Supporting Information

Copper Catalyzed Oxidative [2+2+1] Cycloaddition: Regioselective Synthesis of 1, 3-Oxazoles from Internal Alkynes and Nitriles

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A. General method

^{1}H and ^{13}C NMR spectra were recorded using a Bruker Avance 400 MHz NMR spectrometer. The chemical shifts are referenced to signals at 7.26 and 77.0 ppm, respectively, and chloroform is solvent with TMS as the internal standard. IR spectra were obtained either as potassium bromide pellets or as liquid films between two potassium bromide pellets with a Bruker Vector 22 spectrometer. Mass spectra were recorded on a Shimadzu GCMS-QP5050A spectrometer at an ionization voltage of 70 eV equipped with a DB-WAX capillary column (internal diameter: 0.25 mm, length: 30 m). GC–MS was obtained using electron ionization. HRMS was carried out on a MAT 95XP (Thermo). TLC was performed by using commercially prepared 100–400 mesh silica gel plates (GF_{254}) and visualization was effected at 254 nm. All the other chemicals were purchased from Aldrich Chemicals.

B. General procedure for the synthesis of oxazoles

To a dried Schlenk tube, the mixture of alkyne (0.5 mmol), nitrile (1.5 or 0.6 mmol), H_2O (2.5 mmol), $Cu(OAc)_2$ (10 mol %) and $BF_3{\cdot}Et_2O$ (1 equiv), 2 mL $MeNO_2$ was added successively. Then the mixture was stirred at 80 or 100 ^{o}C for 12 h under 1 atm O_2. After completion, the reaction mixture was purified by preparative TLC (GF_{254}) with petroleum ether/ethyl acetate (50:1 to 20:1) to give the desired products **3aa-3qa**, **3ab-3aj**, **3eb**, **3fb**, **3ce**, **3fe**, **3le**, **3me**, **3re**, **3se**, **3tj**, **3qa**, **and 5**.

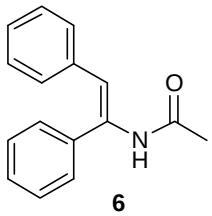
Procedure for the synthesis of 4,5-diphenyl-2-methyloxazole (3aa) from 1,2-diphenylethyne (1a) and acetonitrile (2a). To a dried Schlenk tube, the mixture of 1,2-diphenylethyne (0.5 mmol), acetonitrile (1.5 mmol), H_2O (2.5 mmol), $Cu(OAc)_2$ (10 mol %) and $BF_3{\cdot}Et_2O$ (1 equiv), 2 mL $MeNO_2$ was added successively. Then the mixture was stirred at 80 ^{o}C for 12 h under 1 atm O_2. After completion, the reaction mixture was separated by preparative TLC to give product **3aa** in pure form.

Procedure for the synthesis of 10 from 9.(1) A solution of **9** (0.36 g, 1.4 mmol) in

chlorosulfonic acid (0.42 mL, 6.0 mmol) was stirred at 60 °C for 20 h. The solution was cooled and poured into crash ice carefully. The precipitated product was filtered and washed with abundant cold water than dried in the vacuum-oven at 40 □. sulfuryl chloride (0.04 mL, 1.5 equiv.) was added dropwise and stirred for 18 h at room temperature. After cooling the solution to 0 ˚C, he reaction was quenched with water (5 mL) at 0 °C and was extracted with ethyl acetate (3×5 mL). The organic layer was washed with brine, dried over Na_2SO_4, filtered, and evaporated. The residue was purified over silica gel to give the 4-(5-(4-fluorophenyl)-2-methyloxazol-4-yl)benzene-1-sulfonyl chloride product in 75% yield. Subsequently, conc. aq NH_3 (0.5 mL, 7.3 mmol) was added to a solution of 4-(5-(4-fluorophenyl)-2-methyloxazol-4-yl)benzene-1-sulfonyl chloride (188 mg, 0.54 mmol) in THF (10 mL) at 0 ºC, and the ice bath was removed. The mixture was stirred for 7 min and then Cs_2CO_3 (0.55 g, 1.7 mmol) and MeOH (4 mL) were added. After stirring for a further 15 min, the mixture was diluted with brine and extracted with CH_2Cl_2 (5×3). The combined extracts were dried and evaporated to give **10** (136 mg, 80%) as an orange solid.

C. Control Experiments

(I)



6

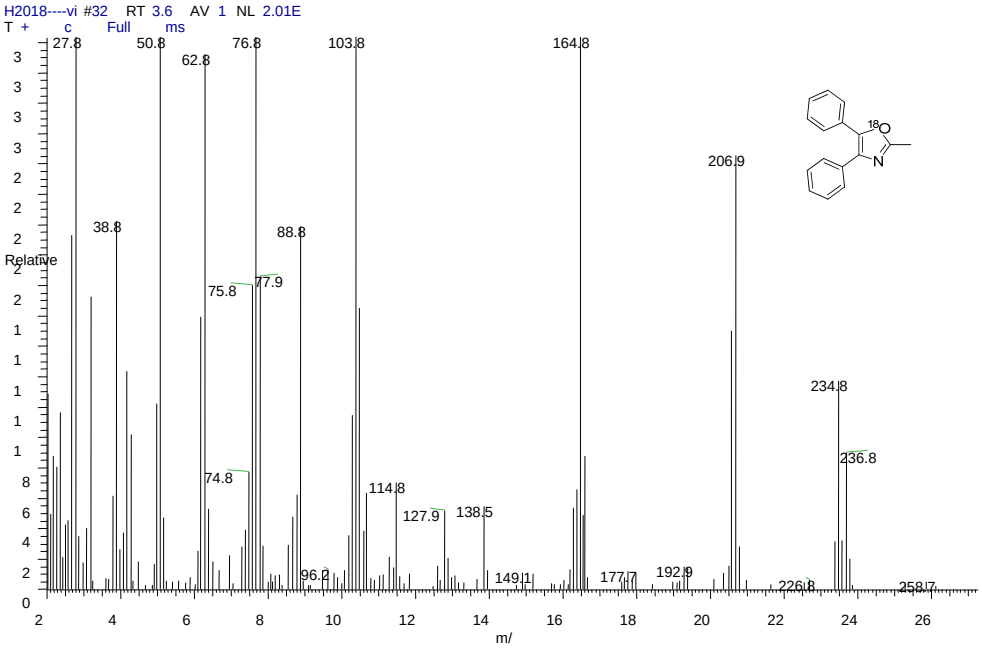
(E)-N-(1,2-diphenylvinyl)acetamide

6 was prepared and its spectroscopic data were in accordance with the literature data.[(2)] ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.45 (s, 1H), 7.31 (s, 5H), 7.07-7.06 (m, 3H), 6.94-6.92 (m, 2H), 6.74 (s, 1H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 168.9, 137.4, 136.7, 135.0, 129.6, 129.4, 129.1, 128.9, 128.1, 126.3, 117.9, 25.0.

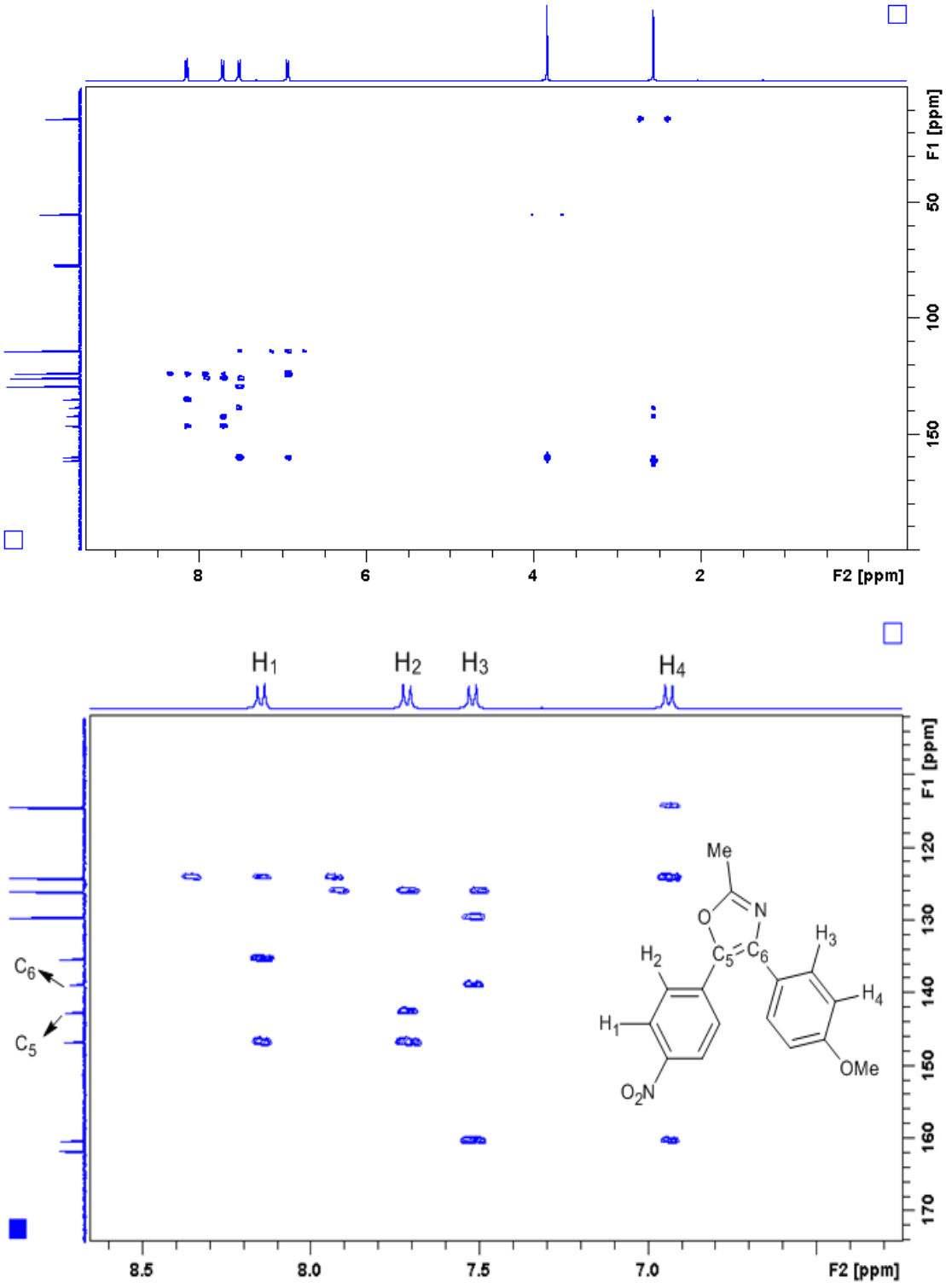
(II) Procedure for ^{18}O-labeling experiment

To a dried Schlenk tube, the mixture of 1,2-diphenylethyne (0.5 mmol), acetonitrile

(1.5 mmol), $H_2{}^{18}O$ (2.5 mmol), $Cu(OAc)_2$ (10 mol %) and $BF_3{\cdot}Et_2O$ (1 equiv), 2 mL $MeNO_2$ was added successively. Then the mixture was stirred at 80 ^oC for 12 h under 1 atm O_2. After completion, the reaction mixture was separated by preparative TLC using light petroleum ether/ethyl acetate (20:1) as eluent to give product in pure form.

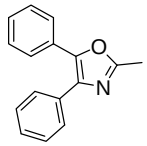


D. The structure determination of 3pa according to HMBC spectrum



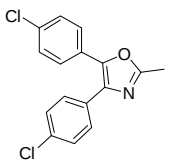
E. Analytical data

4,5-Diphenyl-2-methyloxazole (3aa) [3]



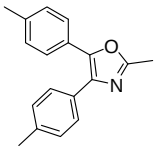
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.65-7.57 (m, 4 H), 7.36-7.32 (m, 6 H), 2.55 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$)** δ = 160.2, 145.3, 128.4, 128.0, 127.8, 126.4, 14.0. **MS** (EI) m/z: 28, 51, 77, 105, 165, 235. **IR** (KBr, cm^{-1}): *v* 3066, 1472, 1227, 1117, 1025, 712.

4,5-Bis(*p*-chlorophenyl)-2-methyl-oxazole (3ba)



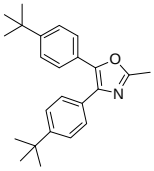
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.54 (d, *J* = 8.0 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.34 (dd, *J* = 2.4 Hz, 8.8 Hz, 4H), 2.54 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 160.6, 144.5, 134.5, 134.4, 134.1, 130.7, 129.1, 129.0, 128.9, 127.7, 127.3, 14.0. **MS** (EI) m/z: 28, 42, 57, 75, 103, 111, 138, 163, 199, 240, 275, 303. **IR** (KBr, cm^{-1}): *v* 3489, 2922, 1650, 1384, 1093, 962, 827, 520. HRMS calc. $C_{16}H_{11}Cl_2NO$ [M^+]: 305.0183, Found: 305.0179.

4,5-Di(4-methyl-phenyl)-2-methyl-oxazole (3ca)



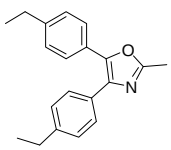
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.53 (d, *J* = 7.6 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.17 (d, *J* = 7.2 Hz, 4H), 2.53 (s, 3H), 2.36 (s, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.9, 145.2, 138.3, 137.7, 129.7, 129.3, 129.2, 127.7, 126.4, 21.4, 21.3, 14.0. **MS** (EI) m/z: 28, 32, 43, 65, 91, 117, 152, 179, 194, 222, 235, 263. **IR** (KBr, cm^{-1}): *v* 3855, 3746, 2923, 1700, 1650, 1513, 1460. HRMS calc. $C_{21}H_{14}NOF$ [M+H]$^+$: 264.1388, Found: 264.1392.

4,5-Bis(4-*tert*-butylphenyl)-2-methyloxazole (3da)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.58 (dd, *J* = 8.8 Hz, 40.0 Hz, 4H), 7.39 (d, *J* = 8.0 Hz, 4H), 2.53 (s, 3 H), 1.33 (d, *J* = 1.6 Hz, 18H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.8, 151.3, 150.8, 145.1, 134.6, 129.7, 128.6, 127.4, 126.4, 126.1, 125.5, 125.4, 34.7, 34.6, 31.3, 31.2, 14.0. **MS** (EI) m/z: 41, 57, 91, 115, 130, 159, 276, 304, 332, 347. **IR** (KBr, cm^{-1}): *v* 3463, 1609, 1472, 1273, 1114, 1017, 851, 778, 706, 545. HRMS calc. $C_{24}H_{29}NO$ [M^+]: 347.2244, Found: 347.2248.

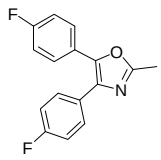
4,5-Bis(4-ethylphenyl)-2-methyl-oxazole (3ea)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.60 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* =8.0 Hz, 2H), 7.22-7.19 (m, 4H), 2.71-2.64 (m, 4H), 2.55 (s, 3H), 1.27 (dt, *J* = 2.8 Hz, 7.8 Hz, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.9, 145.2, 144.6, 144.0, 134.6, 129.9, 128.1, 128.0, 127.7, 126.7, 126.5, 28.7, 15.5, 15.4, 14.0. **MS** (EI) m/z: 29, 43, 77, 115, 117, 132, 165, 178,

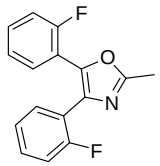
222, 248, 263, 276, 291. **IR** (KBr, cm^{-1}): *v* 3058, 2963, 1587, 1406, 1364, 836. HRMS calc. $C_{19}H_{20}N_2O$ $[M+H]^+$: 292.1570, Found: 292.1596.

4,5-Bis(4-fluorophenyl)2-methyl-oxazole (3fa)



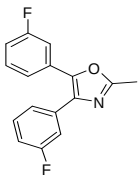
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.59-7.50 (m, 4H), 7.08-7.04 (m, 4H), 2.54 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 163.9, 163.8, 161.4, 161.3, 160.3, 144.4, 128.4, 128.3, 125.1, 116.0, 115.8, 13.9. **MS** (EI) m/z: 57, 75, 95, 122, 181, 201, 243, 271. **IR** (KBr, cm^{-1}): *v* 3464, 1667, 1508, 1232, 1156, 1100, 843. HRMS calc. $C_{16}H_{11}F_2NO$ $[M^+]$: 271.0809, Found: 271.0805.

4,5-Bis(2-fluorophenyl)-2-methyloxazole (3ga)



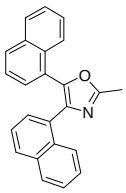
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.69 (dt, J = 1.6 Hz, 7.6 Hz, 1H), 7.49 (dt, J = 1.6 Hz, 7.6 Hz, 1H), 7.28-7.24 (m, 2H), 7.16 (dt, J = 0.8 Hz, 1H), 7.12 (dt, J = 0.8 Hz, 1H), 7.07-7.00 (m, 2H), 2.53 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 161.3, 161.1, 160.6, 106.5, 158.7, 158.6, 158.0, 142.3, 132.1, 130.6, 130.5, 130.4, 13.3, 129.7, 129.2, 129.1, 124.1, 124.0, 123.9, 120.8, 120.7, 120.6, 117.7, 117.6, 117.5, 116.0, 115.8, 115.7, 115.5, 13.9. **MS** (EI) m/z: 28, 57, 75, 95, 122, 175, 181, 201, 243, 271. **IR** (KBr, cm^{-1}): *v* 3068, 1704, 1586, 1448, 1223, 1103, 819, 760, 657. HRMS calc. $C_{16}H_{11}F_2NO$ $[M^+]$: 271.0809, Found: 271.0805.

4,5-Bis(3-fluorophenyl)-2-methyloxazole (3ha)



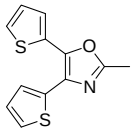
^{1}H NMR (400 MHz, $CDCl_3$): δ =7.68 (dd, J = 7.2 Hz, 1H), 7.11 (dd, J = 7.6 Hz, 1H), 7.36-7.29 (m, 2H), 7.19-7.14(m, 2H), 7.06-7.01 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ = 161.3, 161.1, 161.1, 160.5, 158.6, 142.3, 130.5, 129.8, 129.2, 124, 116, 115.8, 115.7, 115.4, 14.0. **MS** (EI) m/z: 28, 42, 75, 95, 122, 181, 201, 243, 271. **IR** (KBr, cm^{-1}): *v* 2929, 1677, 1589, 1446, 1262, 892, 760. HRMS calc. $C_{16}H_{11}F_2NO$ $[M^+]$: 271.0809, Found: 271.0805.

4,5-Di(naphthalen-1-yl)-2-methyloxazole (3ia)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.20 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 4.4 Hz, 1H), 7.80-7.72 (m, 4H), 7.44-7.31 (m, 6H), 7.24-7.20 (m, 3H), 2.67 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 1171.1, 160.8, 146.8, 136.8, 133.7, 131.1, 129.5, 128.4, 128.1, 126.6, 126.3, 126.0, 125.8, 125.5, 125.2, 125.1, 14.3. **MS** (EI) m/z: 28, 77, 119, 127, 153, 265, 292, 307, 335. **IR** (KBr, cm^{-1}): *v* 1509, 1380, 1240, 1194, 1135, 779. HRMS calc. $C_{24}H_{17}NO$ $[M^+]$: 335.1310, Found: 335.1313.

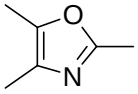
4,5-Di(thiophen-2-yl)-2-methyloxazole (3ja)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.46 (s, 2H), 7.39 (d, J = 4.8 Hz, 1H), 7.33 (d, J = 4.8 Hz, 1H), 7.08 (d, J = 15.6 Hz, 2H), 2.53 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 167.7, 139.9, 134.1, 132.3, 130.9, 129.7,

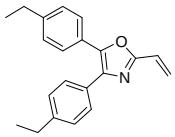
128.9, 127.5, 127.4, 126.6, 125.9, 125.5, 19.2. **MS** (EI) m/z: 39，43，69, 83, 110, 134, 152,178, 219, 247. **IR** (KBr,cm^{-1}): *v* 3833, 3465, 1641, 1381, 746, 466. HRMS calc. $C_{12}H_9NOS_2$, [M^+]: 247.0126, Found: 247.0129.

2,4,5-Trimethyloxazole(3ka) [4]



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 2.31 (s, 3H), 2.14 (s, 3H), 1.99 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 158.6, 142.5, 129.9, 13.7, 11.0, 9.8. **MS** (EI) m/z: 55, 68, 82, 96, 111. **IR** (KBr, cm^{-1}): *v* 3448, 1637, 1381, 1115, 1041, 621, 460.

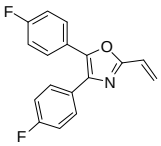
4,5-Bis(4-ethylphenyl)-2-vinyloxazole (3eb)



^{1}H NMR (400 MHz, $CDCl_3$): *δ* ppm 7.58 (t, *J* = 8.8 Hz, 4H), 7.23 (dd, *J* = 2.4 Hz, 8.0 Hz, 4H), 6.51 (dd, *J* = 10.2 Hz, 17.6 Hz, 1H), 6.26 (d, *J* = 17.6 Hz, 1H), 5.66 (d, *J* = 10.8 Hz, 1H), 2.68 (dd, *J* = 7.2 Hz, 14.0 Hz, 4H), 1.26 (t, *J* = 8.8 Hz, 7H). **^{13}C NMR (100 MHz, $CDCl_3$):** *δ* ppm 159.2, 145.2, 145.0, 144.3, 136.0, 129.8, 128.2, 128.1, 127.9, 126.6, 123.4, 121.5, 28.7, 15.5. **MS** (EI) m/z: 39, 51, 77, 126, 143, 165, 189, 233, 259, 275, 287, 303. **IR** (KBr, cm^{-1}): *v* 3401, 3068, 1608, 1407, 1254, 1179, 1020, 843. HRMS calc. $C_{21}H_{21}NO$, [M^+]: 303.1623, Found: 303.1620.

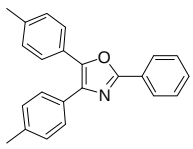
4,5-Bis(4-fluorophenyl)-2-vinyloxazole (3fb)

^{1}H NMR (400 MHz, $CDCl_3$): *δ* ppm 7.62-7.55 (m, 4 H), 7.07 (t, *J* = 8.8 Hz, 4H), 6.65 (dd, *J* = 10.8 Hz, 6.8 Hz, 1H), 6.27 (d, *J* = 18.0 Hz, 1H), 5.69 (d, *J* = 11.2 Hz, 1H).



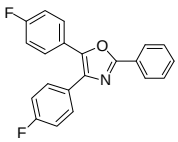
^{13}C NMR (100 MHz, $CDCl_3$): *δ* ppm 164.1, 163.9, 161.6, 161.5, 159.5, 144.3, 135.4, 128.6, 128.5, 128.3, 128.2, 124.9, 124.8, 123.2, 122.2, 116.1, 115.9, 115.6. **MS** (EI) m/z: 39, 57, 75, 95, 107, 123, 134, 201, 255, 283. **IR** (KBr, cm^{-1}): *v* 3060, 2923, 1436, 1369, 976. HRMS calc. $C_{17}H_{11}F_2NO$ [M^+]: 283.0803, Found: 283.0798.

4,5-Di(4-methyl-phenyl)-oxazole (3ce)



^{1}H NMR (400 MHz, $CDCl_3$): *δ* ppm 8.16-8.13 (m, 4H), 7.59 (dd, *J* = 8.0 Hz, 16.0 Hz, 4H), 7.48-7.47 (m, 3H), 7.22-7.19 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** *δ* ppm 159.8, 145.5, 138.5, 137.9, 136.3, 130.2, 129.4, 129.3, 128.7, 128.0, 127.5, 126.4, 126.3, 21.4, 14.1. **MS** (EI) m/z: 28, 32, 51, 77, 105, 165, 196, 222, 284, 327. **IR** (KBr, cm^{-1}): *v* 3460, 1500, 1265, 1114, 764, 695, 495. HRMS calc. $C_{23}H_{19}NO$ [M^+]: 325.1467, Found: 325.1470.

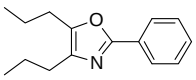
4 ,5-Bis(4-fluorophenyl)-2-phenyloxazole (3fe)



^{1}H NMR (400 MHz, $CDCl_3$): *δ* ppm 8.03-8.01 (m, 2H), 7.58-7.49 (m, 4H), 7.39-7.35 (m, 3H), 7.01-6.95 (m, 4H). **^{13}C NMR (100 MHz, $CDCl_3$):** *δ* ppm 164.0, 161.5, 160.2, 144.6, 135.6, 132.9, 132.8, 130.6, 130.5, 129.9, 128.6, 128.5, 127.2, 126.5, 125.1, 125.0, 116.6, 116.4, 116.1, 116.0, 115.9, 115.7, 115.6. **MS** (EI) m/z: 63, 75, 95, 107, 123, 183, 201,

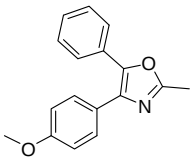
263, 305, 333. **IR** (KBr): *v* 3078, 1683, 1245, 867 cm^{-1}. HRMS calc. $C_{21}H_{13}F_2NO$ [M^+]: 333.0960, Found: 333.0965.

4,5-Dipropyl-2-phenyl oxazole (3le)



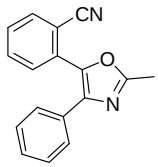
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.00 (d, *J* = 7.6 Hz, 2H), 7.43-7.38 (m, 3H), 2.65-2.61 (m, 2H), 2.49-2.45 (m, 2H), 1.73-1.67 (m, 4H), 1.29-1.26 (m, 2H), 1.00-0.94 (m, 6H), 1.87-1.80 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.2, 147.4, 136.2, 129.6, 128.6, 128.0, 125.9, 27.9, 26.7, 22.6, 21.9, 13.8, 13.7. **MS** (EI) m/z: 67, 73, 79, 95, 105, 133, 151, 159, 161, 179, 201, 211, 229. **IR** (KBr): *v* 3060, 2951, 1442, 1364, 976, 699 cm^{-1}. HRMS calc. $C_{15}H_{19}NO$ [M^+]: 229.1467, Found: 229.1465.

4-(4-Methoxyphenyl)-2-methyl-5-phenyloxazole (3ma)



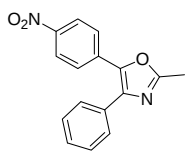
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.59-7.56 (m, 4H), 7.36-7.28 (m, 3H), 6.90 (d, *J* = 8.8 Hz, 2H), 3.81 (s, 3H), 2.53 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 160.1, 159.5, 144.6, 135.0, 129.2, 128.2, 126.2, 125.0, 114.0, 55.3, 14.0. **MS** (EI) m/z: 50, 77, 119, 134, 152, 181, 196, 222, 237, 265. **IR** (KBr, cm^{-1}): *v* 3481, 1603, 1512, 1385, 1254, 1171, 1109, 1028, 840, 769, 699. HRMS calc. $C_{17}H_{15}NO_2$ [M^+]: 265.1103, Found: 265.1106.

2-(2-Methyl-5-phenyloxazol-4-yl)benzonitrile (3na)



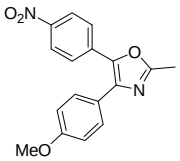
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.75 (d, *J* = 7.6 Hz, 1H), 7.56-7.47 (m, 5H), 7.32 (d, *J* = 5.6 Hz, 3H), 2.59 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 161.8, 141.6, 138.2, 134.1, 132.8, 132.5, 131.4, 130.0, 129.2, 128.7, 128.5, 127.3, 117.5, 111.7, 14.0. **MS** (EI) m/z: 28, 39, 51, 63, 77, 79, 102, 104, 130, 159, 163, 190, 219, 231, 260. **IR** (KBr, cm^{-1}): 3183, 1557, 1388, 1103, 714, 620. HRMS calc. $C_{17}H_{12}N_2O$ [M^+]: 260.0950, Found: 260.0953.

2-Methyl-4-(4-nitrophenyl)-5-phenyloxazole (3oa)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.16 (d, *J* = 8.8 Hz, 2H), 7.72 (d, *J* = 8.8 Hz, 2H), 7.60-7.58 (m, 2H), 7.43-7.40 (m, 3H), 2.58 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 174.6, 161.7, 146.9, 138.8, 135.0, 131.8, 129.0, 128.9, 128.2, 128.1, 127.1, 126.1, 124.1, 123.9, 53.5, 14.1. **MS** (EI) m/z: 28, 32, 77, 89, 104, 165, 280. **IR** (KBr, cm^{-1}): *v* 3042, 2813, 1537, 1342, 851, 632. HRMS calc. $C_{16}H_{12}N_2O_3$ [M^+]: 280.0848, Found: 280.0852.

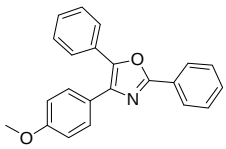
5-(4-Methoxyphenyl)-2-methyl-4-(4-nitrophenyl)oxazole (3pa)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.09 (d, *J* = 8.8 Hz, 2H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 2.52(s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 161.6, 160.1, 146.6, 142.5, 138.7, 135.2, 129.5, 125.8, 124.0, 114.3, 55.3, 14.0. **MS** (EI) m/z: 63, 76, 104, 134, 152, 180, 195, 211, 241, 267, 282. **IR** (KBr, cm^{-1}): 3068, 2839, 1579, 1511, 1340, 1178, 1034, 833, 692, 531. HRMS calc.

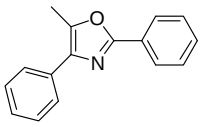
$C_{17}H_{14}N_2O_4$ [M^+]: 310.0954, Found: 310.0958.

2,5-Diphenyl4-(4-methoxyphenyl)oxazole (3me)



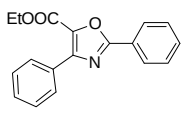
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.17-8.15 (m, 2H), 7.70-7.65 (m, 4H), 7.49-7.47 (m, 3H), 7.41-7.33 (m, 3H), 6.96-6.94 (m, 2H), 3.86 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 160.0, 159.6, 144.9, 136.6, 132.4, 129.5, 128.7, 127.4, 126.4, 125.0, 114.4, 114.1, 55.3. MS (EI) m/z: 28, 51, 77, 91, 105, 120, 163, 181, 209, 225, 235, 255, 299, 327. IR (KBr): *v* 3112,1621, 1465, 1232, 1034 cm^{-1}. HRMS calc. $C_{22}H_{17}NO_2$ [M^+]: 327.1259, Found: 327.1264.

2,4-Diphenyl-5-methyl-oxazole (3re) [5]



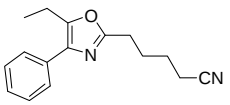
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.10-8.08 (m, 2H), 7.75 (d, *J* = 7.6 Hz, 2H), 7.47-7.45 (m, 5H), 7.35-7.31 (m, 1H), 2.61 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.4, 144.0, 136.0, 132.4, 130.0, 128.7, 128.6, 127.7, 127.3, 126.8, 126.2, 12.0. **MS** (EI) m/z: 43, 63, 89, 103, 165, 192, 220, 235. **IR** (KBr, cm^{-1}): *v* 1671, 1511, 1020, 710.

Ethyl 2,4-diphenyloxazole-5-carboxylate (3se)



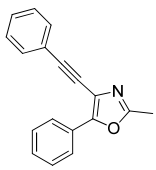
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15- 8.08 (m, 4 H), 7.49-7.45 (m, 6H), 4.44 (q, *J* = 7.2 Hz, 2H), 1.43 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR (75 MHz, $CDCl_3$):** δ 162.3, 159.7, 55.0, 131.0,130.7, 130.3, 128.8, 128.5, 128.4, 127.1, 126.8, 126.4, 61.4, 14.3; **MS** (EI) m/z: 51, 77, 89, 105, 115, 143, 165, 192, 221, 248, 265, 293. **IR** (KBr): *v* 3061, 2970, 1724, 1497, 1327, 1223, 1100, 723,423 cm^{-1}. HRMS calc. $C_{18}H_{15}NO_3$ [M^+]: 293.1052, Found: 293.1056.

5-(5-Ethyl-4-phenyloxazol-2-yl)pentanenitrile (3tj)



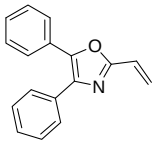
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.61 (d, *J* = 7.6 Hz, 2H), 7.41（dd, *J* = 8.0 Hz, 16.0 Hz, 2H), 7.09 (dd, *J* = 7.6 Hz, 14.8 Hz, 1H), 2.90-2.81 (m, 4H), 2.38 (dd, *J* = 7.6 Hz, 14.8 Hz, 2H), 1.99-1.91(m, 2H), 1.80-1.73 (m, 2H), 1.30 (dd, *J* = 7.6 Hz, 14.8 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 12.63, 16.86, 19.35, 24.78, 25.97, 27.20, 119.45, 126.81, 127.26, 128.31, 128.59, 148.73, 161.54. MS (EI) m/z: 63, 77, 103, 117, 130, 144, 158, 172, 186, 200, 225, 239, 254. IR (KBr, cm^{-1}): *v* 3057, 1591, 1452, 1181, 992, 772, 700. HRMS calc. $C_{16}H_{18}N_2O$ [M^+]: 254.1419, Found: 254.1422.

2-Methyl-5-phenyl-4-(phenylethynyl)oxazole (3qa) [6]



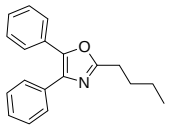
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.13 (d, *J* =7.6 Hz, 2H), 7.58 (dd, *J* = 2.8 Hz, 6.8 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 15.2 Hz, 2H), 7.40 (t, *J* = 3.2 Hz, 6.4 Hz, 3 H), 7.36 (t, *J* = 7.2 Hz, 14.4 Hz, 1H), 2.55(s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 161.4, 142.4, 131.5, 130.9, 129.2, 128.6, 128.5, 126.3, 122.0, 99.7, 14.3. **MS** (EI) m/z: 28, 63, 77, 102, 128, 163, 189, 231, 259. IR (KBr, cm^{-1}): *v* 3053, 2235, 1465, 1212, 1098, 1013, 699. HRMS calc. $C_{18}H_{13}NO$ [M^+]: 259.0997, Found: 259.0995.

4,5-Diphenyl-2-vinyloxazole (3ab) [7]



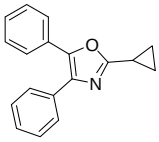
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.65 (dd, J = 8.0 Hz, 12.4 Hz, 4H), 7.40-7.32 (m, 6H), 6.08 (dd, J = 7.2 Hz, 9.6 Hz, 1H), 6.28 (d, J =17.6 Hz, 1H), 5.68 (d, J = 11.2 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 194.6, 134.9, 133.0, 129.9, 129.0. **MS** (EI) m/z: 39, 77, 89, 116, 139, 165, 219, 247. **IR** (KBr, cm^{-1}): v 3472, 3067, 1600, 1509, 1235, 1157, 841, 599.

4,5-Diphenyl-2-butyloxazole (3ac)



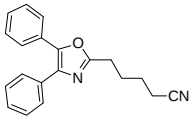
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.67-7.64 (m, 2H). 7.61-7.58 (m, 2H), 7.40-7.30 (m, 6H), 2.87 (dd, J = 8.0 Hz, 16.0 Hz, 2H), 1.89-1.81 (m, 2H), 1.53-1.46 (m, 2H), 0.99 (dd, J = 8.0 Hz, 16.0 Hz, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 163.9, 145.0, 135.0, 133.6, 132.6, 129.2, 129.2, 128.9, 128.6, 128.6, 128.3, 128.0, 126.4, 29.3, 28.0, 22.4, 13.8. **MS** (EI) m/z: 51, 63, 77, 103, 130, 152, 165, 178, 193, 235, 248, 277. **IR** (KBr, cm^{-1}): v 3468, 1599, 1453, 1248, 764, 695. HRMS calc. $C_{18}H_{13}NO$ [M^+]: $C_{19}H_{19}NO$ (M+): 277.1467, Found: 277.1470.

2-Cyclopropyl-4,5-diphenyl-oxazole (3ad)



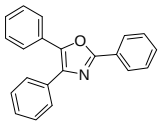
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.65-7.63 (m, 2 H), 7.57-7.55 (m, 2H), 7.39-7.30 (m, 6H), 2.20-2.13 (m, 1H), 1.22-1.18 (m, 2H), 1.12-1.07 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 164.7, 144.4, 135.2, 132.7, 129.2, 128.6, 128.5, 128.2, 128.0, 126.3, 8.99, 8.26. **MS** (EI) m/z: 27, 51, 77, 105, 129, 165, 206, 232, 261. **IR** (KBr, cm^{-1}): v 3061, 2930, 1705, 1443, 1367, 1256, 1172, 930, 697. HRMS calc. $C_{18}H_{15}NO$ $[M+H]^+$: 262.1226, Found: 262.1208.

5-(4,5-diphenyloxazol-2-yl)pentanenitrile (3ae)



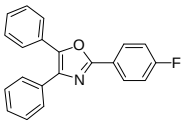
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.65 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.39-7.31 (m, 6H), 2.92 (d, J = 7.2 Hz, 2H), 2.42 (d, J = 7.8 Hz, 2H), 2.01-1.99 (m, 2H), 1.87-1.80 (m, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 162.4, 145.4, 135.1, 132.4, 130.0, 129.0, 128.7, 128.6, 128.5, 128.4, 128.1, 127.9, 126.5, 119.4, 27.3, 26.0, 24.9, 17.0. **MS** (EI) m/z: 51, 77, 89, 103, 117, 130, 143, 165, 178, 193, 235, 248, 262, 274, 302. **IR** (KBr, cm^{-1}): v 1572, 1446, 1244, 1061, 765, 695. HRMS calc. $C_{20}H_{18}N_2O$ $[M+H]^+$: 303.1492, Found: 303.1490.

2,4,5-Triphenyloxazole (3af) [8]



^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.18 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 6.8 Hz, 2H), 7.70-7.68 (m, 2H), 7.51-7.48 (m, 3H), 7.44-7.35 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 160.2, 145.6, 136.8, 132.6, 130.4, 129.9, 128.8, 128.7, 128.6, 128.5, 128.3, 128.2, 127.4, 126.6, 126.5. MS (EI) m/z: 28, 63, 77, 89, 105, 139, 165, 269, 297. IR (KBr, cm^{-1}): v 1638, 1488, 1446, 1244, 1080, 1025.

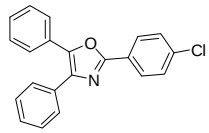
4,5-Diphenyl-2-(4-fluoro -phenyl)-oxazole (3ag)



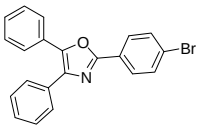
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.17-8.14 (m, 2H), 7.71 (dd, *J* = 7.2 Hz, 23.2 Hz, 4H), 7.44-7.36 (m, 6H), 7.18 (dd, *J* = 7.2 Hz, 8.8 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 165.4, 162.9, 159.4, 145.6, 136.8, 132.5, 129.0, 128.9, 128.7, 128.6, 128.5, 128.3, 128.1, 123.8, 116.1, 115.9. **MS** (EI) m/z: 63, 77, 89, 107, 139, 165, 183, 185, 238, 253, 281, 287, 315. **IR** (KBr, cm^{-1}): *v* 2924, 1700, 1500, 1241, 1117, 843, 694. HRMS calc. $C_{21}H_{14}NOF$ $[M+H]^+$: 316.1136, Found: 316.1165.

4,5-Diphenyl-2-(4-chlorophenyl)-oxazole (3ah)

^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.03 (d, *J* = 7.2Hz, 2H), 7.73-7.62 (m, 6H), 7.44-7.36 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.3, 145.9, 136.9, 133.4, 132.7, 132.3, 132.1, 128.8, 128.7, 128.4, 128.1, 127.9, 126.6, 126.3, 124.8. **MS** (EI) m/z: 63, 77, 89, 123, 139, 165, 190, 200, 226, 268, 290, 303, 331. **IR** (KBr, cm^{-1}): *v* 3746, 2923, 1700, 1482, 1092, 834, 766, 693. HRMS calc. $C_{21}H_{15}ClNO$ $[M+H]^+$: 332.0842, Found: 332.0854.

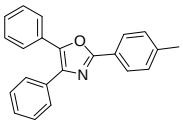


4,5-Diphenyl-2-(4-Bromo-phenyl)-oxazole (3ai)



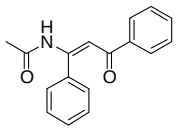
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.10 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 7.40-7.36 (m, 6H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 159.3, 145.9, 136.9, 134.9, 132.3, 132.1, 129.9, 129.0, 128.7, 128.4, 128.1, 127.9, 126.6, 126.3, 124.8. **MS** (EI) m/z: 28, 32, 51, 73, 77, 89, 105, 135, 165, 193, 239, 267, 281, 326, 349, 375. **IR** (KBr): *v* 2920, 1700, 1479, 1236, 1117, 827, 694 cm^{-1}. HRMS calc. $C_{21}H_{14}BrNO$ $[M+H]^+$: 376.0337, Found: 376.0346.

4,5-Diphenyl-2-(4-methyl-phenyl)-oxazole (3aj)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 8.07 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.69 (d, *J* = 7.2 Hz, 2H), 7.44-7.34 (m, 6H), 7.30 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 160.4, 145.3, 140.7, 136.7, 132.7, 129.5, 129.1, 128.7, 128.6, 128.2, 126.5, 124.7, 21.6. **MS** (EI) m/z: 28, 32, 51, 77, 89, 119, 165, 150, 245, 283, 311. **IR** (KBr, cm^{-1}): *v* 2973, 1703, 1600, 1245, 882, 613. HRMS calc. $C_{22}H_{17}NO$ $[M+H]^+$: 312.1388, Found: 312.1396.

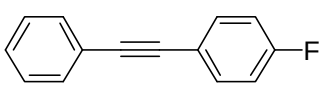
(Z)-N-(3-oxo-1,3-diphenylprop-1-en-1-yl)acetamide



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 12.27 (br. s, 1 H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 7.2 Hz, 1H), 7.50-7.40 (m, 7H), 6.33 (s, 1H), 2.25 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 191.7, 168.9, 156.3, 138.7, 136.3, 132.8, 129.9, 128.7, 128.1, 127.9, 127.4, 104.8, 24.1. **MS** (EI) m/z: 28, 43, 51, 69, 77, 103, 105, 117, 146, 160, 193, 222, 267. **IR**

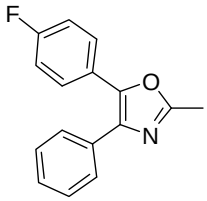
(KBr): *v* 3073, 1720, 1586, 1474, 1294, 1208, 1030, 759 cm^{-1}. $C_{17}H_{15}NO_2$ $[M+H]^+$: 265.1103, Found: 265.1106.

1-Fluoro-4-(phenylethynyl)benzene (8)



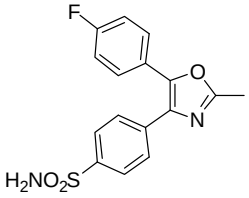
^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.51-7.25 (m, 4 H), 7.30-7.28 (m, 3H), 7.00 (d, *J* = 8.0 Hz, 2H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 163.8, 1161.4, 134.7, 134.6, 133.6, 131.7, 128.5, 128.4, 123.2, 119.5, 116.1, 115.8, 115.6, 89.2, 88.5.

5-(4-Fluorophenyl)-2-methyl-4-phenyloxazole (9)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.61 (dd, *J* = 5.2 Hz, 8.8 Hz, 2H), 7.49 (d, *J* = 7.6 Hz, 2H), 7.37-7.29 (m, 3H), 7.47 (d, *J* = 8.4 Hz, 2H), 2.54 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 163.8, 161.3, 160.3, 145.2, 134.3, 129.7, 129.6, 128.7, 128.6, 128.4, 127.8, 126.4, 115.9, 115.7, 115.5, 13.9. **MS** (EI) m/z: 28, 43, 51, 69, 77, 103, 105, 117, 146, 160, 193, 222, 253.

4-(5-(4-Fluorophenyl)-2-methyloxazol-4-yl)benzenesulfonamide (10)



^{1}H NMR (400 MHz, $CDCl_3$): δ ppm 7.68 (d, *J* = 7.6 Hz, 2H), 7.51 (d, *J* = 7.6 Hz, 2H), 7.36-7.29 (m, 2H), 7.21-7.14 (m, 2H), 7.10-7.01 (m, 2H), 2.58 (s, 3H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ ppm 167.7, 161.3, 161.1, 161.1, 158.6, 158.0, 142.3, 134.9, 132.0, 131.6, 130.5, 129.7, 129.2, 124.8, 124.1, 124.0, 120.7, 117.6, 117.5, 116.2, 116.0, 115.8, 115.7, 115.5, 14.0.

F. References

(1) W. Zeng, S. R. Chemler, *J. Org. Chem*., **2008**, *73*, 6045–6047.
(2) J. Chen, W. Zhang, H. Geng, W. Li, G. Hou, A. Lei, X. Zhang, *Angew. Chem., Int. Ed.,* **2009**, *48*, 800-802.
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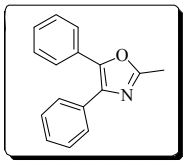
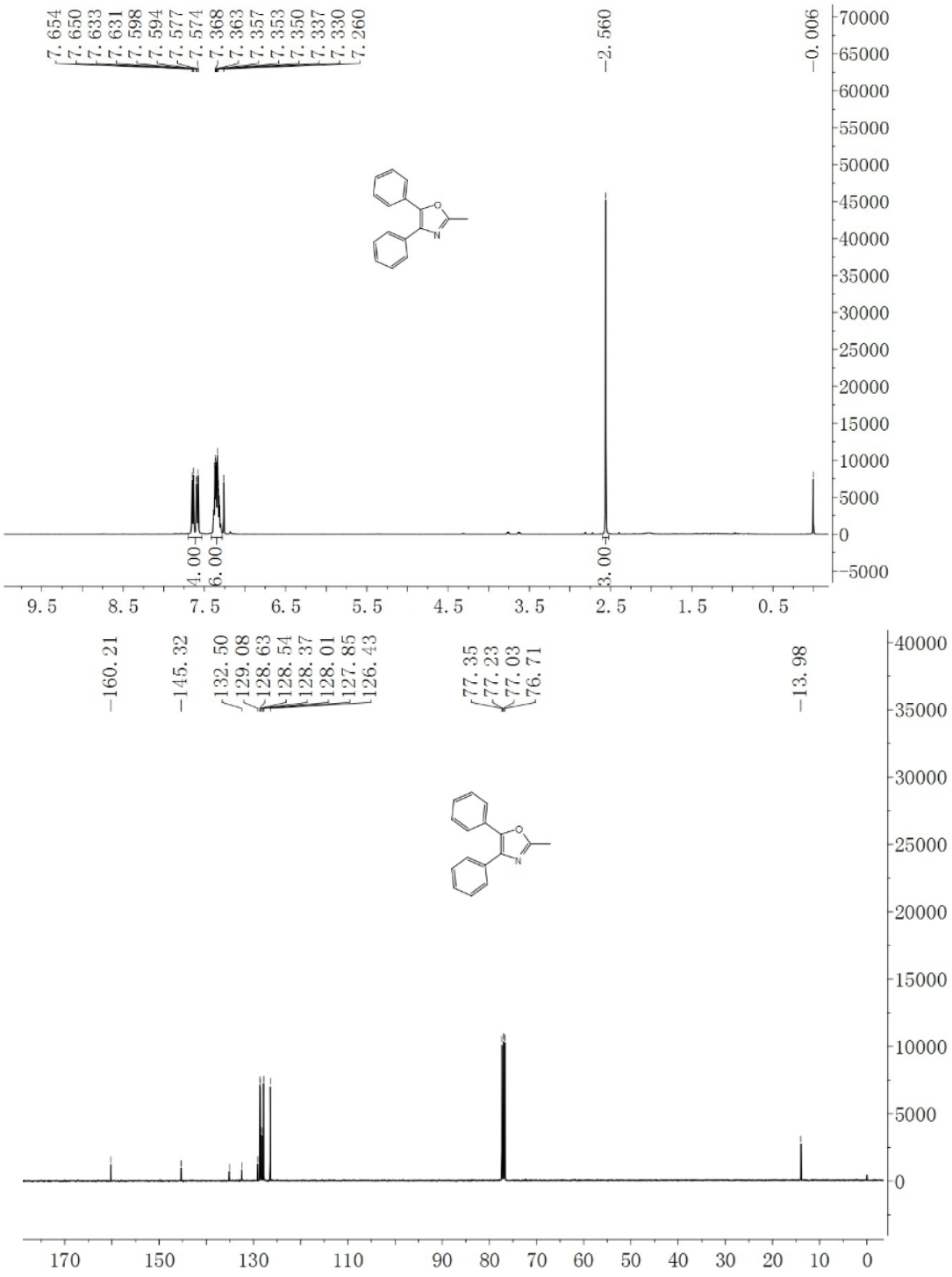
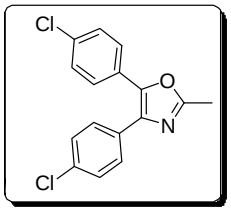
(6) I. Cano, E. Álvarez, M. C. Nicasio, P. J. Pérez, *J. Am. Chem. Soc.,* **2011**, *133*, 191-193
(7) P. Albert, L. A. Cohen. *J. Org. Chem.,* **1984**, *49*, 399-406.
(8) H. F. Jiang, H. W. Huang, H. Cao, C. R. Qi. *Org. Lett.,* **2010**, *12*, 5561-5563.

G. NMR Spectra

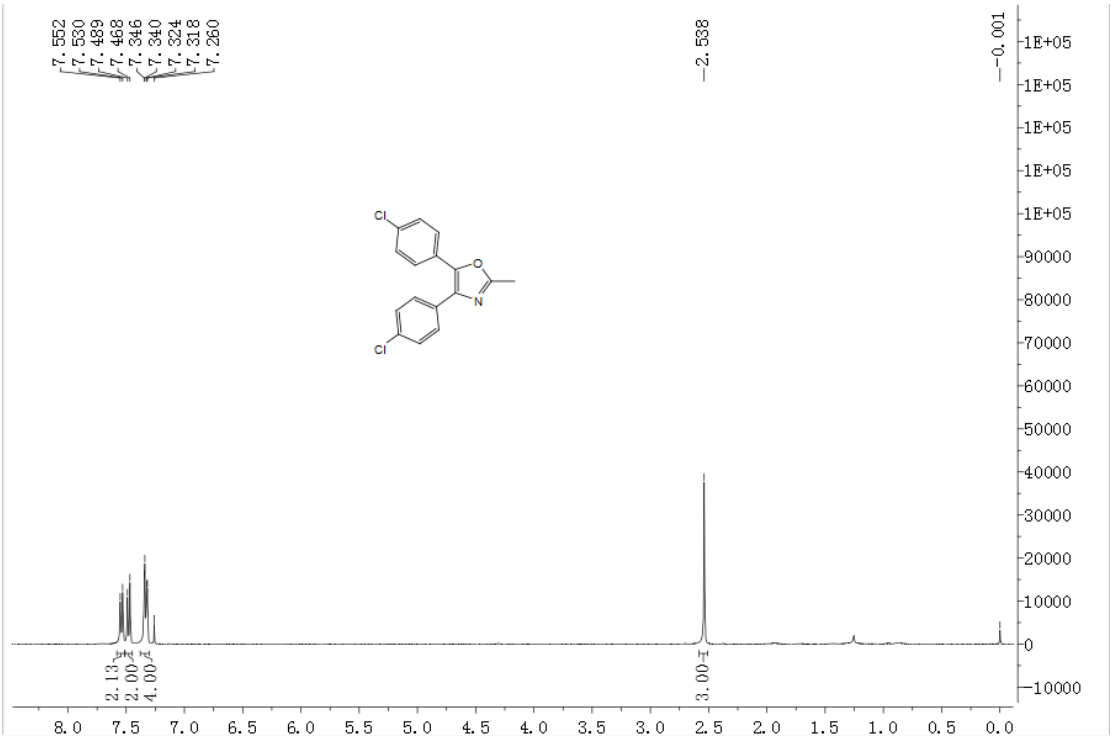


(**3aa**)




Cl
O
N
Cl

(3ba)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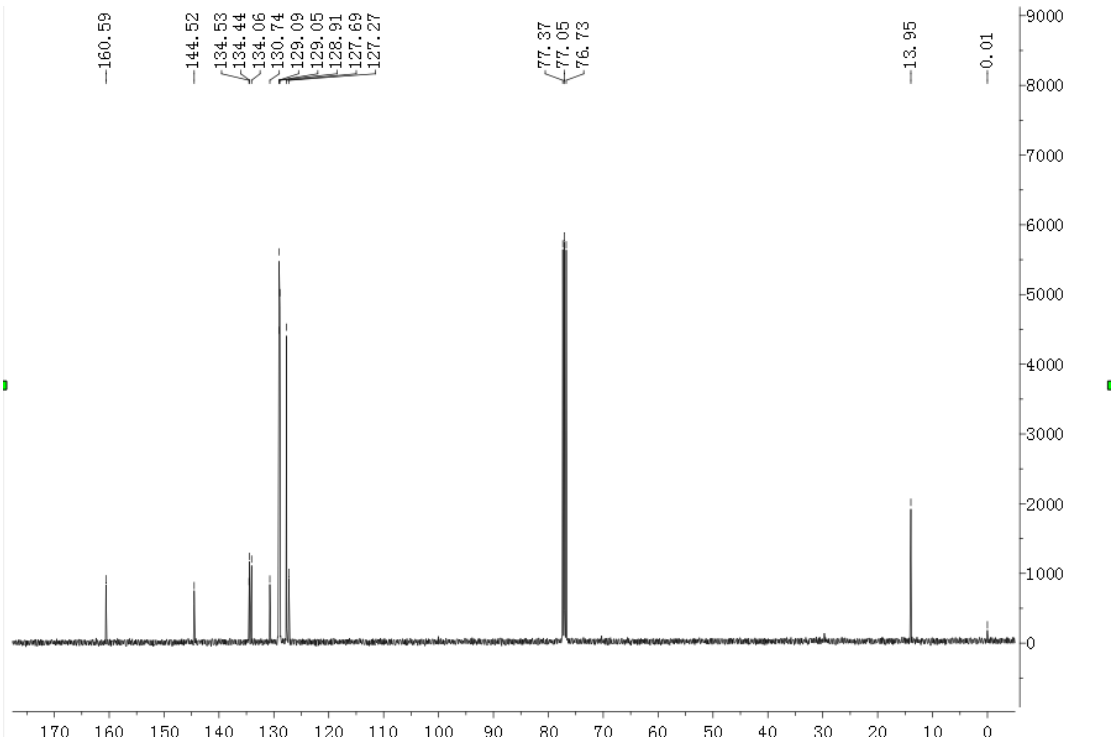
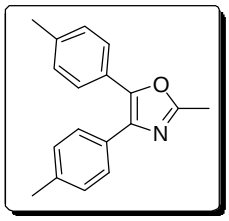
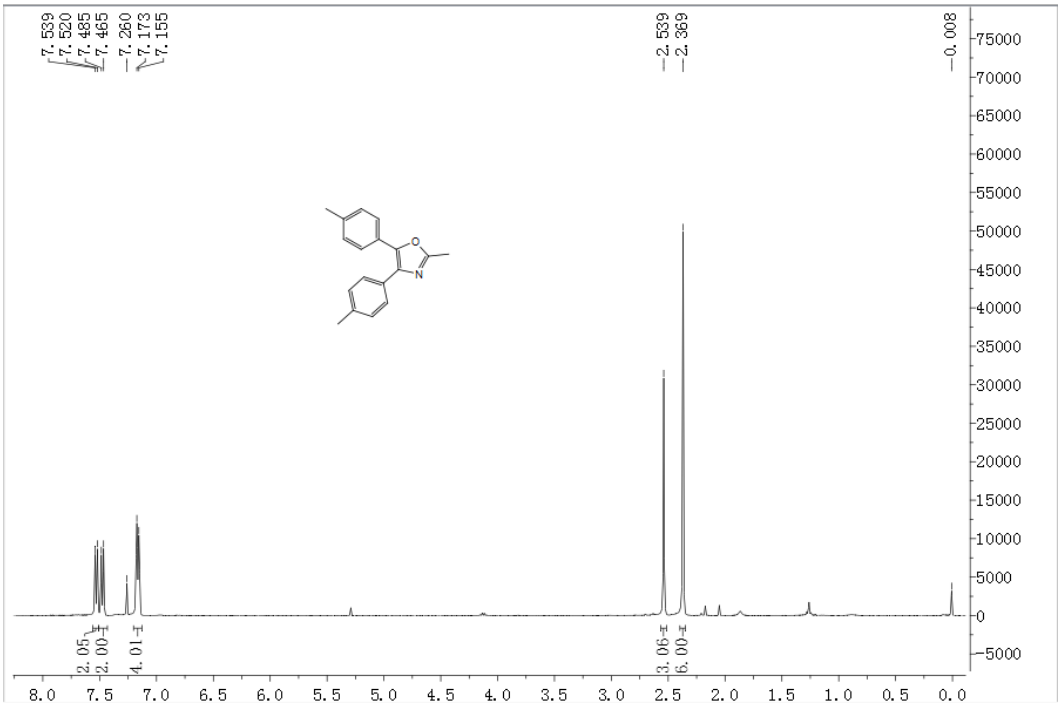
7.530
7.489
7.468
7.346
7.340
7.324
7.318
7.260
2.538
0.001
2.13
2.00
4.00
3.00


160.59
144.52
134.53
134.44
134.06
130.74
129.09
129.05
128.91
127.69
127.27
77.37
77.05
76.73
13.95
0.01



(3ca)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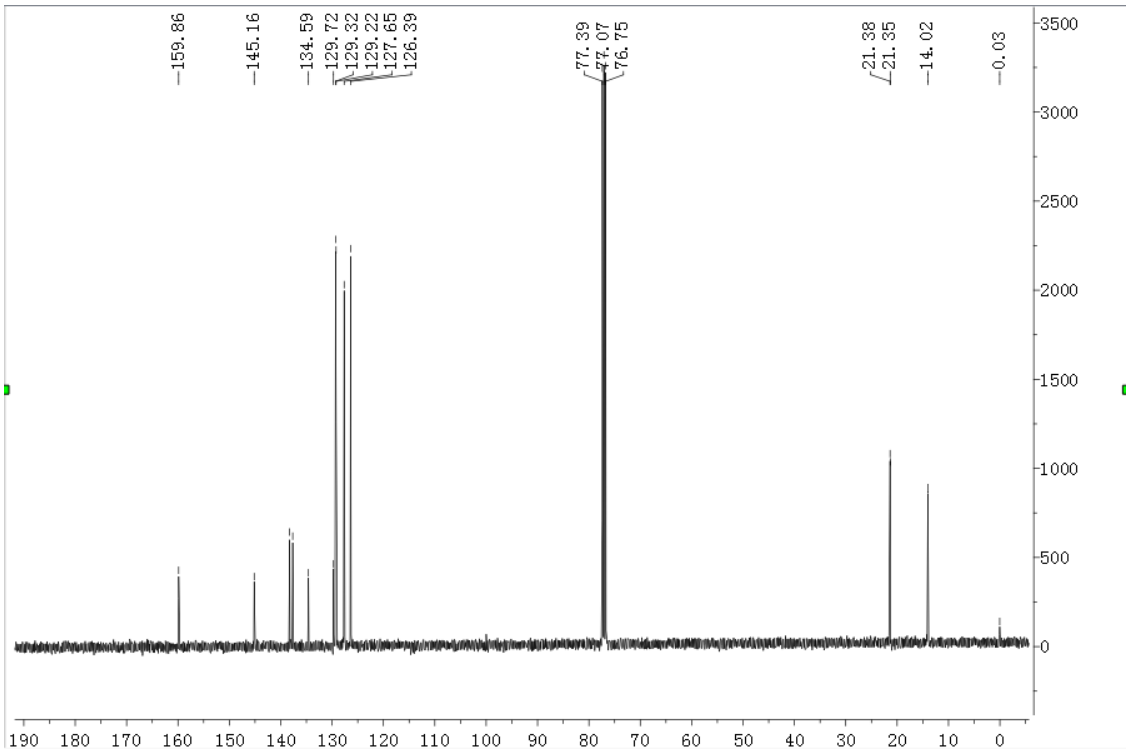
2.539
2.369
0.008
2.05
2.00
4.01
3.06
6.00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145.16
134.59
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129.22
127.65
126.39
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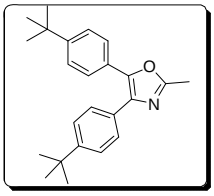
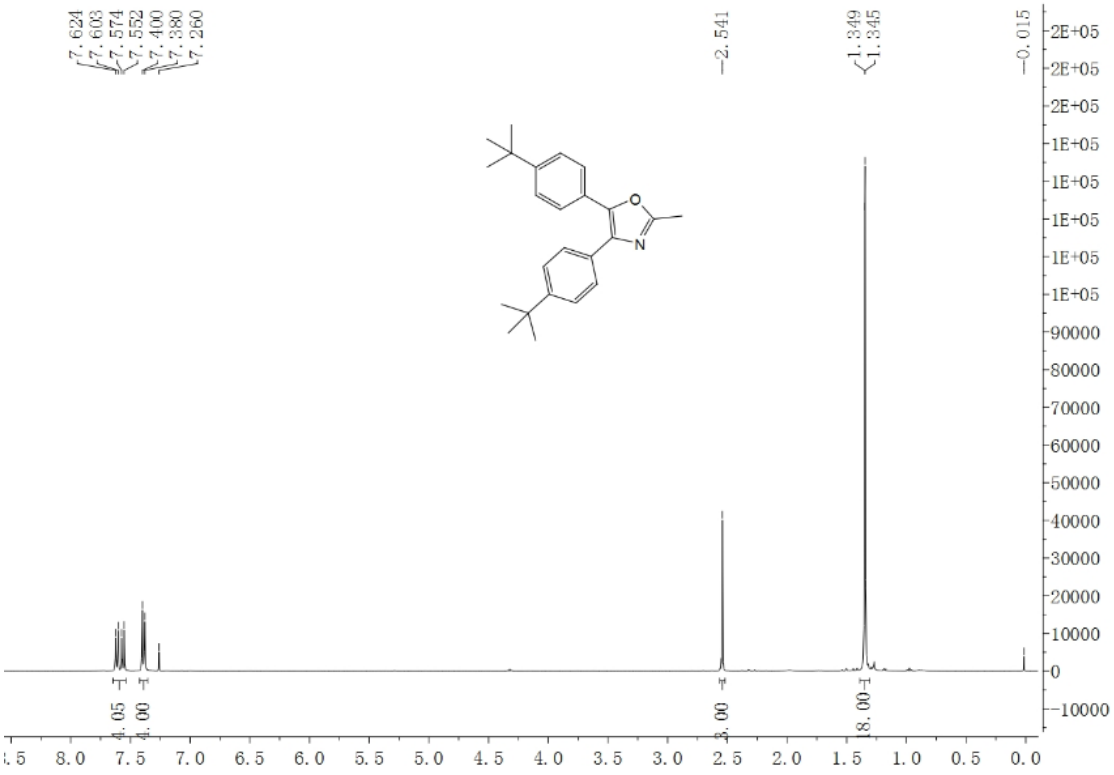
77.07
76.75
21.38
21.35
14.02
0.03



(3da)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7.260
2.541
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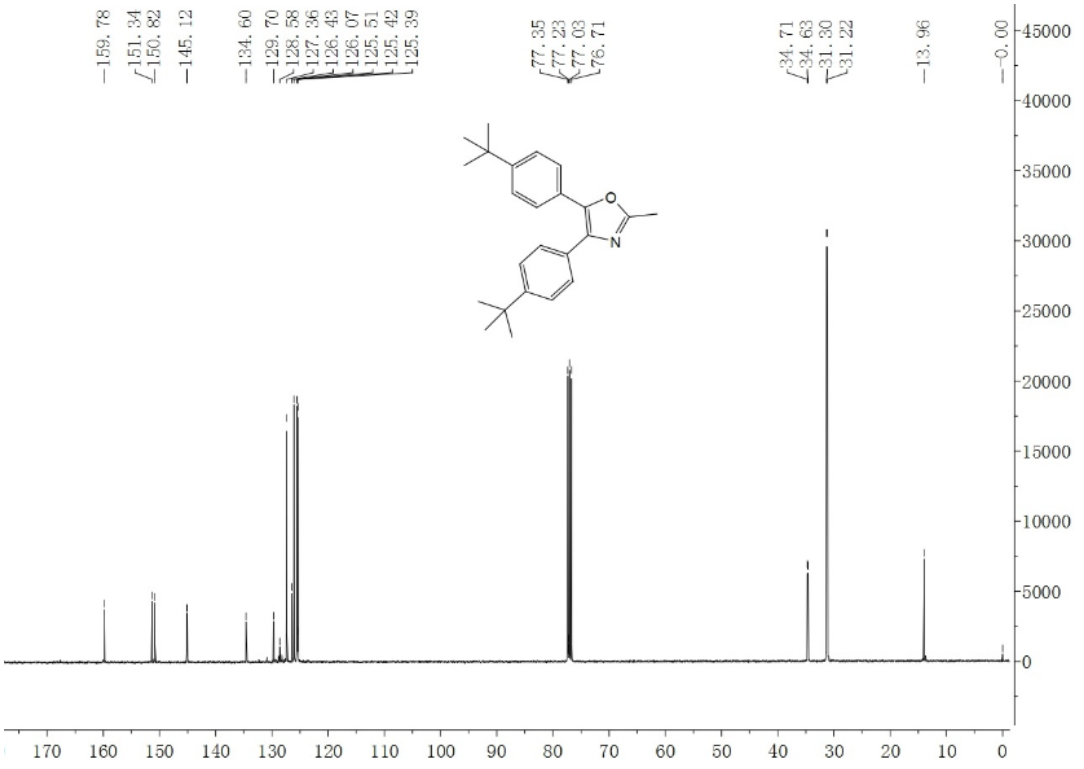
1.345
0.015
4.05
4.00
3.00
18.00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150.82
145.12
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129.70
128.58
127.36
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126.07
125.51
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77.23
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34.71
34.63
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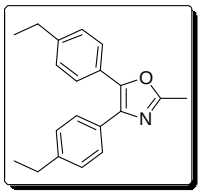
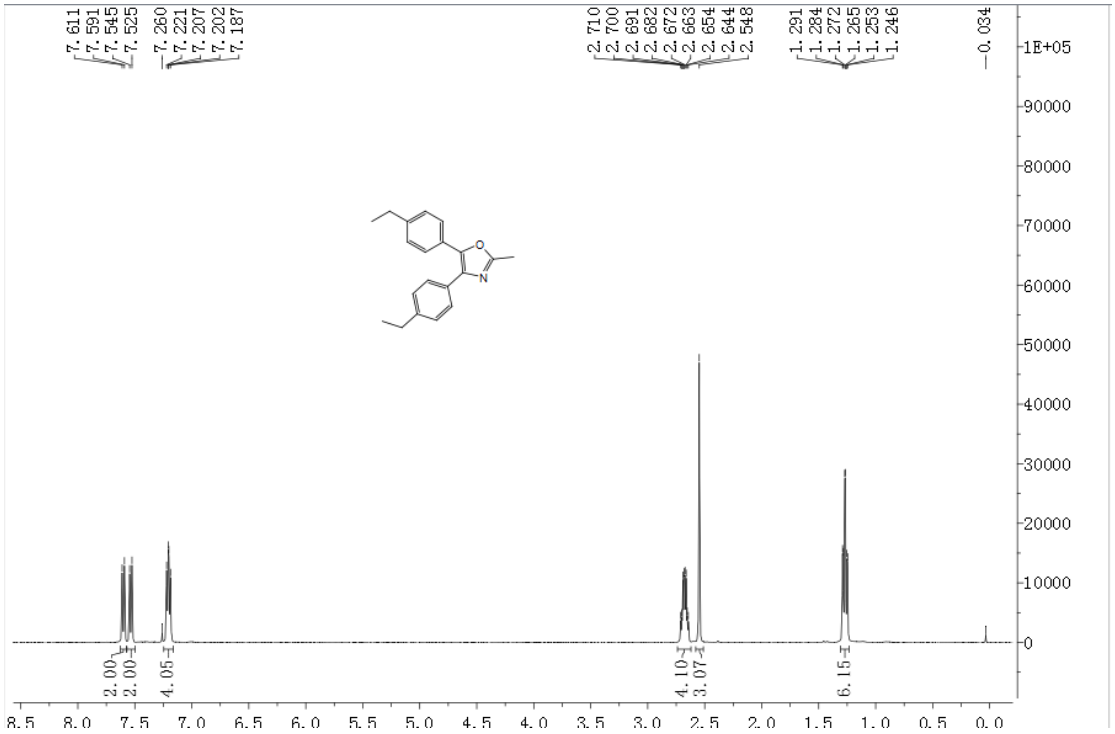
31.22
13.96
0.00



(3ea)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7.207
7.202
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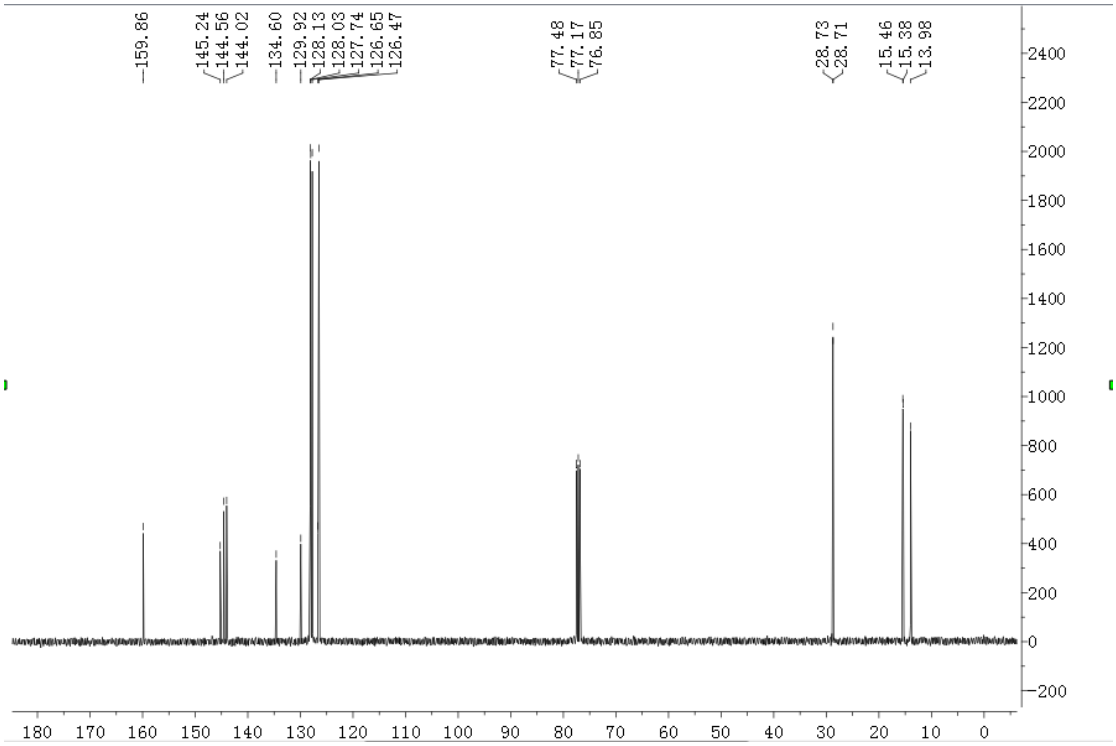
2.710
2.700
2.691
2.682
2.672
2.663
2.654
2.644
2.548
1.291
1.284
1.272
1.265
1.253
1.246
0.034
2.00
2.00
4.05
4.10
3.07
6.15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144.56
144.02
134.60
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128.13
128.03
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126.65
126.47
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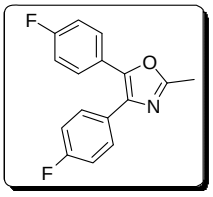
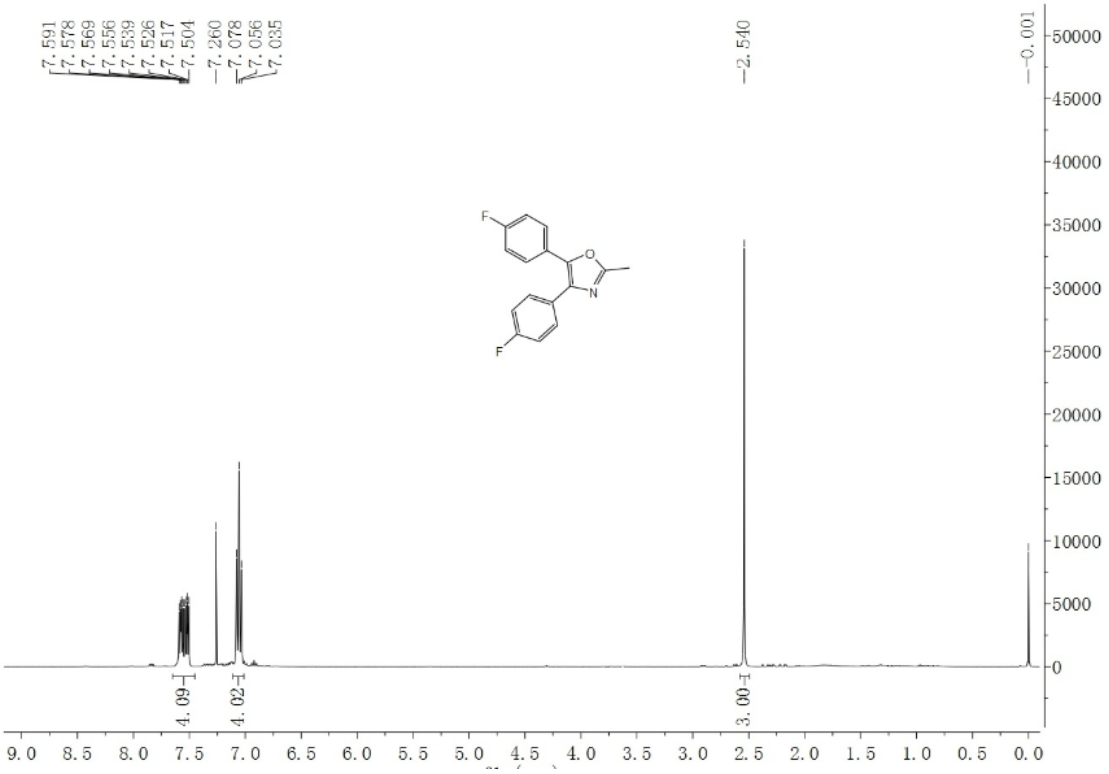
76.85
28.73
28.71
15.46
15.38
13.98


F
O
N
F

(**3fa**)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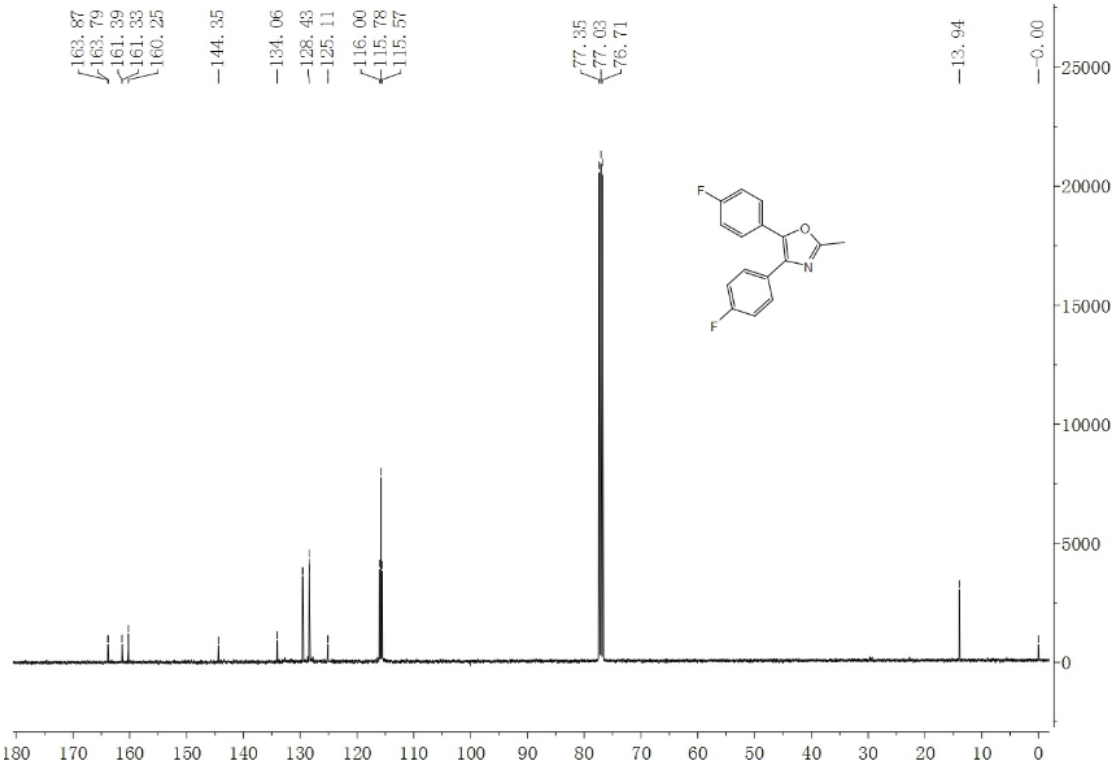
0.001
4.09
4.02
3.00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160.25
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77.03
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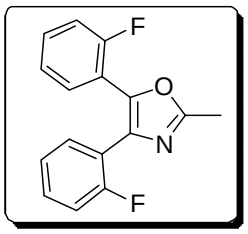
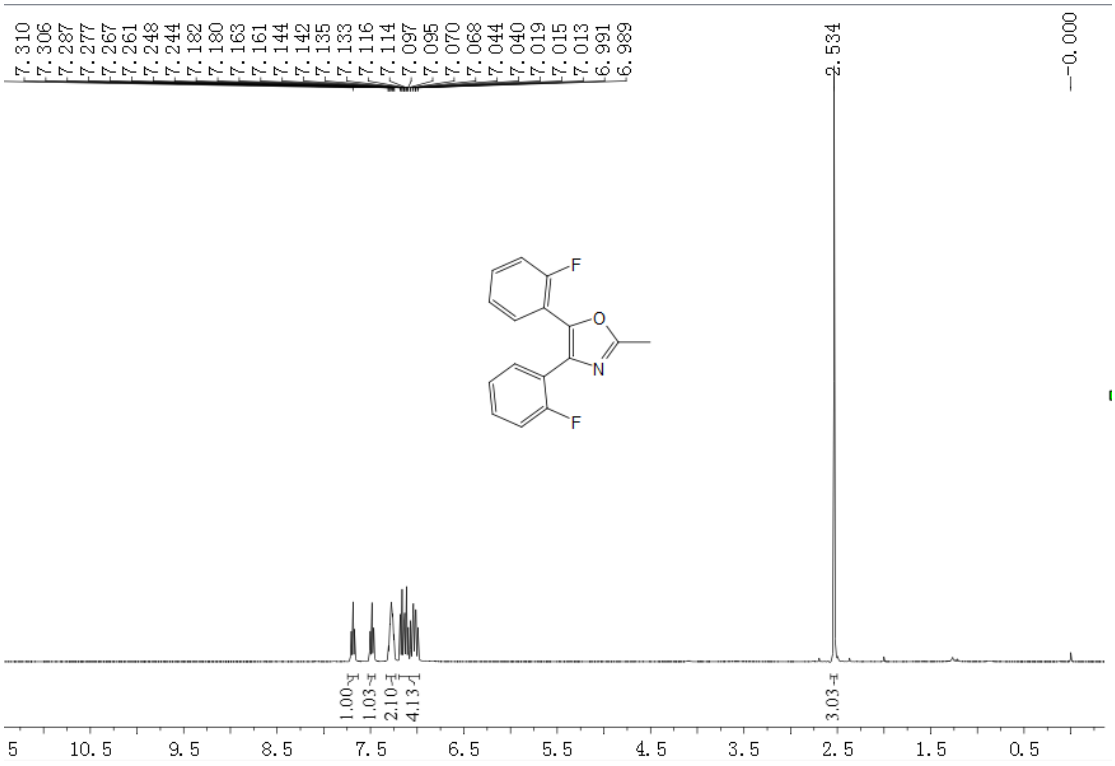

F
O
N
F

(3ga)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7.097
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7.015
7.013
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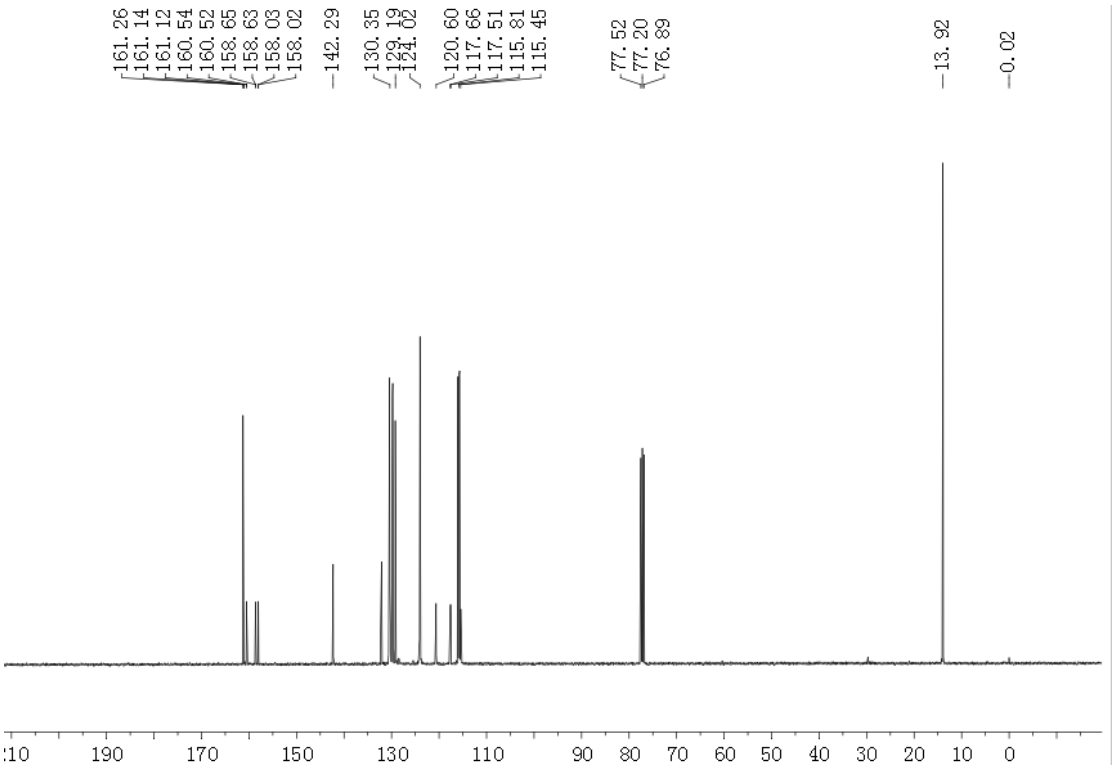
4.13
3.03
F
O
N
F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115.45
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77.20
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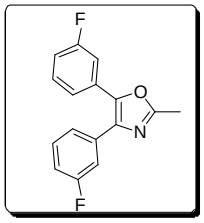
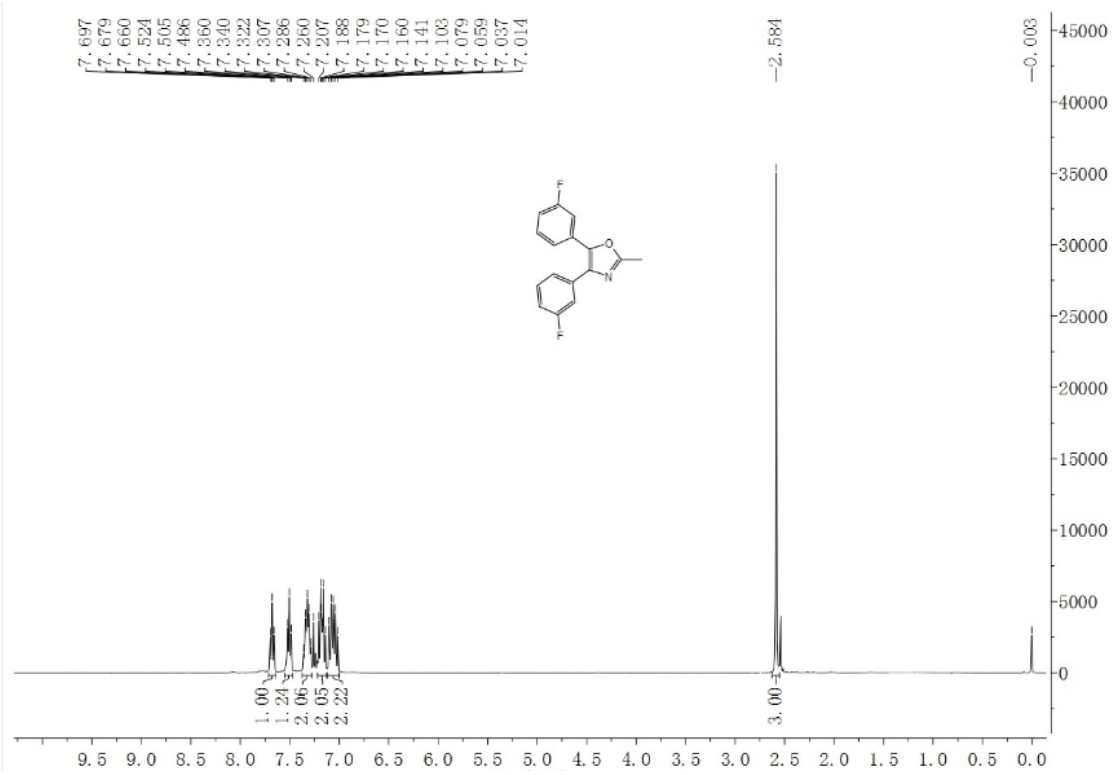
0.02

(3ha)


F
O
N
F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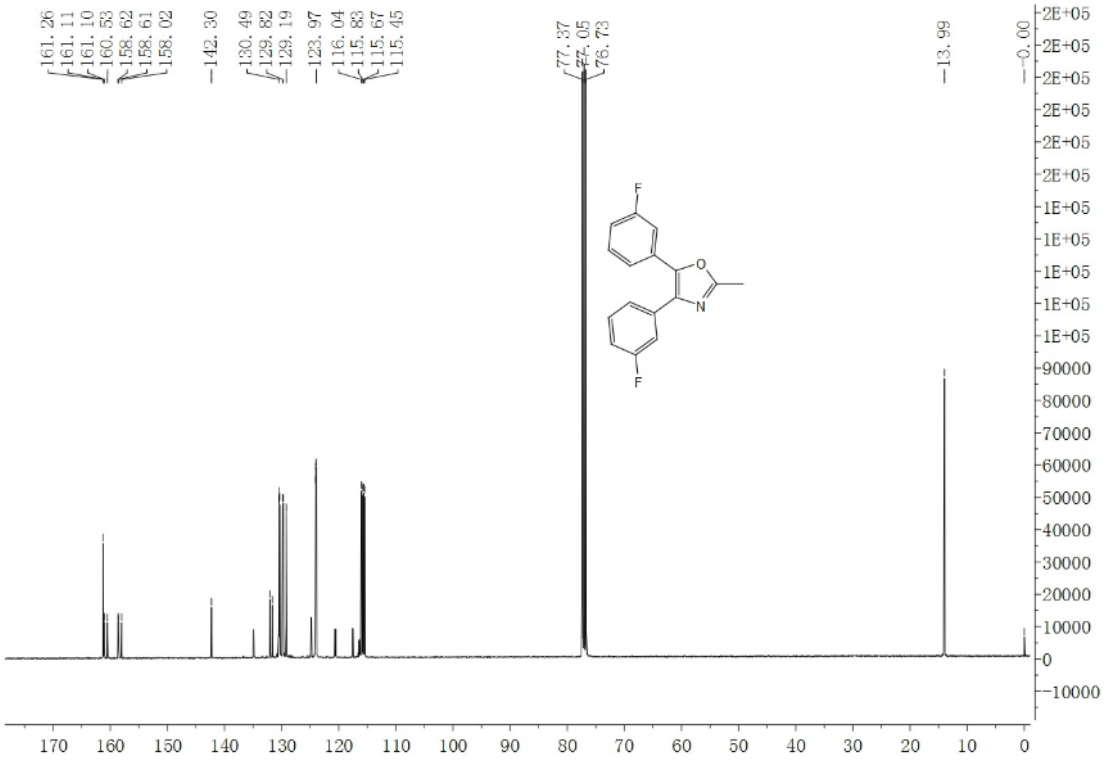
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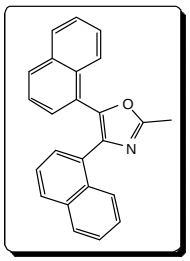

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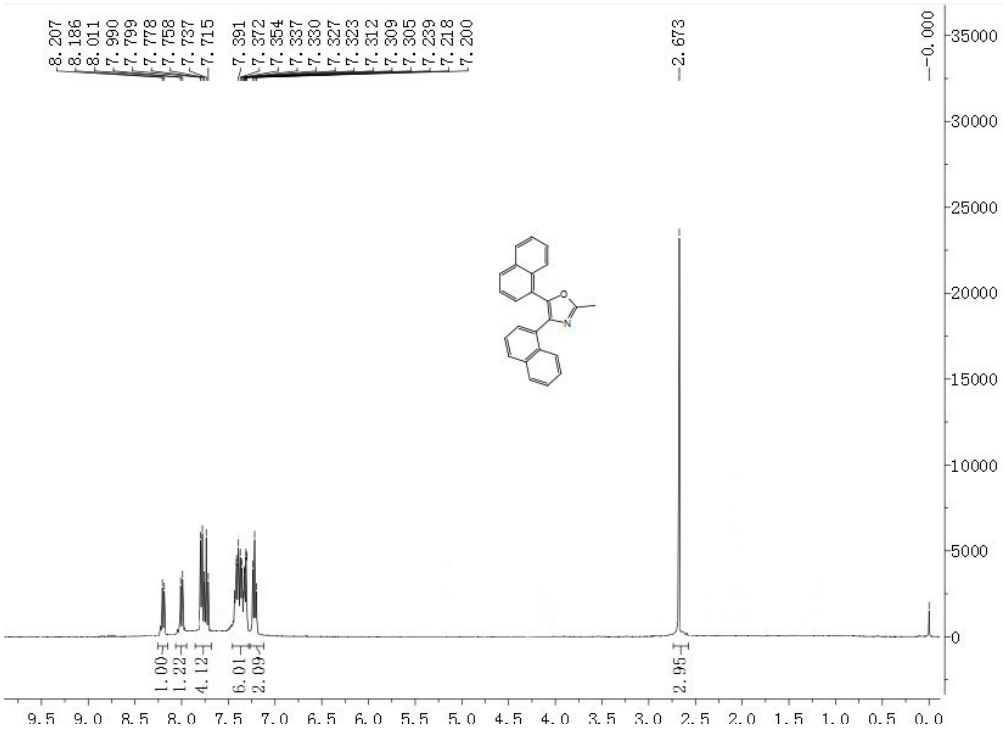
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7.309
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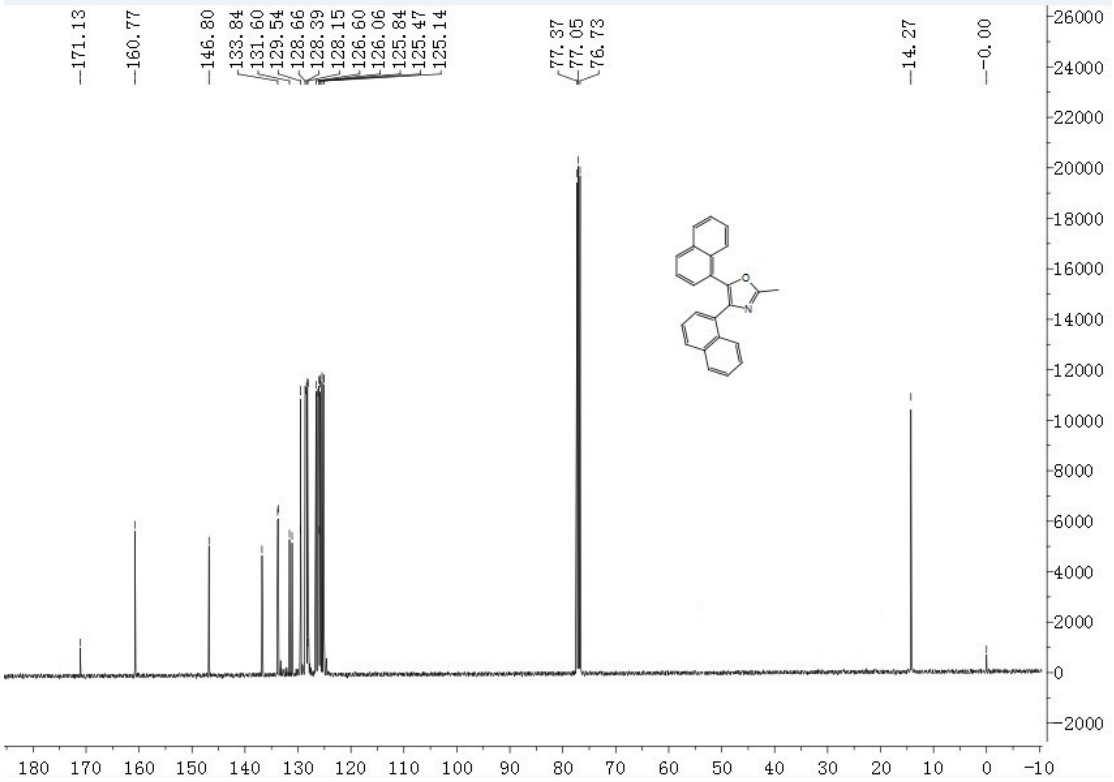
2.09
2.95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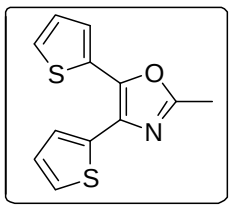
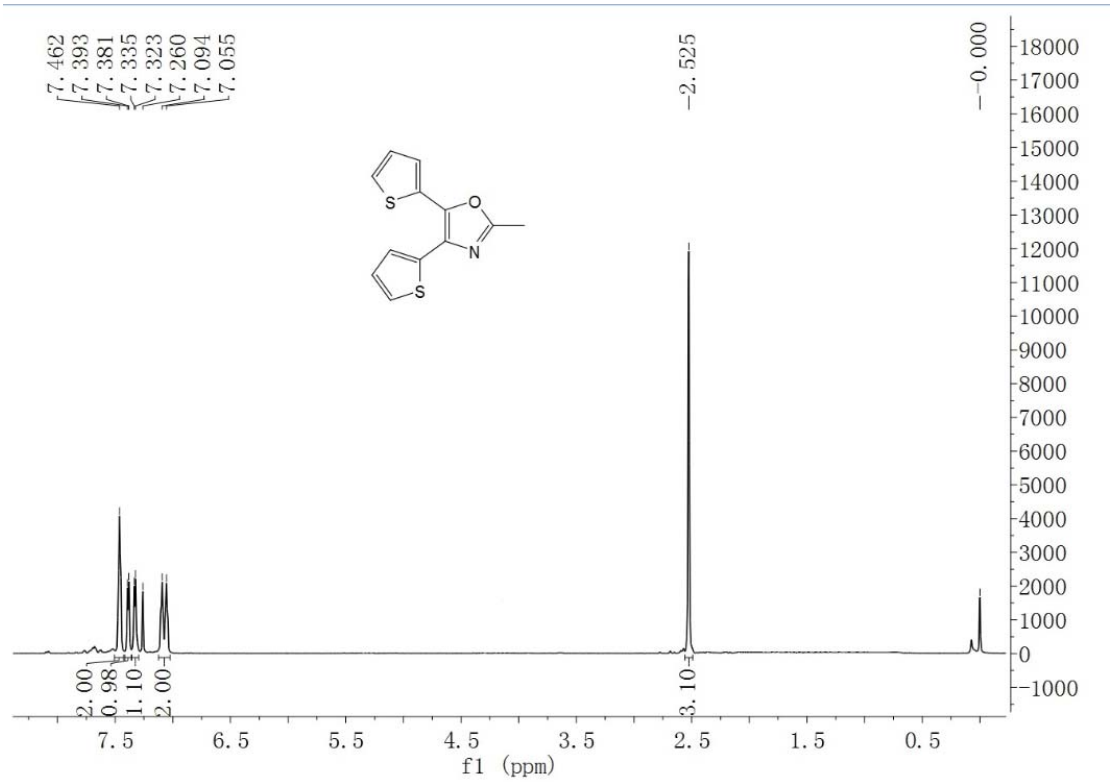


(3ja)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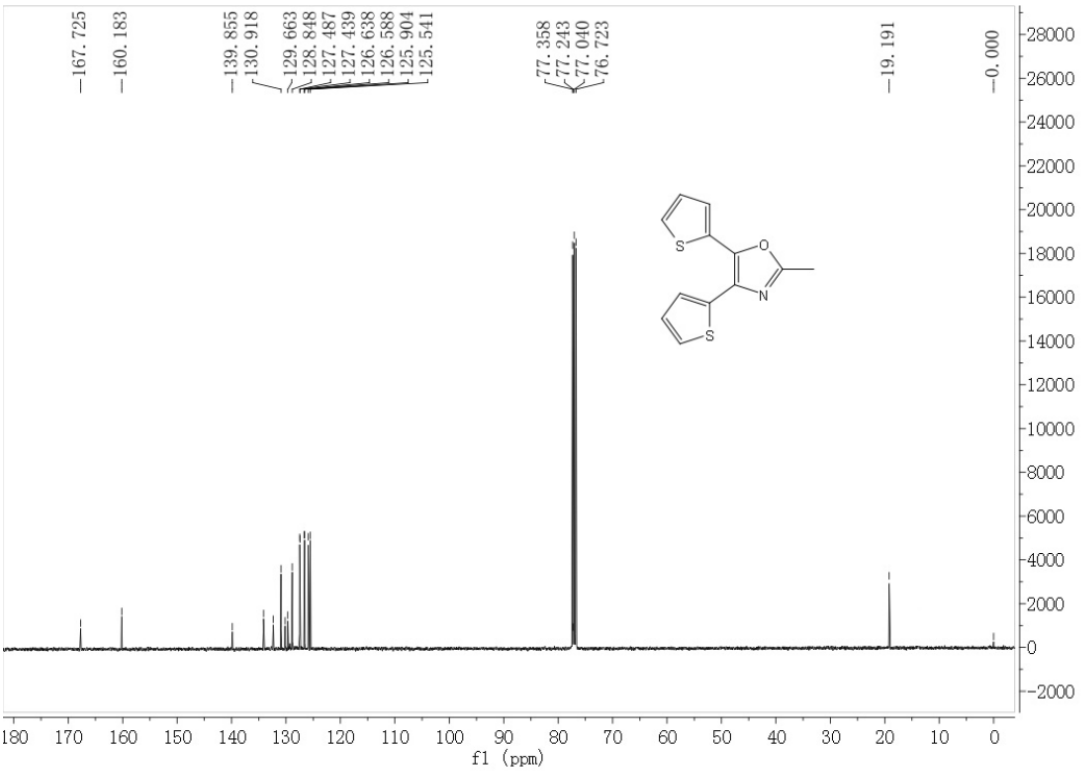
f1 (ppm)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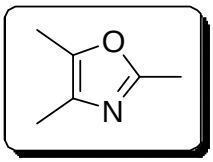
f1 (ppm)



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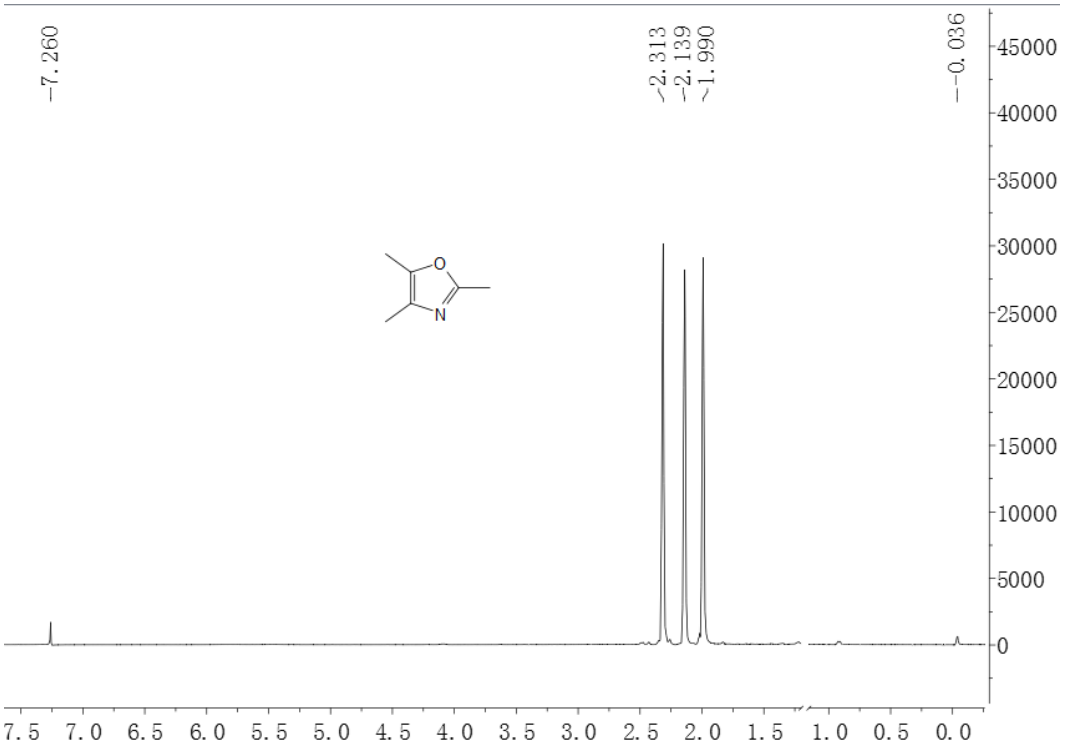

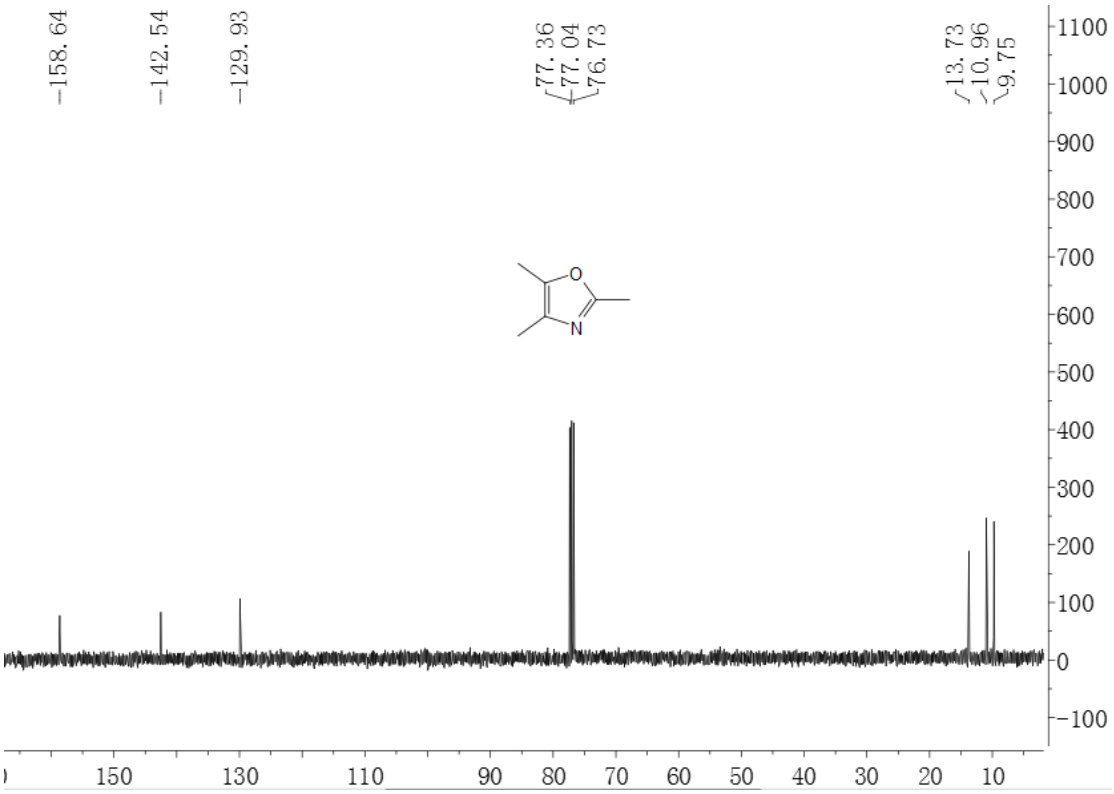

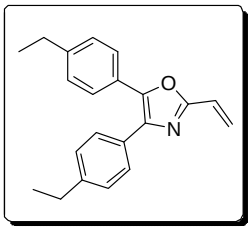

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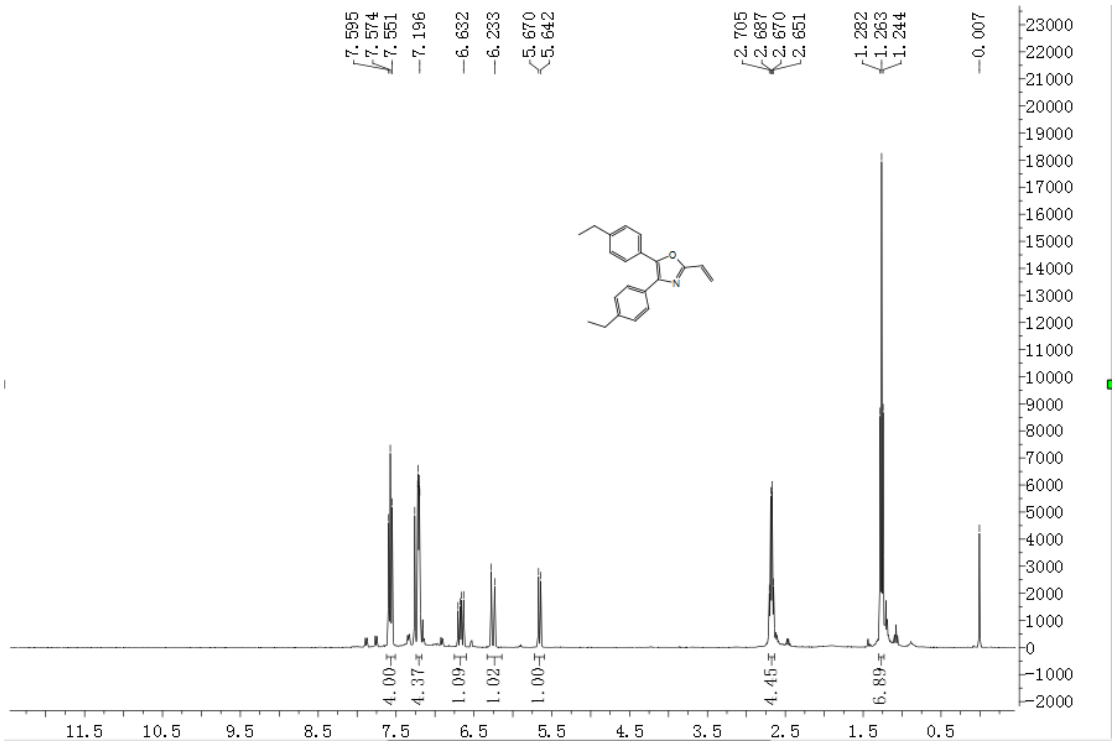
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1.02
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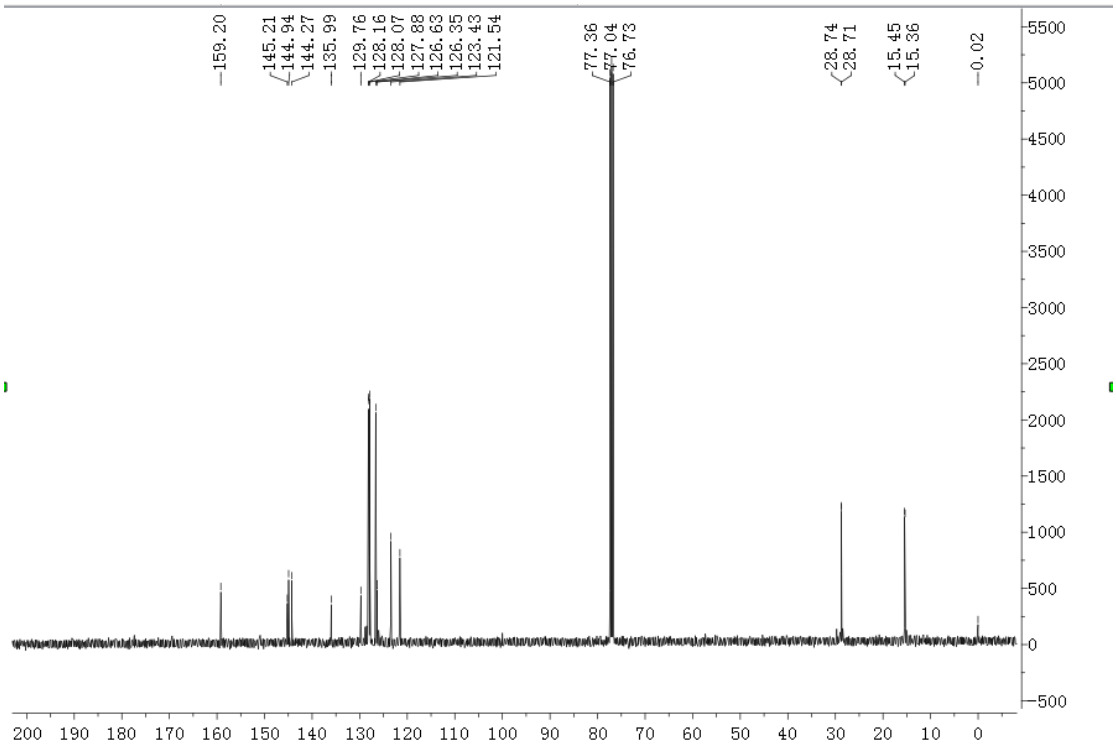
6.89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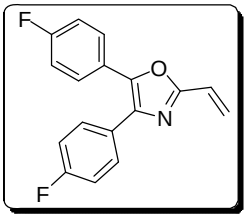
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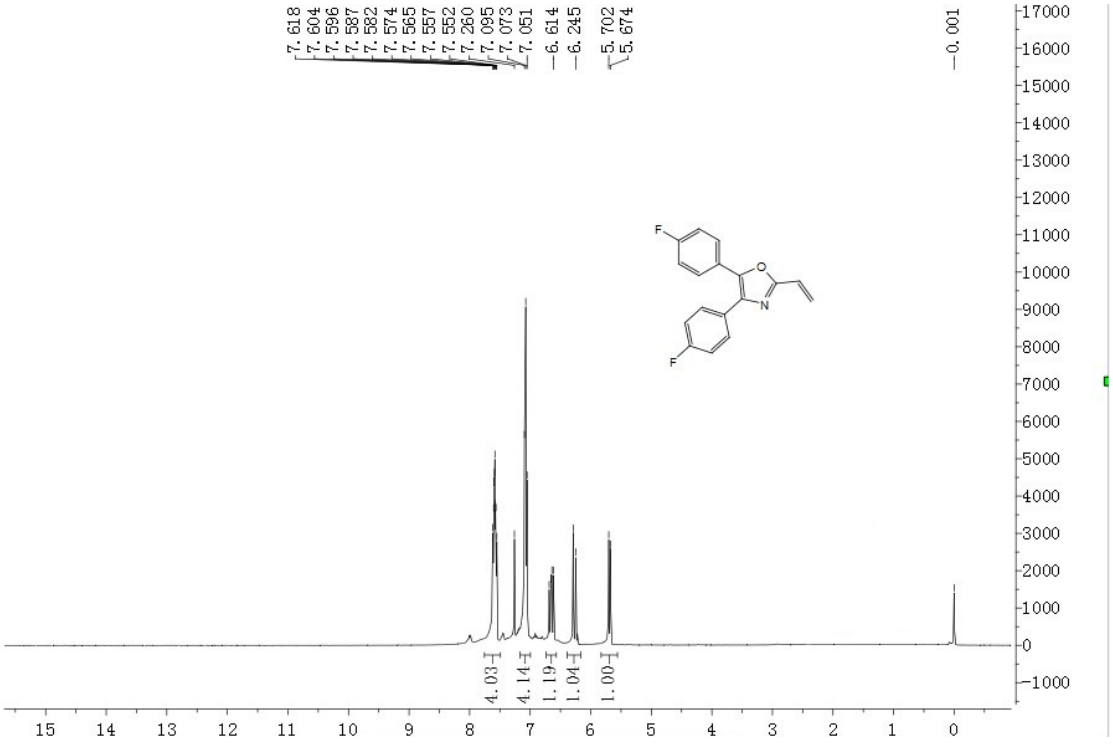
(3fb)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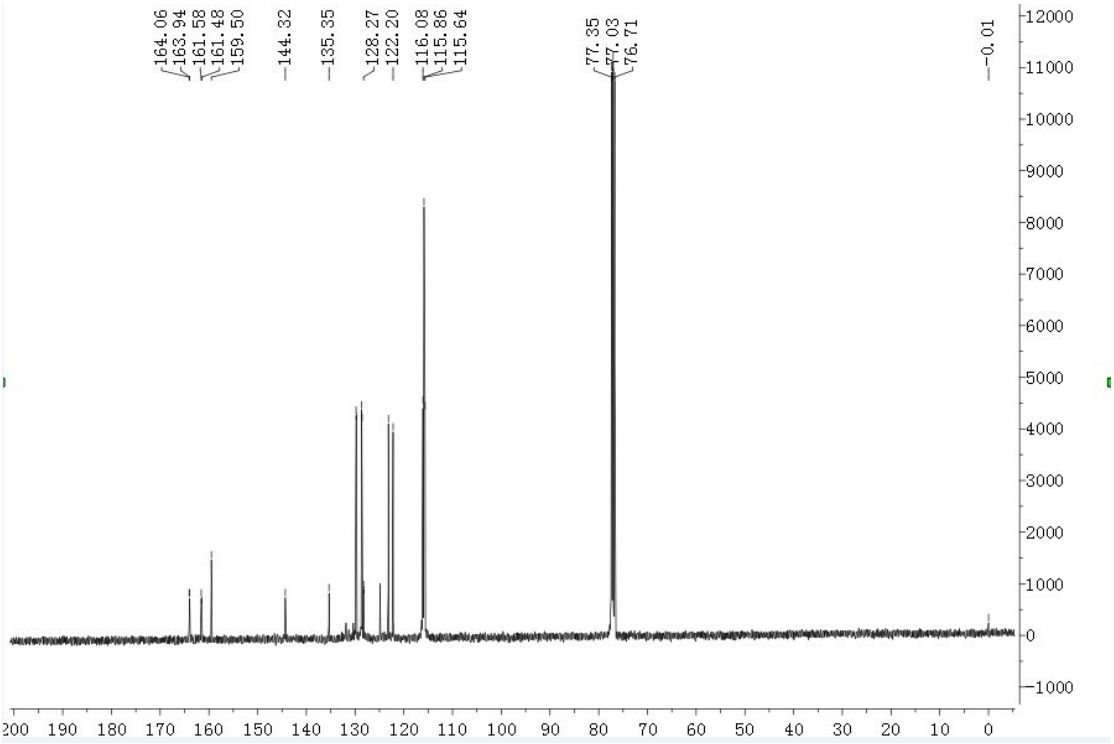
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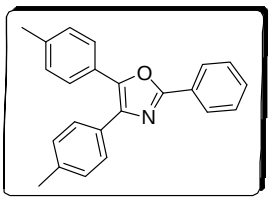

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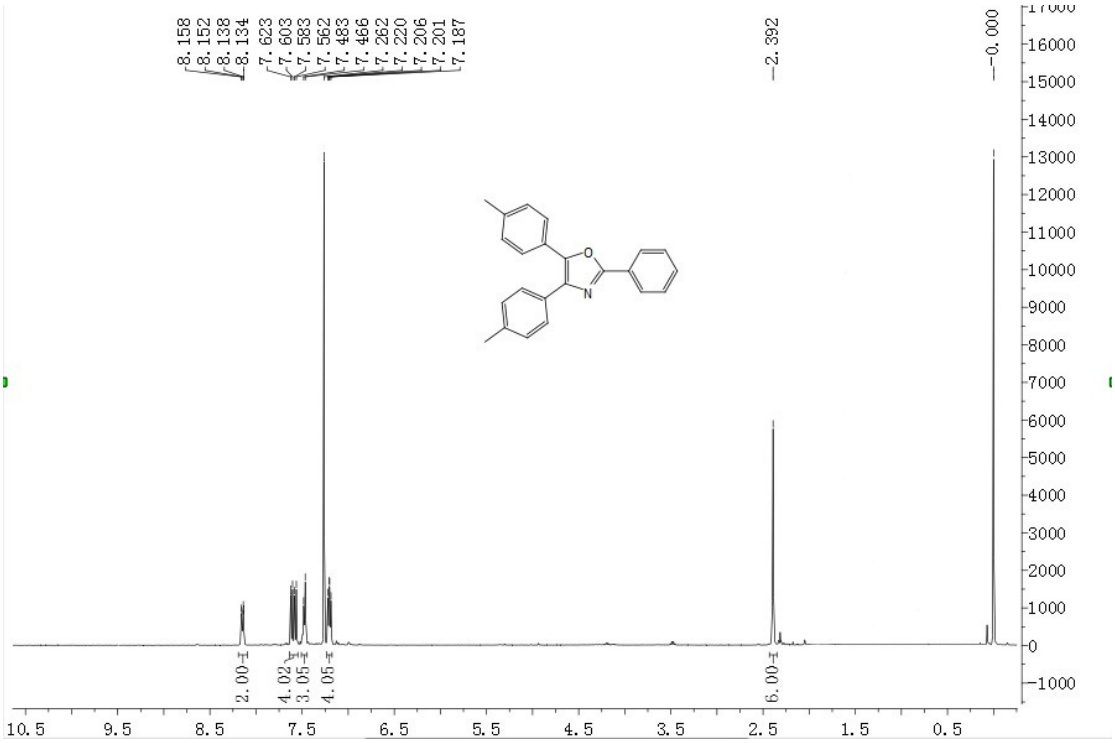
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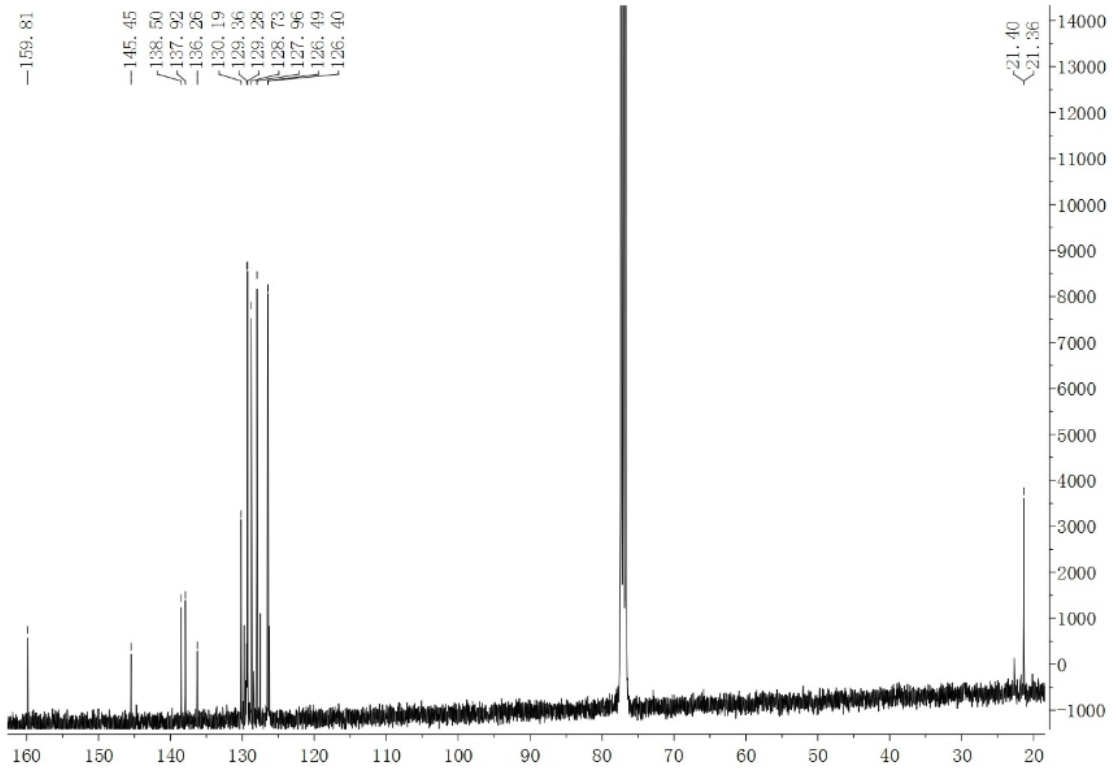
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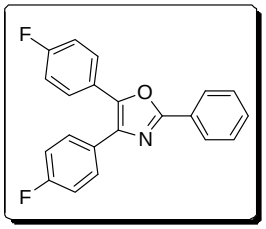
(3fe)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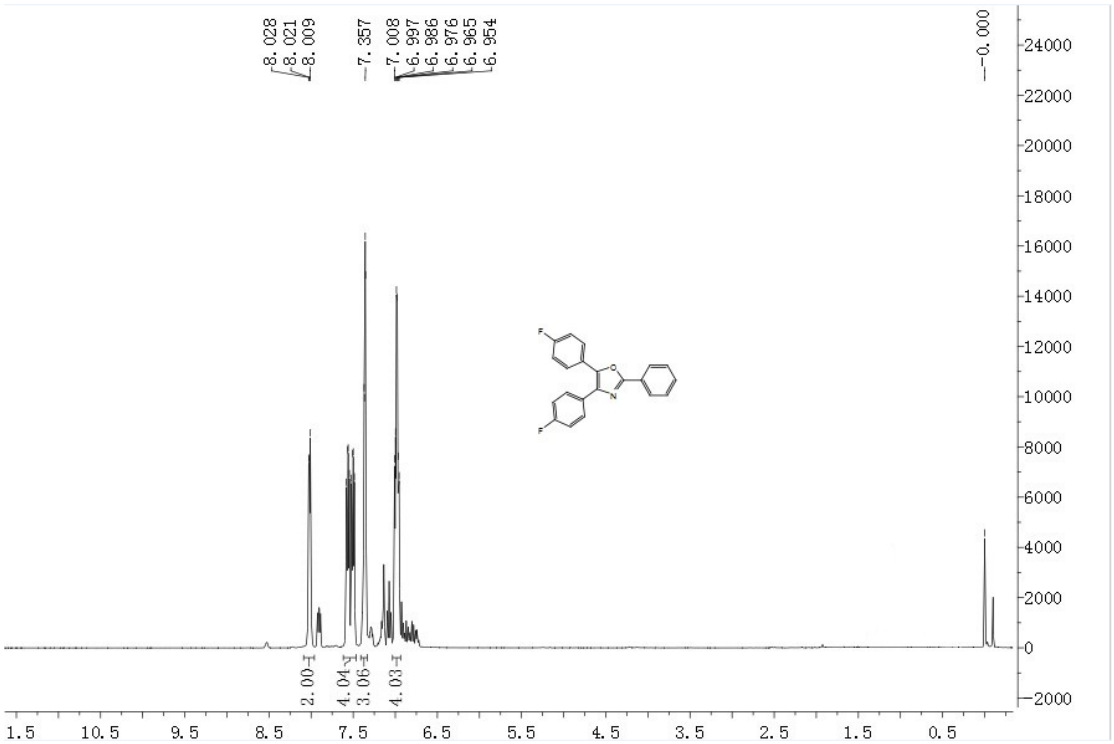
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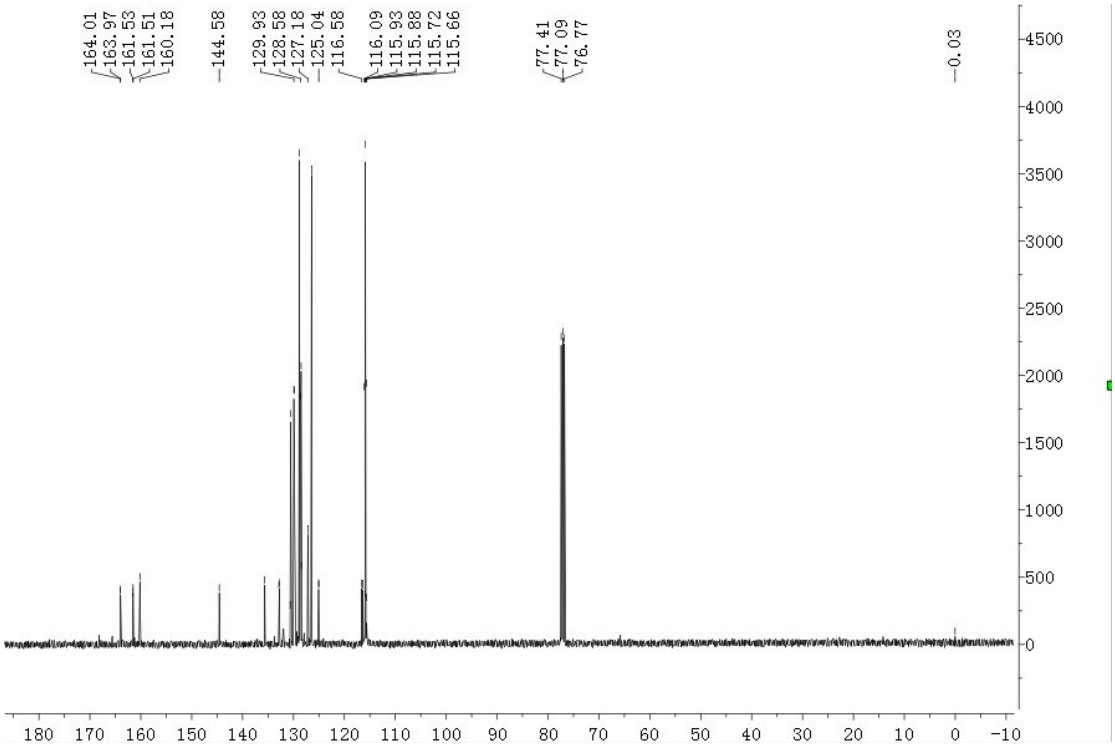
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76.77
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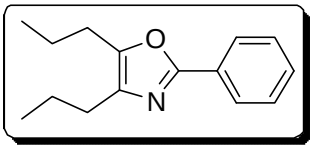

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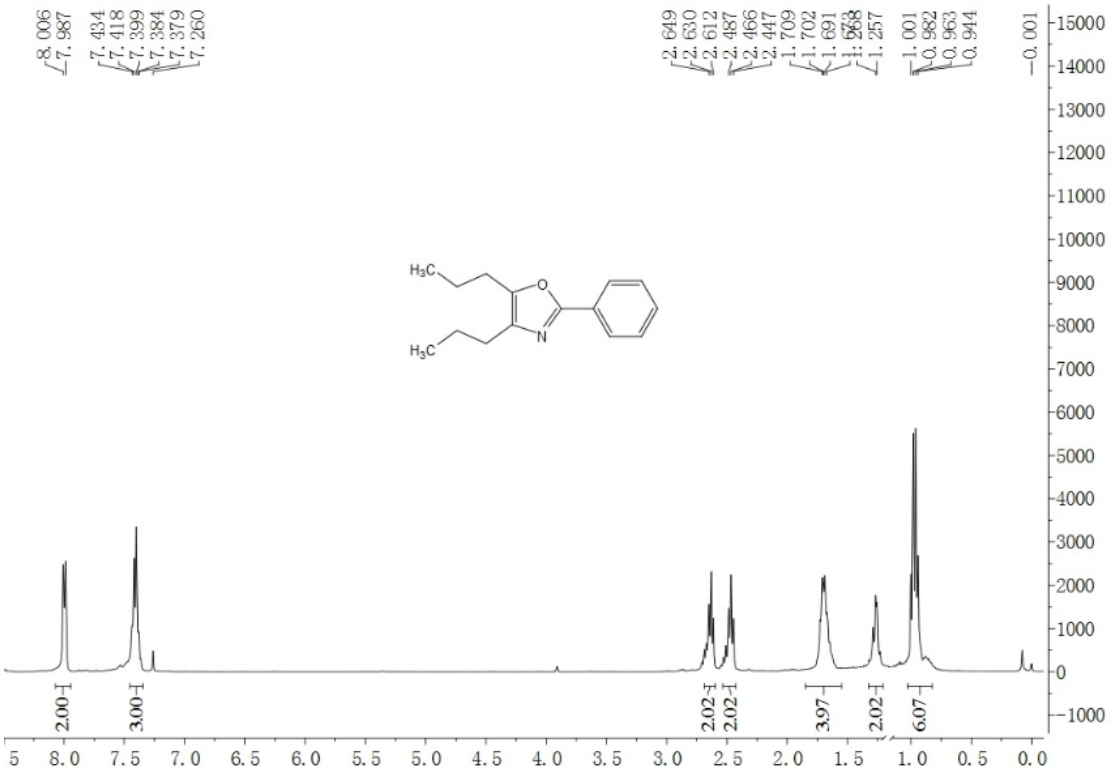
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2.02
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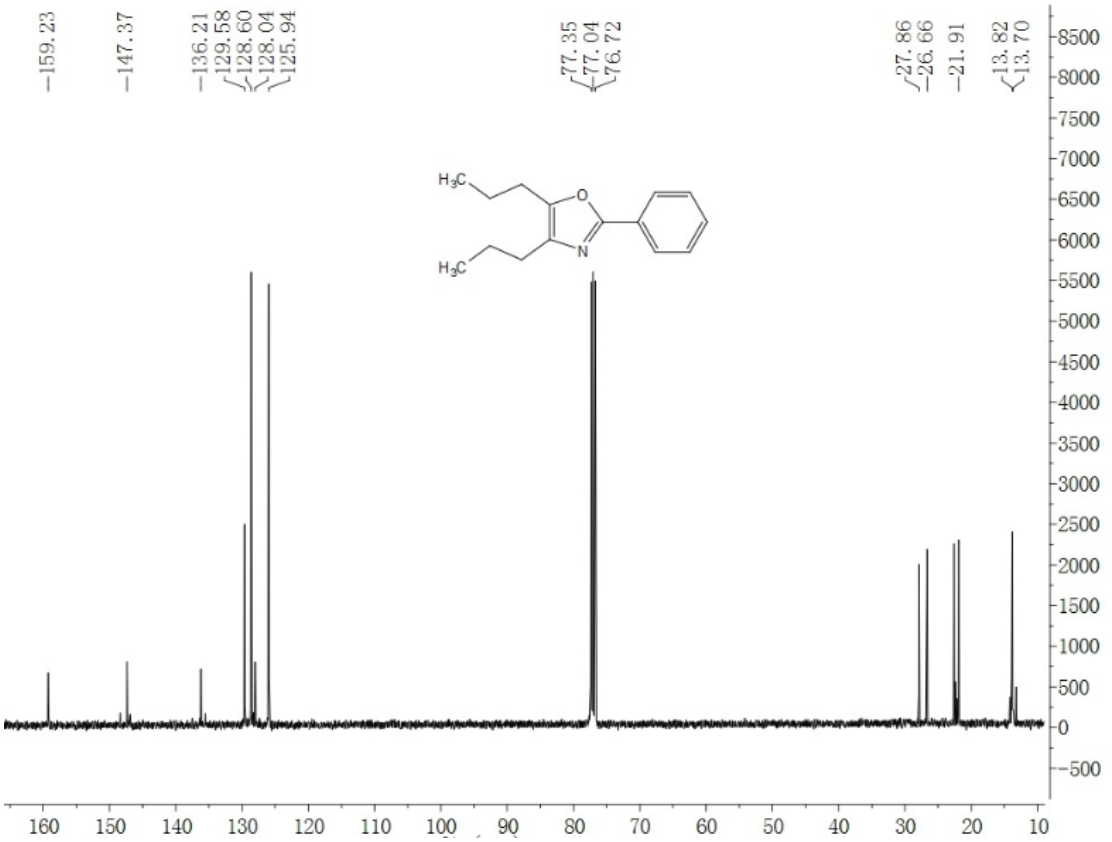
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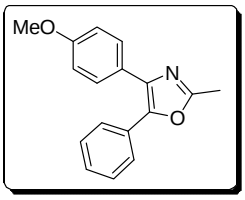
13.70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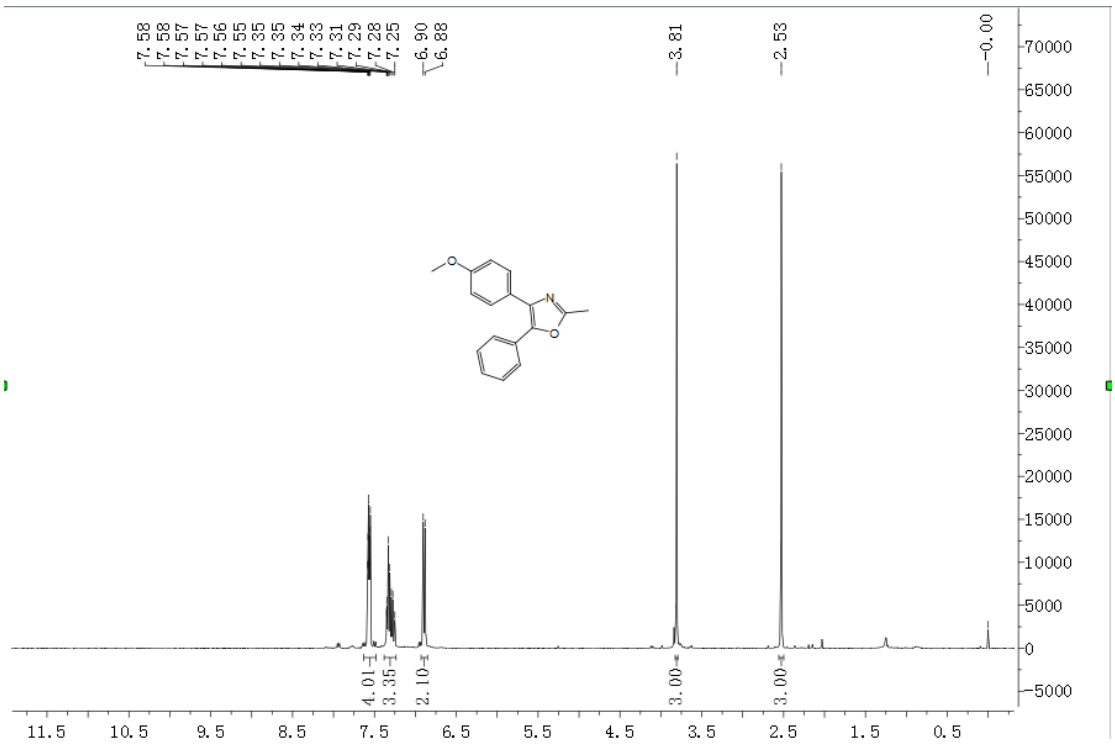
(3ma)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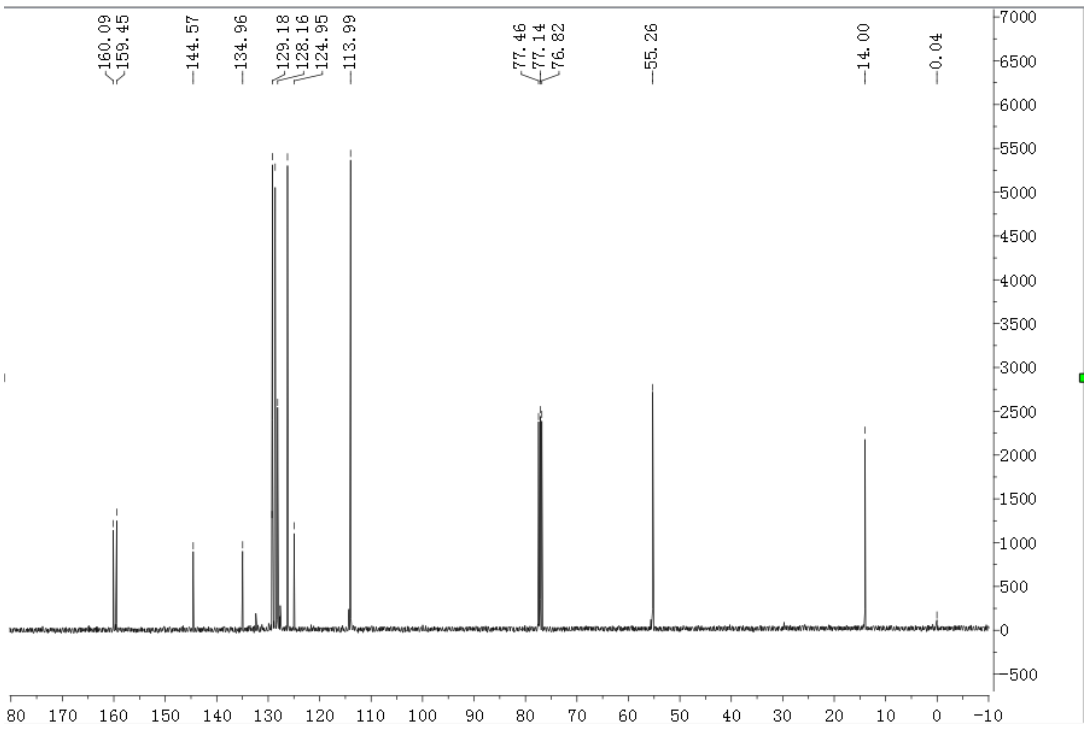
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14.00
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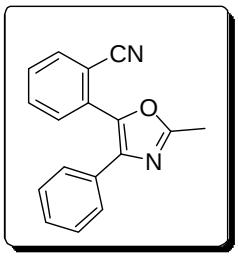
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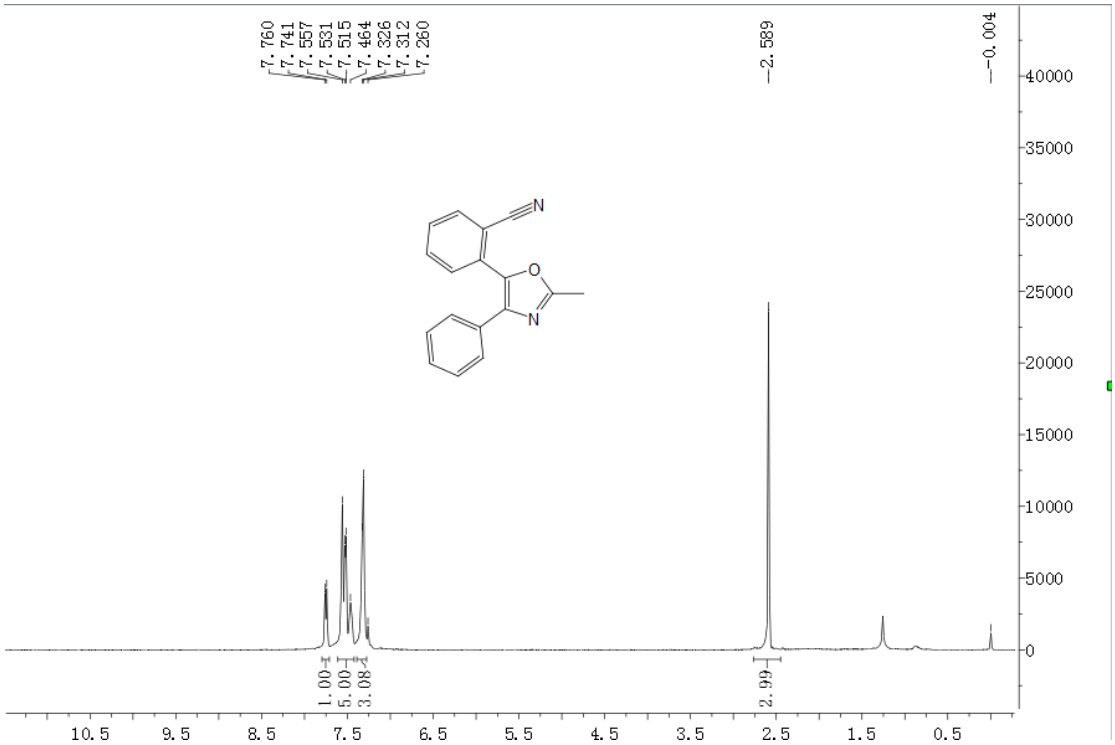
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O
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6.5
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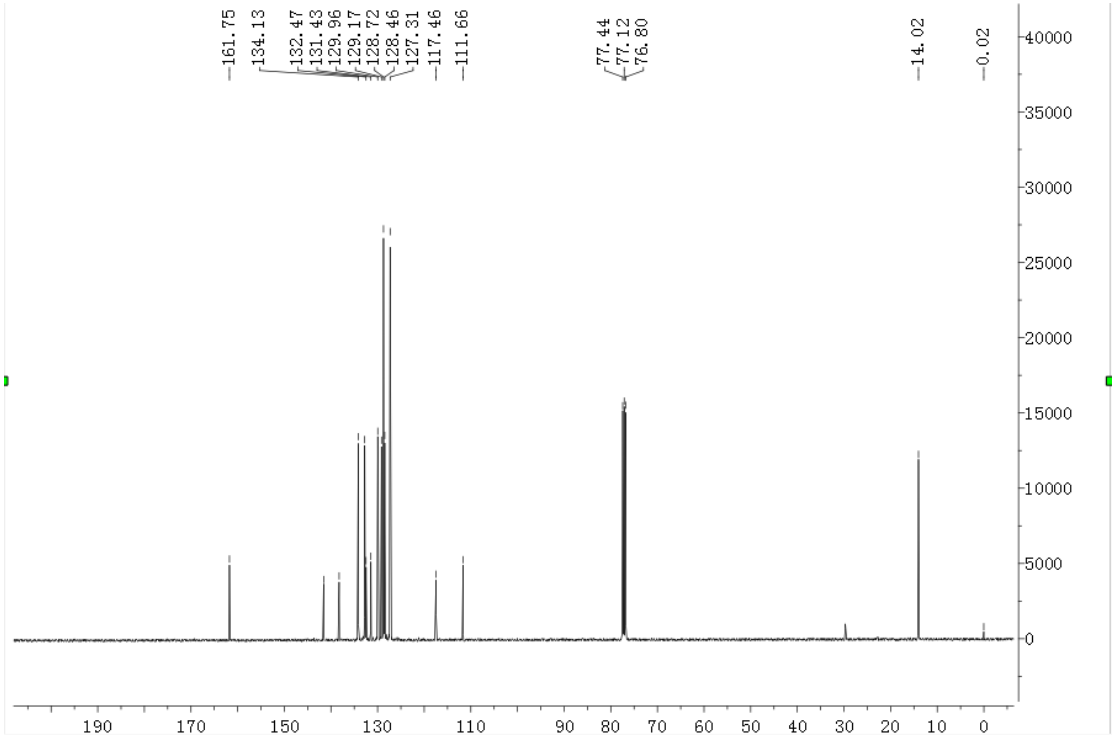
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150
130
110
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30000
25000
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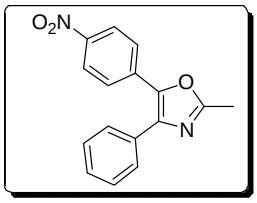
10000
5000
0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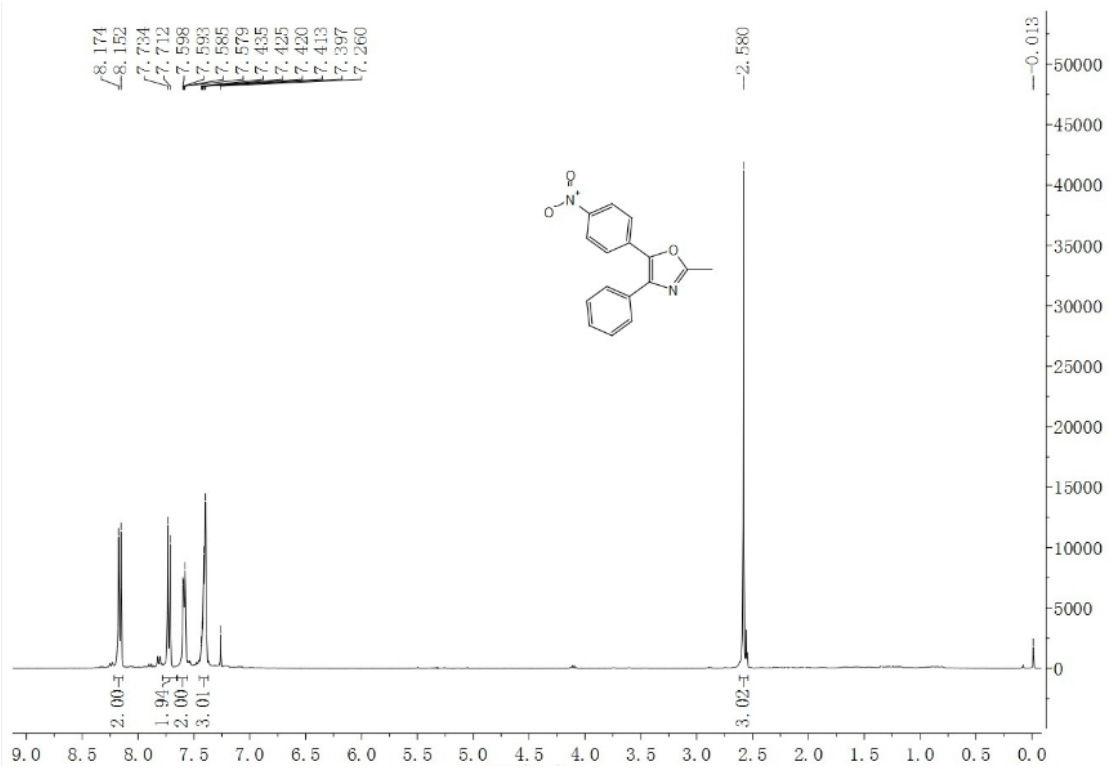
(3oa)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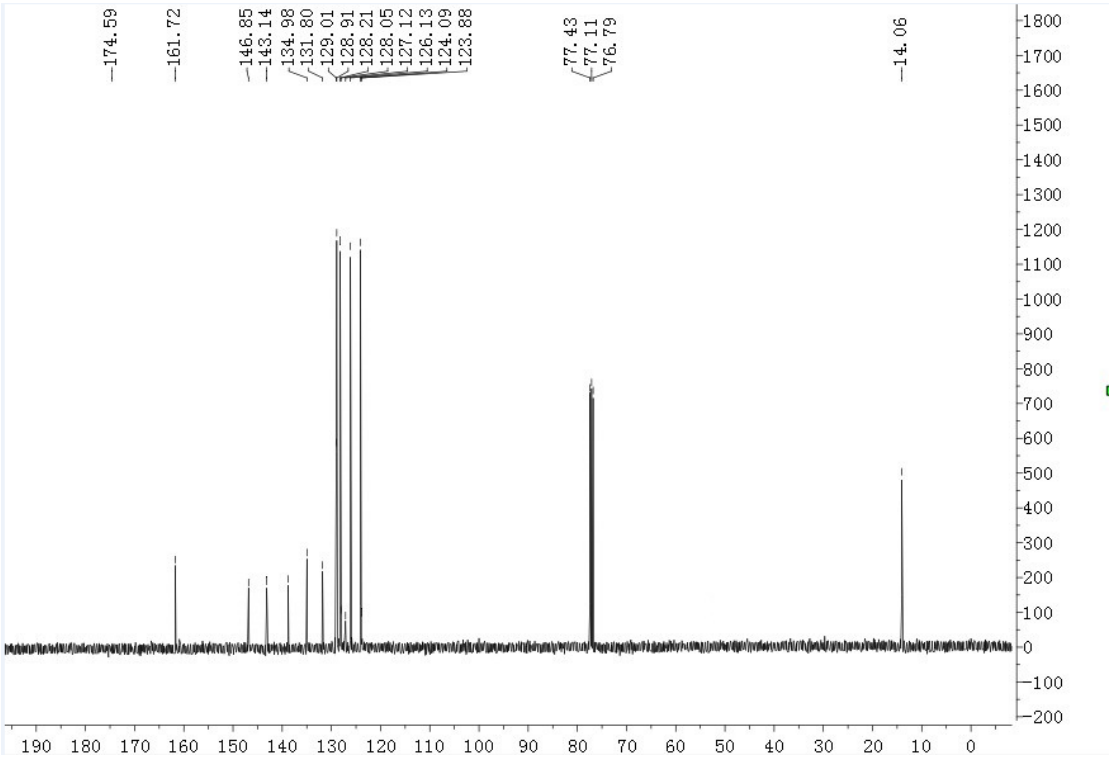
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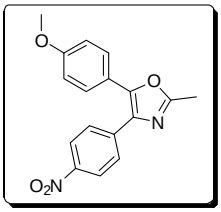

(3pa)


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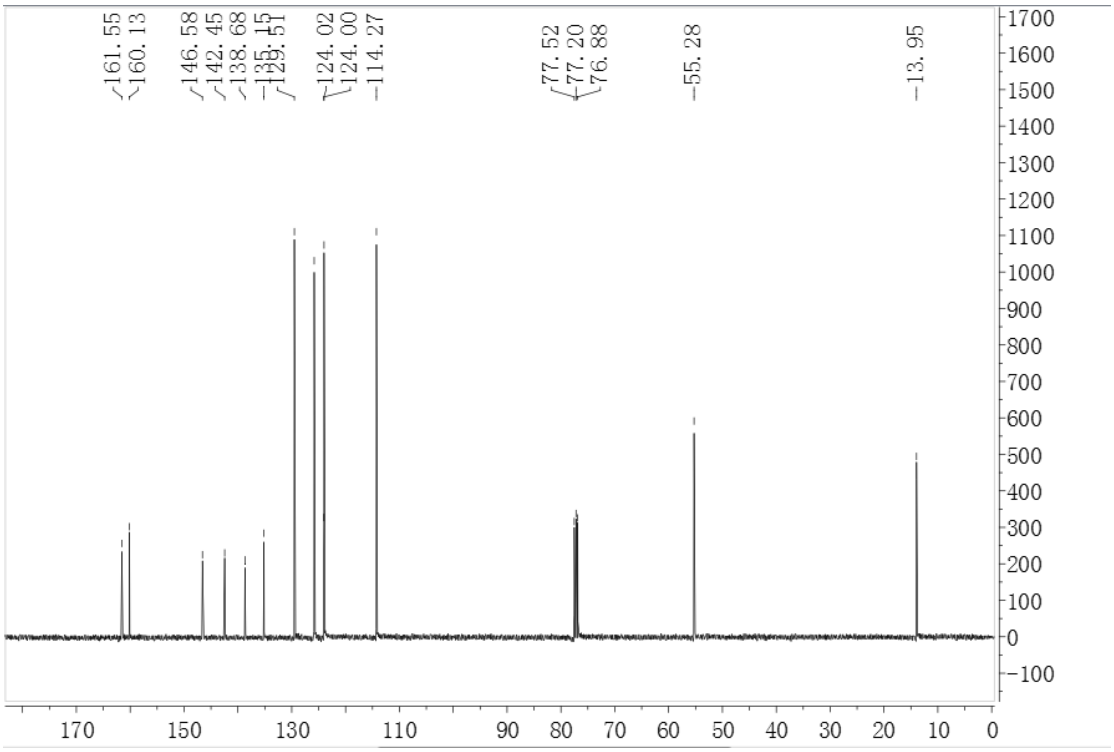
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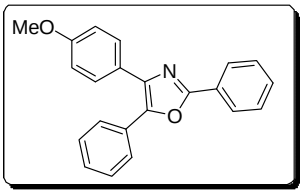
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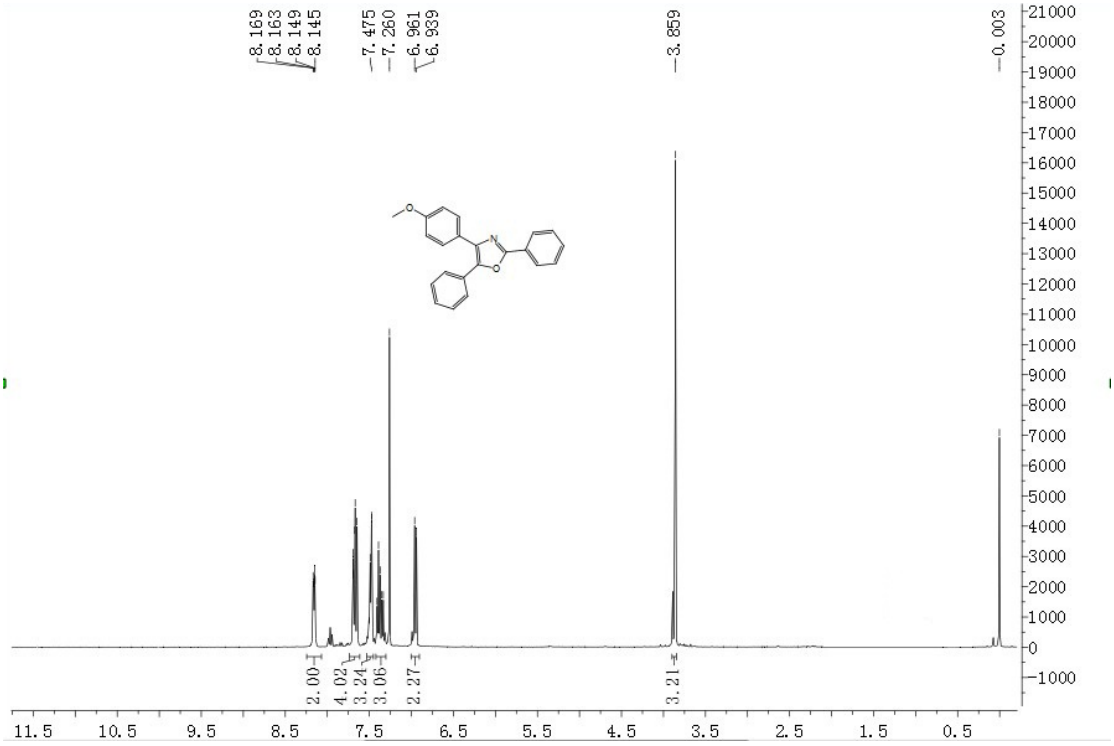
(3me)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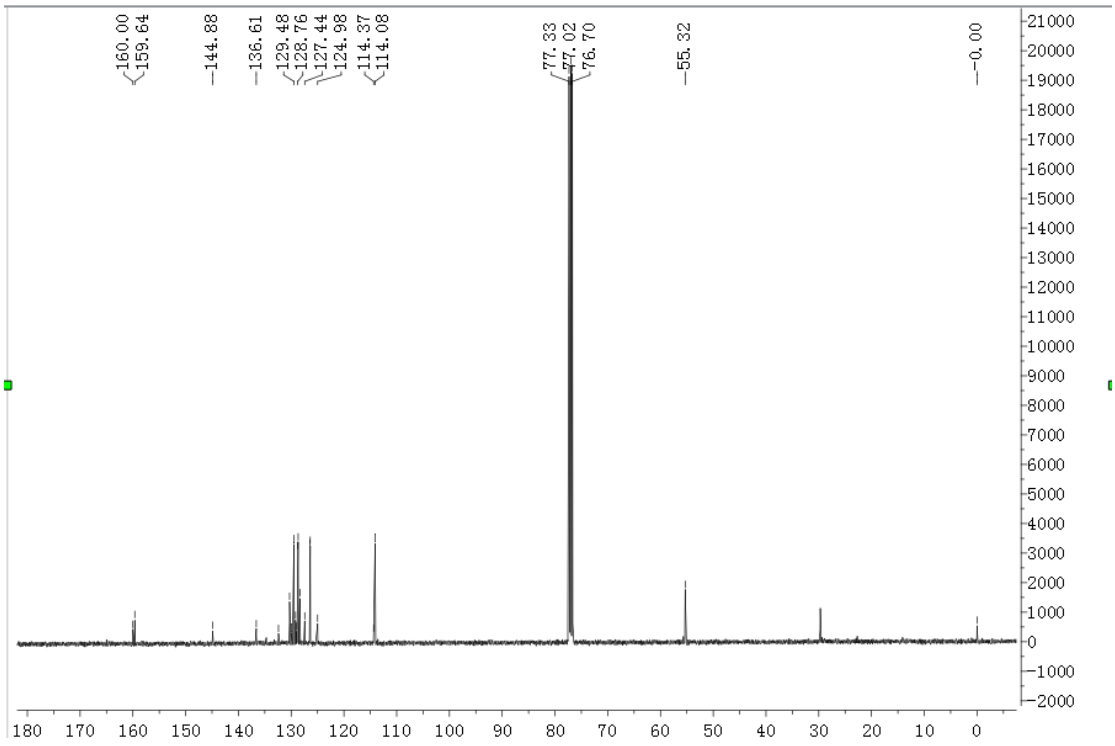
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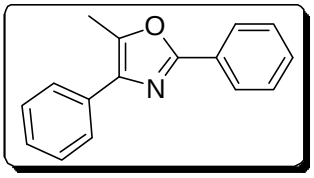
55.32
0.00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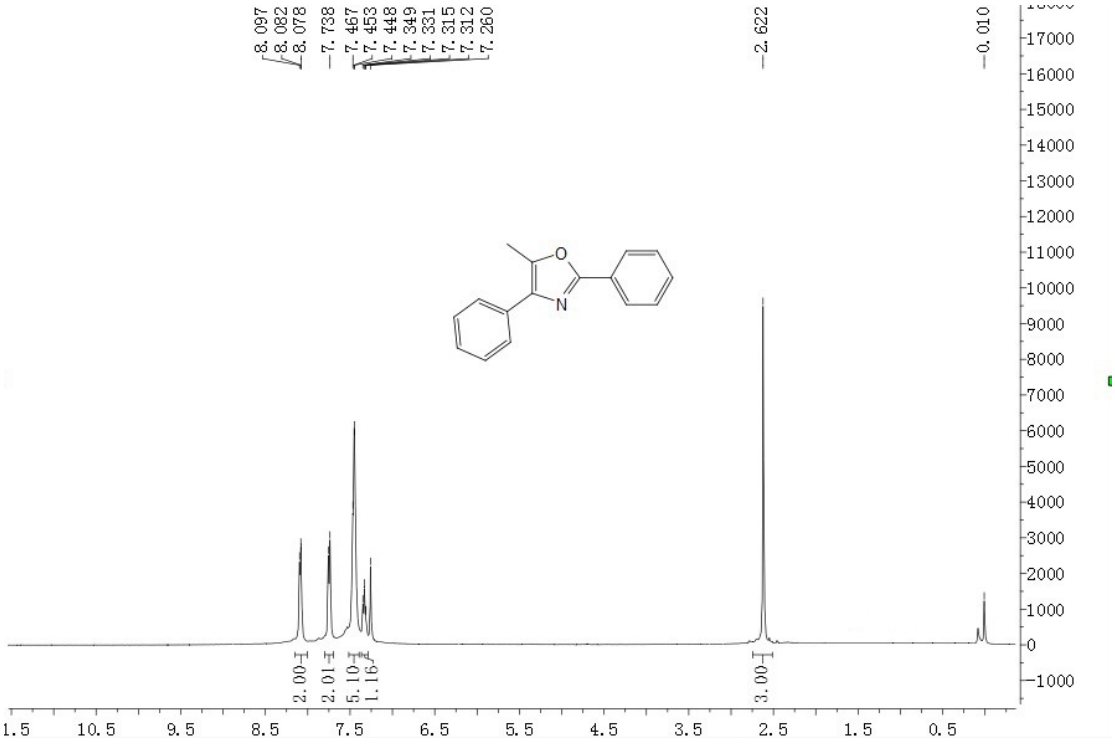
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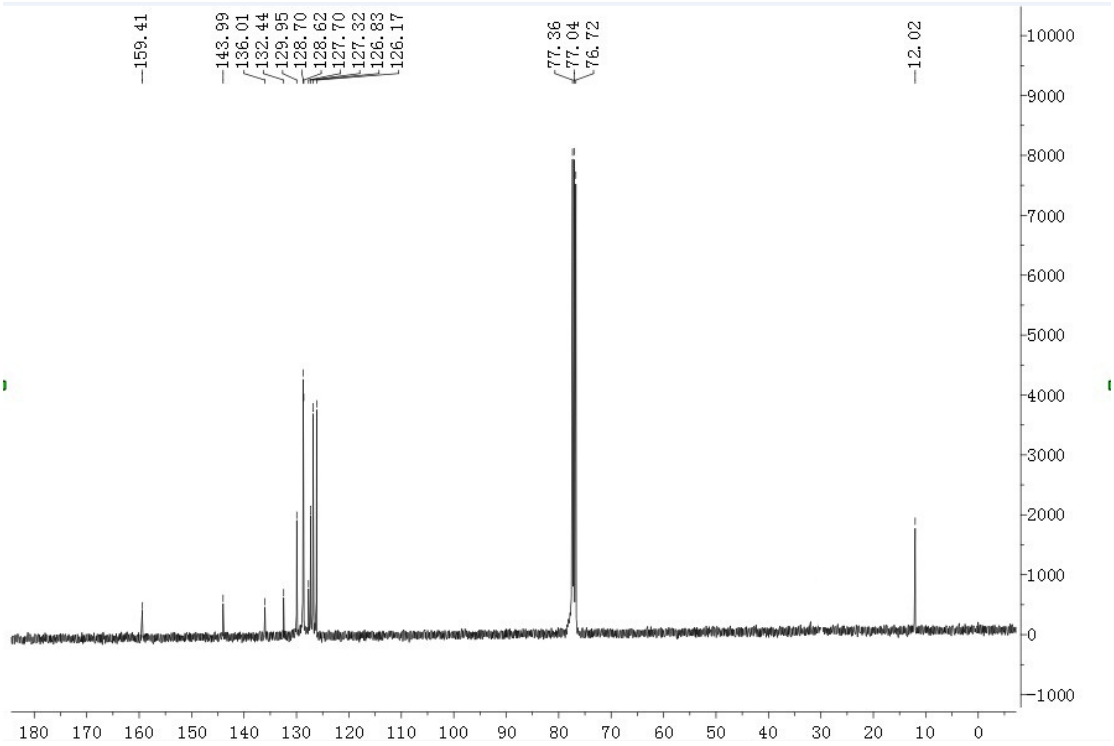
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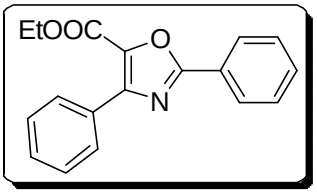
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(3se)


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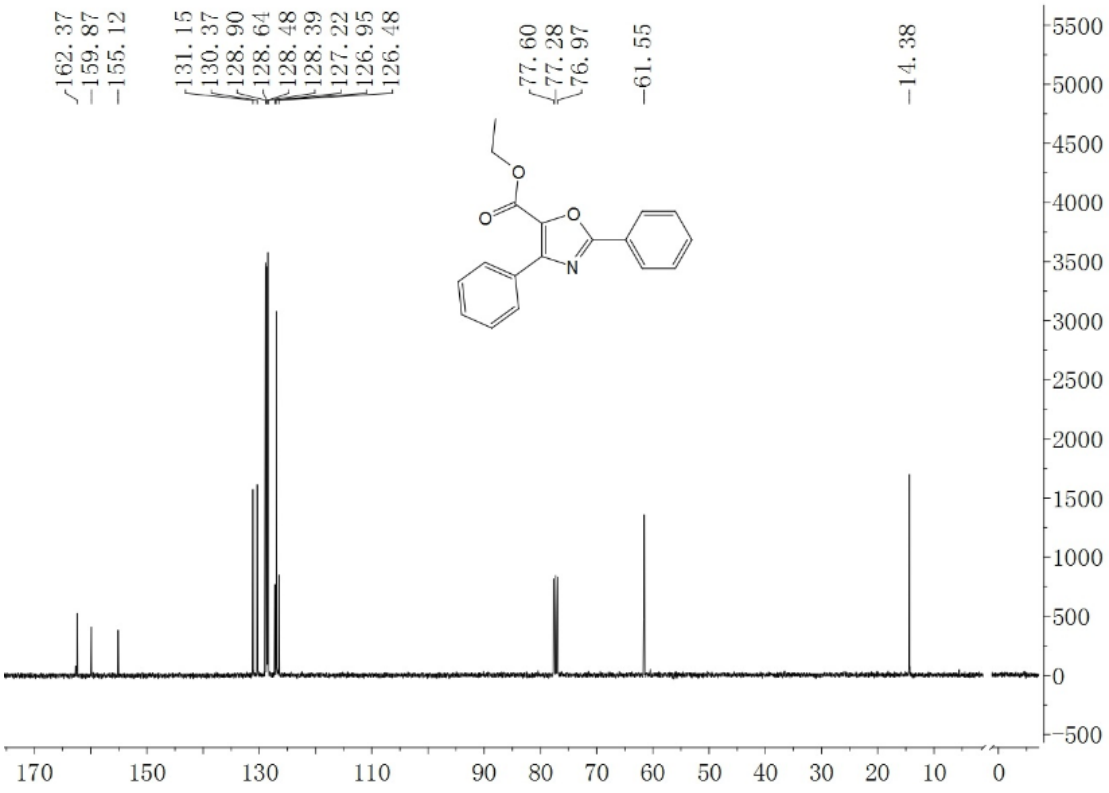
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O
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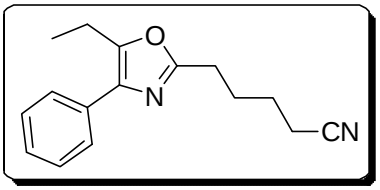
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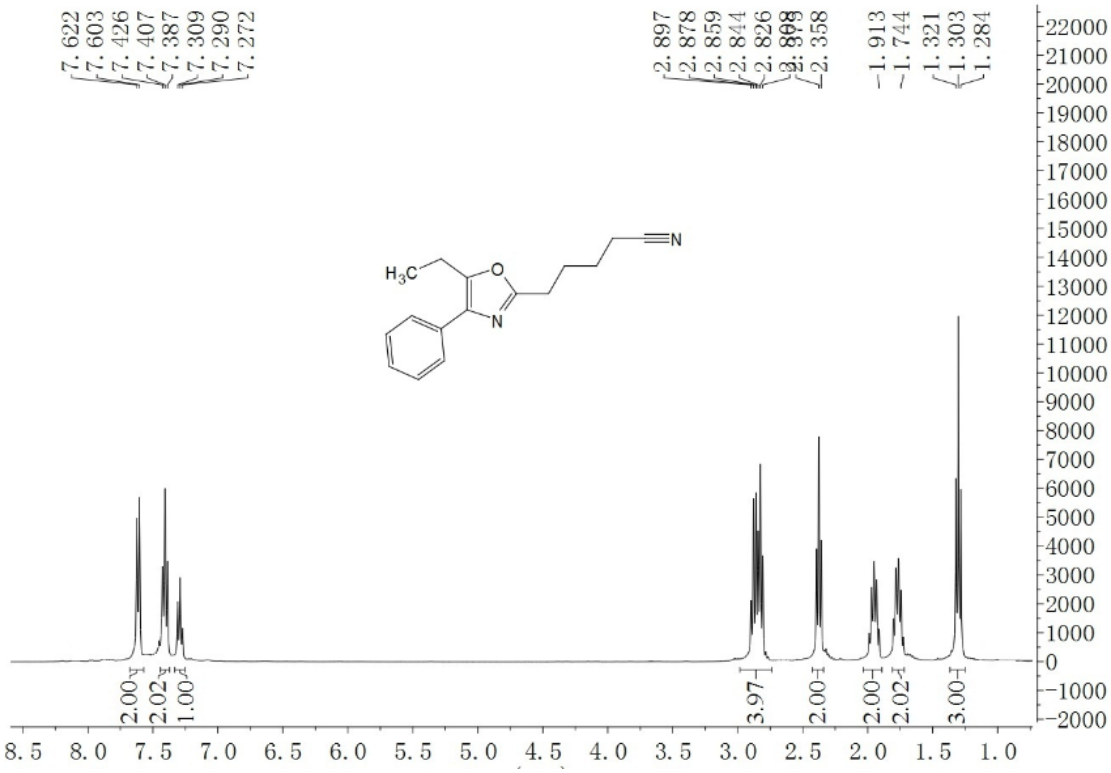
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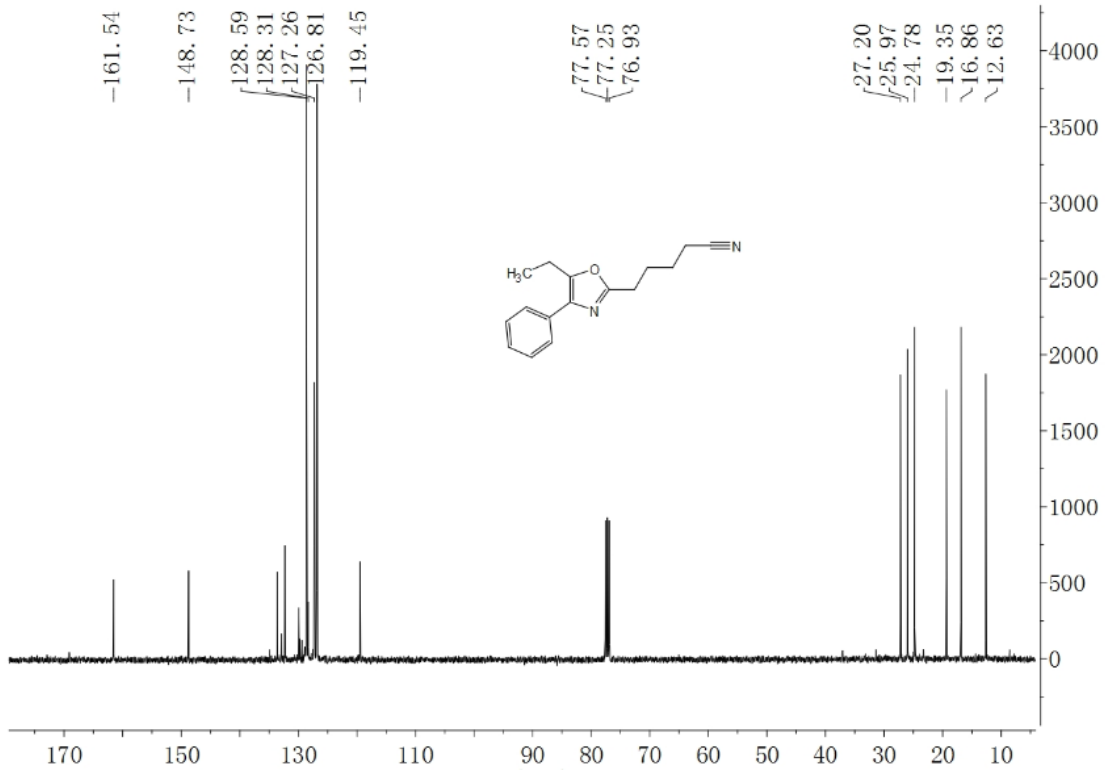
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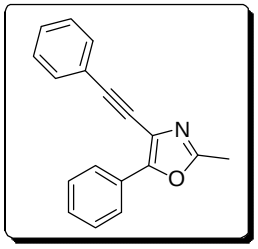
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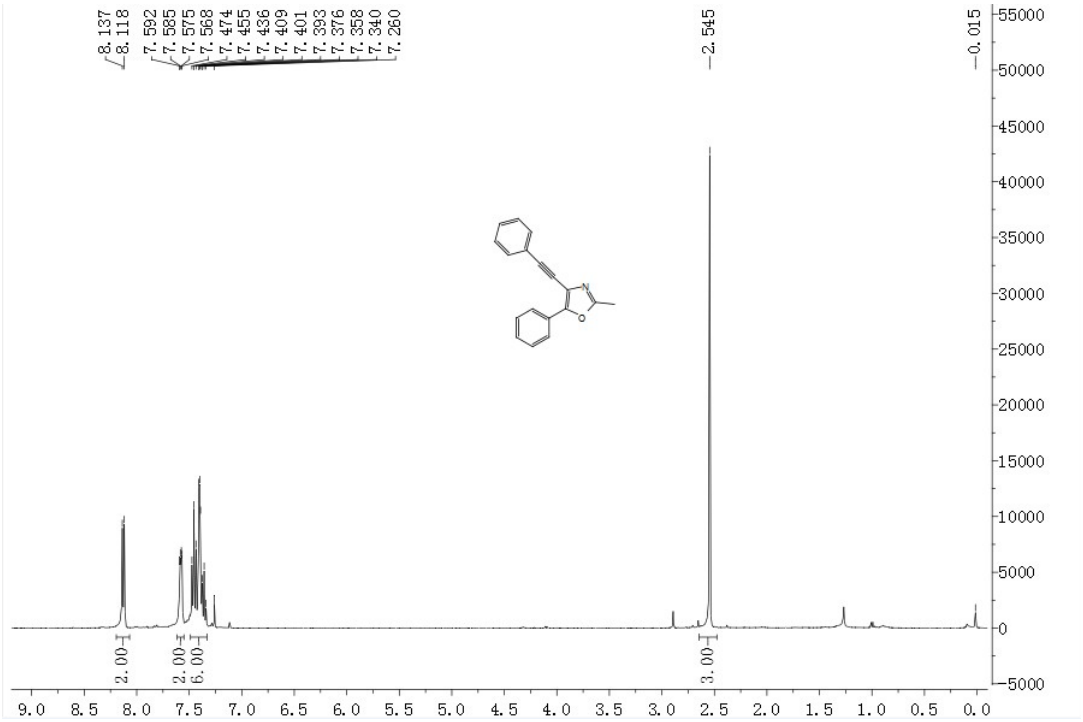
(3qa)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7.401
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7.340
7.260
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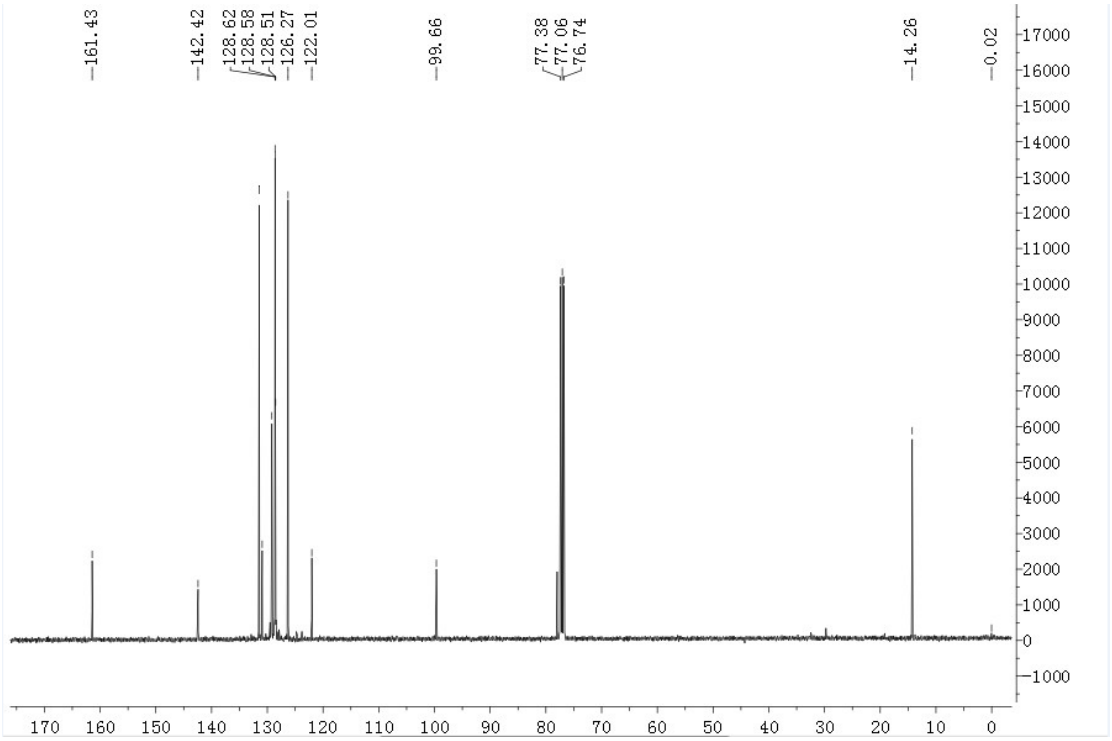
2.00
6.00
3.00
N
O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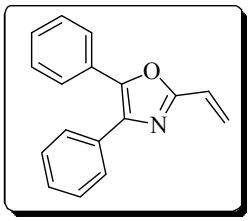
128.58
128.51
126.27
122.01
99.66
77.38
77.06
76.74
14.26
0.02



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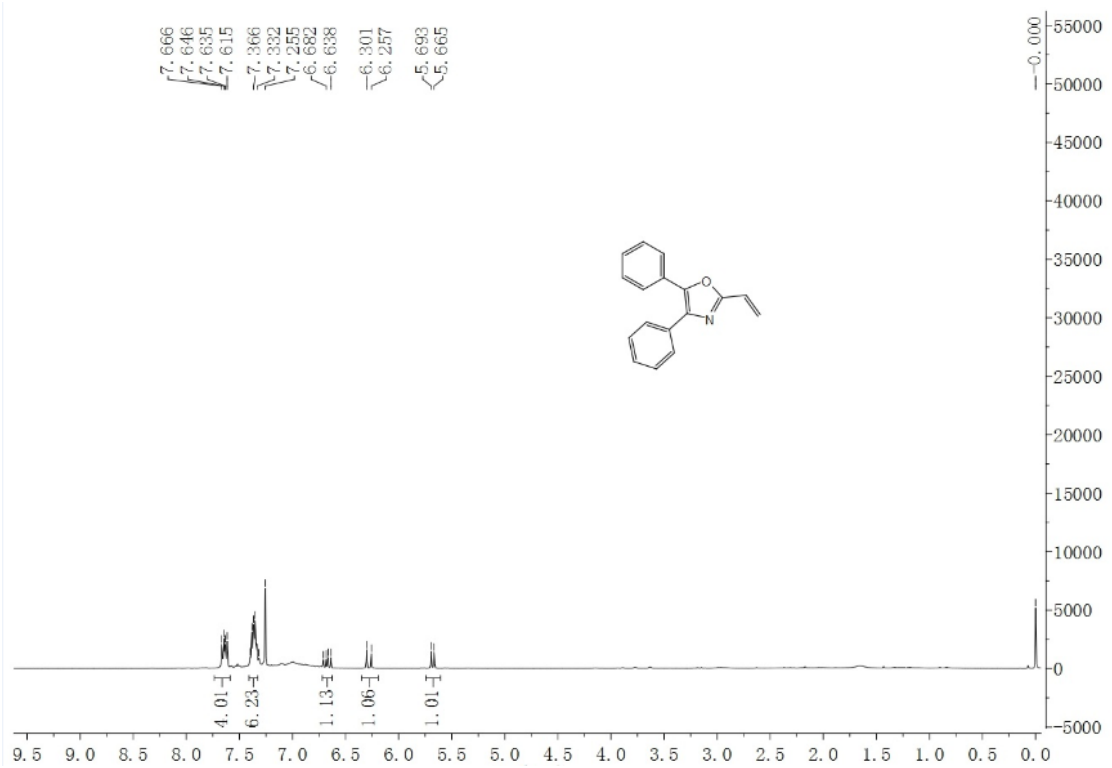
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7.332
7.255
6.682
6.638
6.301
6.257
5.693
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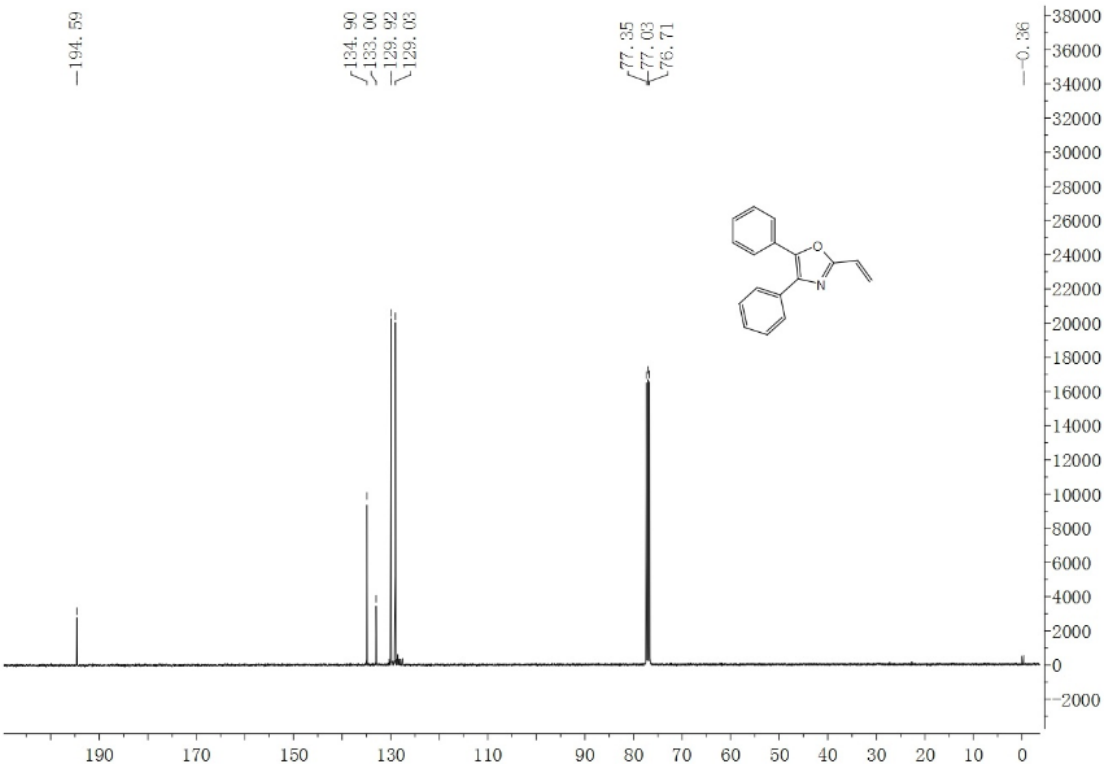
0.000
4.01
6.23
1.13
1.06
1.01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76.71
0.36
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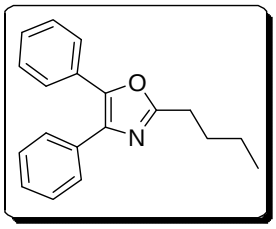
N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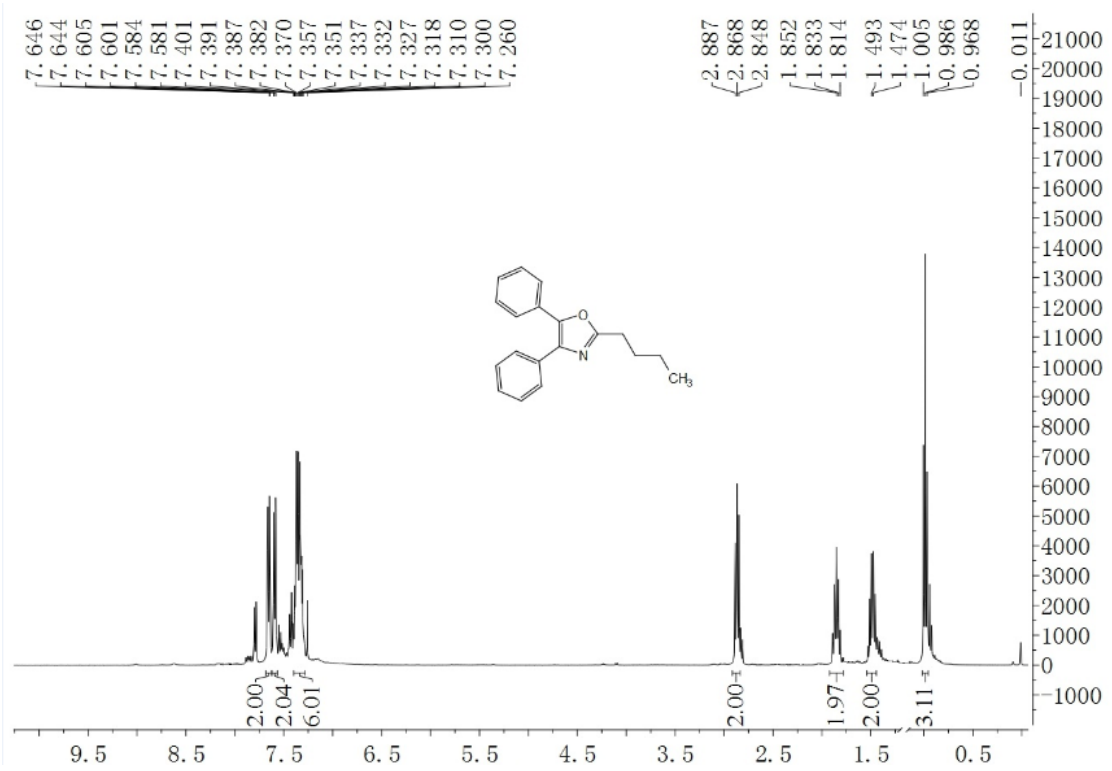
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7.581
7.401
7.391
7.387
7.382
7.370
7.357
7.351
7.337
7.332
7.327
7.318
7.310
7.300
7.260
2.887
2.868
2.848
1.852
1.833
1.814
1.493
1.474
1.005
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0.968
0.011
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6.01
2.00
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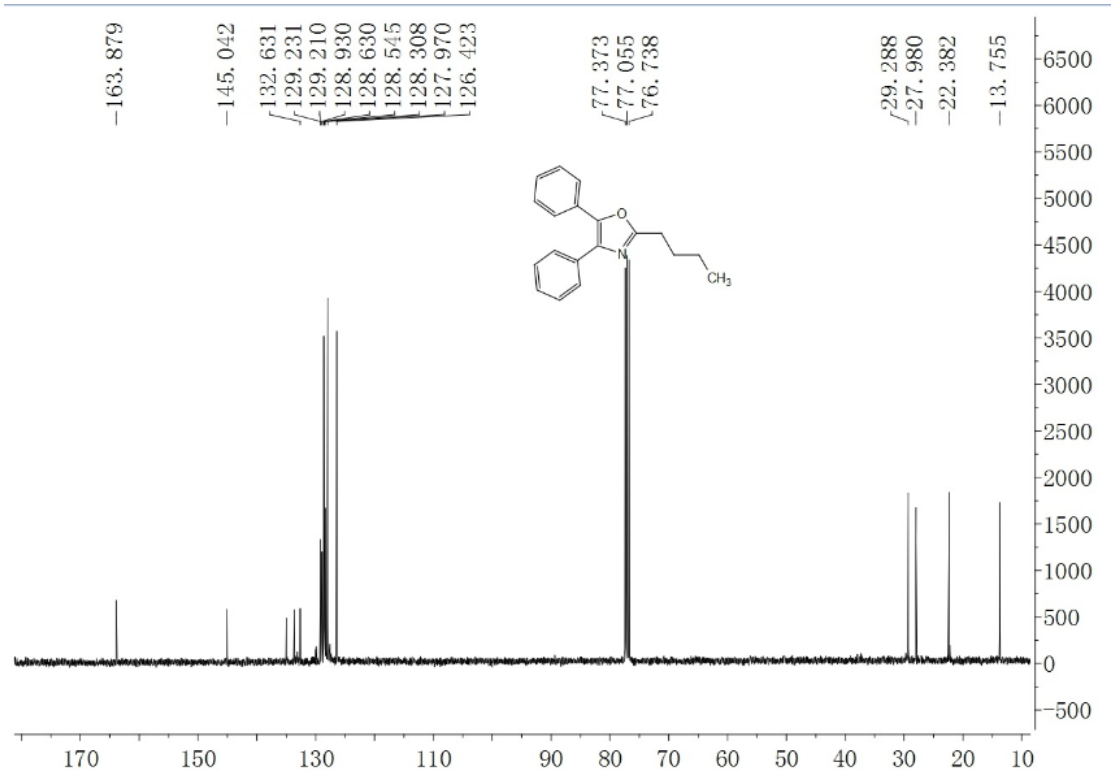
2.00
3.11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22.382
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O
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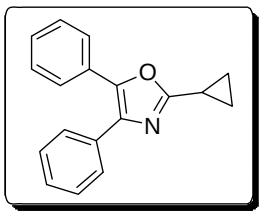
CH3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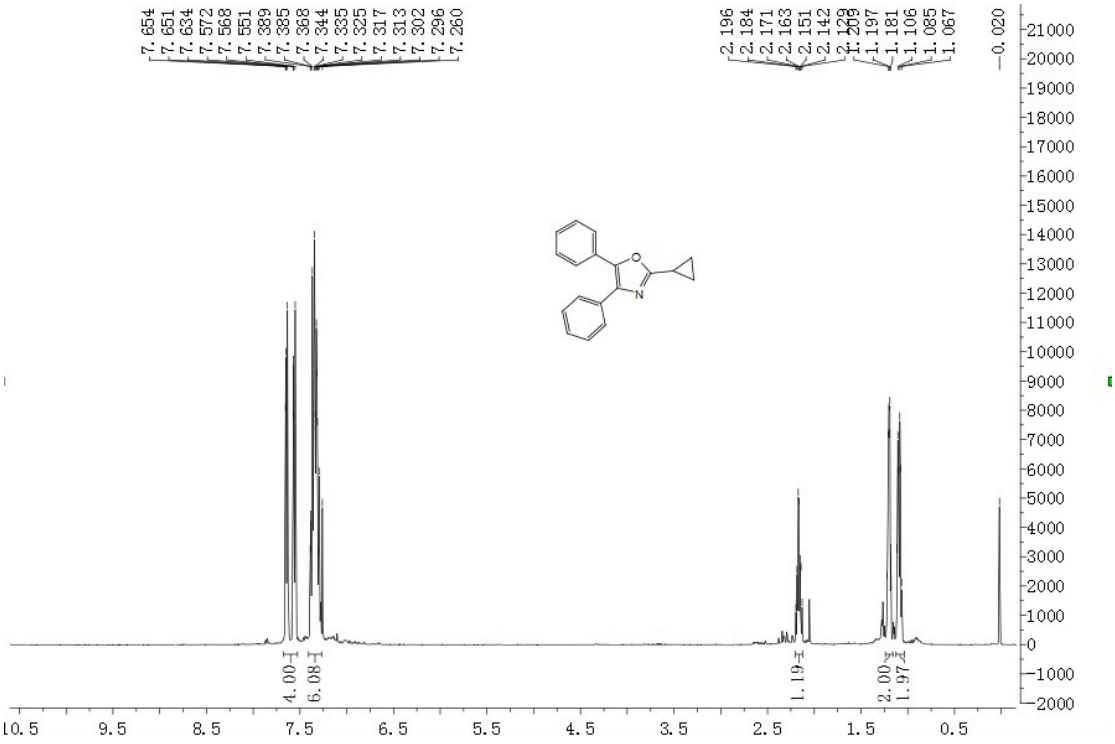
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7.385
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7.317
7.313
7.302
7.296
7.260
2.196
2.184
2.171
2.163
2.151
2.142
1.197
1.181
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1.085
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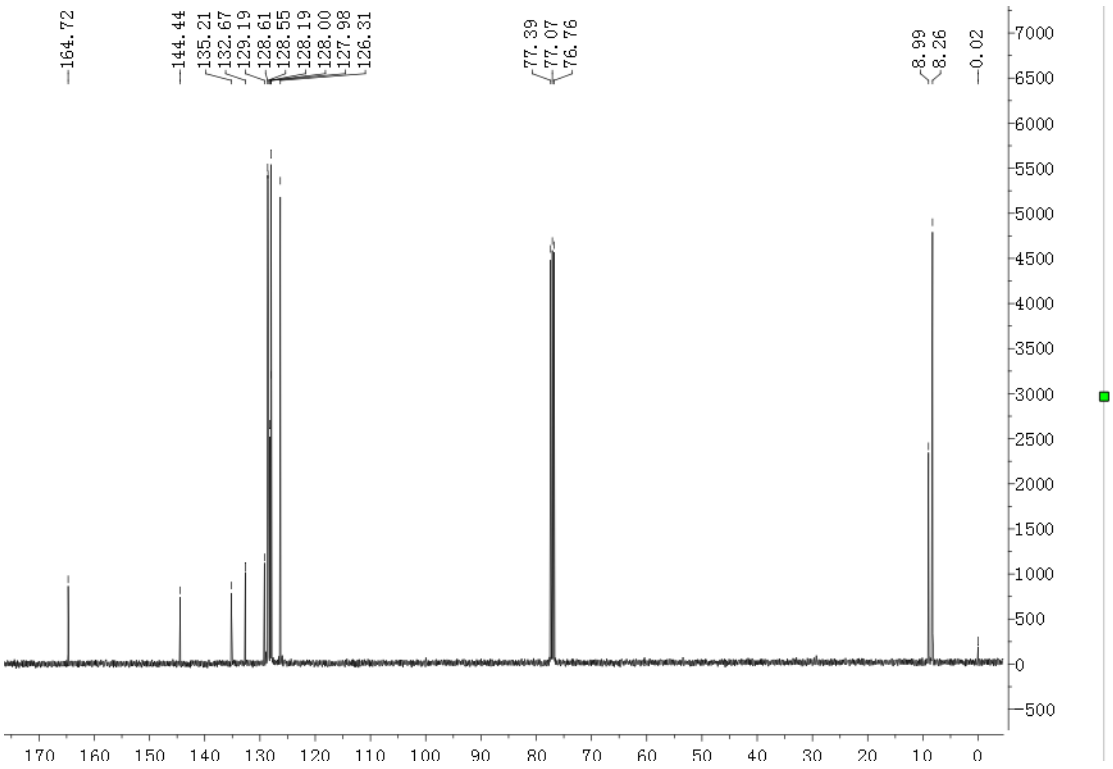
6.08
1.19
2.00
1.97
O
N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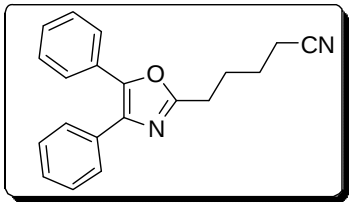
128.55
128.19
128.00
127.98
126.31
77.39
77.07
76.76
8.99
8.26
0.02
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0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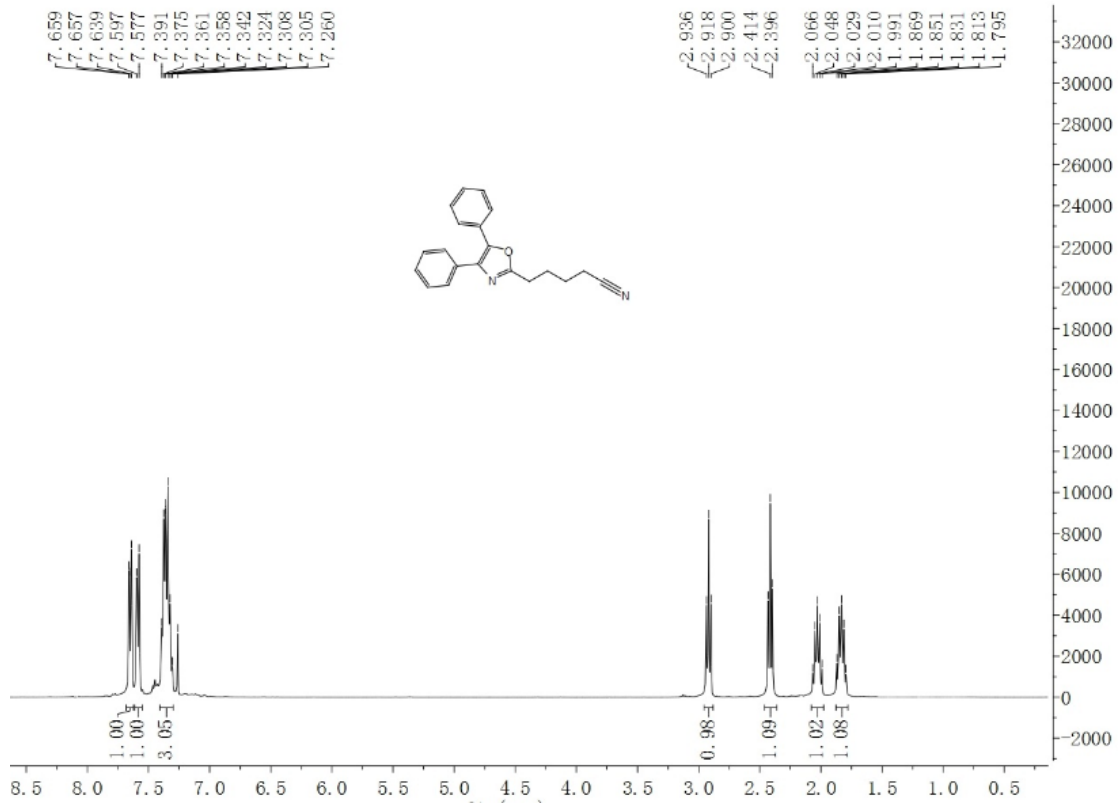
(3ae)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7.324
7.308
7.305
7.260
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2.918
2.900
2.414
2.396
2.066
2.048
2.029
2.010
1.991
1.869
1.851
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1.00
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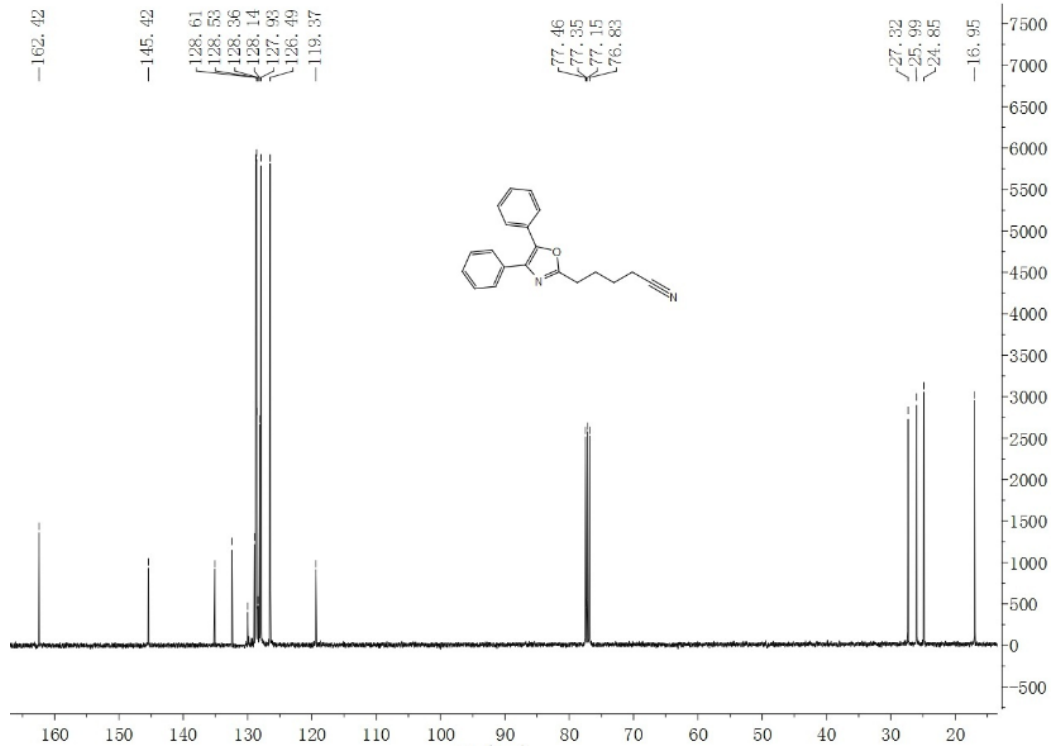
0.98
1.09
1.02
1.08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77.15
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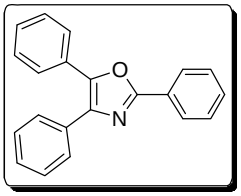
24.85
16.95



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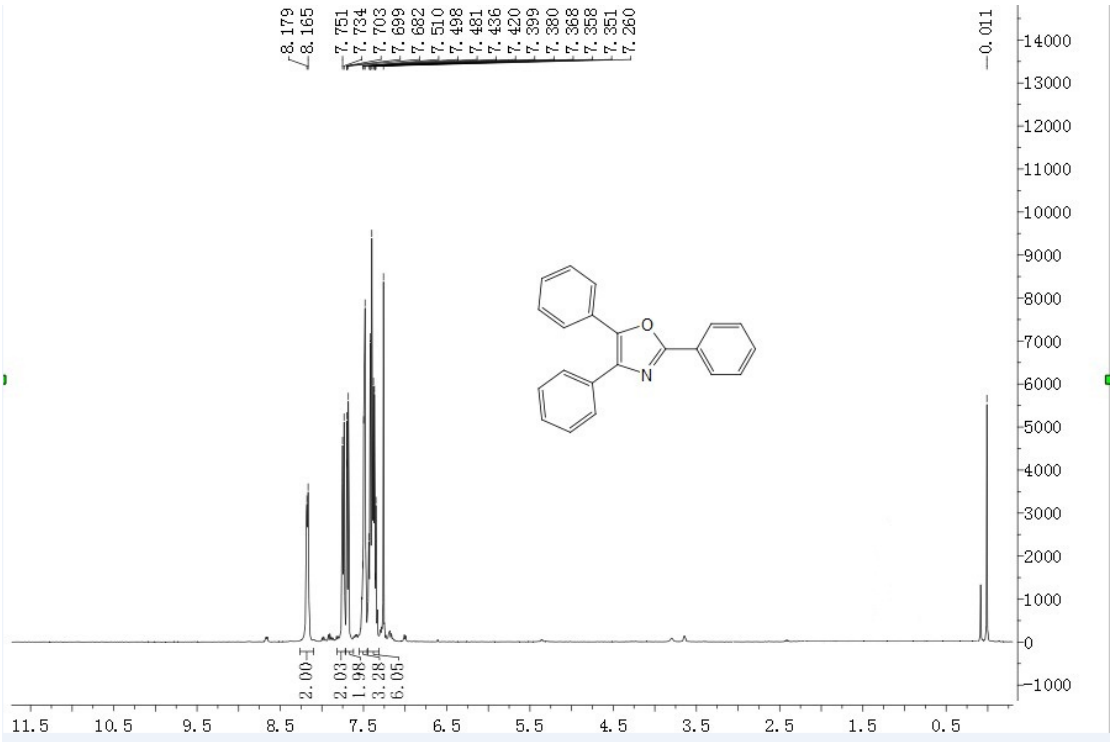
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7.699
7.682
7.510
7.498
7.481
7.436
7.420
7.399
7.380
7.368
7.358
7.351
7.260
0.011
O
N
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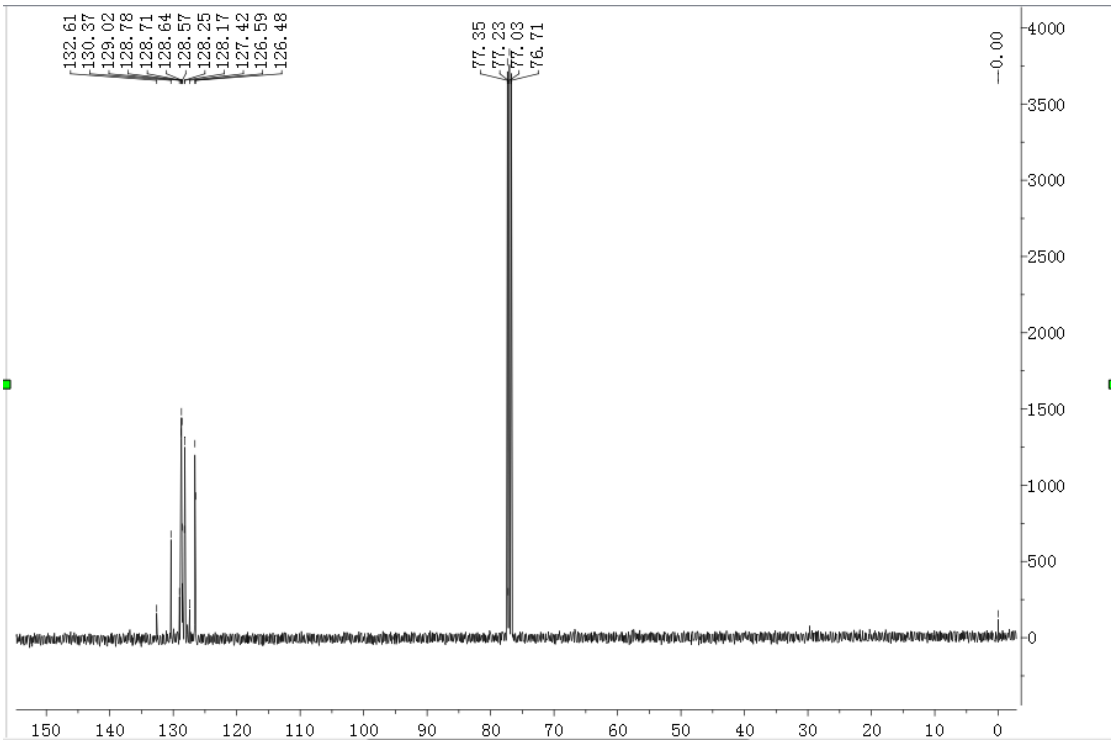
2.03
1.98
3.28
6.05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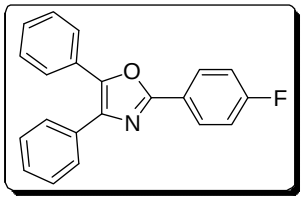
77.35
77.23
77.03
76.71
0.00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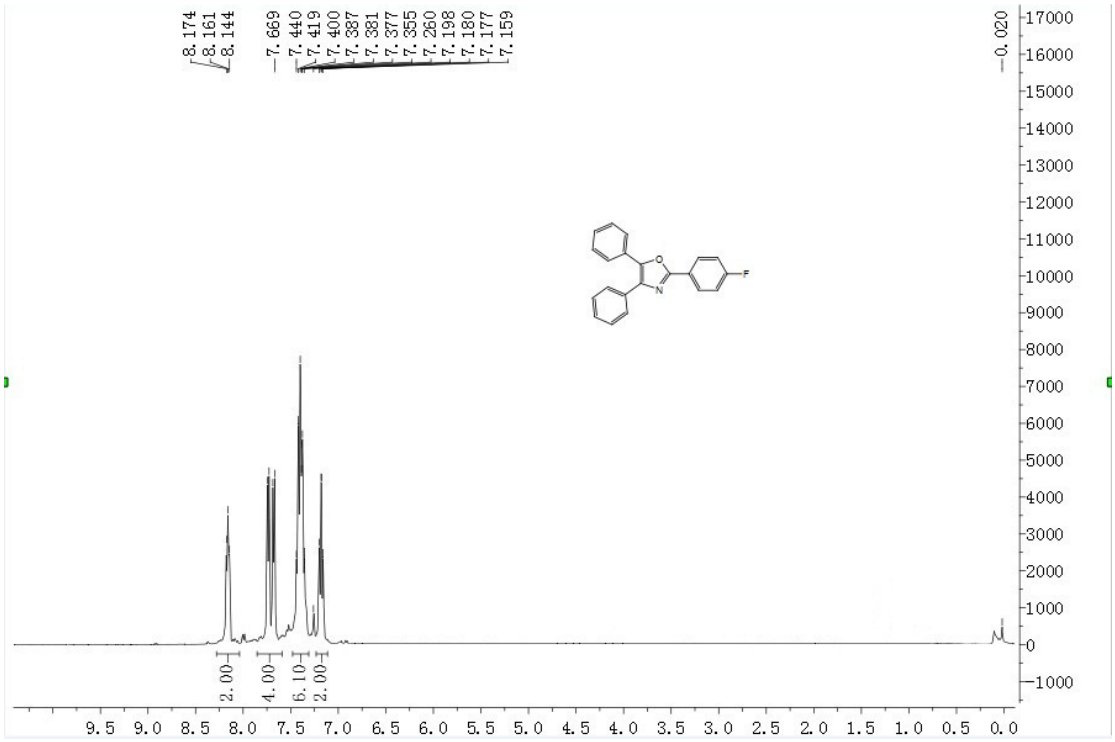
(3ag)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7.400
7.387
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7.177
7.159
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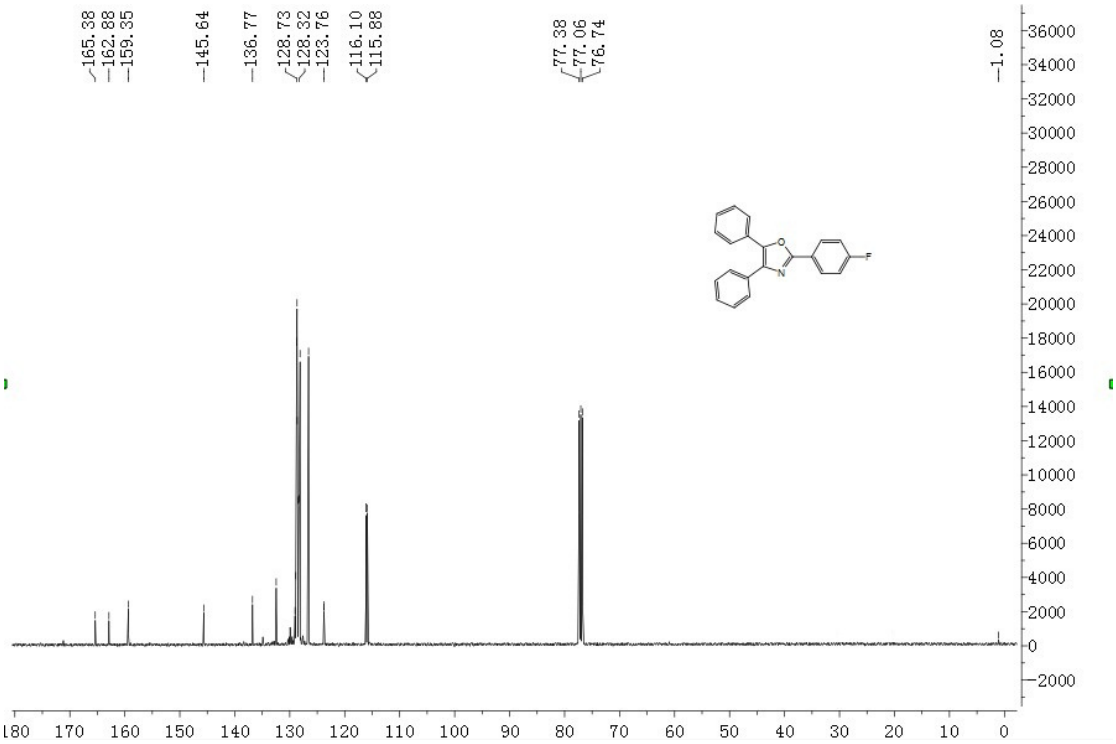
4.00
6.10
2.00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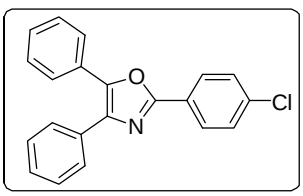
115.88
77.38
77.06
76.74
1.08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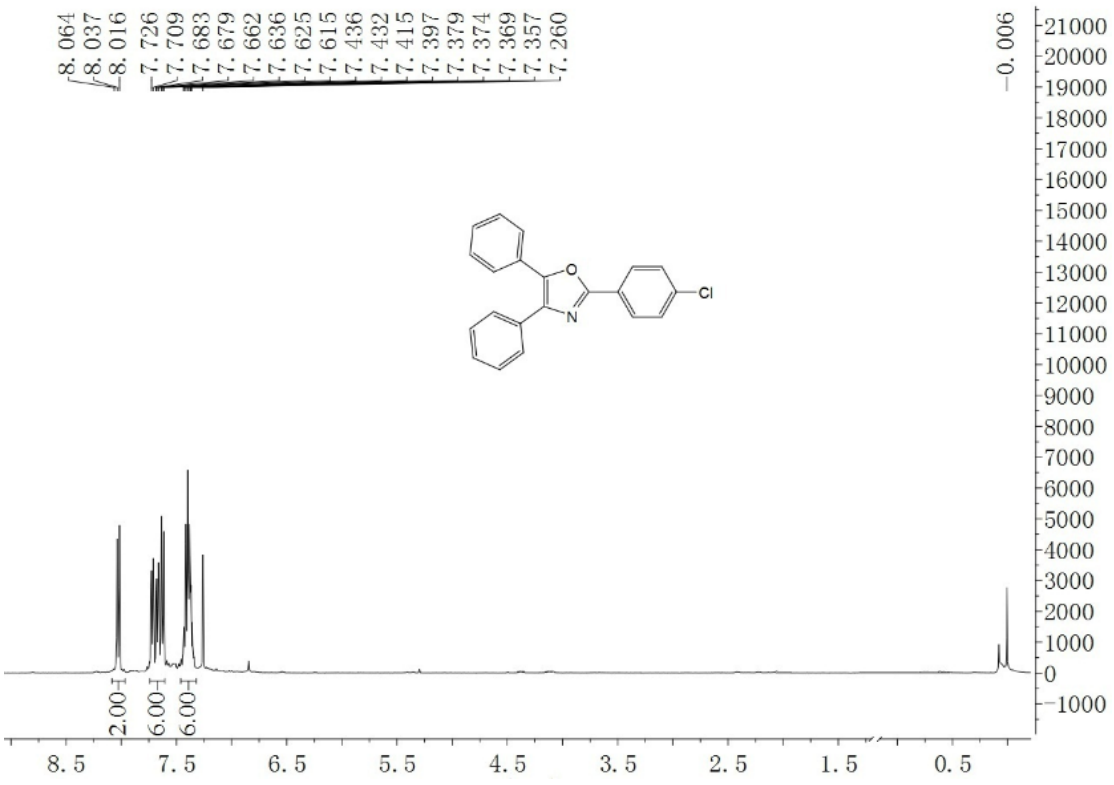
N
Cl

(3ah)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7.662
7.636
7.625
7.615
7.436
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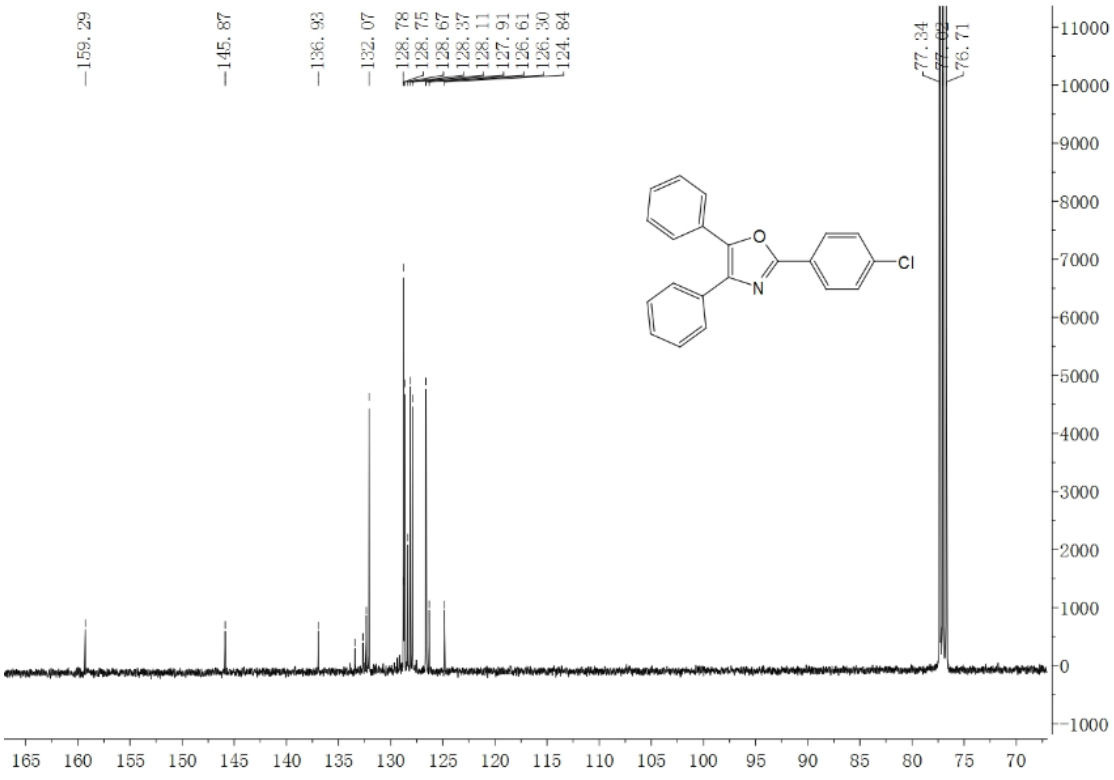
7.415
7.397
7.379
7.374
7.369
7.357
7.260
-0.006
2.00
6.00
6.00
Cl
N
O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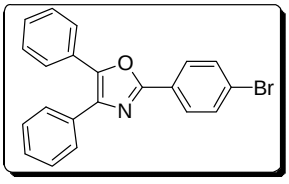
124.84
77.34
77.03
76.71
Cl
N
O


Br
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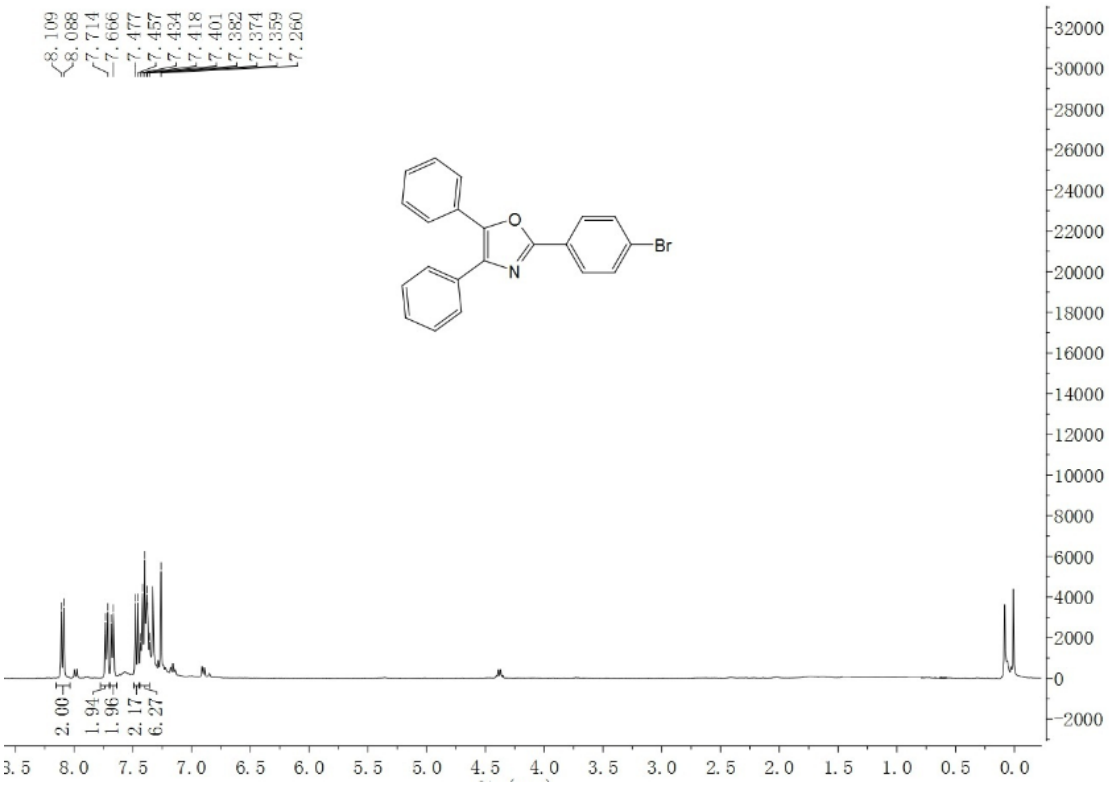
(3ai)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7.434
7.418
7.401
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7.374
7.359
7.260
Br
O
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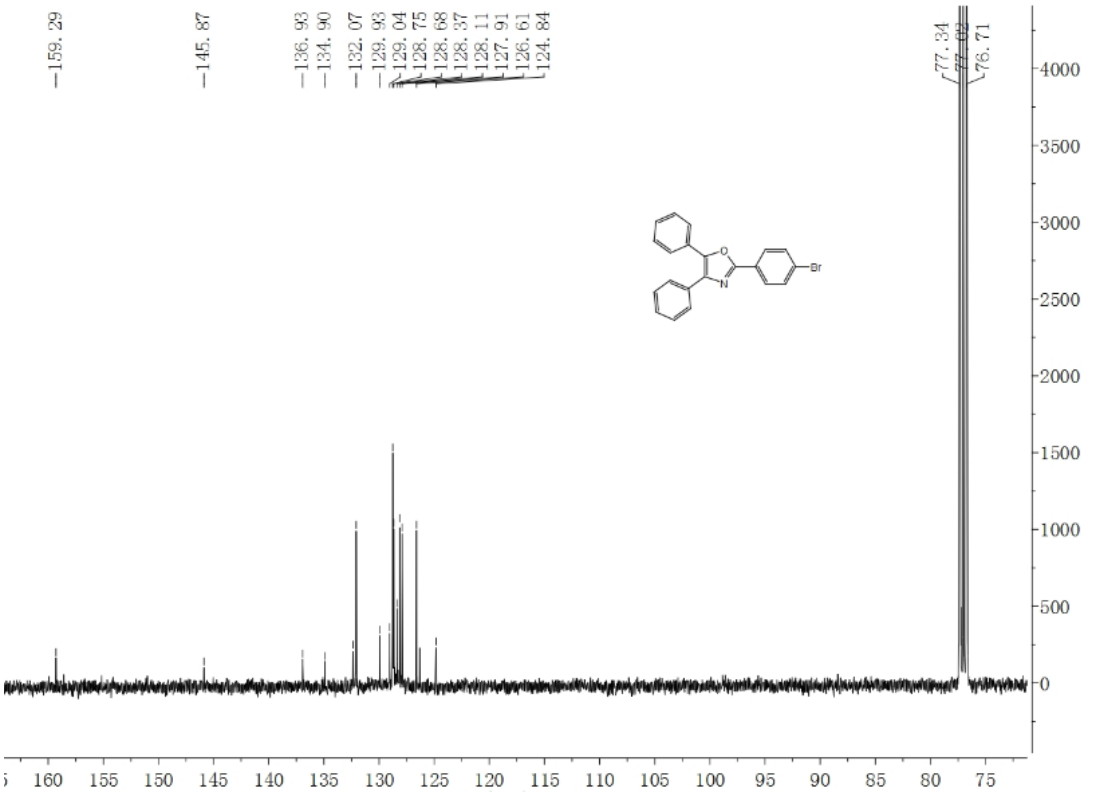
6.27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136.93
134.90
132.07
129.93
129.04
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128.68
128.37
128.11
127.91
126.61
124.84
77.34
77.00
76.71
Br
O
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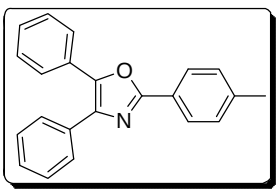
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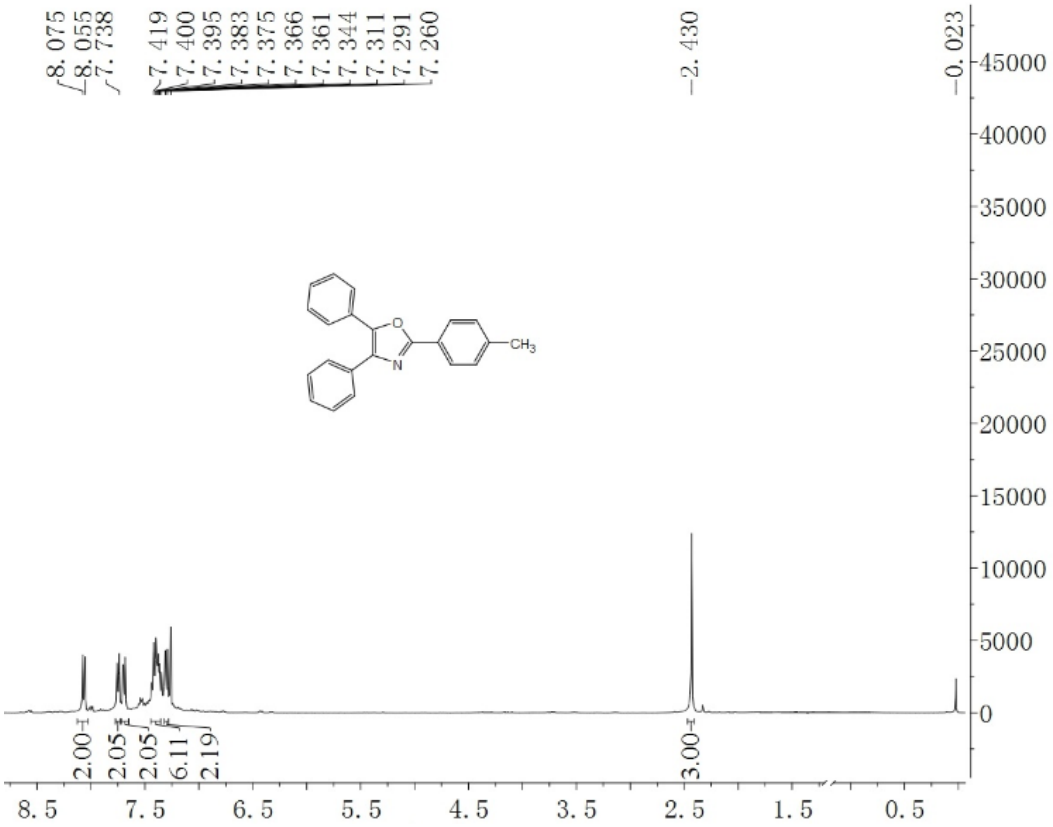
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7.395
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7.375
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7.361
7.344
7.311
7.291
7.260
2.430
0.023
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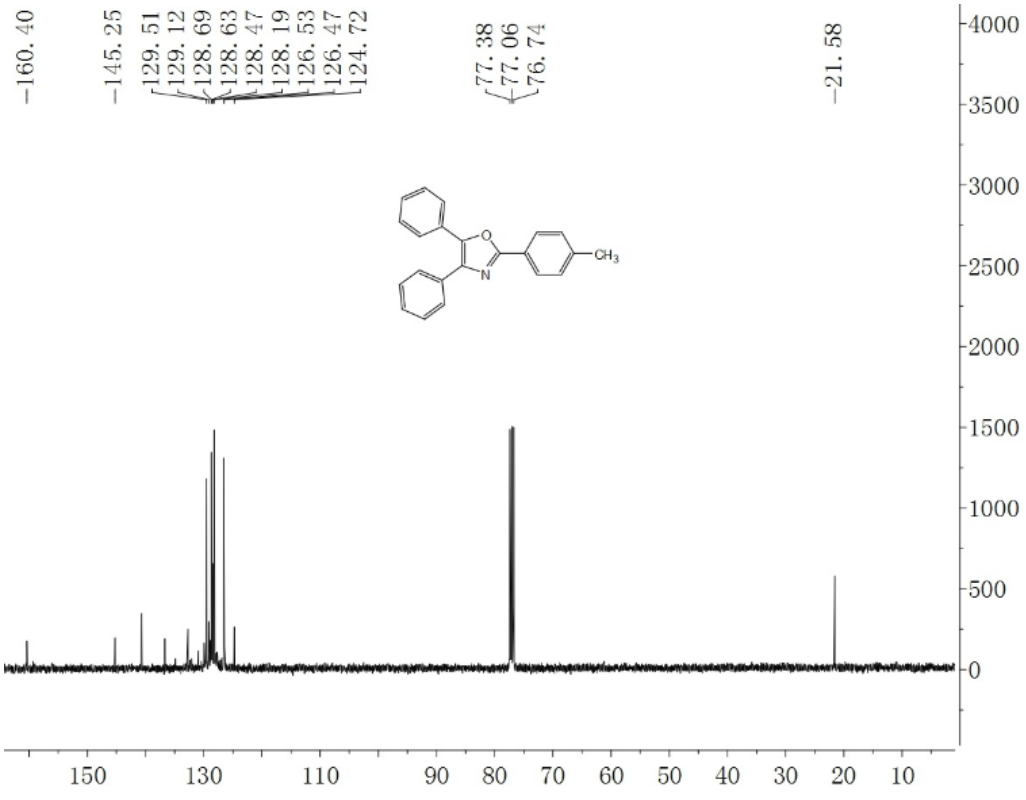
2.05
2.05
6.11
2.19
3.00
CH3
O
N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124.72
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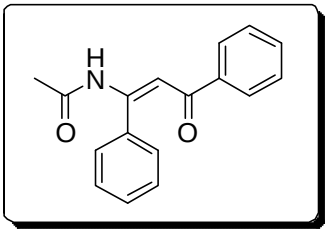
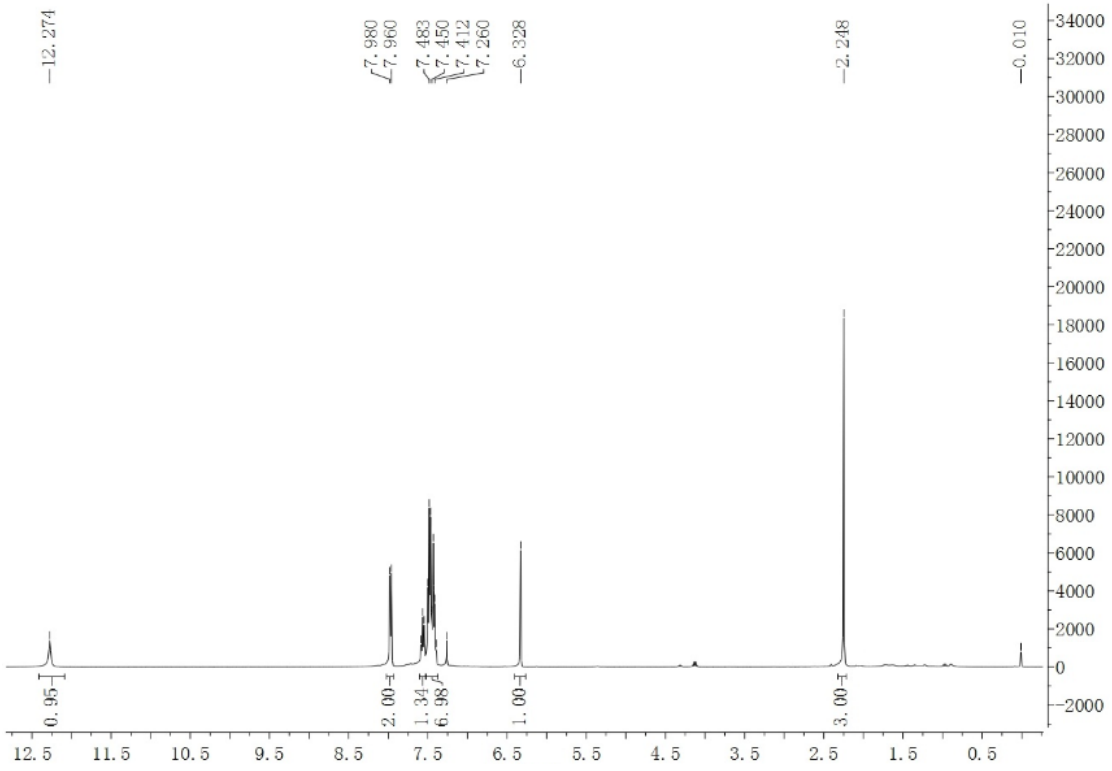
77.06
76.74
21.58
CH3
O
N


H
N
O
O

5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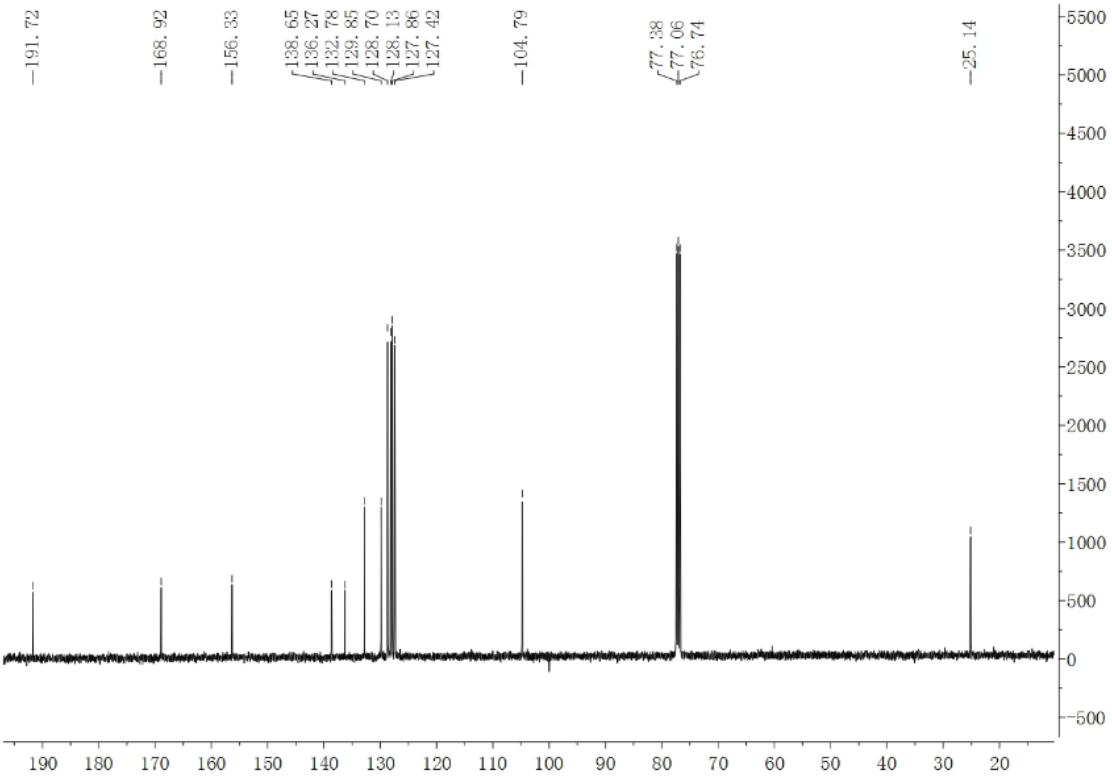
1.34
6.98
1.00
3.00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168.92
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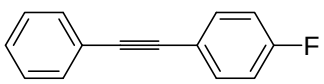
77.06
76.74
25.14

(**8**)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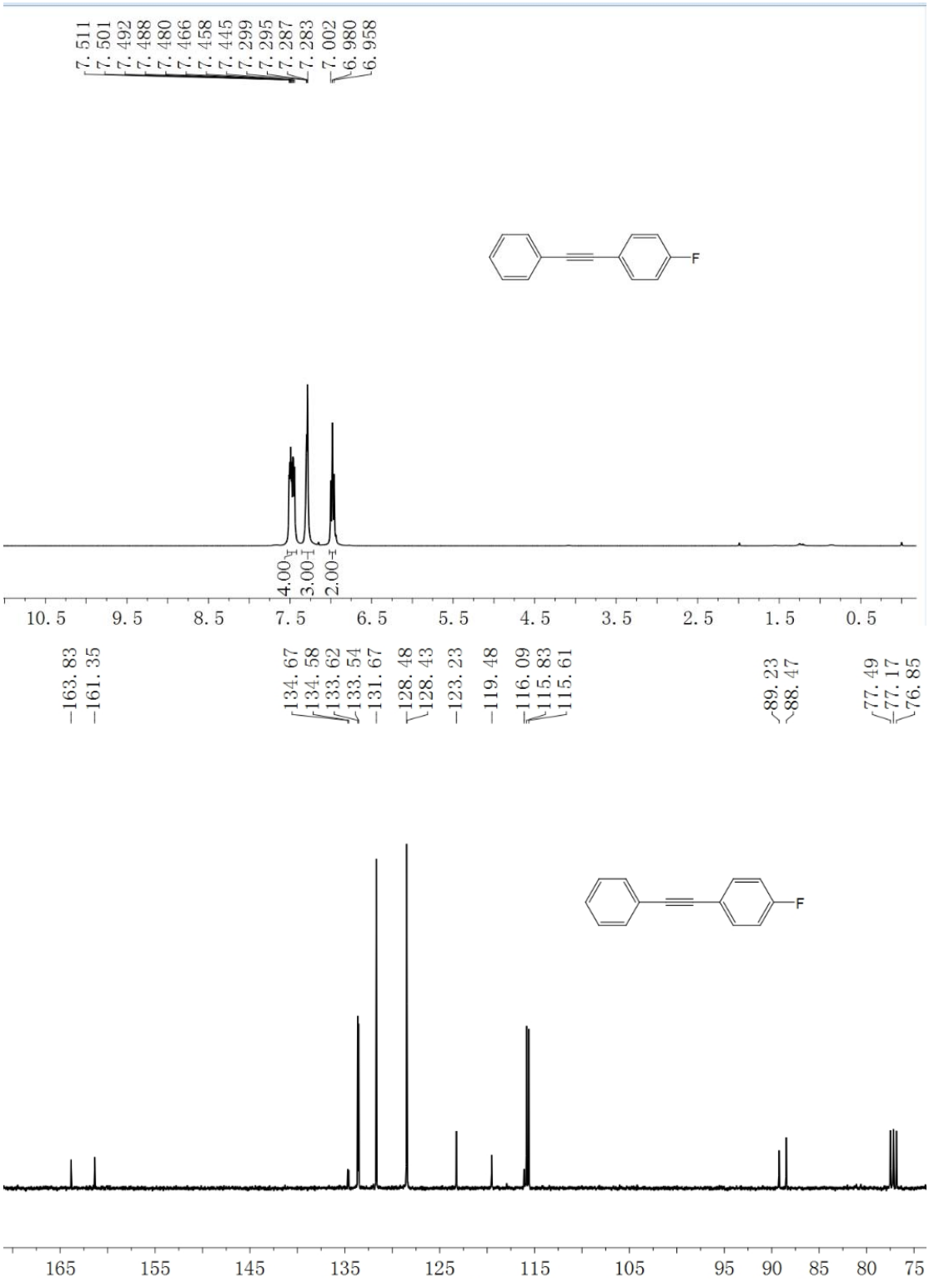
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7.295
7.287
7.283
7.002
6.980
6.958
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3.00
2.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
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161.35
134.67
134.58
133.62
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128.48
128.43
123.23
119.48
116.09
115.83
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90
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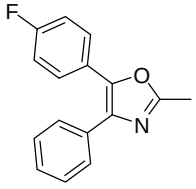
80
75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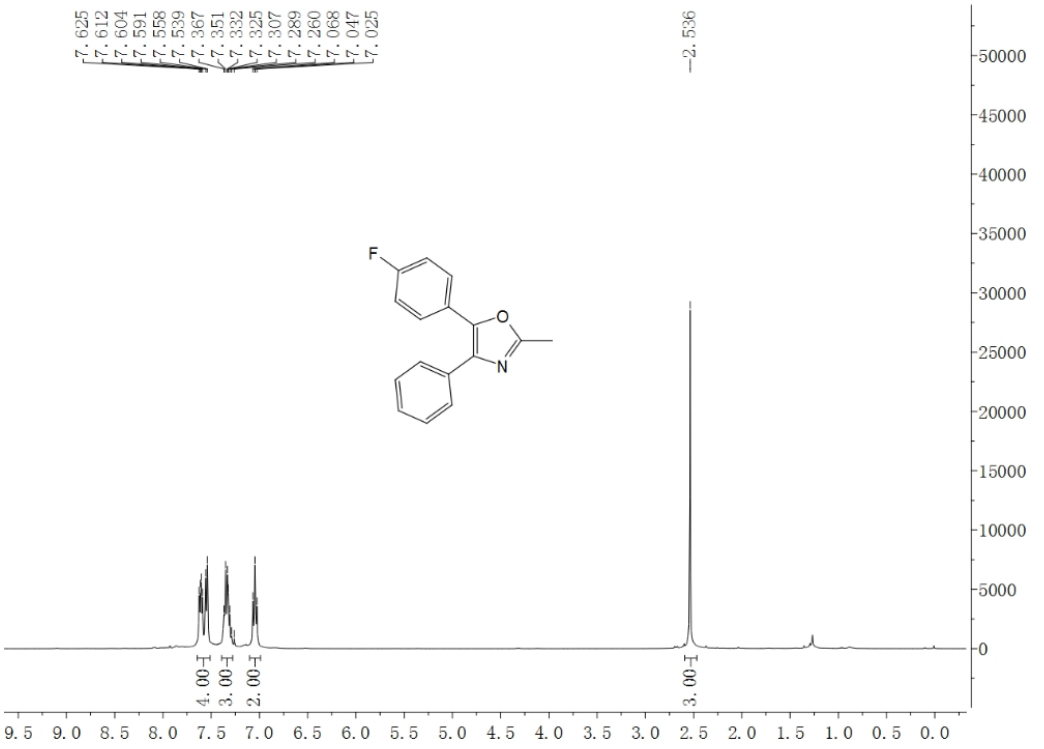
(**9**)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7.325
7.307
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7.068
7.047
7.025
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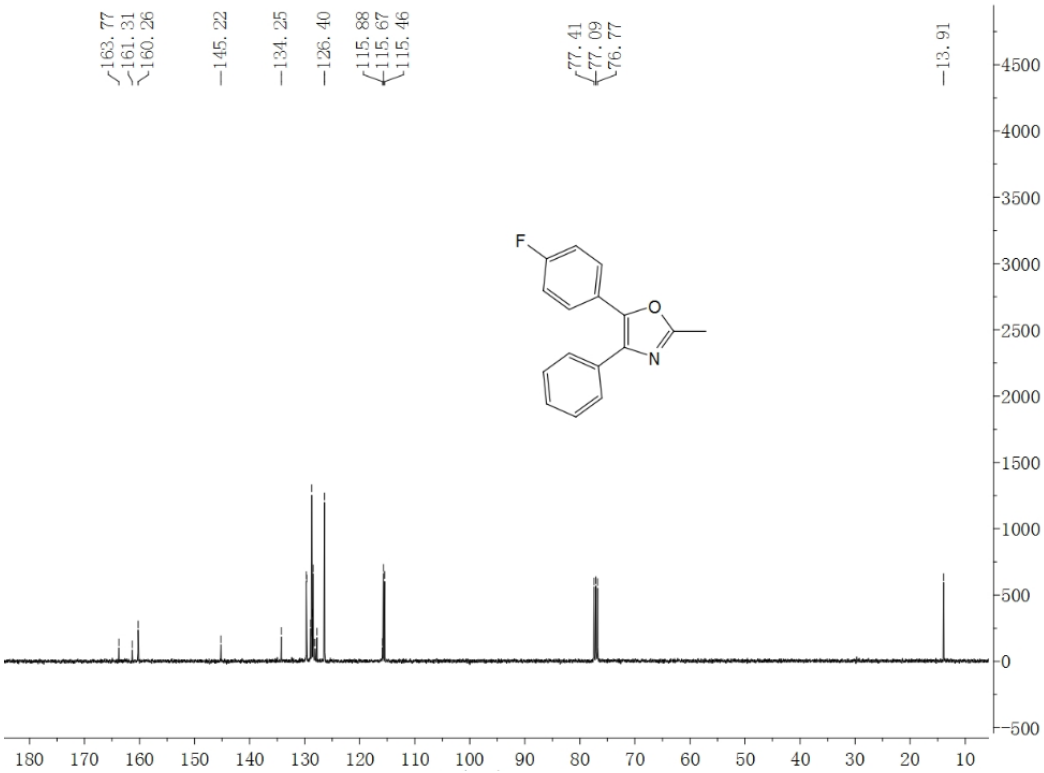
3.00
2.00
3.00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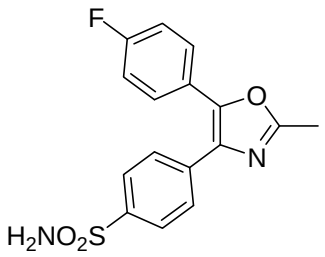
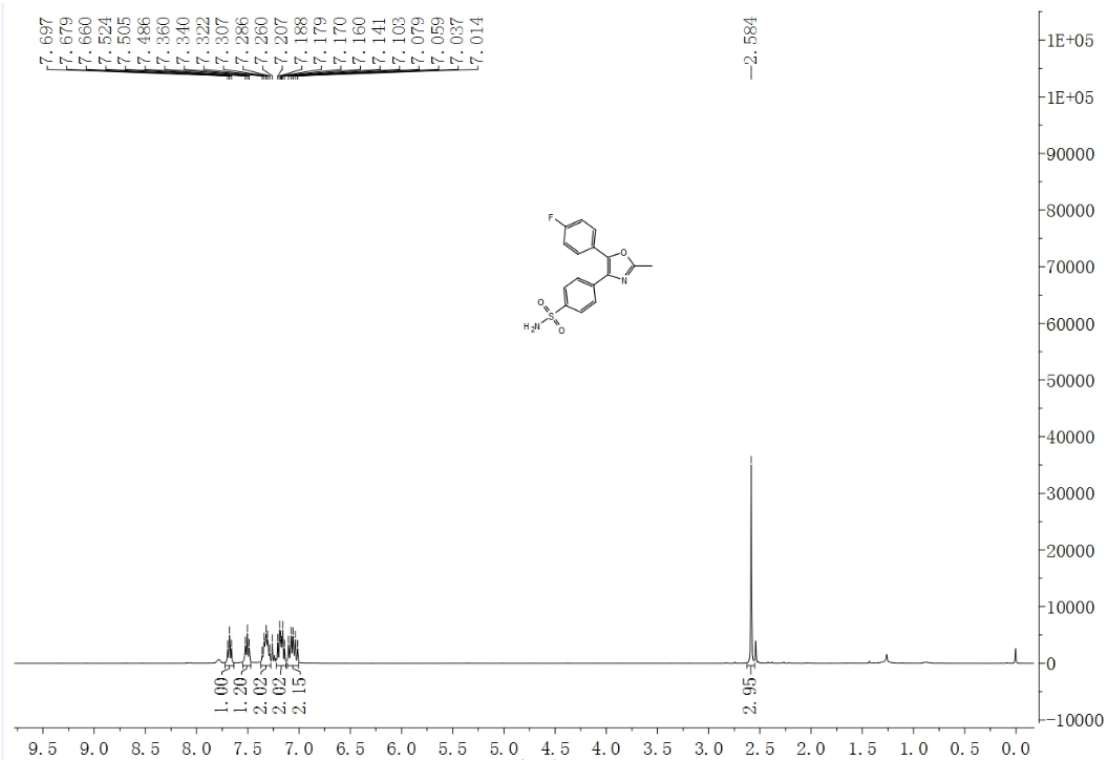
115.67
115.46
77.41
77.09
76.77
13.91
F
O
N


F
O
N
H2NO2S

(**10**)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7.322
7.307
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7.260
7.207
7.188
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7.170
7.160
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7.014
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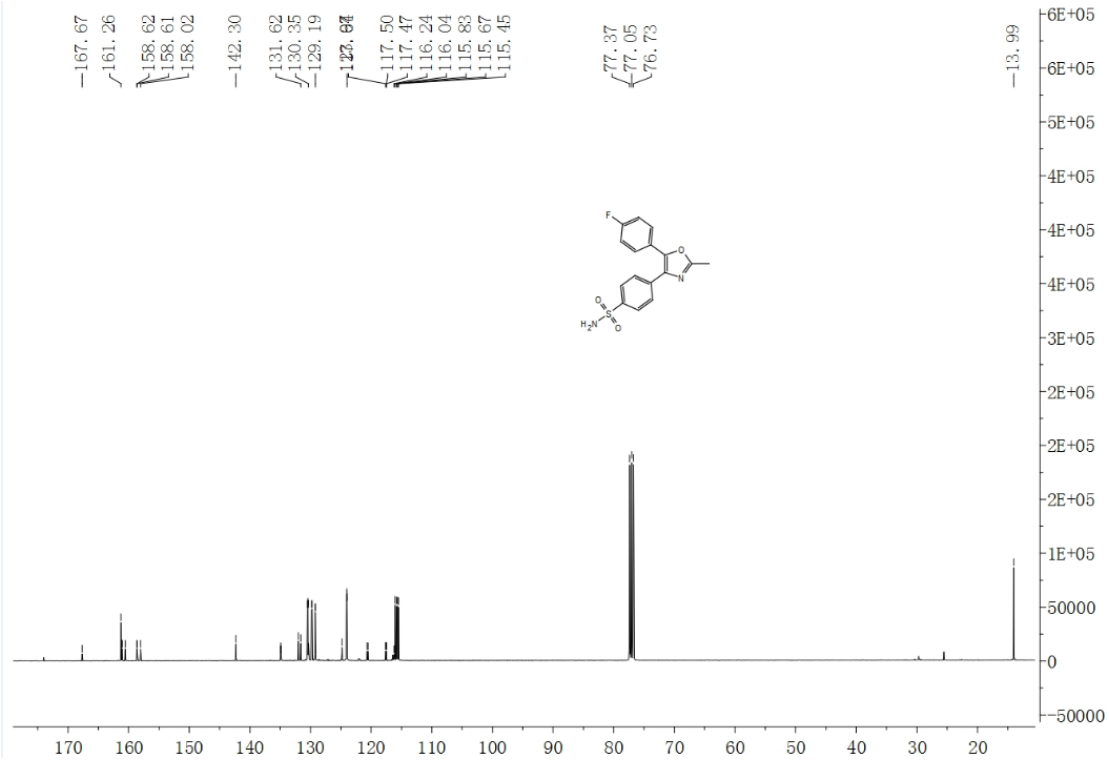
1.00
1.20
2.02
2.02
2.15
2.95


167.67
161.26
158.62
158.61
158.02
142.30
131.62
130.35
129.19
117.50
117.47
116.24
116.04
115.83
115.67
115.45
77.37
77.05
76.73
13.99