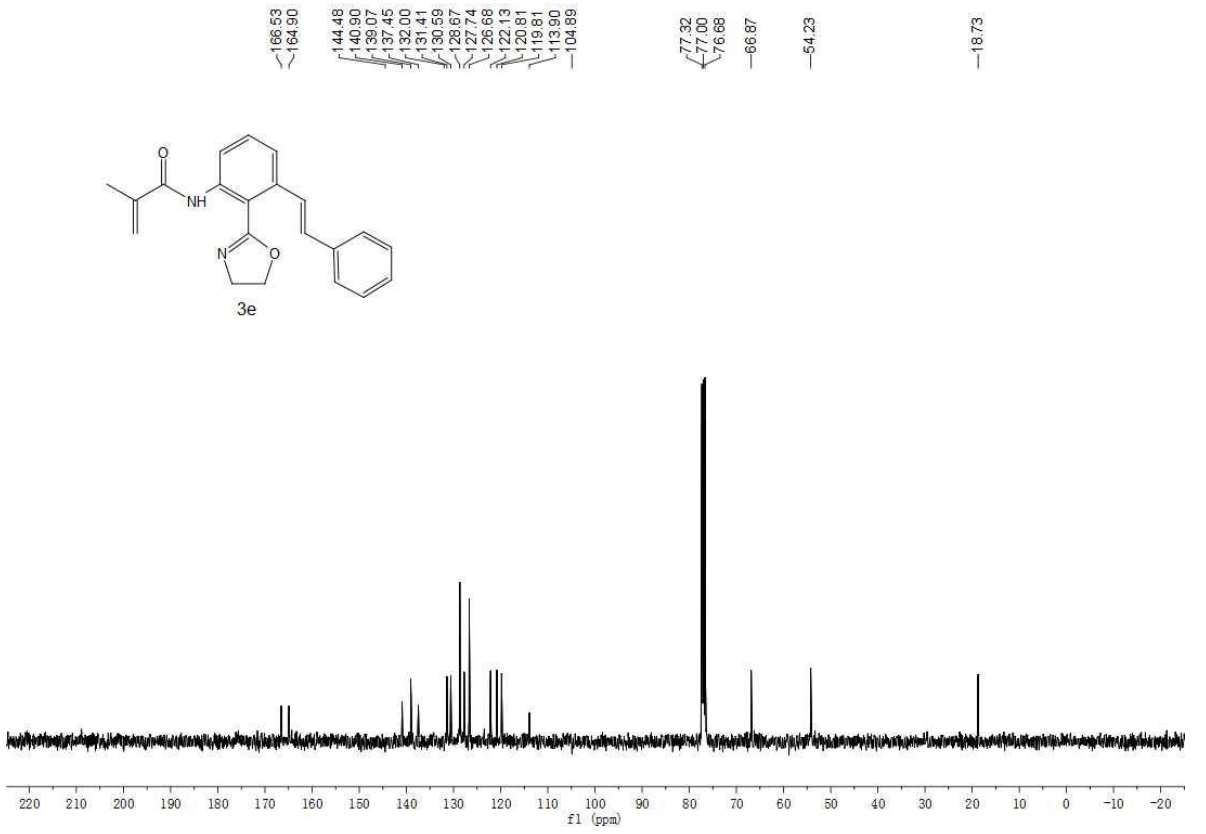
7.50
7.50
7.48
7.44
7.42
7.38
7.38
7.36
7.34
7.27
7.25
6.94
6.90
5.49
5.49
4.48
4.45
4.43
4.18
4.15
4.13
2.08
0.00
NH
O
N
O
3e
5.95
6.94
6.90
3.97
3.00
0.96
0.98
1.00
f1 (ppm)
1.00
1.06
3.97
3.00
0.96
0.98
1.00
1.01
2.01
2.05
3.03
f1 (ppm)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144.48
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139.07
137.45
132.00
131.41
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128.67
127.74
126.68
122.13
120.81
119.81
113.90
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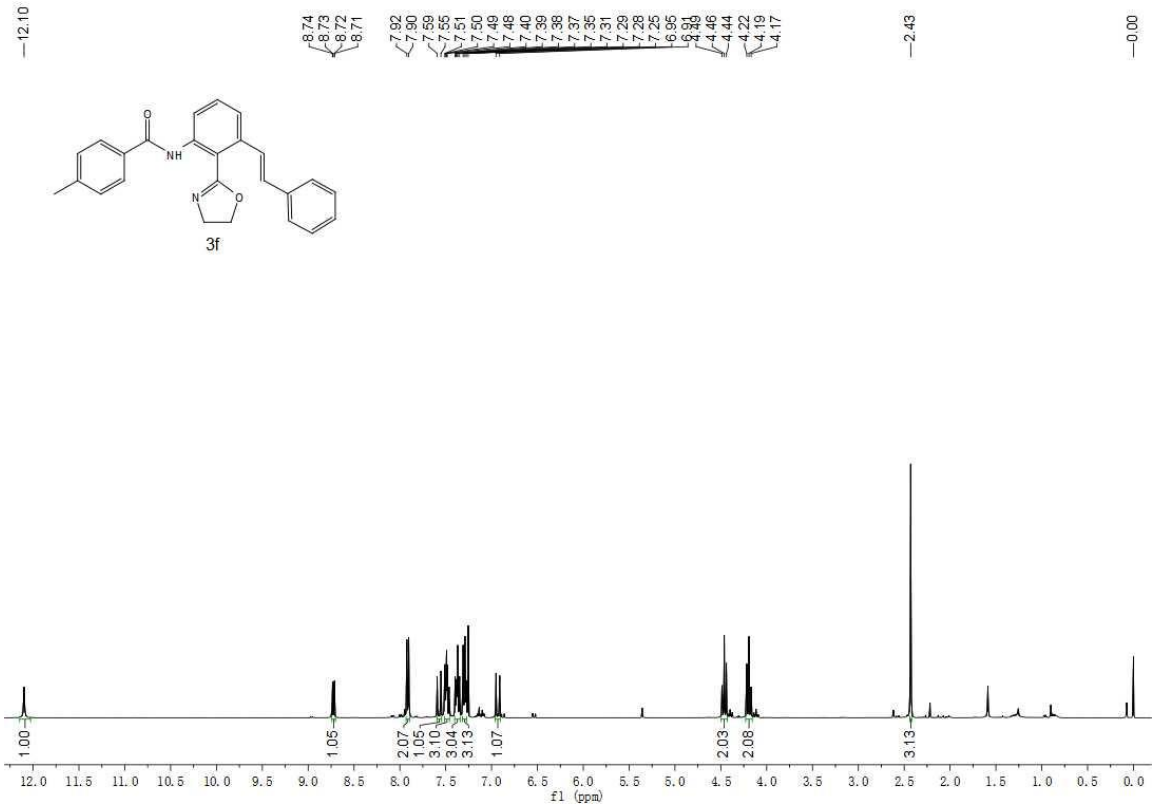
77.00
76.68
66.87
54.23
18.73
NH
O
N
O
3e
f1 (ppm)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8.73
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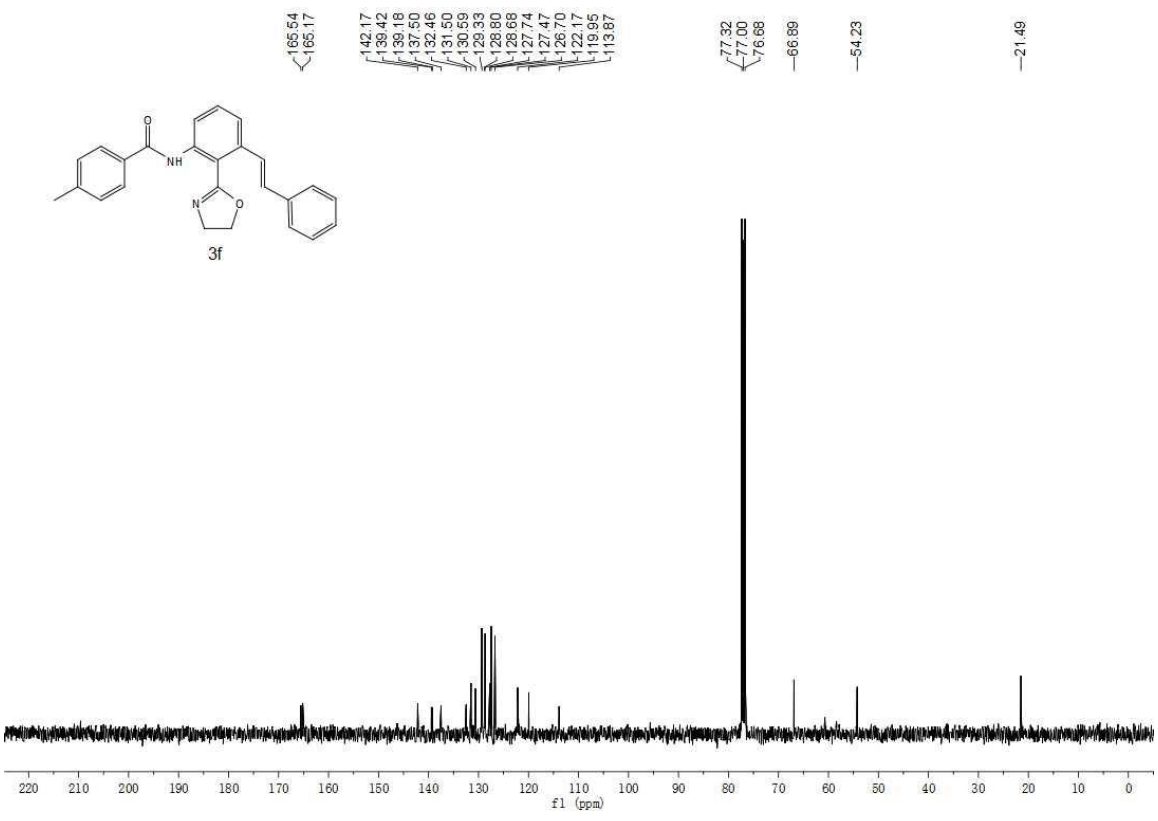
7.92
7.90
7.59
7.55
7.51
7.50
7.49
7.48
7.40
7.39
7.38
7.37
7.35
7.31
7.29
7.28
7.25
6.95
6.91
4.46
4.44
4.22
4.19
4.17
2.43
0.00
3f
1.00
1.05
2.07
1.05
3.10
3.04
3.13
1.07
2.03
2.08
3.13
f1 (ppm)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165.17
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131.50
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129.33
128.80
128.68
127.74
127.47
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122.17
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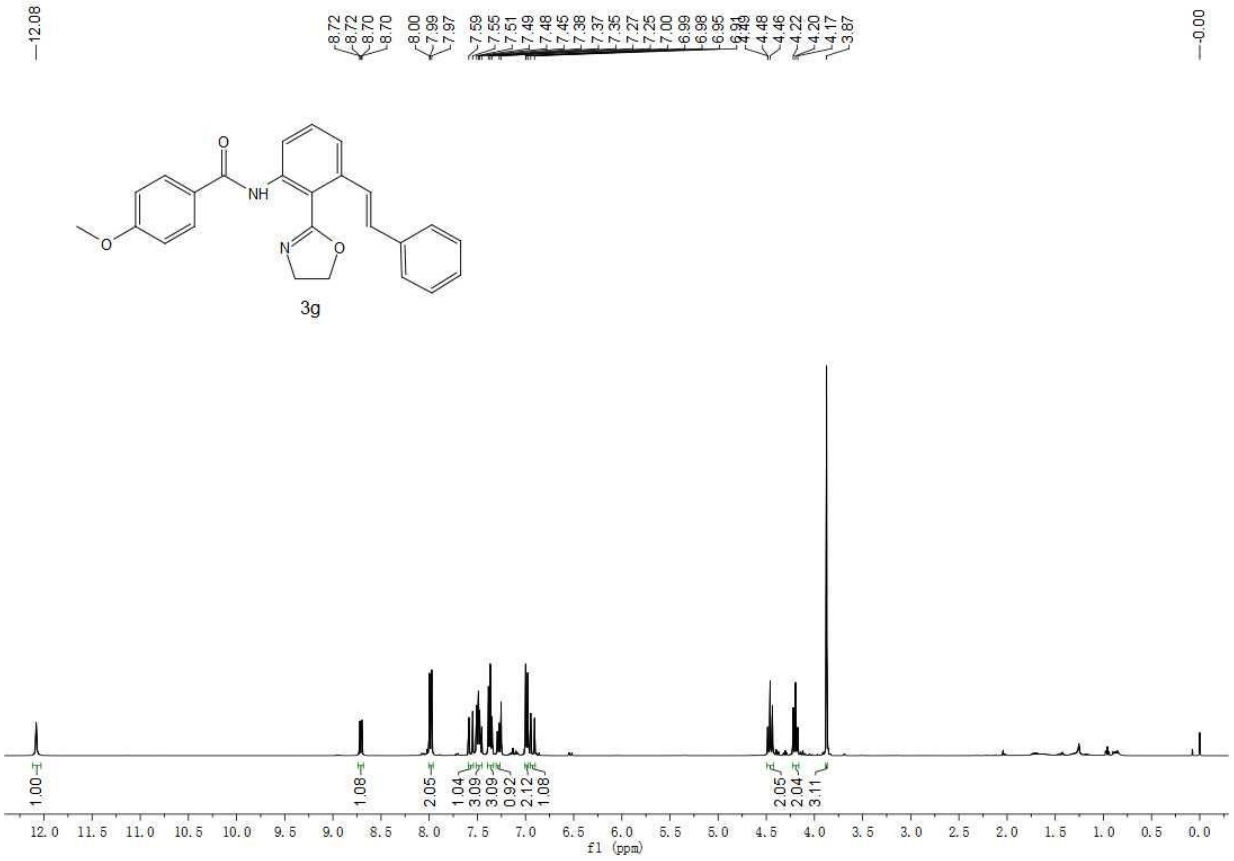
113.87
77.32
77.00
76.68
66.89
54.23
21.49
3f
f1 (ppm)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7.97
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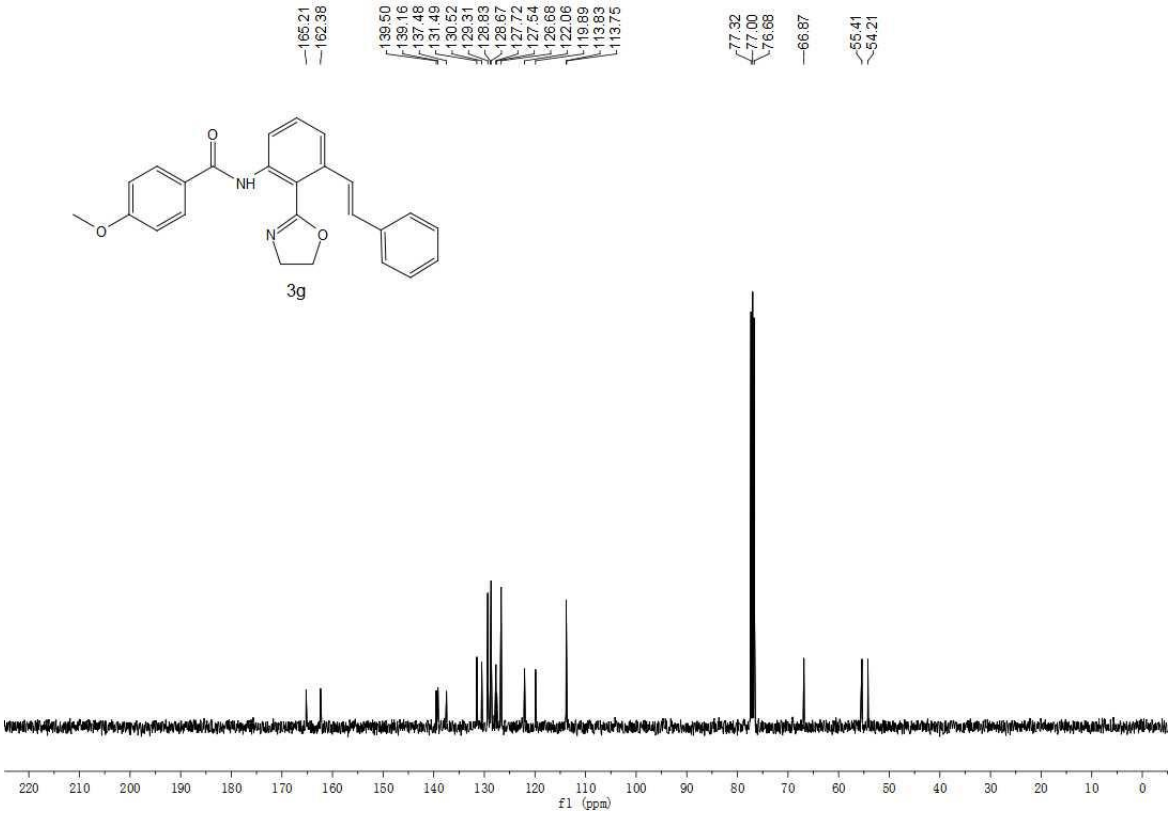
7.55
7.51
7.49
7.48
7.45
7.38
7.37
7.35
7.27
7.25
7.00
6.99
6.98
6.95
4.48
4.46
4.22
4.20
4.17
3.87
0.00
O
NH
O
N
O
3g
1.00
1.08
2.05
1.04
3.09
3.09
0.92
2.12
1.08
2.05
2.04
3.11
f1 (ppm)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162.38
139.50
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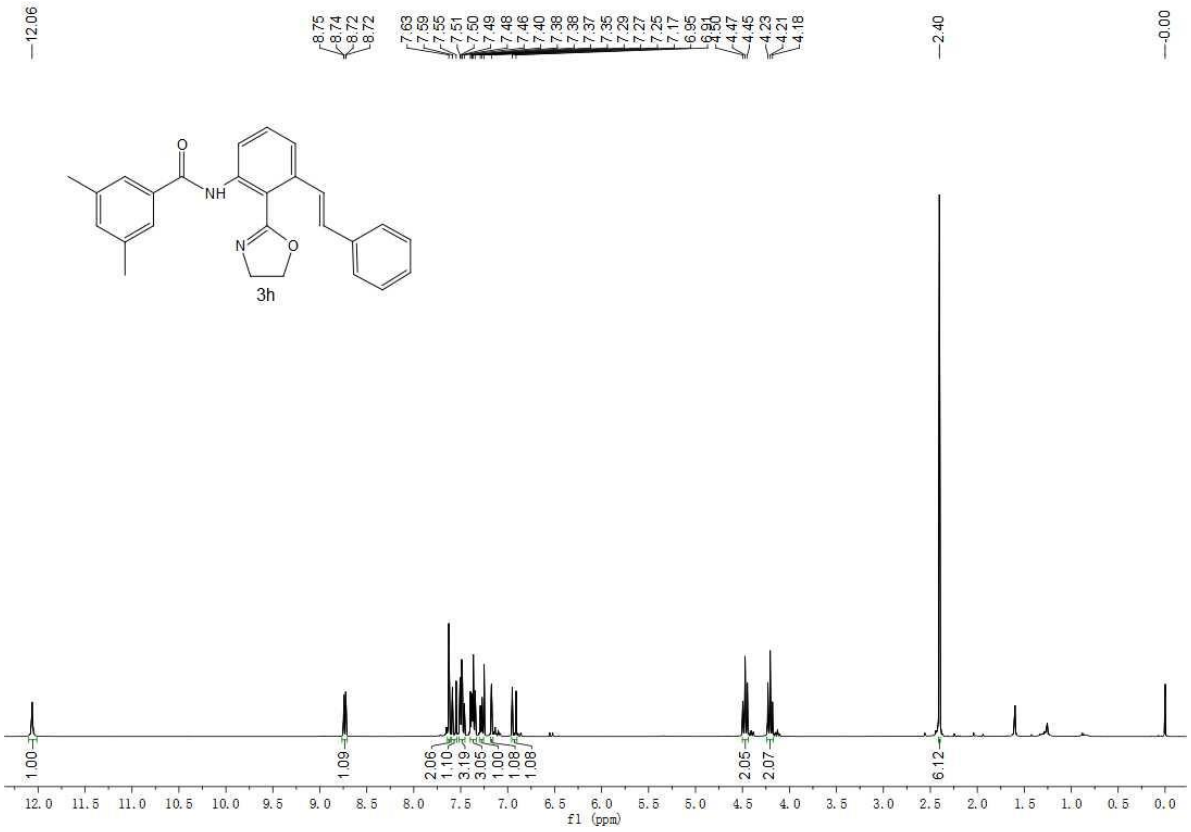
131.49
130.52
129.31
128.83
128.67
127.72
127.54
126.68
122.06
119.89
113.83
113.75
77.32
77.00
76.68
66.87
55.41
54.21
O
NH
O
N
O
3g
f1 (ppm)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7.63
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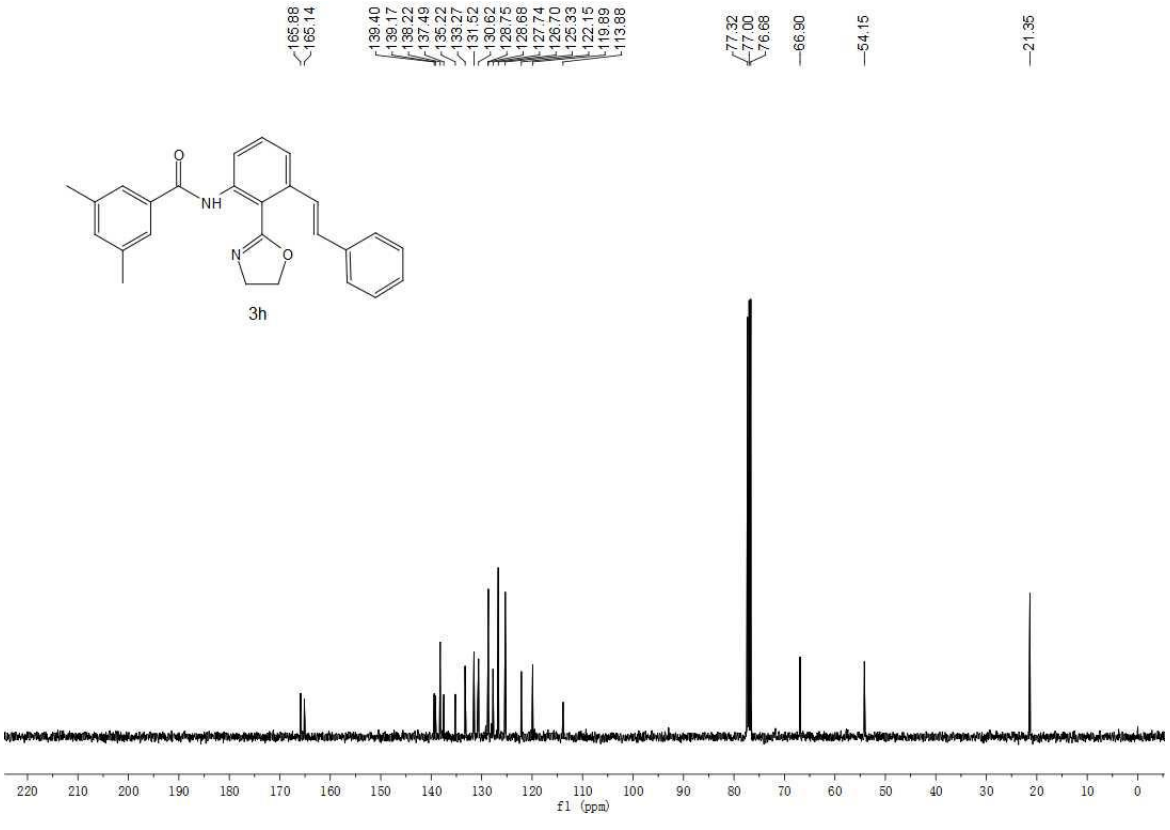
7.55
7.51
7.50
7.49
7.48
7.46
7.40
7.38
7.38
7.37
7.35
7.29
7.27
7.25
7.17
6.95
6.91
4.50
4.47
4.45
4.23
4.21
4.18
2.40
0.00
O
NH
N
O
3h
1.00
1.09
2.06
1.10
3.19
3.05
1.00
1.08
1.08
2.05
2.07
6.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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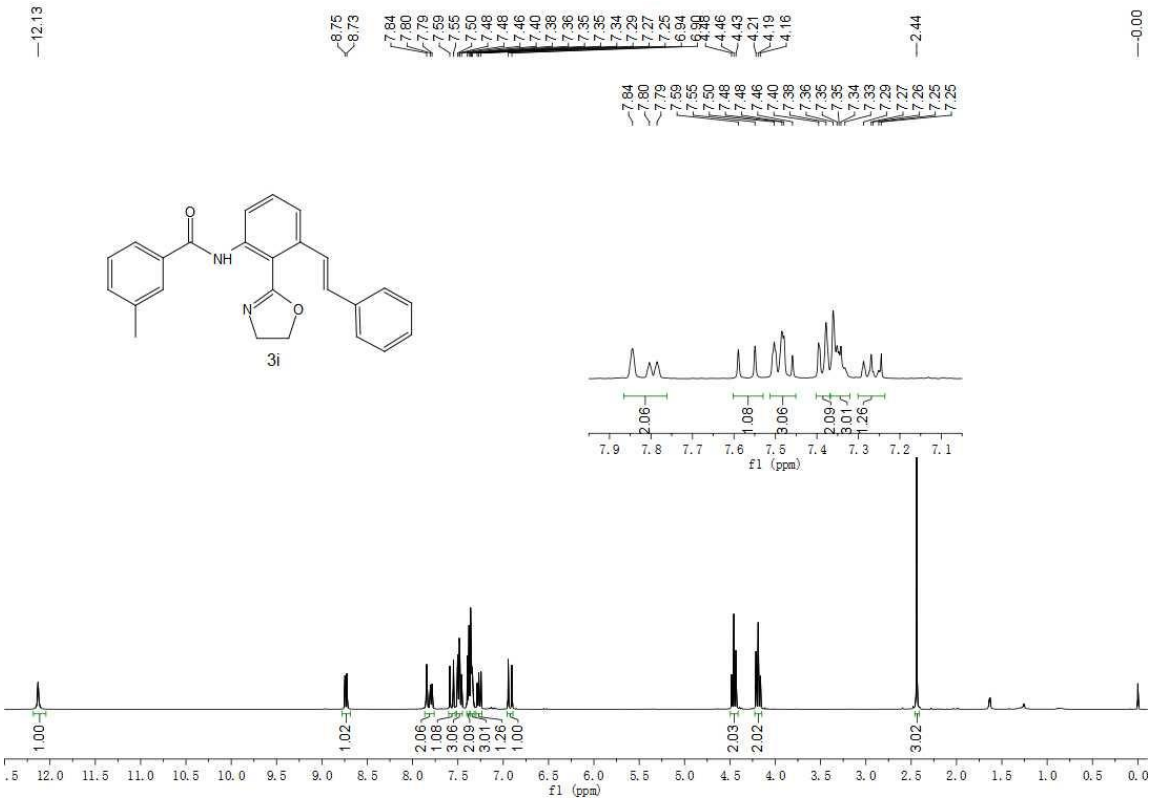
165.14
139.40
139.17
138.22
137.49
135.22
133.27
131.52
130.62
128.75
128.68
127.74
126.70
125.33
122.15
119.89
113.88
77.32
77.00
76.68
66.90
54.15
21.35
O
NH
N
O
3h
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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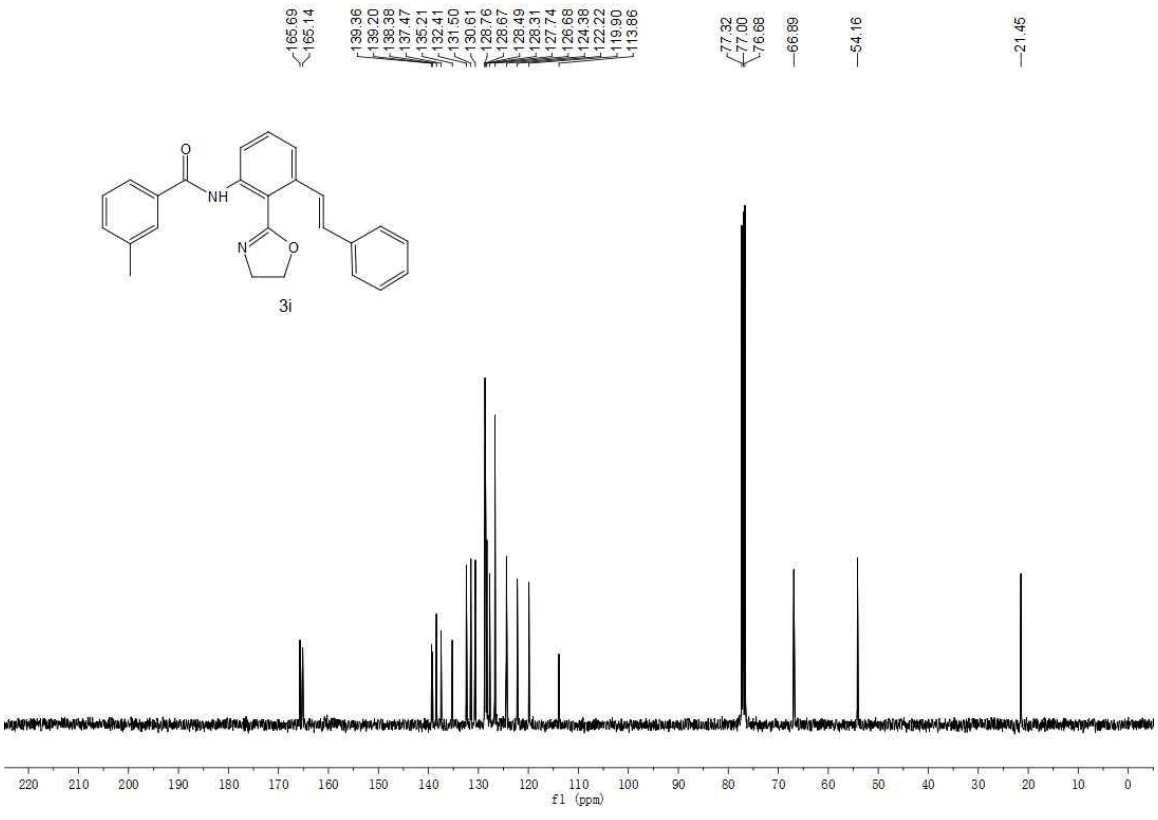
7.79
7.59
7.55
7.50
7.48
7.48
7.46
7.40
7.38
7.36
7.35
7.35
7.34
7.29
7.27
7.25
6.94
6.90
4.46
4.43
4.21
4.19
4.16
2.44
0.00
NH
O
N
O
3i
2.06
1.08
3.06
2.09
3.01
1.26
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
1.00
1.02
2.06
1.08
3.06
2.09
3.01
1.26
1.00
2.03
2.02
3.02
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.47
135.21
132.41
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130.61
128.76
128.67
128.49
128.31
127.74
126.68
124.38
122.22
119.90
113.86
77.32
77.00
76.68
66.89
54.16
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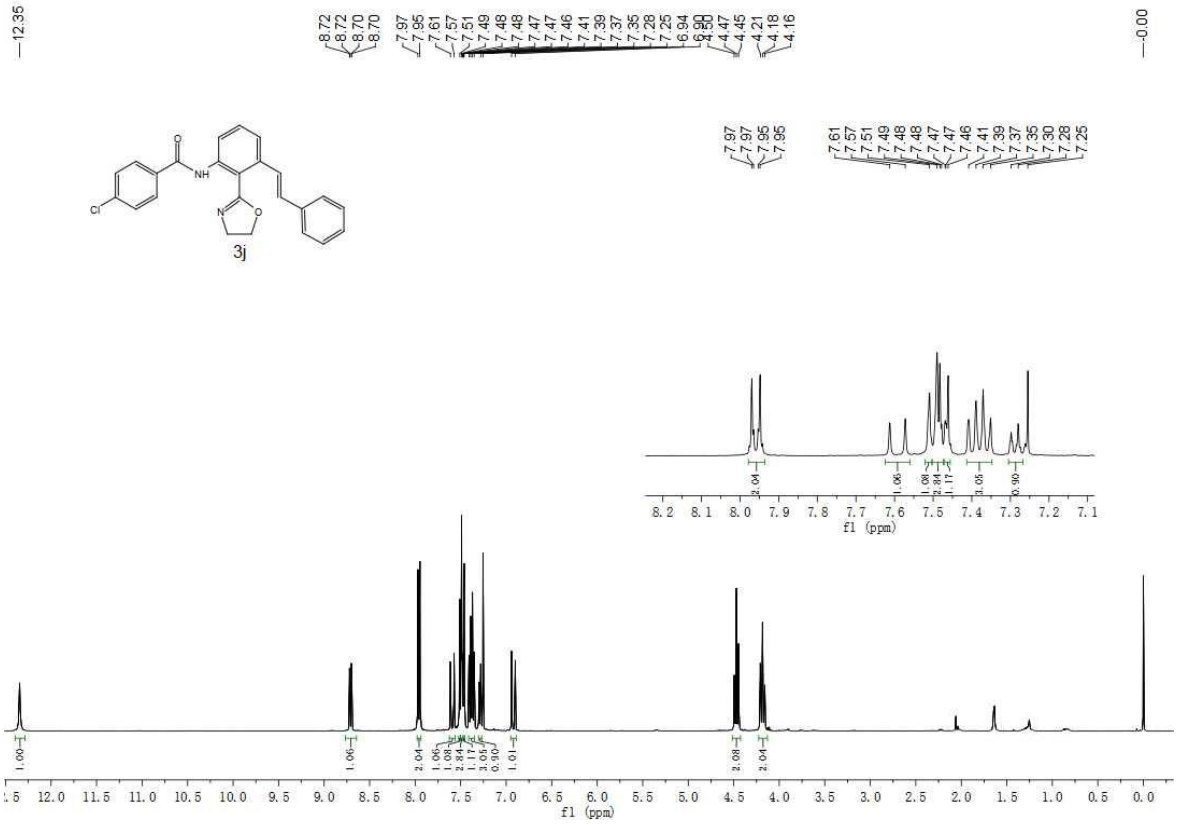
NH
O
N
O
3i
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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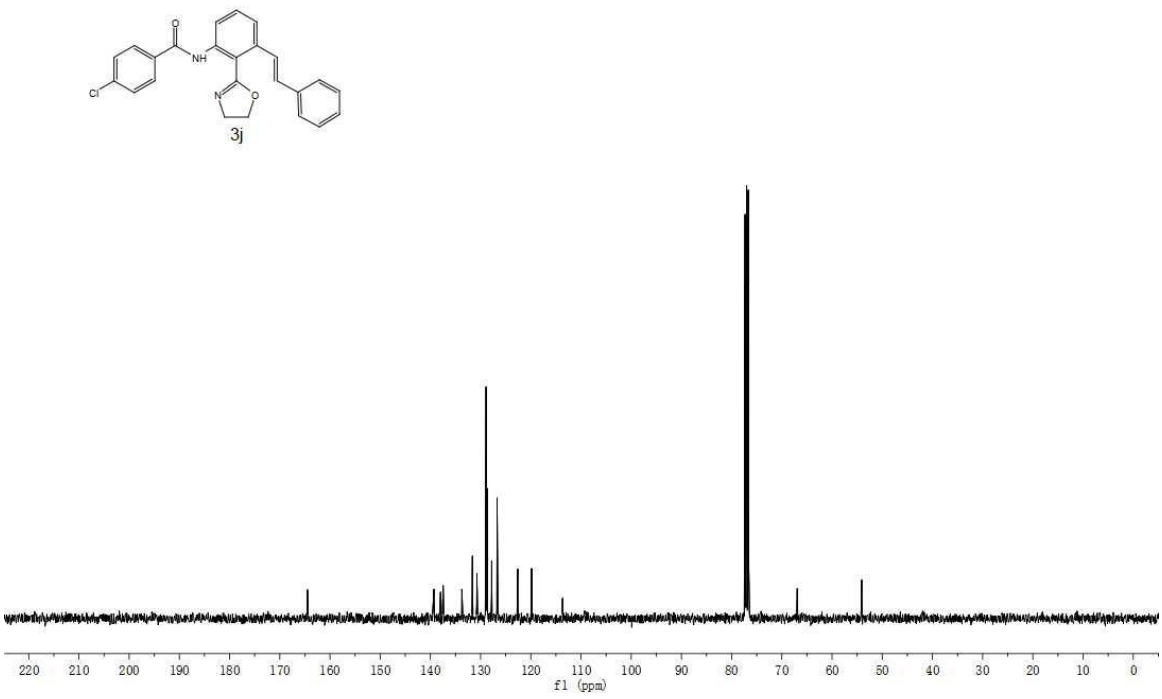
7.57
7.51
7.49
7.48
7.48
7.47
7.47
7.46
7.41
7.39
7.37
7.35
7.28
7.25
6.94
6.90
4.50
4.47
4.45
4.21
4.18
4.16
0.00
3j
f1 (ppm)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139.28
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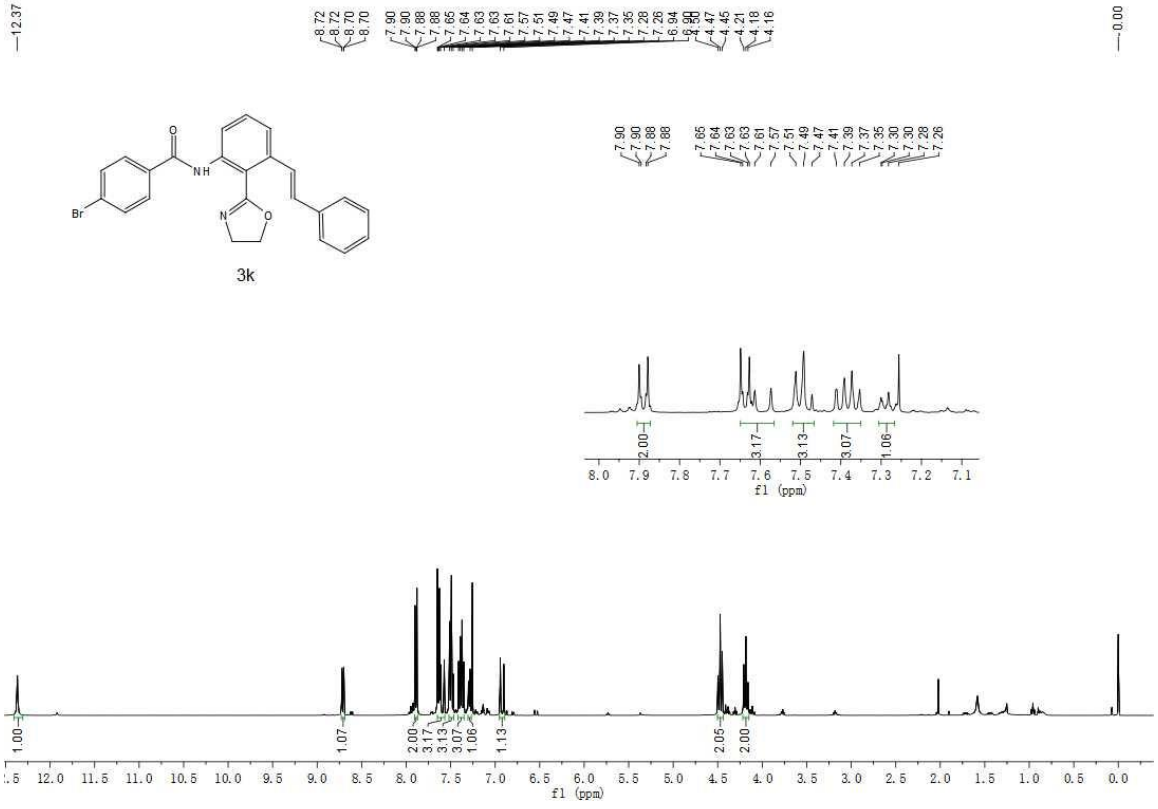
137.46
133.73
131.62
130.75
128.90
128.70
127.80
126.71
122.61
119.84
113.66
77.32
77.00
76.68
66.93
54.10
3j
f1 (ppm)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7.88
7.88
7.65
7.64
7.63
7.63
7.61
7.57
7.51
7.49
7.47
7.41
7.39
7.37
7.35
7.28
7.26
6.94
6.90
4.50
4.47
4.45
4.21
4.18
4.16
0.00
O
NH
Br
N
O
3k
2.00
3.17
3.13
3.07
1.06
f1 (ppm)
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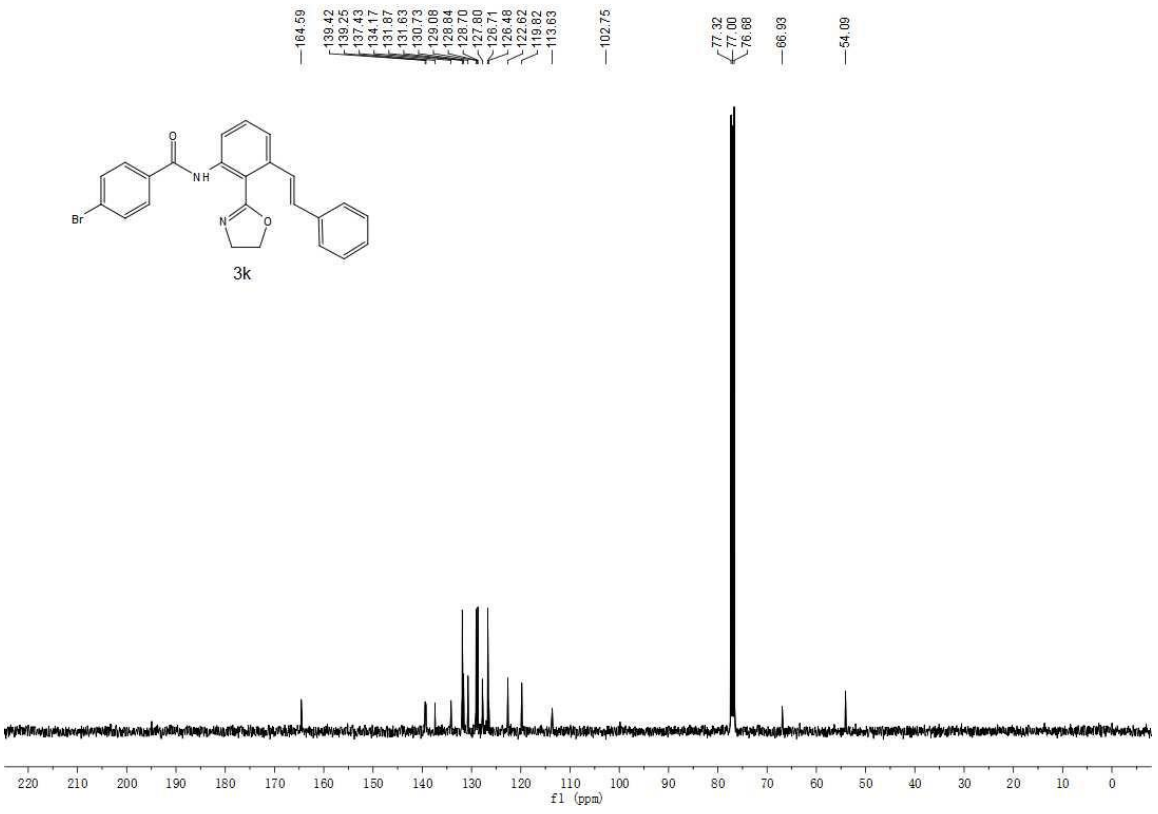
1.07
2.00
3.17
3.13
3.07
1.06
1.13
2.05
2.00
f1 (ppm)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131.87
131.63
130.73
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128.84
128.70
127.80
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126.48
122.62
119.82
113.63
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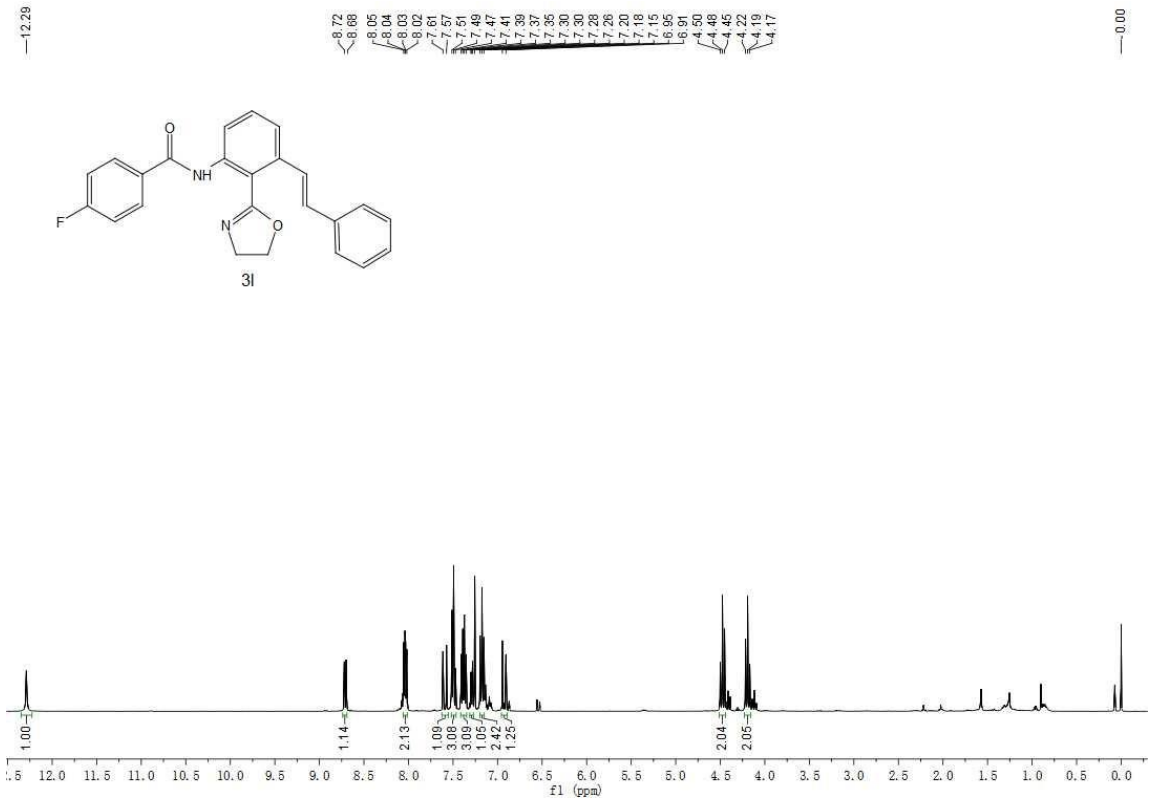
77.00
76.68
66.93
54.09
O
NH
Br
N
O
3k
f1 (ppm)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8.02
7.61
7.57
7.51
7.49
7.47
7.41
7.39
7.37
7.35
7.30
7.30
7.28
7.26
7.20
7.18
7.15
6.95
6.91
4.50
4.48
4.45
4.22
4.19
4.17
0.00
O
NH
F
N
O
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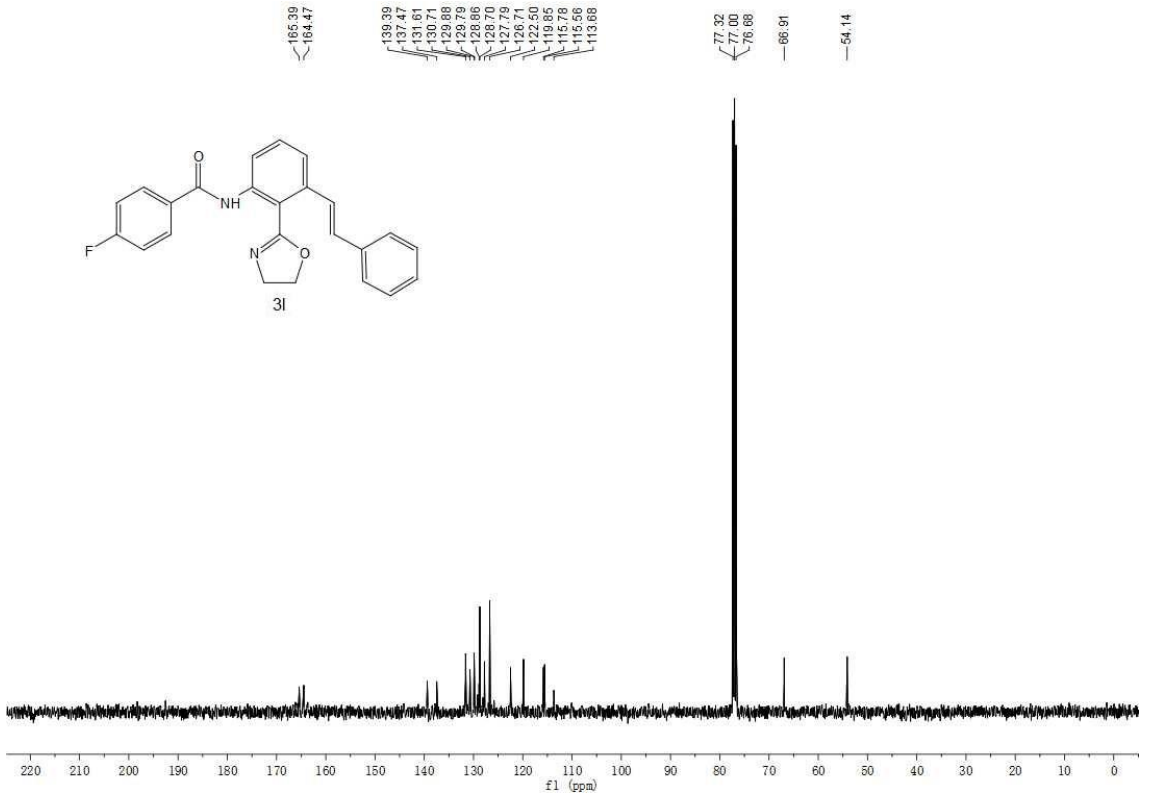
2.42
1.25
2.04
2.05
f1 (ppm)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129.79
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126.71
122.50
119.85
115.78
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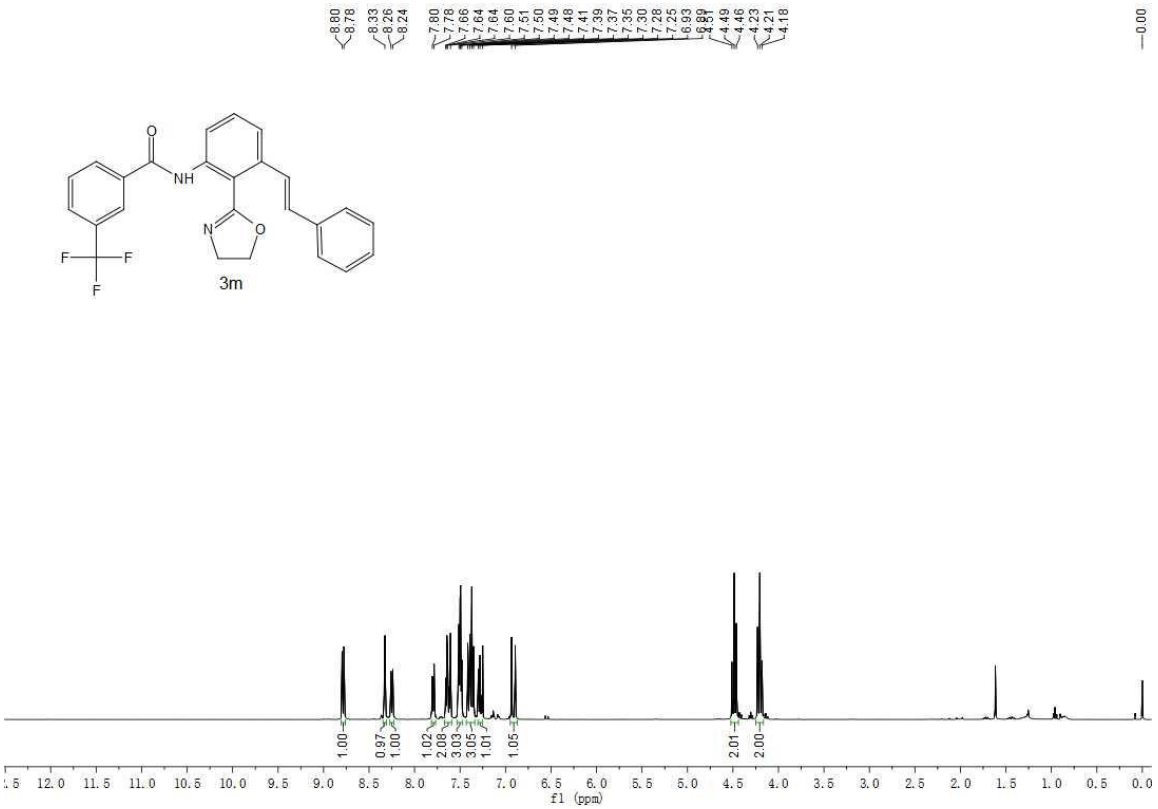
77.00
76.68
66.91
54.14
O
NH
F
N
O
3l
f1 (ppm)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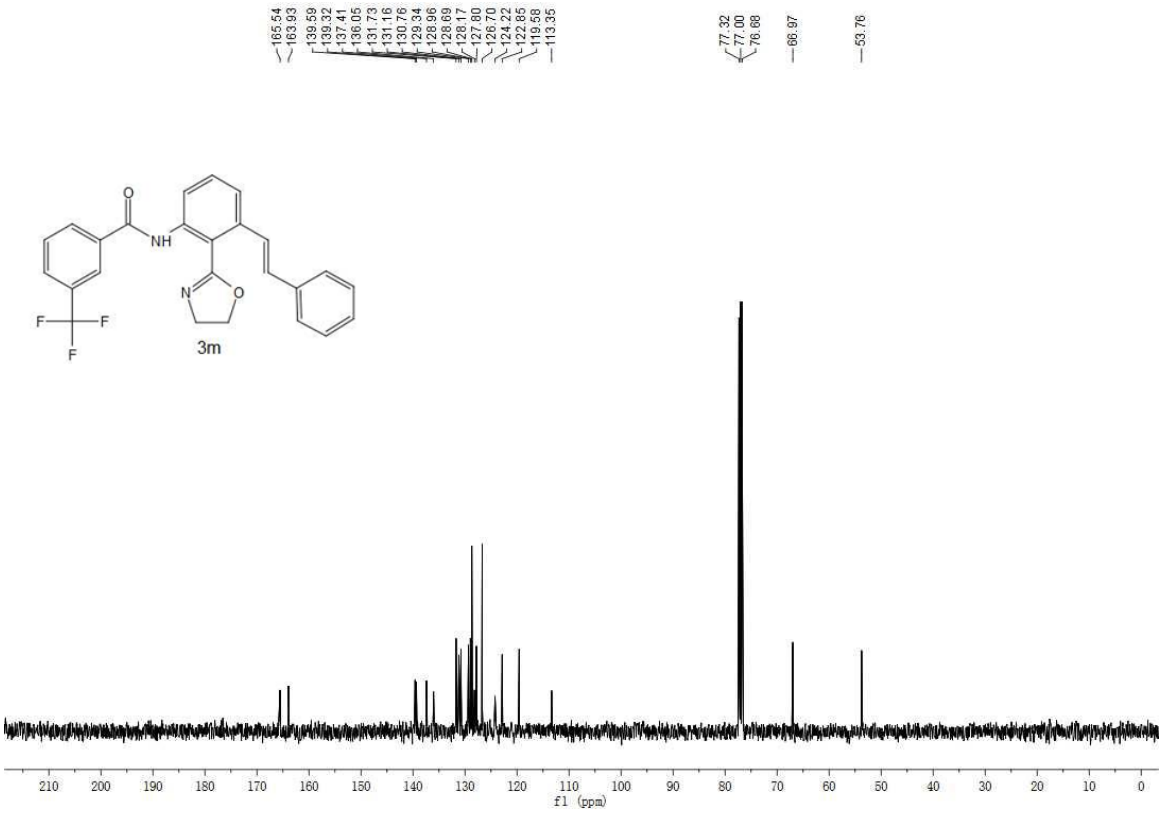
7.78
7.66
7.64
7.64
7.60
7.51
7.50
7.49
7.48
7.41
7.39
7.37
7.35
7.30
7.28
7.25
6.93
6.89
4.51
4.49
4.46
4.23
4.21
4.18
0.00
O
NH
N
O
F
F
F
3m
1.00
0.97
1.00
1.02
2.08
3.03
3.05
1.01
1.05
2.01
2.00
f1 (ppm)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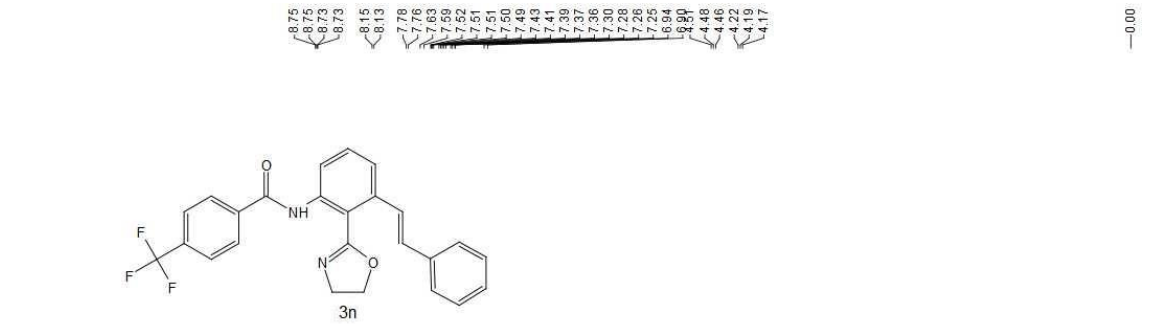
139.32
137.41
136.05
131.73
131.16
130.76
129.34
128.96
128.69
128.17
127.80
126.70
124.22
122.65
119.58
113.35
77.32
77.00
76.68
66.97
53.76
O
NH
N
O
F
F
F
3m
f1 (ppm)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8.73
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7.76
7.63
7.59
7.52
7.51
7.51
7.50
7.49
7.43
7.41
7.39
7.37
7.36
7.30
7.28
7.26
7.25
6.94
6.90
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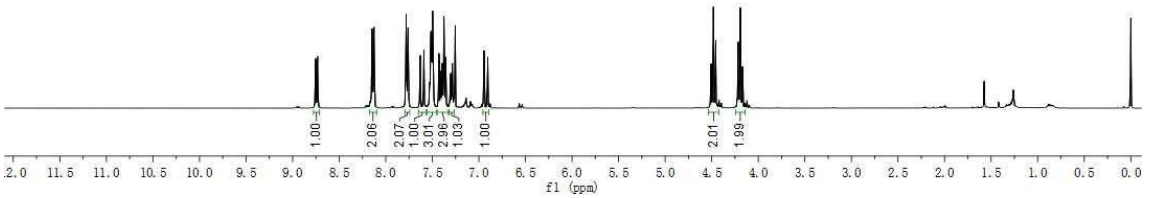
4.48
4.46
4.22
4.19
4.17
0.00

O
NH
F
F
F
N
O

3n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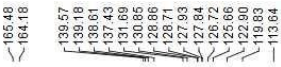
2.07
1.00
3.01
2.96
1.03
1.00
2.01
1.99
f1 (ppm)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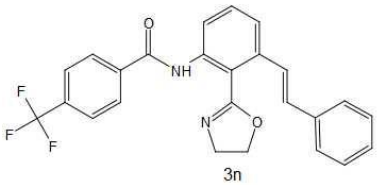
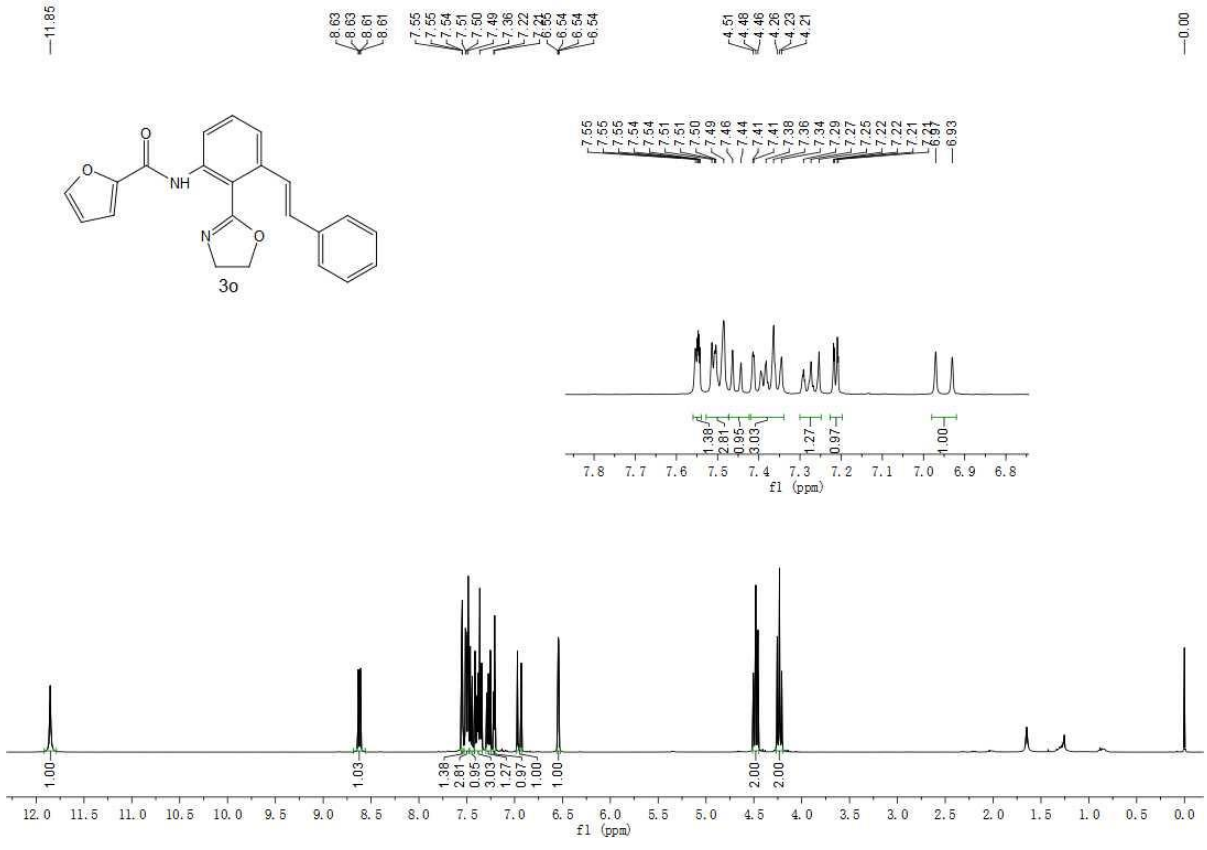
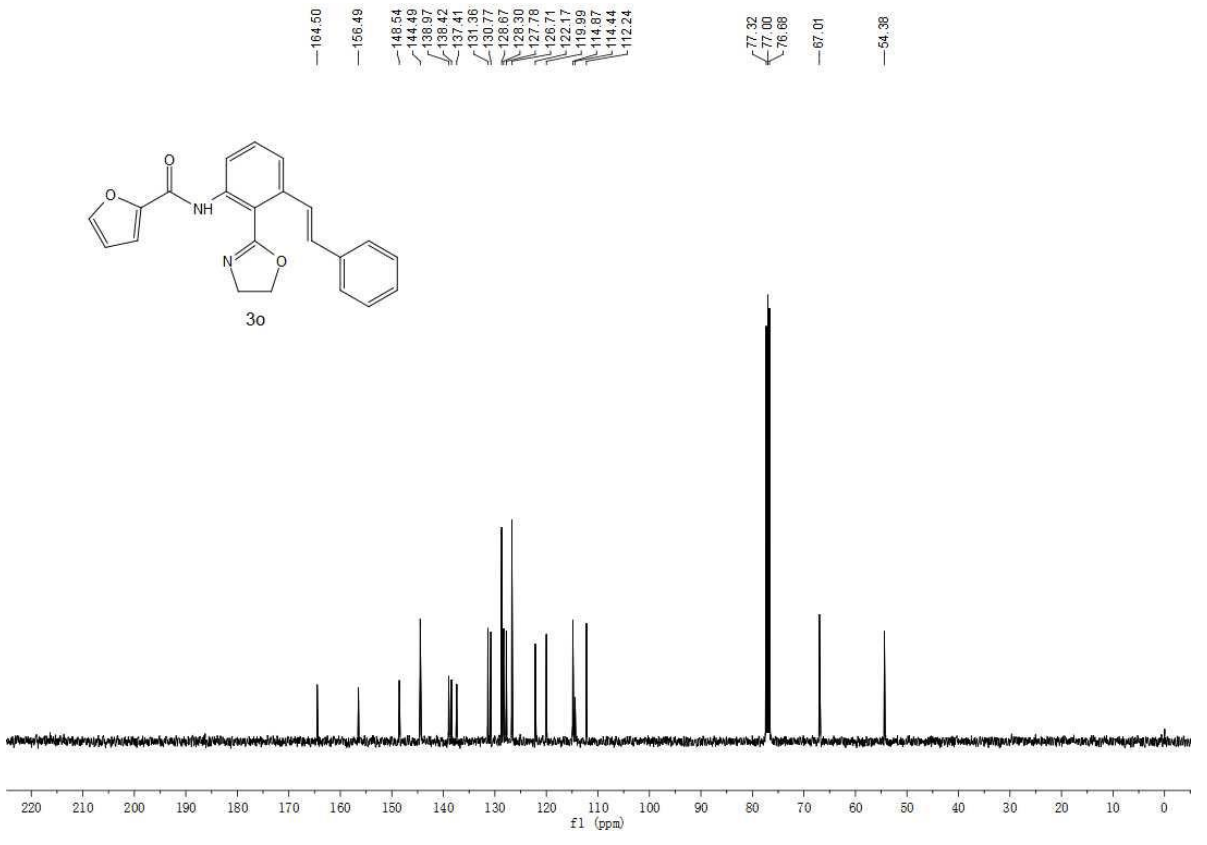
138.61
137.43
131.69
130.85
128.86
128.71
127.93
127.84
126.72
125.66
122.90
119.83
113.64
77.32
77.00
76.68
66.95
54.06

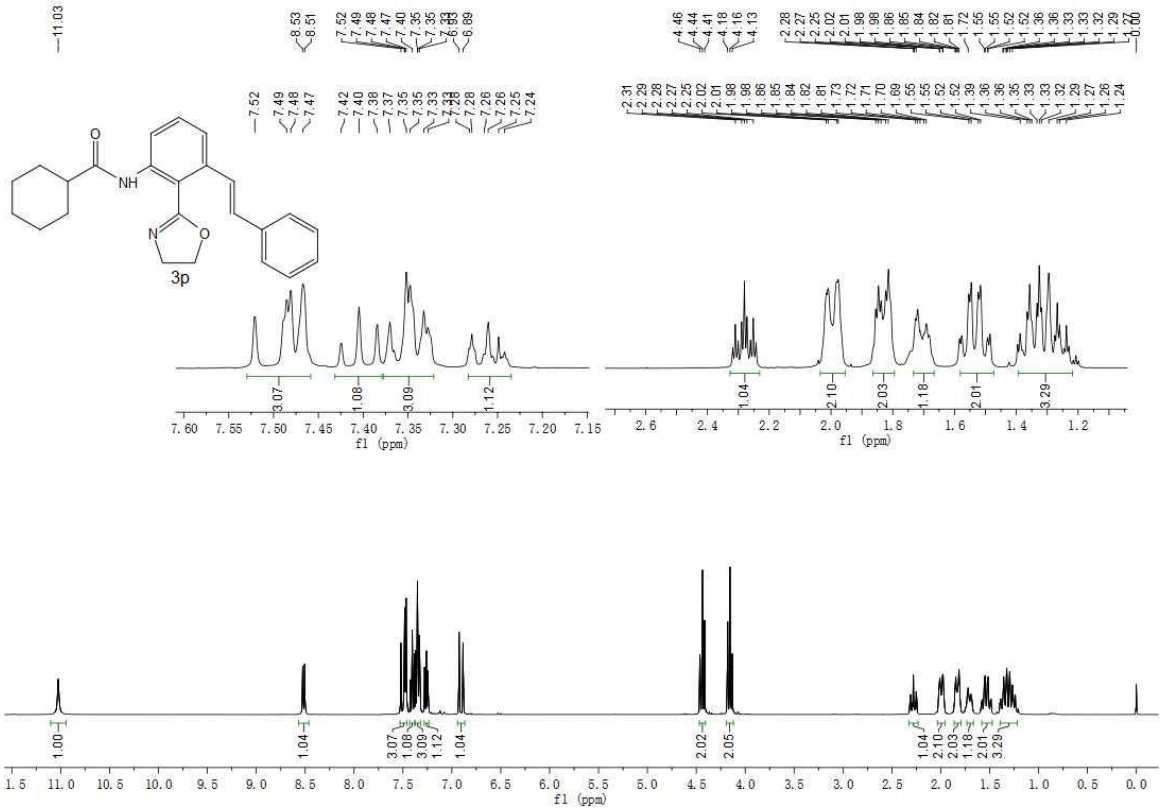

O
NH
F
F
F
N
O

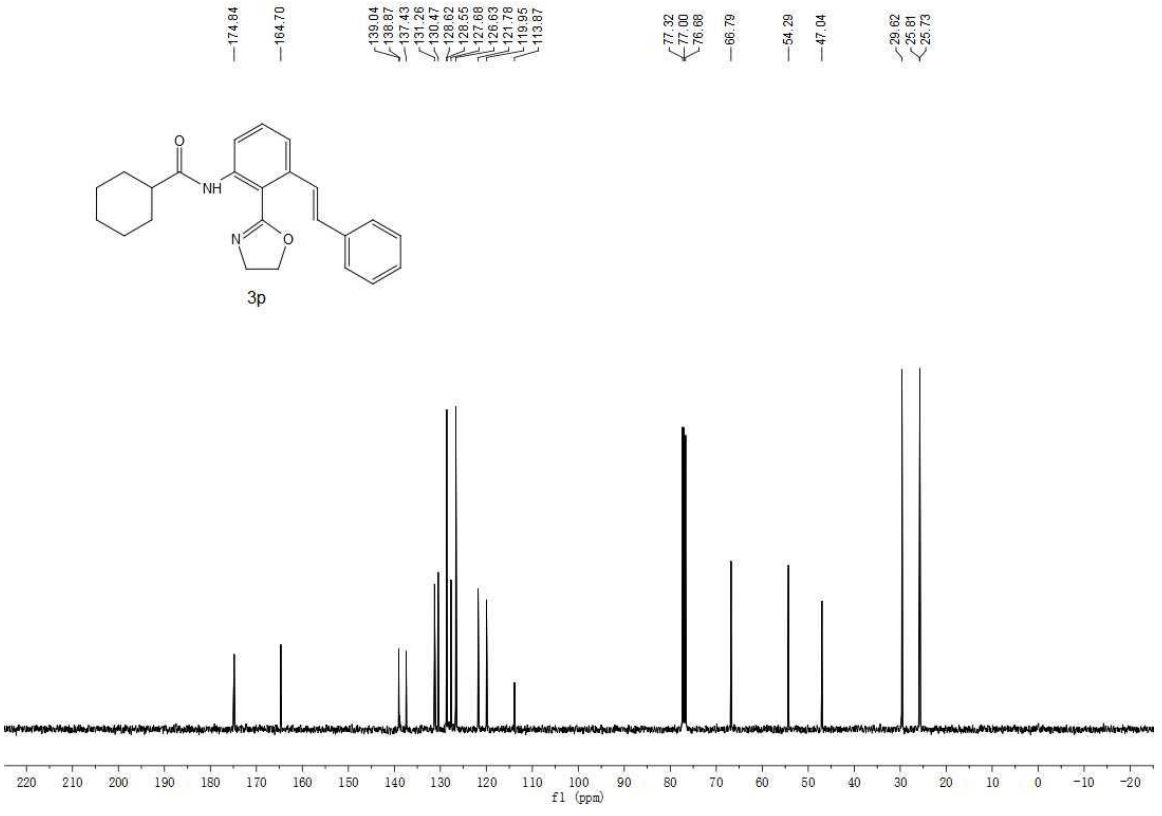
3n

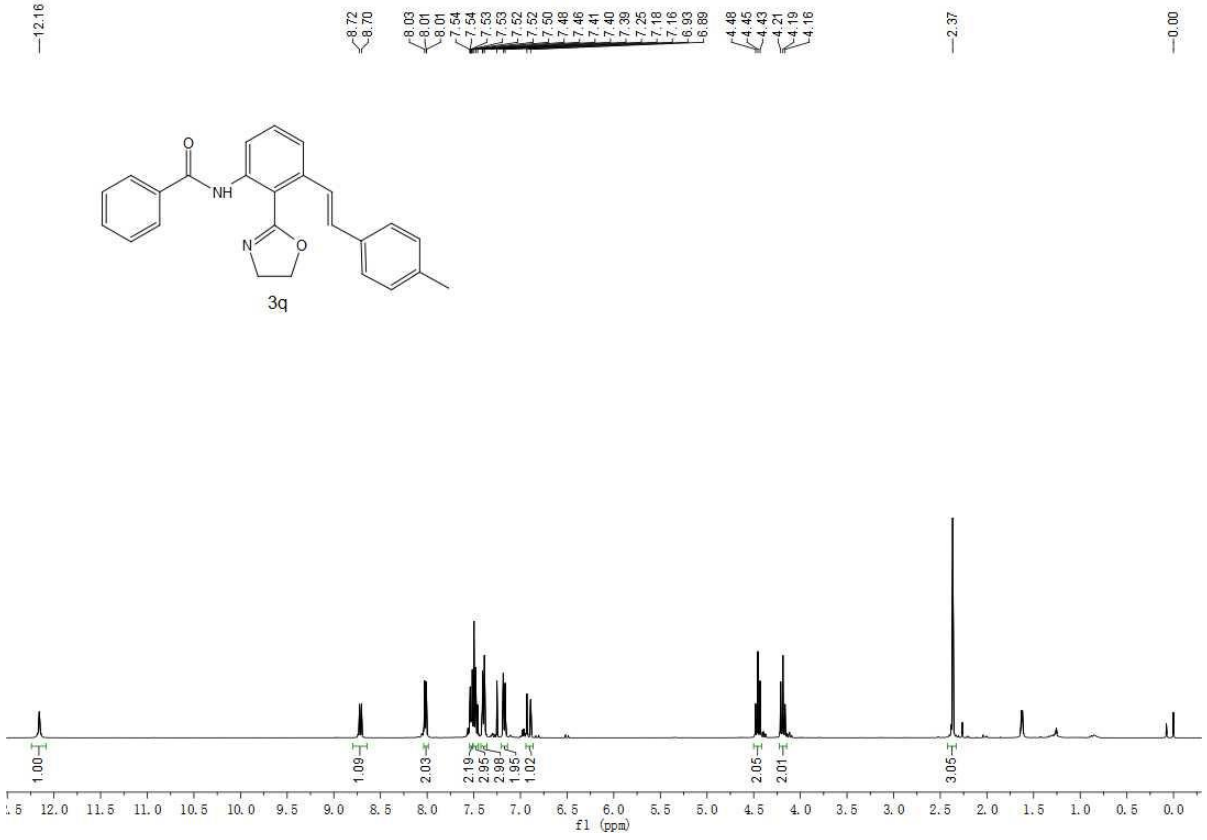
f1 (ppm)


3o
f1 (ppm)


3o
f1 (ppm)


3p
f1 (ppm)


3p
f1 (ppm)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8.72
8.70
8.03
8.01
8.01
7.54
7.53
7.53
7.52
7.52
7.50
7.48
7.46
7.41
7.40
7.39
7.25
7.18
7.16
6.93
6.89
4.48
4.45
4.43
4.21
4.19
4.16
2.37
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O
NH
N
O
3q
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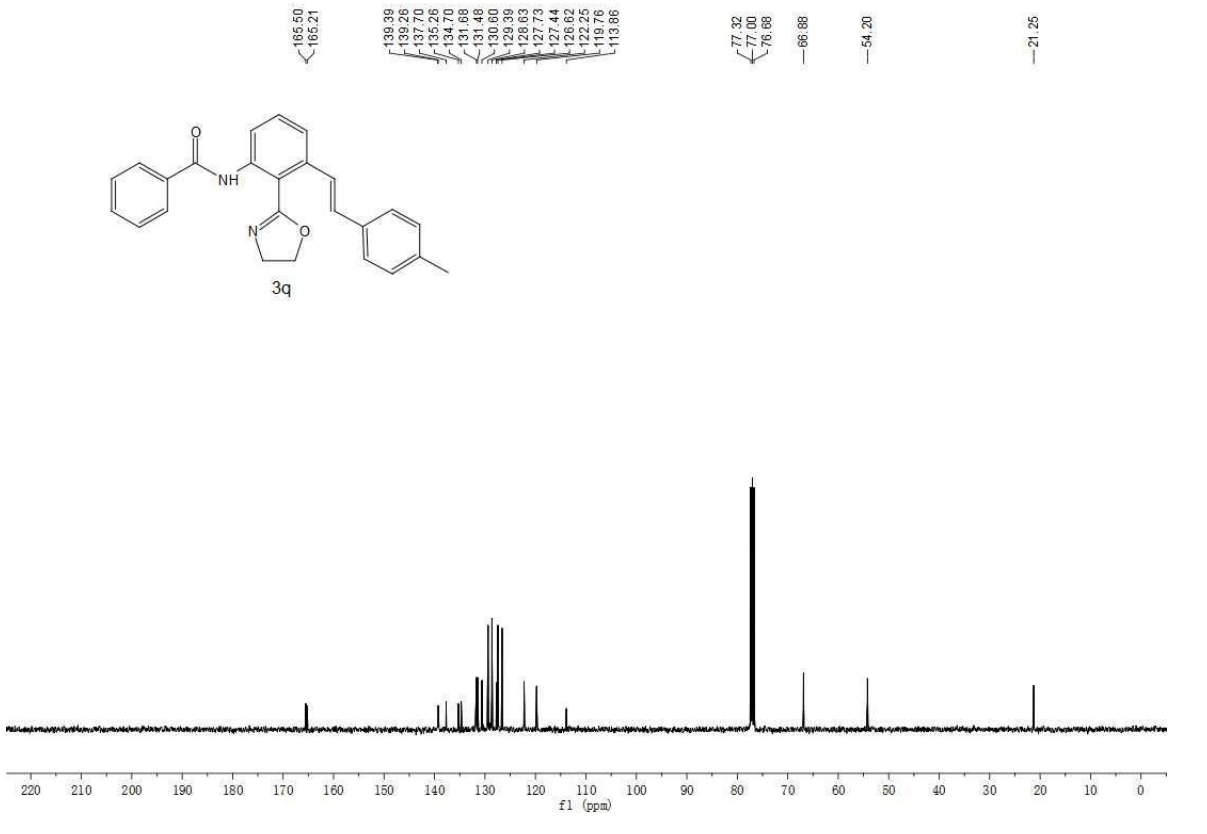
2.05
2.01
3.05
f1 (ppm)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127.44
126.62
122.25
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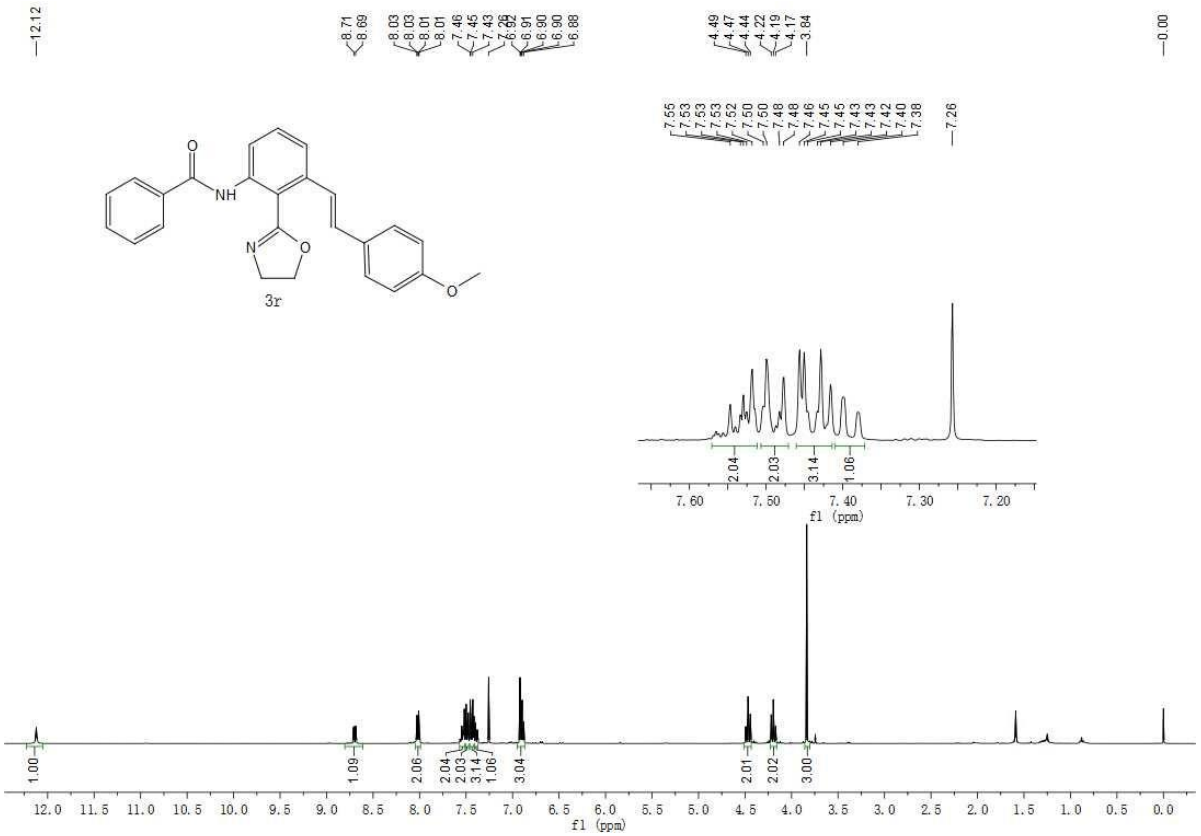
77.00
76.68
66.88
54.20
21.25
O
NH
N
O
3q
f1 (ppm)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8.01
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7.28
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6.91
6.90
6.90
6.88
4.49
4.47
4.44
4.22
4.19
4.17
3.84
0.00
7.55
7.53
7.53
7.53
7.52
7.50
7.50
7.48
7.48
7.46
7.45
7.45
7.43
7.43
7.42
7.40
7.38
7.26
O
NH
N
O
O
3r
2.04
2.03
3.14
1.06
7.60
7.50
7.40
7.30
7.20
f1 (ppm)
1.00
1.09
2.06
2.04
2.03
3.14
1.06
3.04
2.01
2.02
3.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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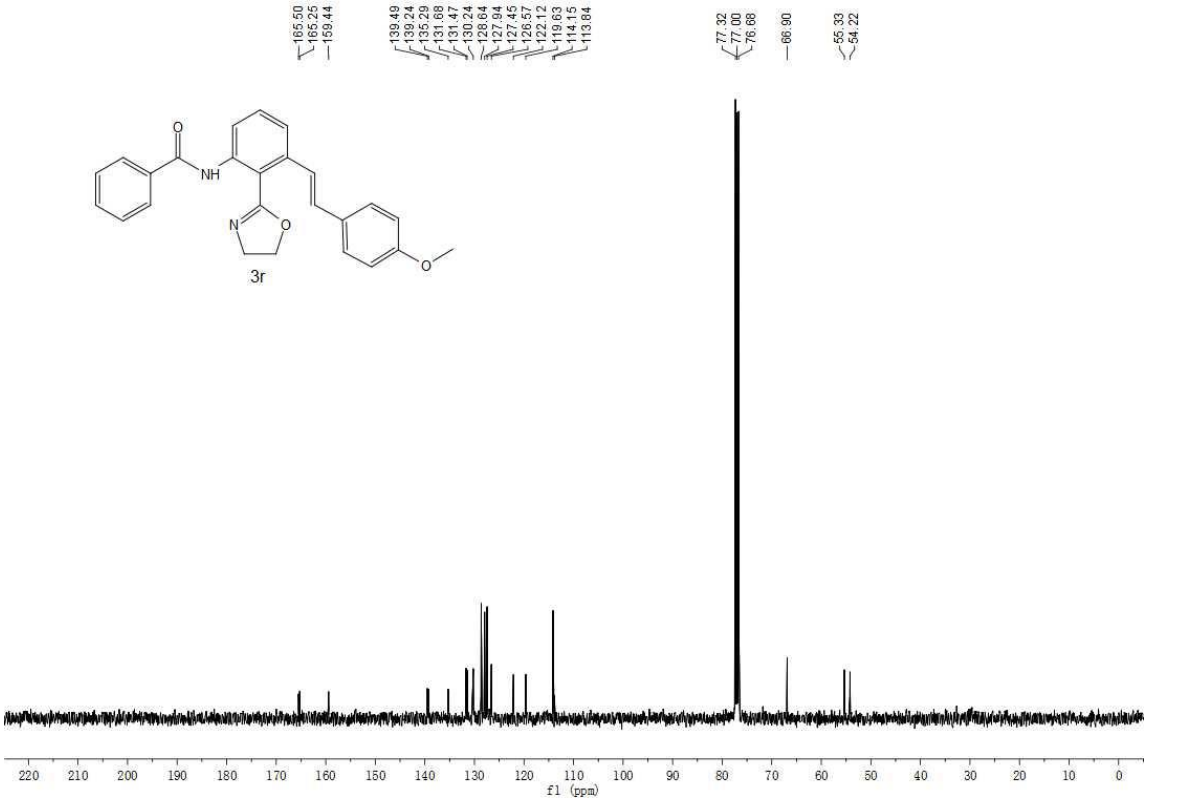
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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135.29
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127.94
127.45
126.57
122.12
119.63
114.15
113.84
77.32
77.00
76.68
66.90
55.33
54.22
O
NH
N
O
O
3r
220
210
200
190
180
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130
120
110
100
90
80
70
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50
40
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20
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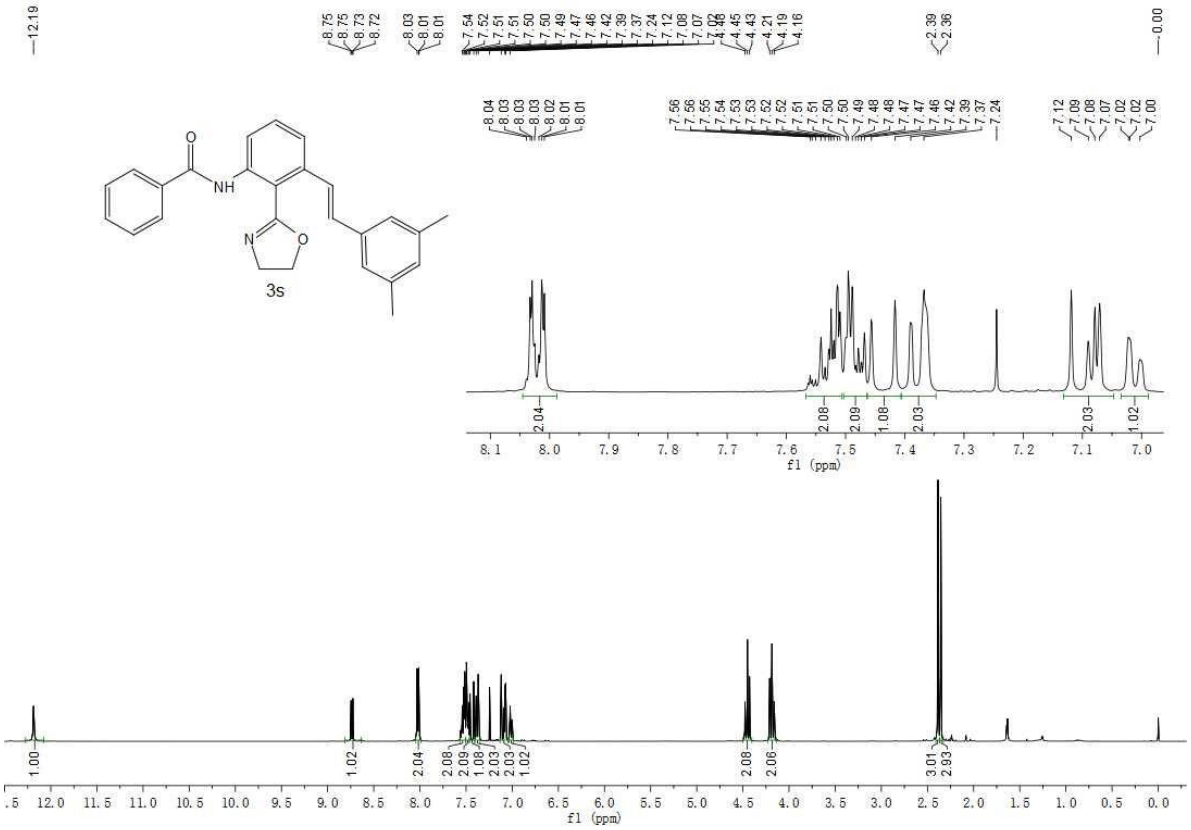
f1 (ppm)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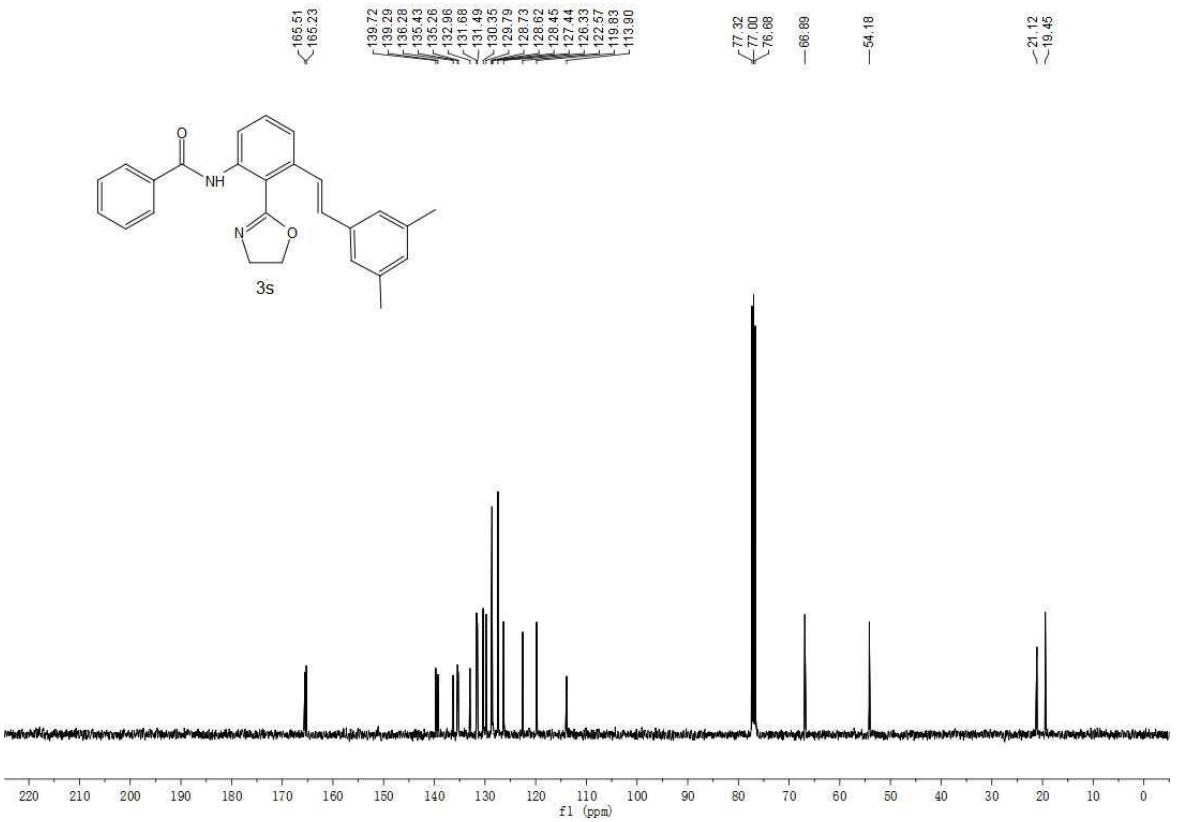
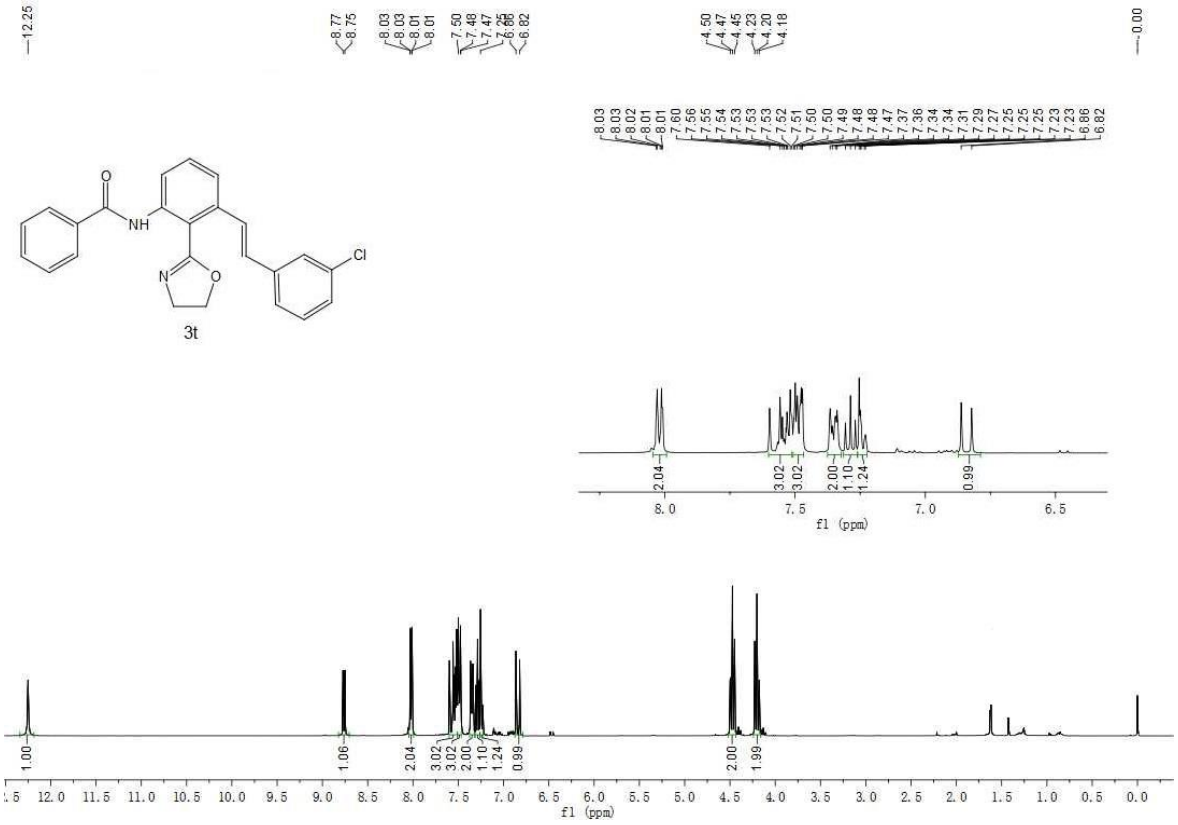
f1 (ppm)


3s
f1 (ppm)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8.75
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8.01
8.01
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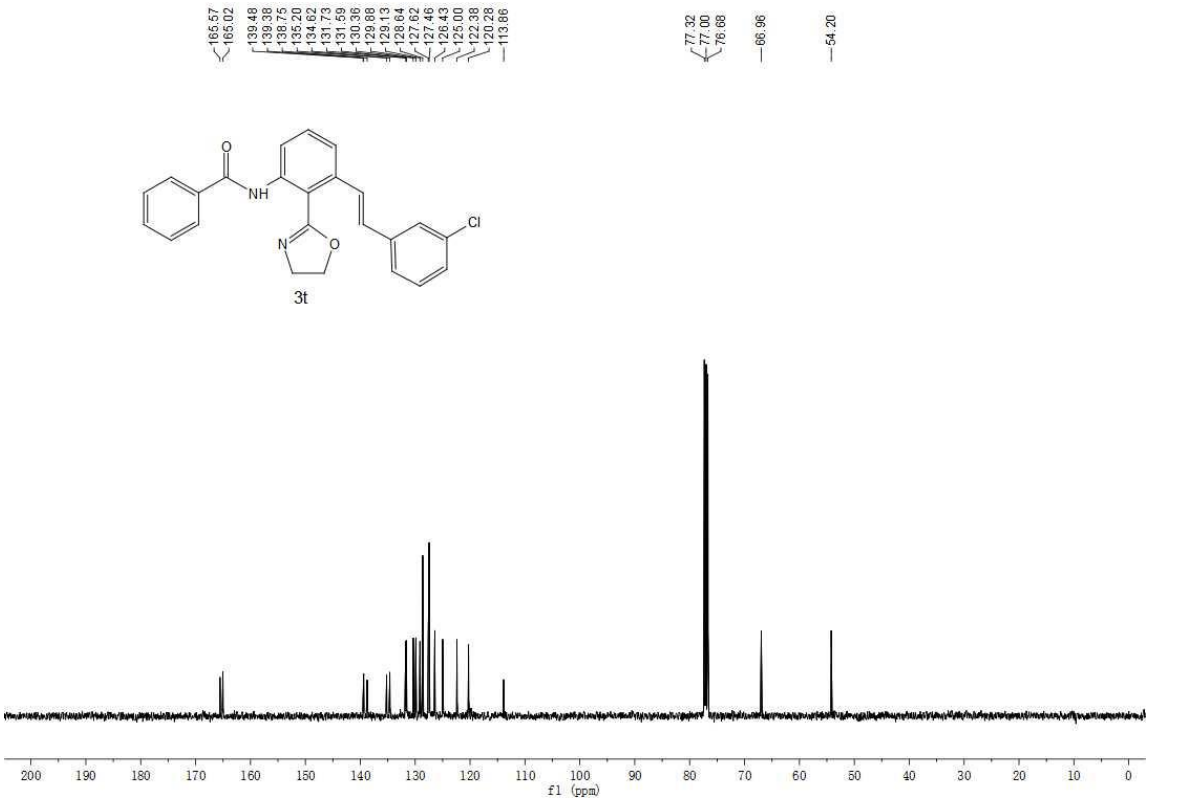
7.48
7.47
6.86
6.82
4.50
4.47
4.45
4.23
4.20
4.18
0.00
O
NH
N
O
Cl
3t
2.04
3.02
3.02
2.00
1.10
1.24
0.99
8.0
7.5
7.0
6.5
f1 (ppm)
1.00
1.06
2.04
3.02
3.02
2.00
1.10
1.24
0.99
2.00
1.99
f1 (ppm)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127.62
127.46
126.43
125.00
122.38
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77.00
76.68
66.96
54.20
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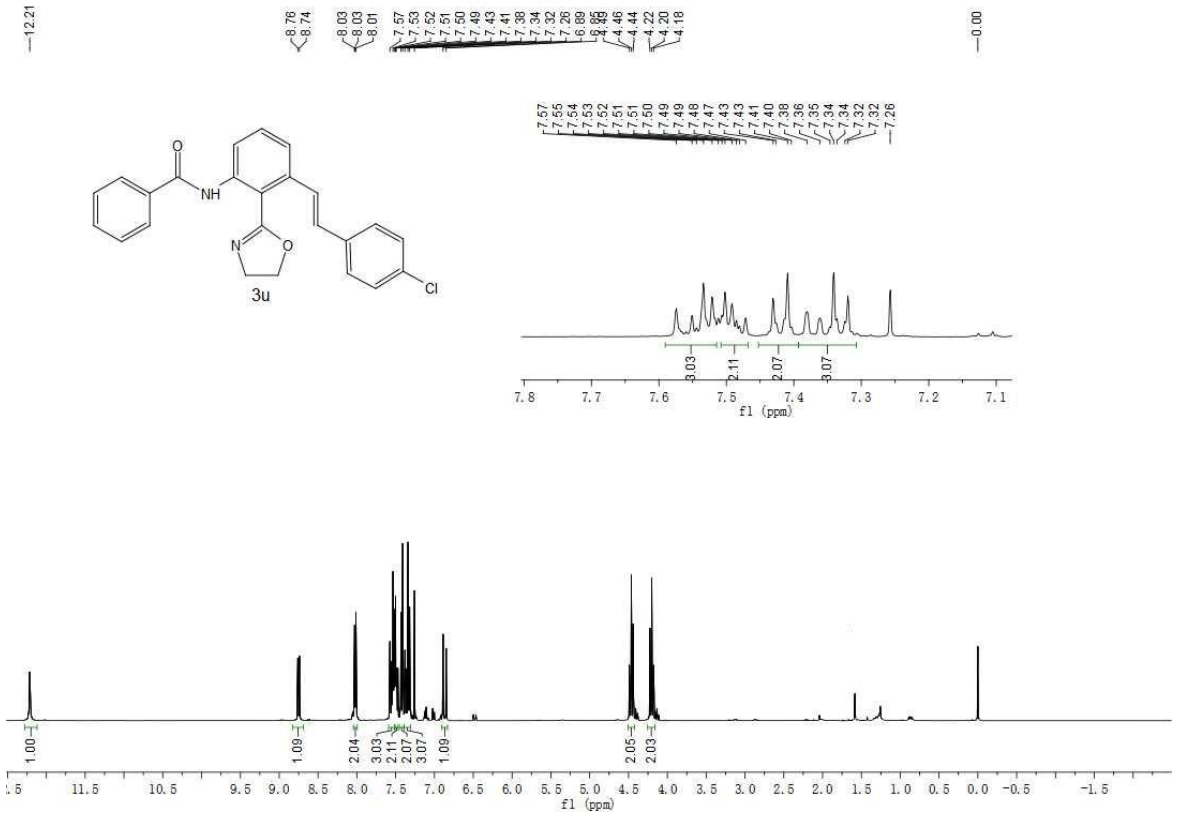
NH
N
O
Cl
3t
f1 (ppm)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8.01
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7.53
7.52
7.51
7.50
7.49
7.43
7.41
7.38
7.34
7.32
7.26
6.89
4.46
4.44
4.22
4.20
4.18
0.00
O
NH
N
O
Cl
3u
7.57
7.55
7.54
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.48
7.47
7.43
7.43
7.41
7.40
7.38
7.36
7.35
7.34
7.34
7.32
7.32
7.26
3.03
2.11
2.07
3.07
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
1.00
1.09
2.04
3.03
2.11
2.07
3.07
1.09
2.05
2.03
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
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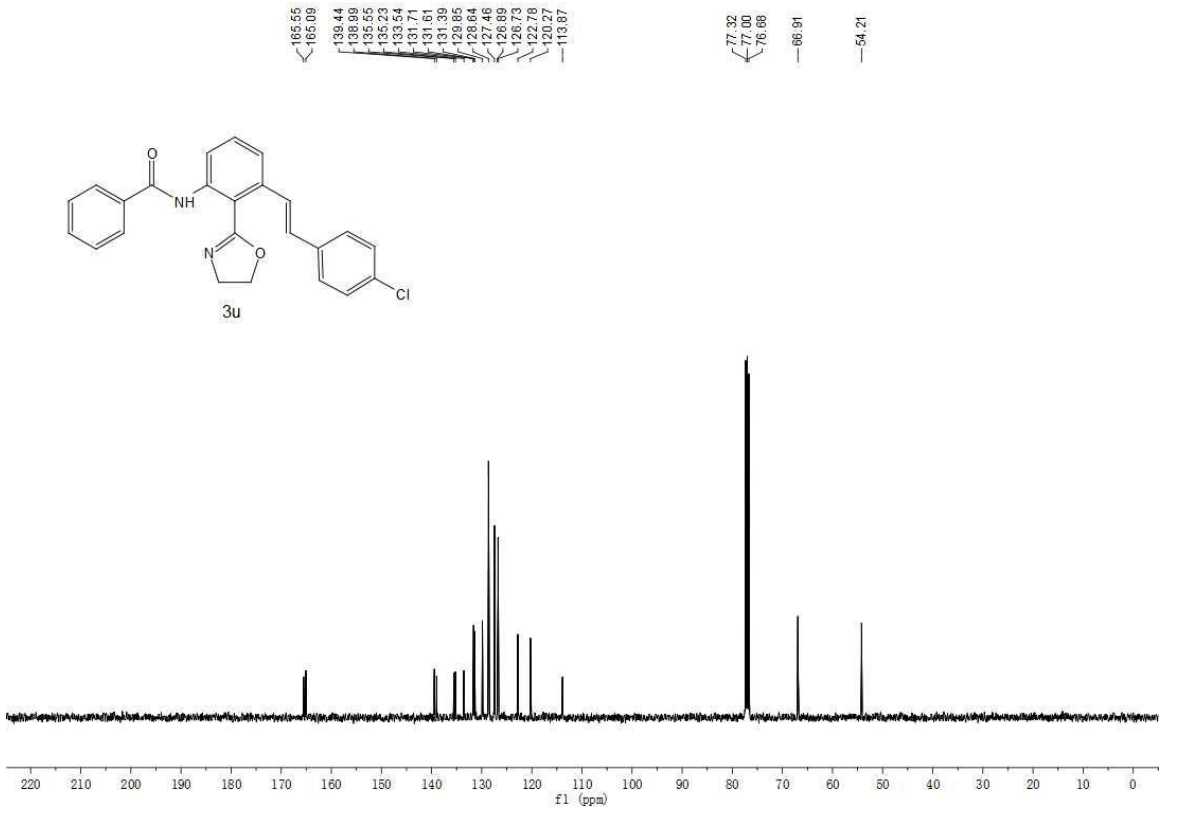
0.0
-0.5
-1.5
f1 (ppm)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127.46
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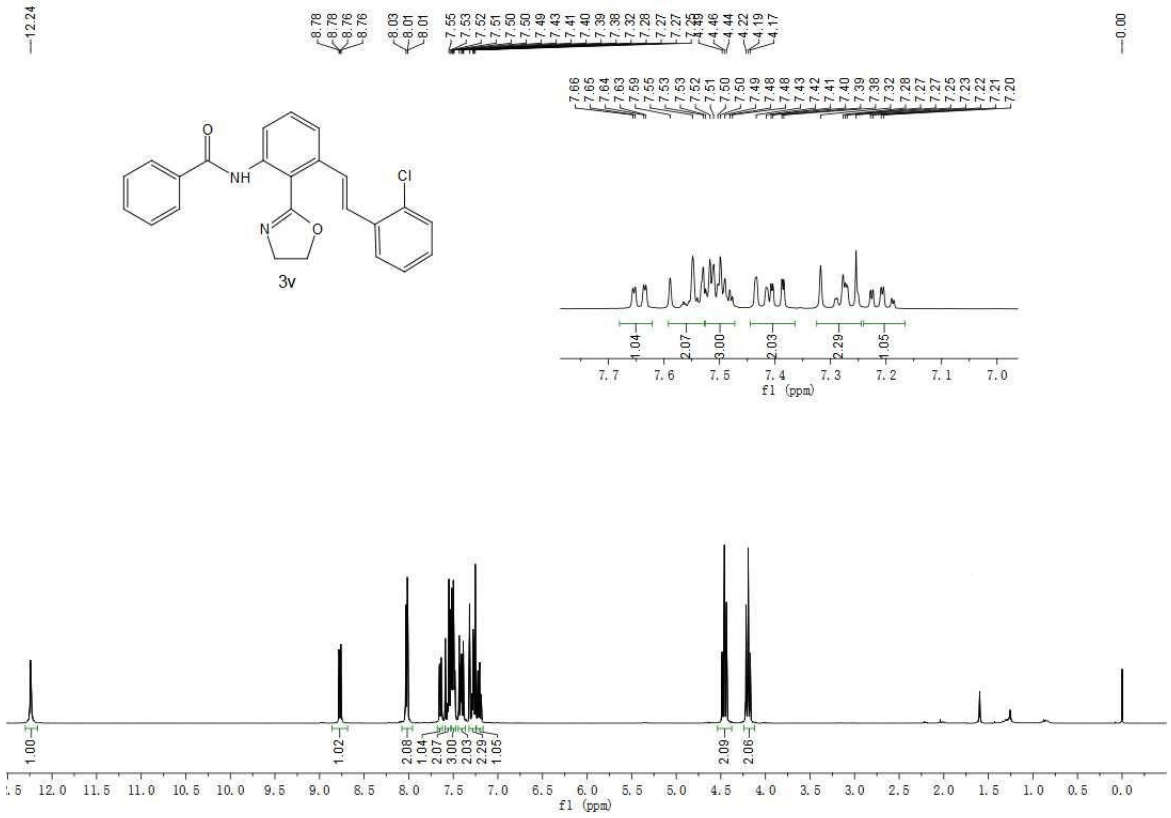
126.73
122.78
120.27
113.87
77.32
77.00
76.68
66.91
54.21
O
NH
N
O
Cl
3u
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.78
8.76
8.76
8.03
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7.53
7.52
7.51
7.50
7.50
7.49
7.43
7.41
7.40
7.39
7.38
7.32
7.28
7.27
7.27
4.46
4.44
4.22
4.19
4.17
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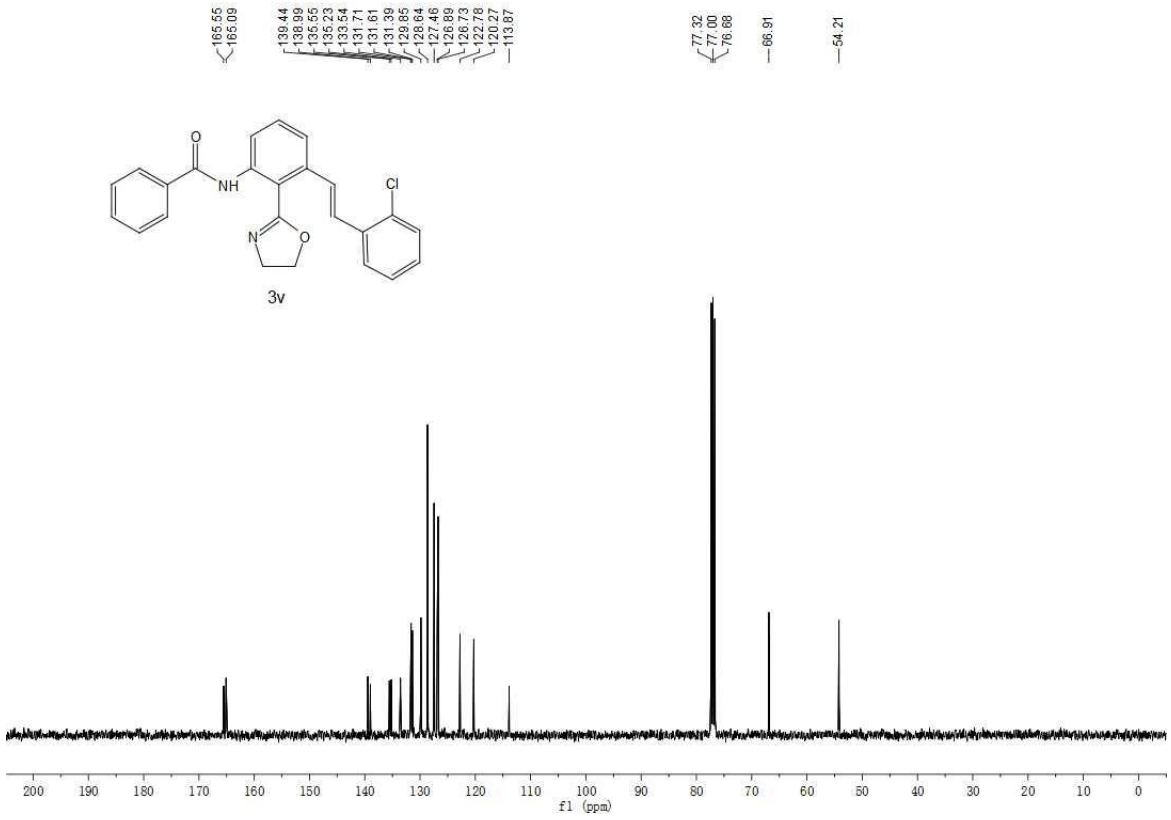
7.66
7.65
7.64
7.63
7.59
7.55
7.53
7.53
7.52
7.51
7.50
7.50
7.49
7.48
7.48
7.43
7.42
7.41
7.40
7.39
7.38
7.32
7.28
7.27
7.27
7.25
7.23
7.22
7.21
7.20
O
NH
Cl
N
O
3v
1.04
2.07
3.00
2.03
2.29
1.05
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
1.00
1.02
2.08
1.04
2.07
3.00
2.03
2.29
1.05
2.09
2.06
f1 (ppm)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131.71
131.61
131.39
129.85
128.64
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126.89
126.73
122.78
120.27
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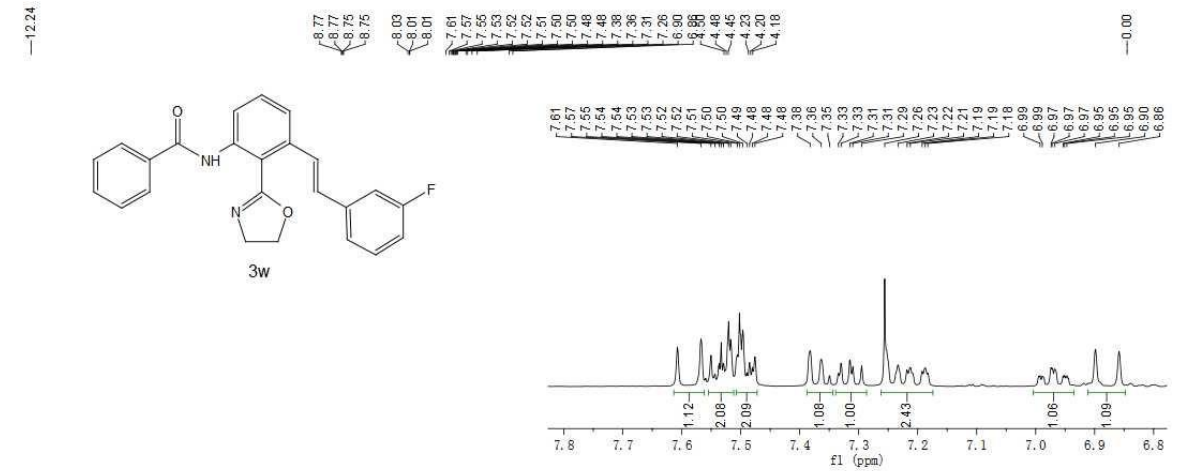
77.32
77.00
76.68
66.91
54.21
O
NH
Cl
N
O
3v
f1 (ppm)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8.01
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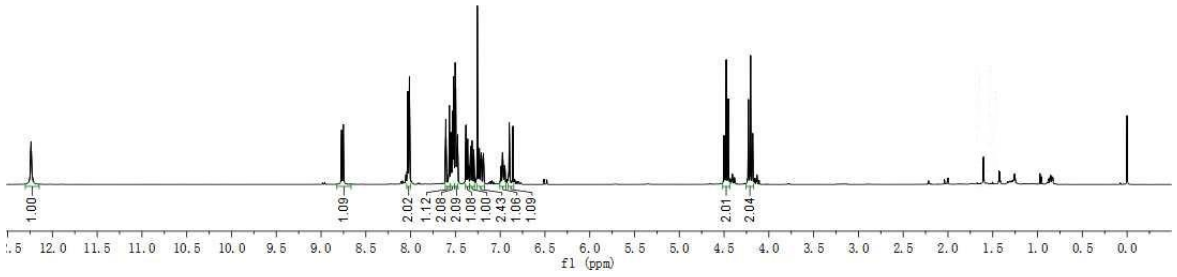
7.53
7.52
7.52
7.51
7.50
7.50
7.48
7.48
7.38
7.36
7.31
7.26
6.90
4.48
4.45
4.23
4.20
4.18
0.00
O
NH
N
O
F
3w
7.61
7.57
7.55
7.54
7.54
7.53
7.53
7.52
7.52
7.51
7.50
7.50
7.49
7.48
7.48
7.48
7.38
7.36
7.35
7.33
7.33
7.31
7.31
7.29
7.26
7.23
7.22
7.21
7.19
7.19
7.18
6.99
6.99
6.97
6.97
6.97
6.95
6.95
6.95
6.90
6.86
1.12
2.08
2.09
1.08
1.00
2.43
1.06
1.09
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
f1 (ppm)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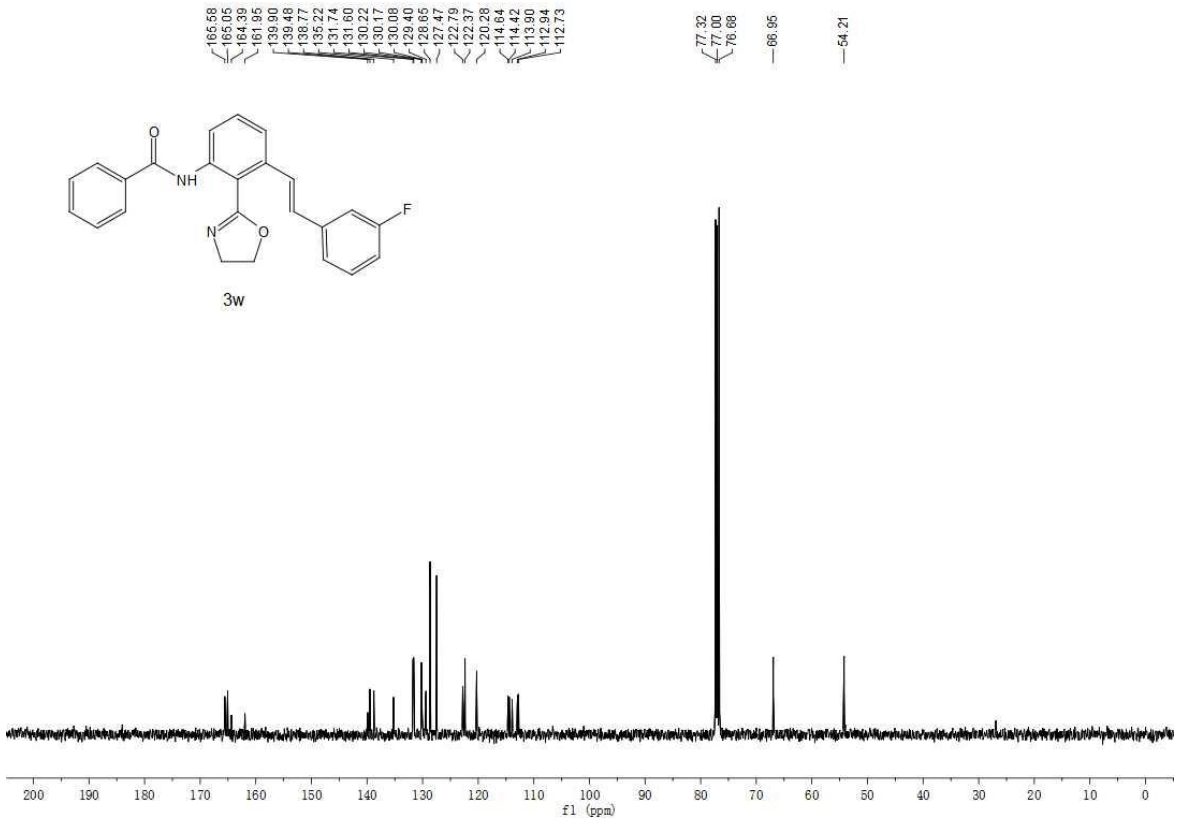
1.12
2.08
2.09
1.08
1.00
2.43
1.06
1.09
2.01
2.04
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.60
130.22
130.17
130.08
129.40
128.65
127.47
122.79
122.37
120.28
114.64
114.42
113.90
112.94
112.73
77.32
77.00
76.68
66.95
54.21
O
NH
N
O
F
3w
200
190
180
170
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150
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130
120
110
100
90
80
70
60
50
40
30
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10
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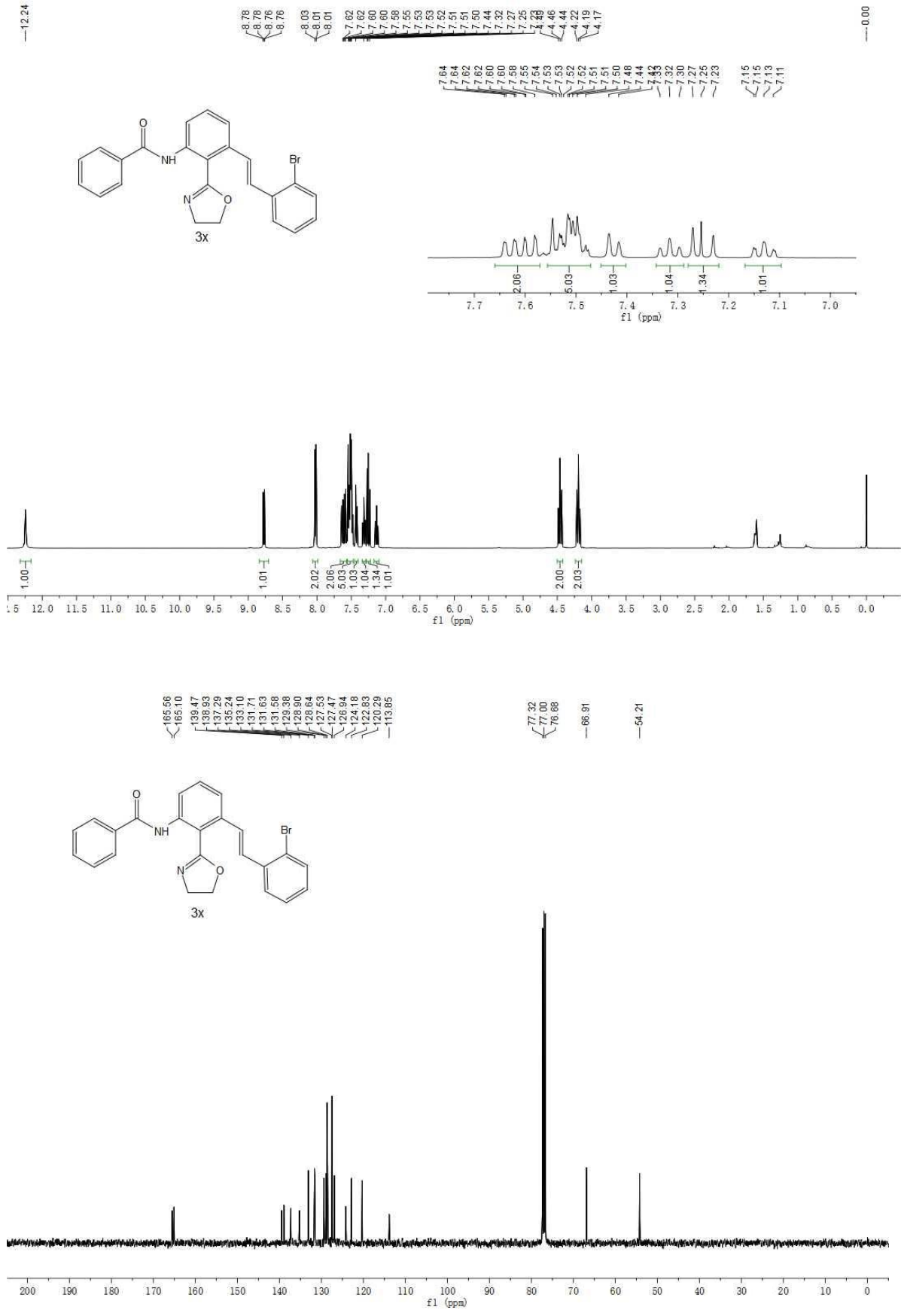
f1 (ppm)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8.76
8.76
8.03
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8.01
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7.62
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7.55
7.53
7.53
7.52
7.51
7.51
7.50
7.44
7.32
7.27
7.25
4.46
4.44
4.22
4.19
4.17
0.00
7.64
7.64
7.62
7.62
7.60
7.60
7.58
7.55
7.54
7.53
7.53
7.52
7.52
7.51
7.51
7.50
7.48
7.44
7.32
7.30
7.27
7.25
7.23
7.15
7.15
7.13
7.11
O
NH
Br
N
O
3x
2.06
5.03
1.03
1.04
1.34
1.01
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
1.00
1.01
2.02
2.06
5.03
1.03
1.04
1.34
1.01
2.00
2.03
f1 (ppm)
165.56
165.10
139.47
138.93
137.29
135.24
133.10
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131.63
131.58
129.38
128.90
128.64
127.53
127.47
126.94
124.18
122.83
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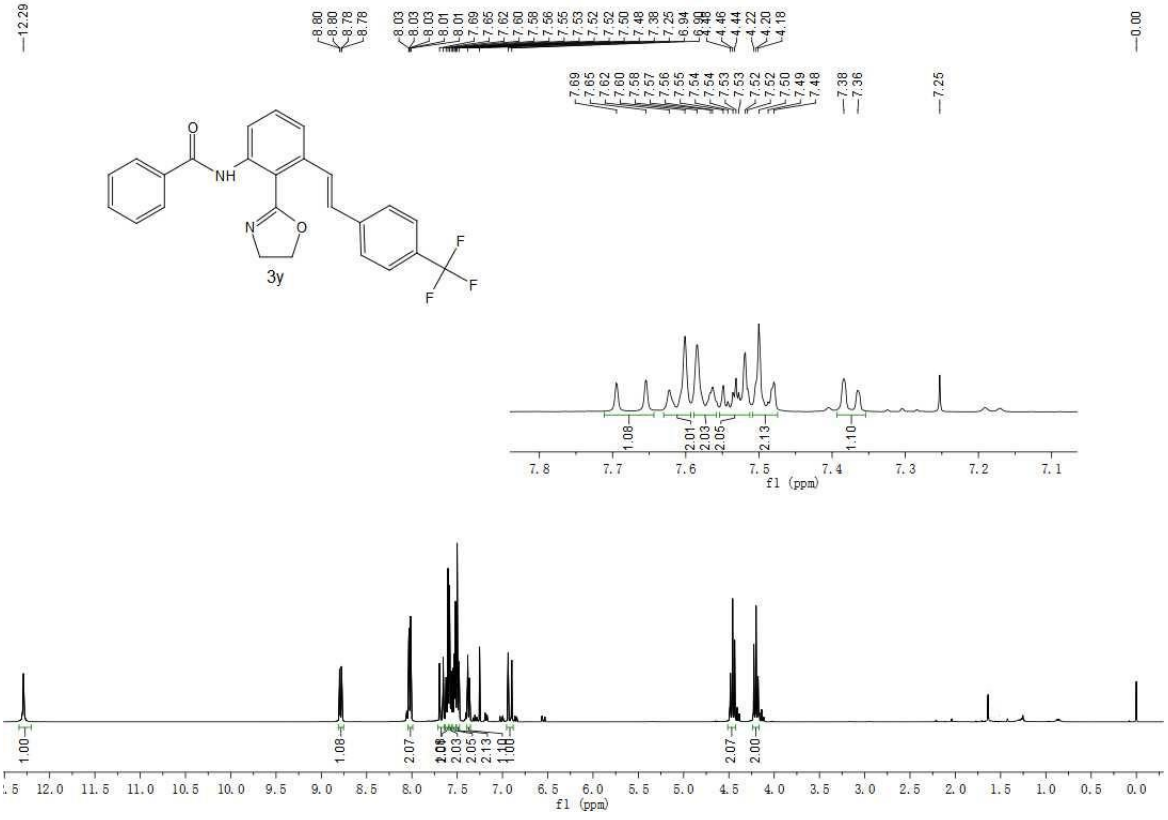
77.00
76.68
66.91
54.21
O
NH
Br
N
O
3x
f1 (ppm)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8.03
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8.01
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7.62
7.60
7.59
7.56
7.55
7.53
7.52
7.52
7.50
7.48
7.38
7.25
6.94
4.46
4.44
4.22
4.20
4.18
0.00
7.69
7.65
7.62
7.60
7.58
7.57
7.56
7.55
7.54
7.54
7.53
7.53
7.52
7.52
7.50
7.49
7.48
7.38
7.36
7.25
O
NH
N
O
F
F
F
3y
1.08
2.01
2.03
2.05
2.13
1.10
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
f1 (ppm)
1.00
1.08
2.07
2.03
2.05
2.13
1.10
2.07
2.00
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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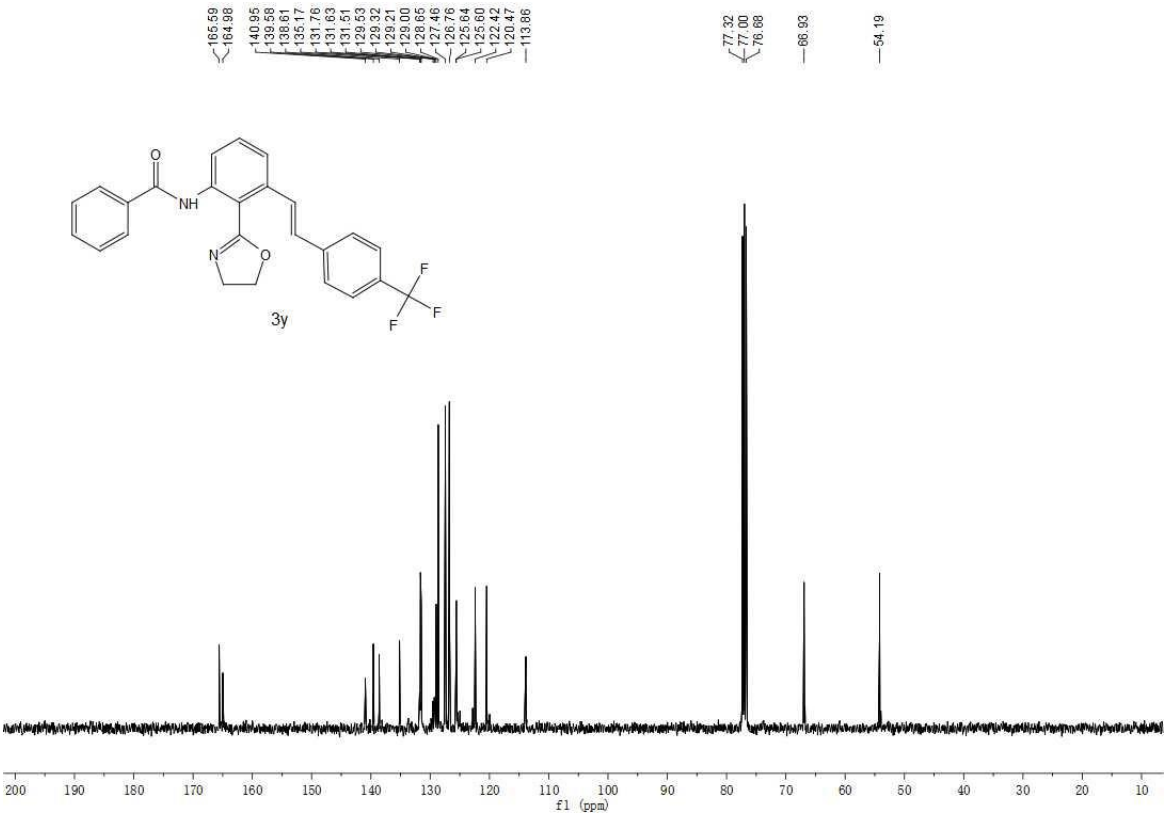
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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131.63
131.51
129.53
129.32
129.21
129.00
128.65
127.46
126.76
125.64
125.60
122.42
120.47
113.86
77.32
77.00
76.68
66.93
54.19
O
NH
N
O
F
F
F
3y
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)