# Supporting Information

## Metal-Free Iodine(III)-Promoted Synthesis of 2,5-Diaryloxazoles

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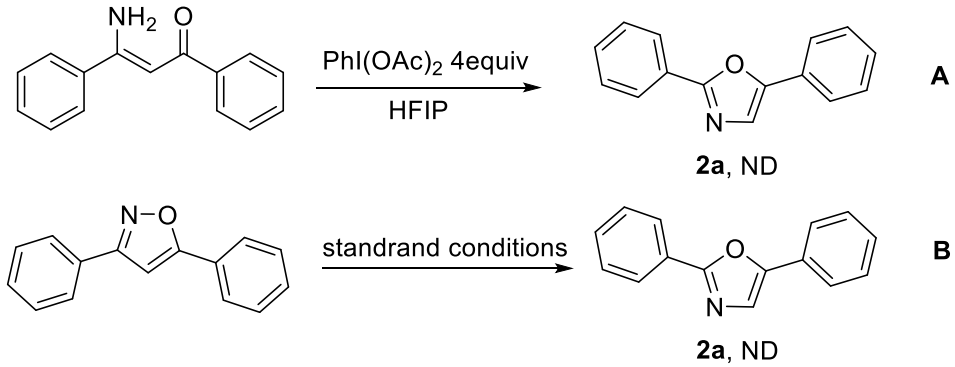
## 1. General information

$^{1}H$ NMR and $^{13}C$ NMR spectra were recorded on 300MHz and 75MHz in $CDCl_3$. All chemical shifts are given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. The high-resolution mass spectra (HRMS) were recorded on an FT-ICR mass spectrometer using electrospray ionization (ESI). Products were purified by flash chromatogrgraphy on 200-300 mesh silica gel. Unless otherwise noted, commercially reagents were used without further purification

General procedure for the synthesis of 2 (2a as an example)

Synthesis of 2a: A test tube was charged with chalcone (0.2 mmol), $PhI(OAc)_2$ (0.8 mmol), $NH_4OAc$ (2 mmol) in HFIP (0.5 mL). The mixture was stirred at room temperature for 5 h under air atmosphere. When the reaction was completed, the mixture was concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 20:1) to yield the isolated product 2a.

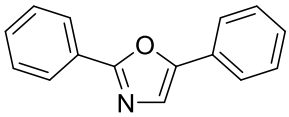
## 2. Experiments for Mechanistic Studies



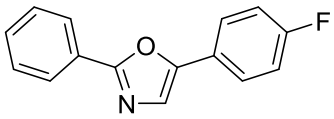

In order to elucidate the possible mechanism of this reaction, more

control experiments were investigated. We first use enaminone[1] as substrate to start the reaction with 4 equiv of $PhI(OAc)_2$, unfortunately, we did not get the desirable product. Then we got the 3,5-disubstituted isoxazole.[2] Unfortunately, we did not get 2,5-disubstituted oxazole under standard conditions by using 3,5-disubstituted isoxazole as substrate . The experimental results indicated that the reaction process did not experience such intermediates.

**3. Characterization data for isolated compounds**

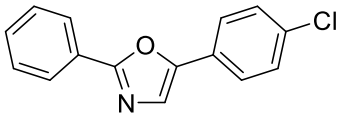


**2,5-Diphenyloxazole 2a.** White solid (35.7 mg 86%); m. p. = 64-67 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.17 – 8.06 (m, 2H), 7.71 (dd, J = 7.4, 1.0 Hz, 2H), 7.53 – 7.39 (m, 6H), 7.37 – 7.28 (m, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 161.1, 151.2, 130.3, 128.8, 128.4, 127.9, 127.3, 126.2, 124.1, 123.4; HRMS (ESI) calcd for $C_{15}H_{12}NO$ $[M+H]^+$ 222.0914 ; found: 222.0916. The $^1$H and $^{13}$C NMR spectra of 2a were identical to data reported in the literature.[3]

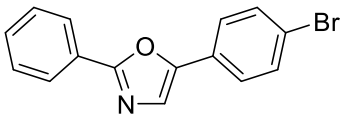


**5-(4-Fluorophenyl)-2-phenyloxazole 2b.** White solid (37.7 mg 79%); m. p. = 87-89 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.10 (dd, J = 7.3, 2.3 Hz, 2H), 7.70 (dd, J = 8.8, 5.3 Hz, 2H), 7.48 (dd, J = 5.2, 1.8 Hz, 3H), 7.39 (s, 1H), 7.15 (t, J = 8.7 Hz, 2H).$^{13}$C NMR (75 MHz, CDCl3) δ 164.13, 160.88 (d, J = 7.5 Hz), 150.23, 130.25, 128.70, 127.15,

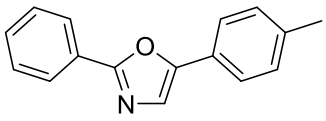
126.09, 125.89 (d, J = 8.2 Hz), 124.15, 122.94, 116.09, 115.79; HRMS (ESI) calcd for $C_{15}H_{11}FNO$ $[M+H]^+$ 240.0819 ; found: 240.0820. The $^1H$ and $^{13}C$ NMR spectra of 2b were identical to data reported in the literature.[4]



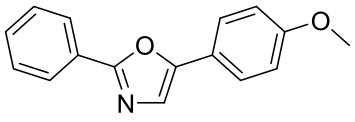

**5-(4-Chlorophenyl)-2-phenyloxazole 2c.** Light yellow solid (38.2 mg 75%); m. p. =102-104 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.08 (ddd, J = 8.6, 3.7, 2.1 Hz, 2H), 7.67 – 7.58 (m, 2H), 7.51 – 7.44 (m, 3H), 7.44 – 7.36 (m, 3H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.2, 150.1, 134.0, 130.4, 129.1, 128.8, 127.1, 126.4, 126.2, 125.3, 123.7; HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524 ; found: 256.0522. The $^1H$ and $^{13}C$ NMR spectra of 2c were identical to data reported in the literature.[5]



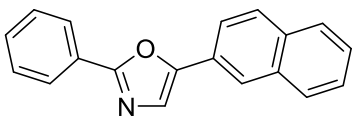

**5-(4-Bromophenyl)-2-phenyloxazole 2d.** Light yellow solid (35.8 mg 60%); m. p. = 99-100 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.06 (dd, J = 6.6, 3.2 Hz, 2H), 7.52 (s, 4H), 7.48 – 7.42 (m, 3H), 7.41 (s, 1H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.2, 150.1, 132.0, 130.4, 128.7, 127.0, 126.7, 126.2, 125.4, 123.8, 122.1. HRMS (ESI) calcd for $C_{15}H_{11}BrNO$ $[M+H]^+$ 300.0019 ; found: 300.0018. The $^1H$ and $^{13}C$ NMR spectra of 2d were identical to data reported in the literature.[3]



**2-phenyl-5-(p-tolyl)oxazole 2e.** White solid (19.2 mg 41%); m. p. = 76-78 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, J = 6.1 Hz, 2H), 7.60 (d, J = 7.3 Hz, 2H), 7.45 (s, 3H), 7.39 (s, 1H), 7.23 (d, J = 7.3 Hz, 2H), 2.37 (s, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 160.7, 151.3, 138.4, 130.1, 129.5, 128.7, 127.4, 126.1, 125.1, 124.0, 122.7, 21.3; HRMS (ESI) calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070 ; found: 236.1070. The $^{1}$H and $^{13}$C NMR spectra of 2e were identical to data reported in the literature.[4]

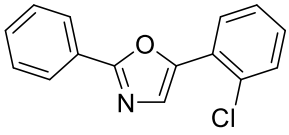


**5-(4-Meth phenyl)-2-phenyloxazole 2f.** Light yellow solid(35.6 mg 71%); m. p. = 78-79 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.08 (dt, J = 12.6, 6.5 Hz, 2H), 7.64 (d, J = 8.9 Hz, 2H), 7.53 – 7.40 (m, 3H), 7.32 (s, 1H), 6.96 (d, J = 8.9 Hz, 2H), 3.83 (d, J = 5.7 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 160.4, 159.7, 151.2, 130.0, 128.7, 127.4, 126.0, 125.6, 121.8, 120.7, 114.3, 77.4, 77.0, 76.6 , 55.3. HRMS (ESI) calcd for $C_{16}H_{14}NO_2$ $[M+H]^+$ 252.1019 ; found: 252.1020. The $^{1}$H and $^{13}$C NMR spectra of 2f were identical to data reported in the literature.[3]

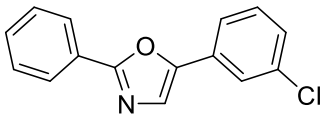


**5-(Naphthalen-2-yl)-2-phenyloxazole 2g.** White solid(22.7 mg 42%); m. p. = 98-99 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ

8.16 (d, J = 7.9 Hz, 3H), 7.88 (dd, J = 7.6, 4.0 Hz, 2H), 7.82 (d, J = 7.2 Hz, 1H), 7.75 (d, J = 8.6 Hz, 1H), 7.54 (s, 1H), 7.50 (dd, J = 6.0, 4.6 Hz, 5H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 161.2, 151.3, 133.3, 133.0, 130.3, 128.8, 128.7, 128.1, 127.8, 127.3, 126.8, 126.4, 126.3, 125.2, 123.9, 122.8, 122.0; HRMS (ESI) calcd for $C_{19}H_{14}NO$ $[M+H]^+$ 272.1070 ; found: 272.1071. The $^1$H and $^{13}$C NMR spectra of 2g were identical to data reported in the literature.[5]

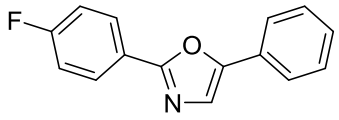



**5-(2-chlorophenyl)-2-phenyloxazole 2h.** White solid(37.2 mg 73%); m. p. = 108-110 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.11 (dd, J = 6.6, 3.2 Hz, 2H), 7.70 (d, J = 1.5 Hz, 1H), 7.59 (d, J = 7.6 Hz, 1H), 7.52 – 7.43 (m, 4H), 7.38 (dd, J = 9.7, 5.8 Hz, 1H), 7.33 – 7.27 (m, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 161.4, 149.7 (s), 134.9, 130.5, 130.1, 129.5, 128.8, 128.2, 127.0, 126.3, 124.3, 124.0, 122.1; HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524 ; found: 256.0523. The $^1$H and $^{13}$C NMR spectra of 2h were identical to data reported in the literature.[8]

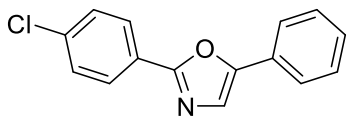



**5-(3-chlorophenyl)-2-phenyloxazole 2i.** White solid(29.6 mg 58%); m. p. = 103-106 °C; $^1$H NMR (300 MHz, $CDCl_3$) δ 8.12 (dd, J = 6.5, 3.2 Hz, 2H), 7.72 (t, J = 1.7 Hz, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.53 – 7.46 (m, 4H), 7.40 (dd, J = 7.9, 2.9 Hz, 1H), 7.35 – 7.29 (m,

1H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.4, 149.7, 134.9, 130.5, 130.1, 129.5, 128.8, 128.2, 127.0, 126.3, 124.3, 124.0, 122.1; HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524 ; found: 256.0522. The $^1H$ and $^{13}C$ NMR spectra of 2i were identical to data reported in the literature.[8]

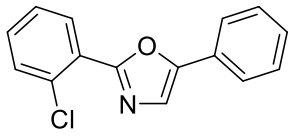


**2-(4-Fluorophenyl)-5-phenyloxazole 2j.** Light yellow solid(42.5 mg 89%); m. p. = 71-73 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.07 (ddd, J = 16.1, 9.1, 6.5 Hz, 2H), 7.70 (dd, J = 5.2, 3.3 Hz, 2H), 7.50 – 7.38 (m, 3H), 7.33 (ddd, J = 7.4, 3.8, 1.2 Hz, 1H), 7.22 – 7.09 (m, 2H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 165.6, 162.3, 160.2, 151.2, 128.9, 128.4 (d, J = 6.1 Hz), 128.2, 127.8, 124.1, 123.7, 123.3, 116.1, 115.8. HRMS (ESI) calcd for $C_{15}H_{11}FNO$ $[M+H]^+$ 239.0746 ; found: 239.0750. The $^1H$ and $^{13}C$ NMR spectra of 2j were identical to data reported in the literature.[3]

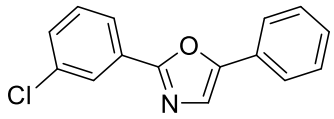


**2-(4-Chlorophenyl)-5-phenyloxazole 2k.** Light yellow solid (39.7 mg 78%), m. p. = 115-117 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.00 (d, J = 8.5 Hz, 2H), 7.68 (d, J = 7.3 Hz, 2H), 7.49 – 7.37 (m, 5H), 7.33 (t, J = 7.3 Hz, 1H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 160.0, 151.4, 136.3, 129.0, 128.9, 128.5, 127.7, 127.4, 125.8, 124.1, 123.4. HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 255.0524 ; found: 255.0522. The $^1H$ and $^{13}C$ NMR spectra of 2k were identical to data reported in the

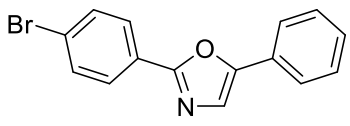
literature.[4]




**2-(2-Chlorophenyl)-5-phenyloxazole 2l.** Light yellow solid(38.7 mg 76%); m. p. = 81-83 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.07 (ddd, J = 16.1, 9.1, 6.5 Hz, 2H), 7.70 (dd, J = 5.2, 3.3 Hz, 2H), 7.50 – 7.38 (m, 3H), 7.33 (ddd, J = 7.4, 3.8, 1.2 Hz, 1H), 7.22 – 7.09 (m, 2H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 158.9, 151.6, 132.2, 131.3, 130.9, 130.6, 128.9, 128.6, 127.7, 126.8, 126.0, 124.3, 123.1. HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524 ; found: 256.0521. The $^{1}$H and $^{13}$C NMR spectra of 2l were identical to data reported in the literature.[6]

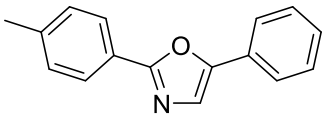



**2-(3-chlorophenyl)-5-phenyloxazole 2m.** White solid(28.5 mg 56%); m. p. = 101-103 °C; $^{1}$H NMR (300 MHz, $CDCl_3$) δ 8.09 (s, 1H), 8.00 (dd, J = 4.9, 2.5 Hz, 1H), 7.73 (d, J = 7.3 Hz, 2H), 7.50 – 7.41 (m, 5H), 7.38 (d, J = 7.5 Hz, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 159.7, 151.7, 134.9, 130.3, 130.1, 129.0, 128.7, 127.6, 126.2, 124.3, 124.2, 123.5; HRMS (ESI) calcd for $C_{15}H_{11}ClNO$ $[M+H]^+$ 256.0524 ; found: 256.0520. The $^{1}$H and $^{13}$C NMR spectra of 2m were identical to data reported in the literature.[7]

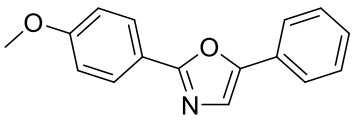



**2-(4-bromophenyl)-5-phenyloxazole 2n.** Light yellow solid(43.0 mg 72%); m. p. = 104-106 °C; $^{1}$H NMR (300 MHz,

$CDCl_3$) δ 7.98 – 7.89 (m, 2H), 7.68 (dd, J = 5.2, 3.4 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.46 – 7.38 (m, 3H), 7.33 (ddd, J = 7.4, 3.7, 1.2 Hz, 1H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 160.1, 151.4, 132.0, 128.9, 128.5, 127.6, 127.6, 126.2, 124.6, 124.1, 123.4;HRMS (ESI) calcd for $C_{15}H_{11}BrNO$ $[M+H]^+$ 300.0019 ; found: 300.0018. The $^1H$ and $^{13}C$ NMR spectra of 2n were identical to data reported in the literature.[9]

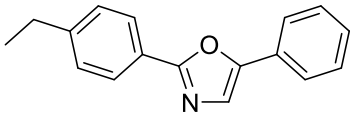


**5-Phenyl-2-p-tolyloxazole 2o.** White solid(33.4 mg 71%); m. p. = 69-71 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 2H), 7.75 – 7.66 (m, 2H), 7.43 (dt, J = 13.1, 3.7 Hz, 3H), 7.37 – 7.31 (m, 1H), 7.31 – 7.24 (m, 2H), 2.40 (s, 3H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.3, 150.8, 140.6, 129.5, 128.8, 128.2, 128.0, 126.2, 124.6, 124.0, 123.2, 21.5; HRMS (ESI) calcd for $C_{16}H_{14}NO$ $[M+H]^+$ 236.1070 ; found: 236.1073. The $^1H$ and $^{13}C$ NMR spectra of 2o were identical to data reported in the literature.[3]

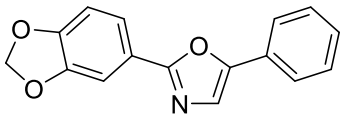


**2-(4-Methoxyphenyl)-5-phenyloxazole 2p.** White solid(25.6 mg 58%); m. p. = 92-94 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 2H), 7.75 – 7.66 (m, 2H), 7.43 (dt, J = 13.1, 3.7 Hz, 3H), 7.37 – 7.31 (m, 1H), 7.31 – 7.24 (m, 2H), 2.40 (s, 3H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.2, 150.6, 128.8, 128.1, 128.0, 127.9, 123.9, 123.1, 120.1, 114.1, 55.3; HRMS (ESI) calcd for $C_{16}H_{14}NO_2$ $[M+H]^+$ 252.1019 ;

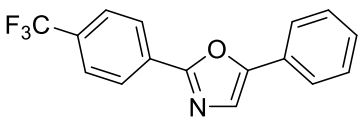
found: 252.1015. The $^{1}H$ and $^{13}C$ NMR spectra of 2p were identical to data reported in the literature.[3]



**2-(4-ethylphenyl)-5-phenyloxazole 2q.** White solid(34.3 mg 69%); m. p. = 85-87 °C; $^{1}H$ NMR (300 MHz, $CDCl_3$) δ 8.02 (d, J = 8.2 Hz, 2H), 7.70 (d, J = 7.3 Hz, 2H), 7.47 – 7.38 (m, 3H), 7.31 (t, J = 7.7 Hz, 3H), 2.69 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H).$^{13}C$ NMR (75 MHz, $CDCl_3$) δ 161.3, 150.8, 146.8, 128.8, 128.3, 128.2, 126.2, 124.8, 124.0, 123.3, 28.8, 15.3; HRMS (ESI) calcd for $C_{17}H_{16}NO$ $[M+H]^+$ 250.1227 ; found: 250.1223. The $^{1}H$ and $^{13}C$ NMR spectra of 2q were identical to data reported in the literature.[9]

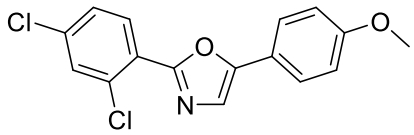


**2-(benzo[d][1,3]dioxol-5-yl)-5-phenyloxazole 2r.** White solid(32.8 mg 62%); m. p. = 110-112 °C; $^{1}H$ NMR (300 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 3H), 7.53 (d, J = 1.6 Hz, 1H), 7.47 – 7.36 (m, 3H), 7.35 – 7.26 (m, 1H), 6.86 (t, J = 10.4 Hz, 1H), 6.00 (s, 2H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 160.8, 150.7, 149.4, 148.0, 128.8, 128.2, 127.9, 123.9, 123.2, 121.5, 120.9, 108.5, 106.5, 101.5; HRMS (ESI) calcd for $C_{16}H_{12}NO_3$ $[M+H]^+$ 266.0812 ; found: 266.0815.

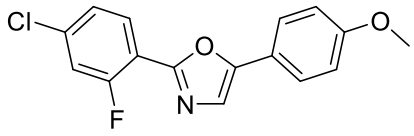


**5-phenyl-2-(4-(trifluoromethyl)phenyl)oxazole 2u.** Light yellow solid(30.0 mg 52%); m. p. = 109-111 °C; $^{1}H$ NMR (300

MHz, $CDCl_3$) δ 8.20 (d, J = 8.0 Hz, 2H), 7.73 (d, J = 7.7 Hz, 4H), 7.54 – 7.42 (m, 3H), 7.41 – 7.31 (m, 1H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 159.60 (s), 152.01 (s), 131.95 (s), 130.44 (s), 128.98 (s), 128.81 (s), 127.52 (s), 126.38 (s), 126.18 – 125.60 (m), 124.29 (s), 123.72 (s), 122.01 (s). HRMS (ESI) calcd for $C_{16}H_{11}F_3NO$ $[M+H]^+$ 290.0787 ; found: 290.0786. The $^1H$ and $^{13}C$ NMR spectra of 2u were identical to data reported in the literature.[4]




**2-(2,4-dichlorophenyl)-5-(4-methoxyphenyl)oxazole 2w.** Light yellow solid(26.7 mg 42%); m. p. = 121-122 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.03 (d, J = 8.5 Hz, 1H), 7.65 (d, J = 8.5 Hz, 2H), 7.52 (s, 1H), 7.47 – 7.29 (m, 2H), 6.97 (d, J = 8.6 Hz, 2H), 3.88 (d, J = 18.9 Hz, 3H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 159.9, 151.9, 136.0, 132.7, 131.2, 131.1, 127.3, 125.9, 124.6, 121.8, 120.3, 114.4, 55.3; HRMS (ESI) calcd for $C_{16}H_{12}Cl_2NO_2$ $[M+H]^+$ 320.0240 ; found: 320.0241.




**2-(4-chloro-2-fluorophenyl)-5-(4-methoxyphenyl)oxazole 2x.** Light yellow solid(41.8 mg 69%); m. p. = 105-107 °C; $^1H$ NMR (300 MHz, $CDCl_3$) δ 8.01 (dd, J = 19.5, 11.3 Hz, 1H), 7.63 (dd, J = 17.4, 10.4 Hz, 2H), 7.38 (s, 1H), 7.25 (d, J = 8.7 Hz, 2H), 6.95 (t, J = 9.8 Hz, 2H), 3.98 –

3.77 (m, 3H). $^{13}C$ NMR (75 MHz, $CDCl_3$) δ 160.0, 151.7, 136.6 (d, J = 9.6 Hz), 129.8, 125.9, 124.9, 121.9, 120.3, 117.8, 117.5, 114.4, 55.3; HRMS (ESI) calcd for $C_{16}H_{12}ClFNO_2$ $[M+H]^+$ 304.0535 ; found: 304.0538.

(1) Z. Zhu, X. Tang, J. Li, X. Li, W. Wu, G. Deng and H. Jiang, *Chem. Commun.* 2017, **53**, 3228.

(2) A. M. Jawalekar, E. Reubsaet, F. P. Rutjes and F. L. van Delft, *Chem. Commun.* 2011, **47**, 3198.

(3) W. C. Gao, R. L. Wang and C. Zhang, Org. *Biomol. Chem.* 2013, **11**, 7123.

(4) Z. Xu, C. Zhang and N. Jiao, *Angew. Chem.* 2012, **51**, 11367.

(5) T. Chatterjee, J. Y. Cho and E. J. Cho, *J. Org. Chem.* 2016, **81**, 6995.

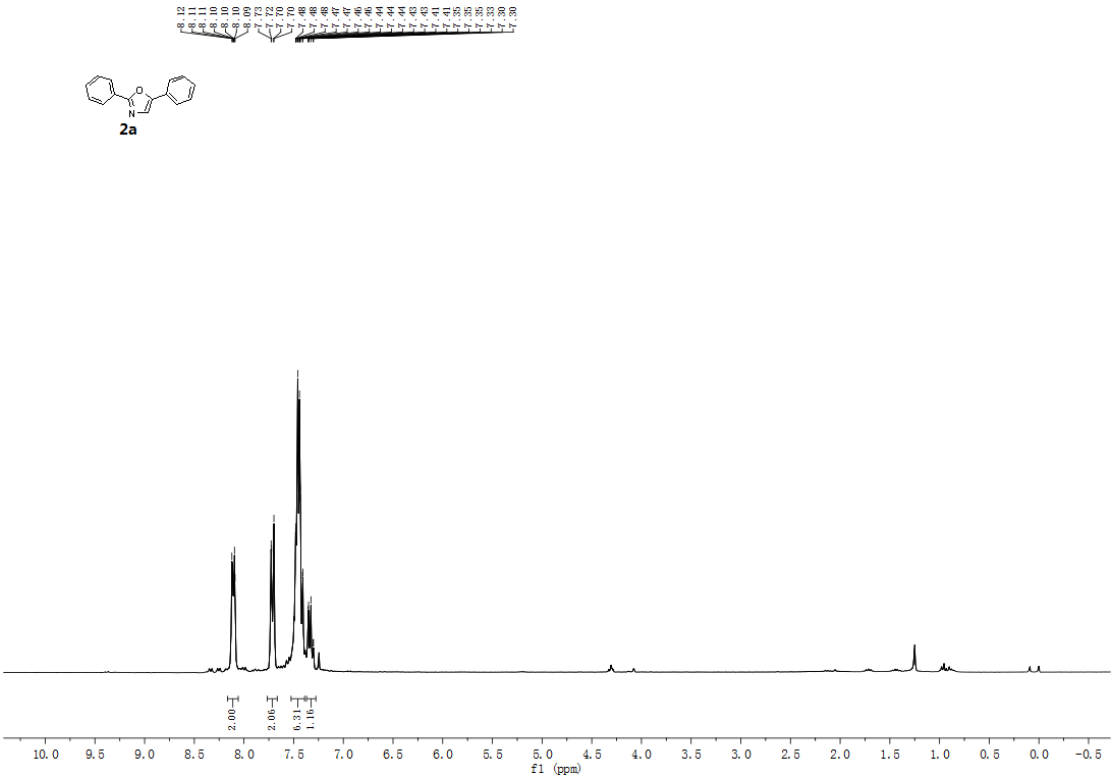
(6) D. Liu, J. Yu and J. Cheng, *Tetrahedron*, 2014, **70**, 1149.

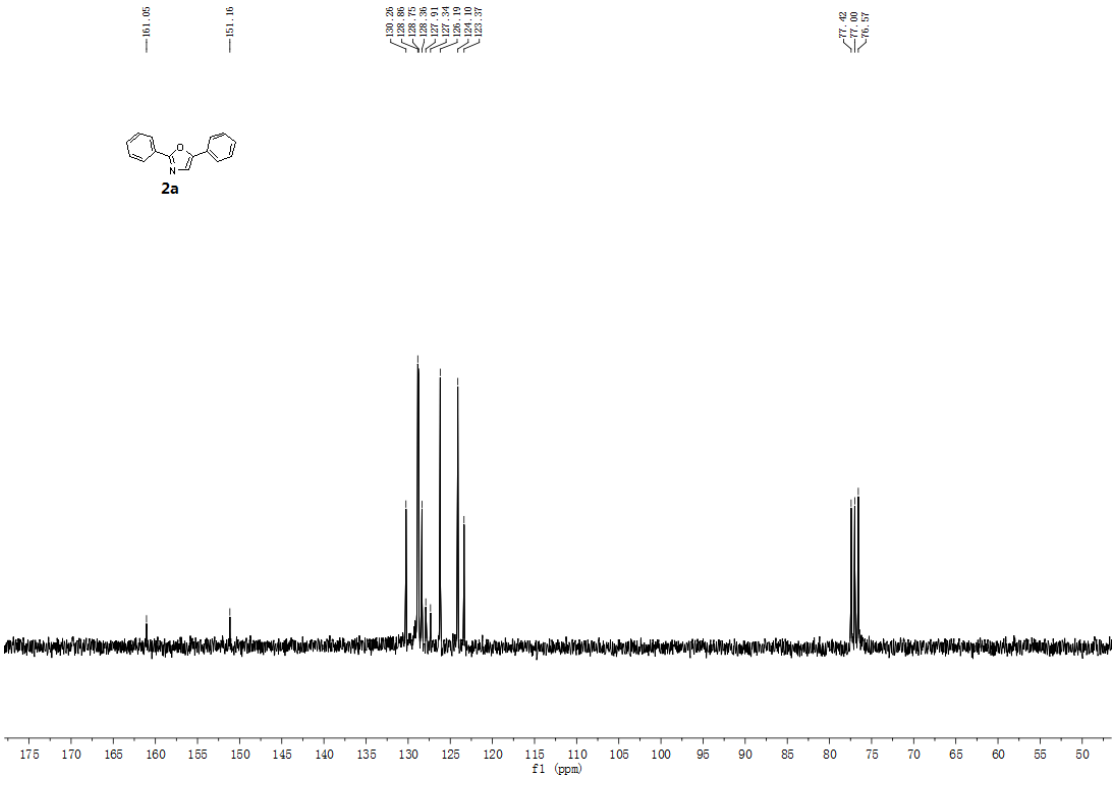
(7) C. Wan, L. Gao, Q. Wang, J. Zhang and Z. Wang, *Org. Lett.* 2010, **12**, 3902.

(8) J. J. Lee, J. Kim, Y. M. Jun, B. M. Lee and B. H. Kim, *Tetrahedron*, 2009, **65**, 8821.

(9) D. J. Ritson, C. Spiteri and J. E. Moses, *J. Org. Chem.* 2011, **76**, 3519.

# 4. Copies of $^{1}H$ and $^{13}C$ NMR spectra

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130.26
128.86
128.75
128.36
127.91
127.34
126.19
124.10
123.37
77.42
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2a
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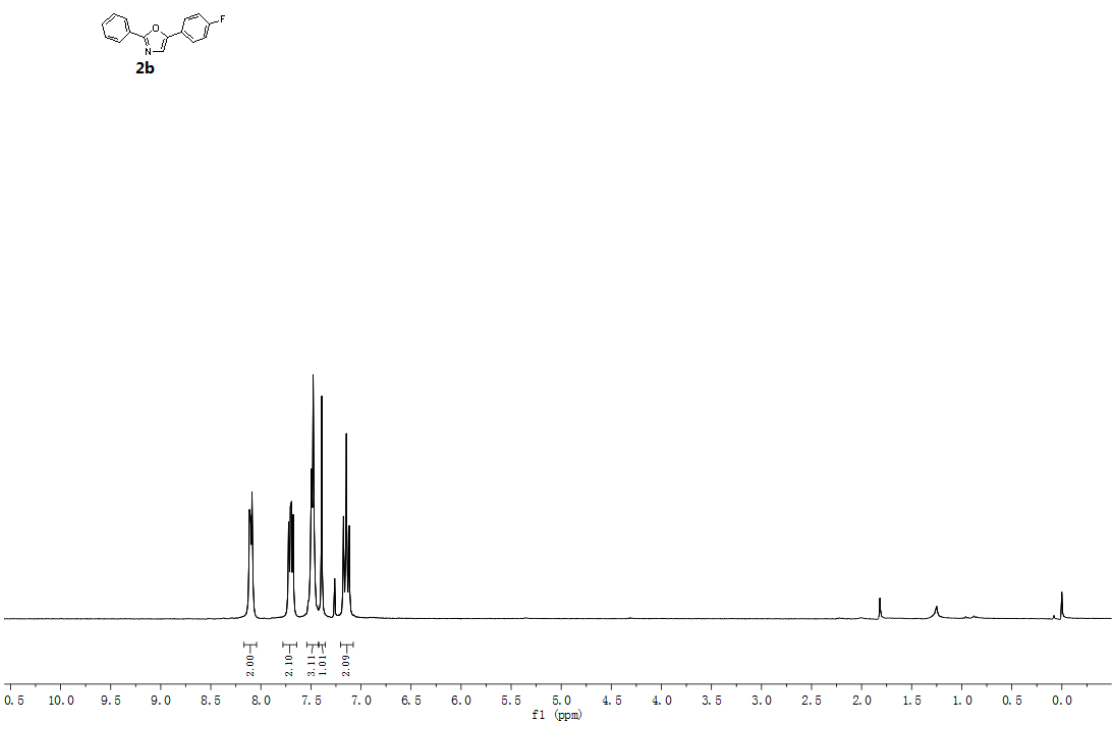
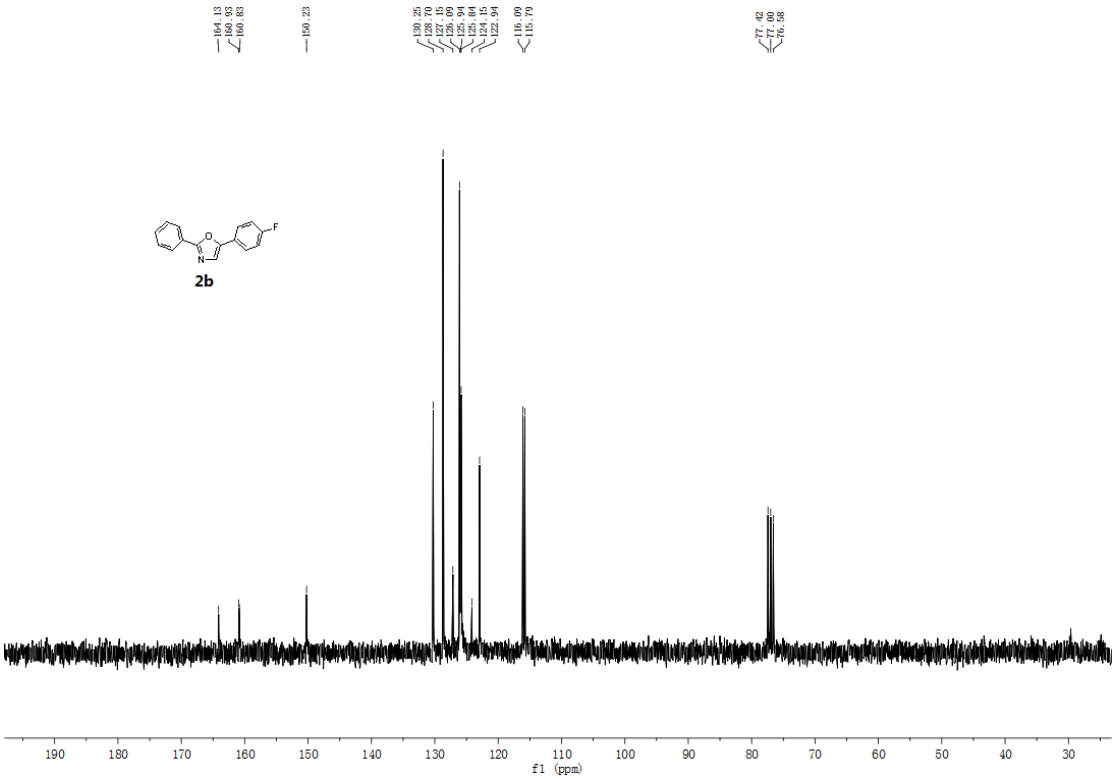
f1 (ppm)


F
2b
2.00
2.10
3.11
1.01
2.09
0.5 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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130.25
128.70
127.15
126.09
125.94
125.84
124.15
122.94
116.09
115.79
77.42
77.00
76.58
F
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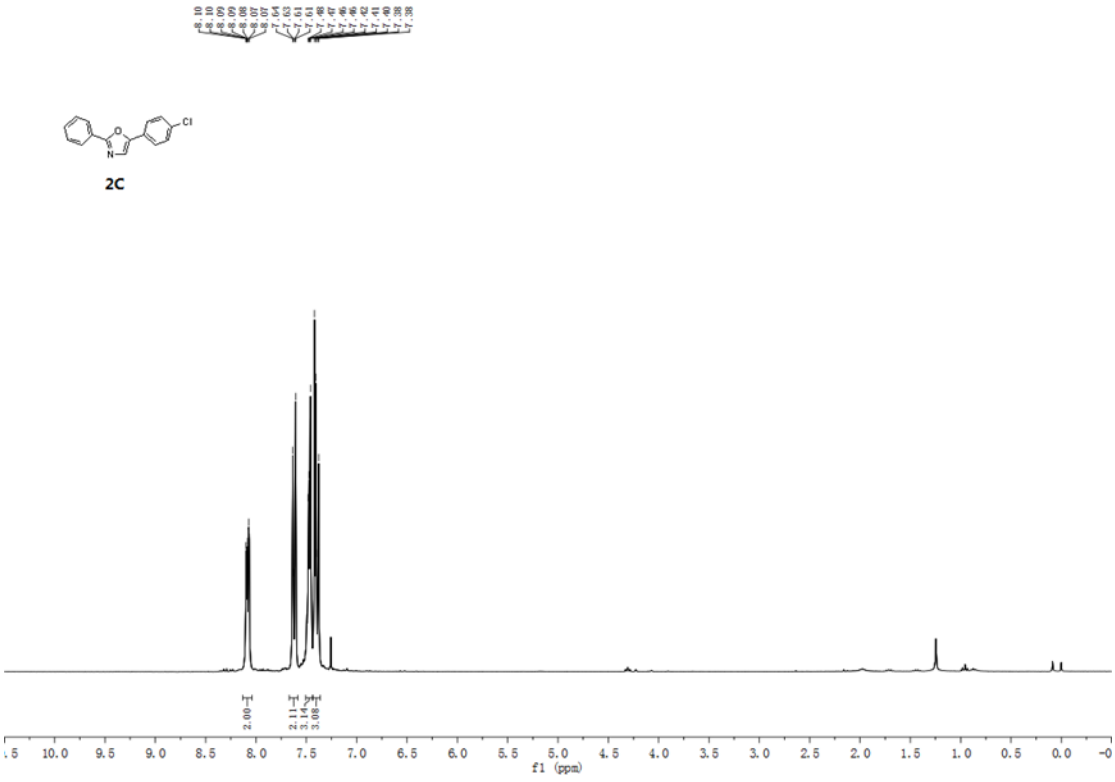
90
80
70
60
50
40
30
f1 (ppm)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8.10
8.09
8.09
8.08
8.08
8.07
8.07
7.64
7.63
7.61
7.61
7.48
7.47
7.46
7.46
7.45
7.45
7.41
7.40
7.38
7.38
Cl
2C
2.00
2.11
3.14
3.08
.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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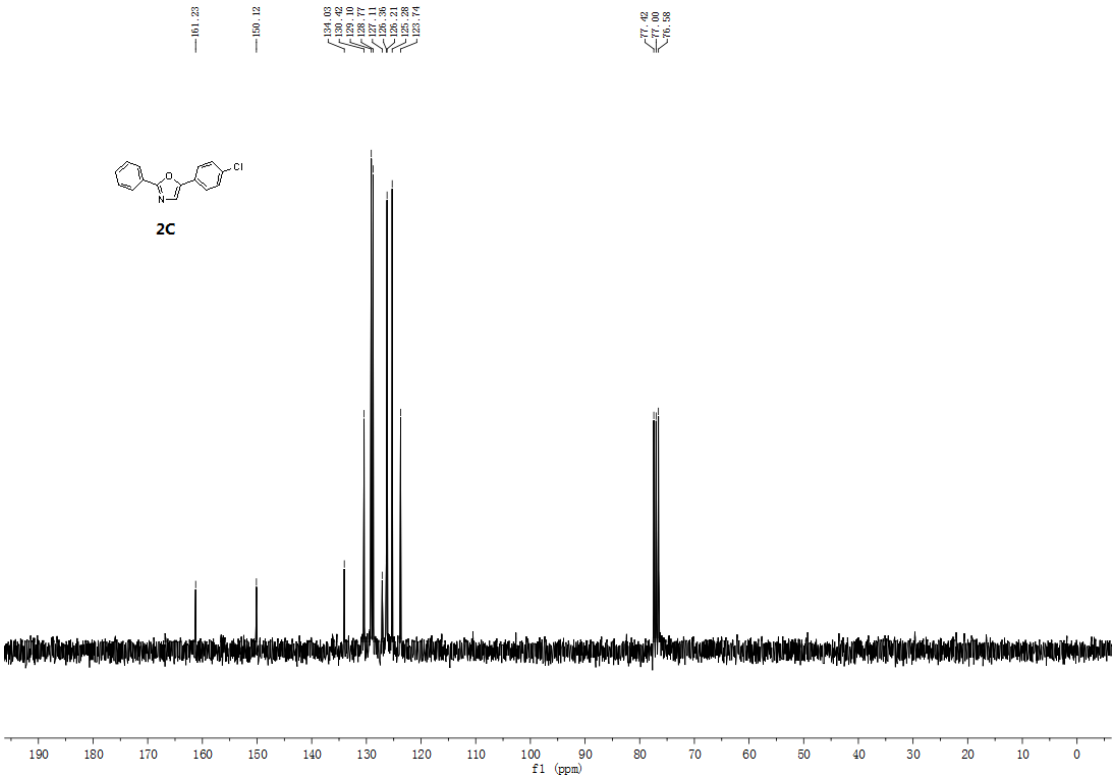
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)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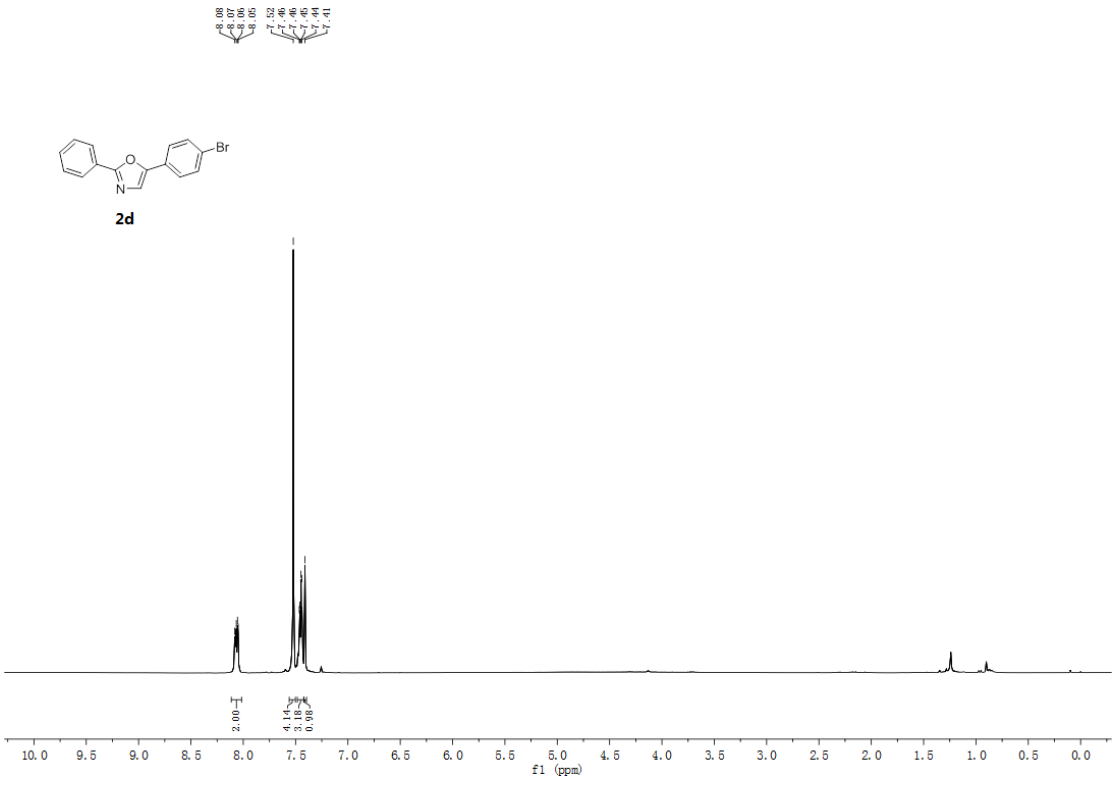
150.12
134.03
130.42
129.10
128.77
127.11
126.36
125.21
125.28
123.74
77.42
77.00
76.58
Cl
O
N
2C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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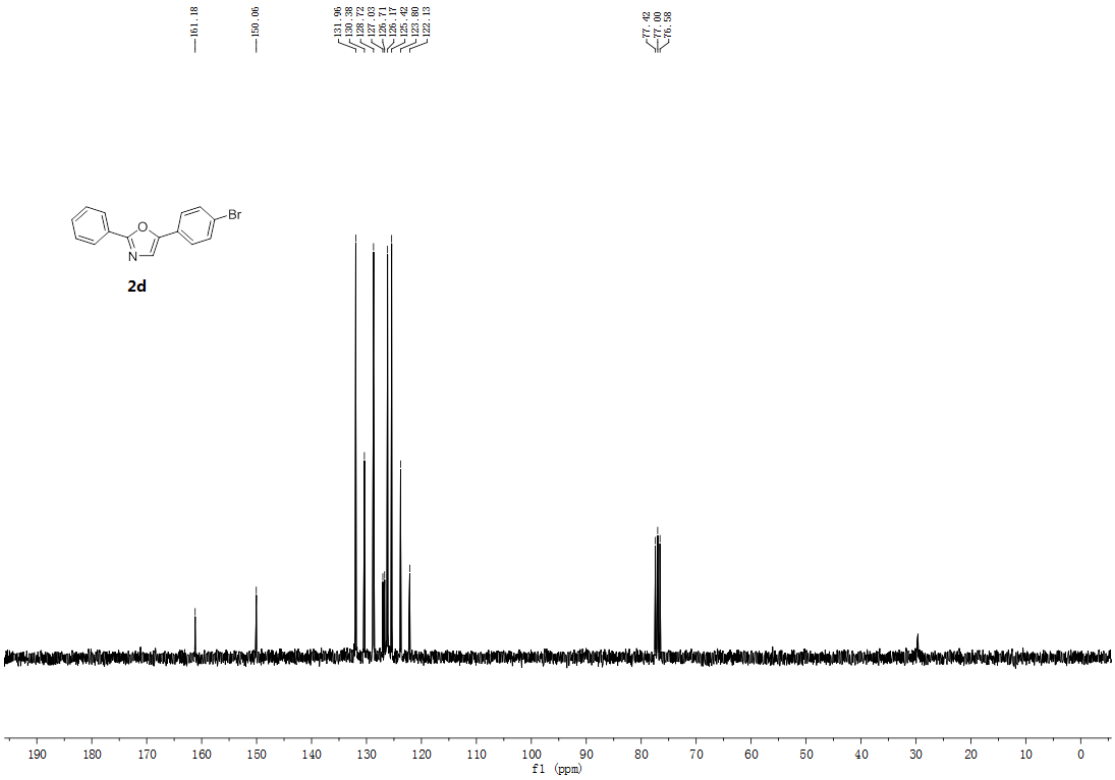
8.07
8.06
8.05
7.52
7.46
7.46
7.45
7.44
7.41
Br
O
N
2d
2.00
4.14
3.18
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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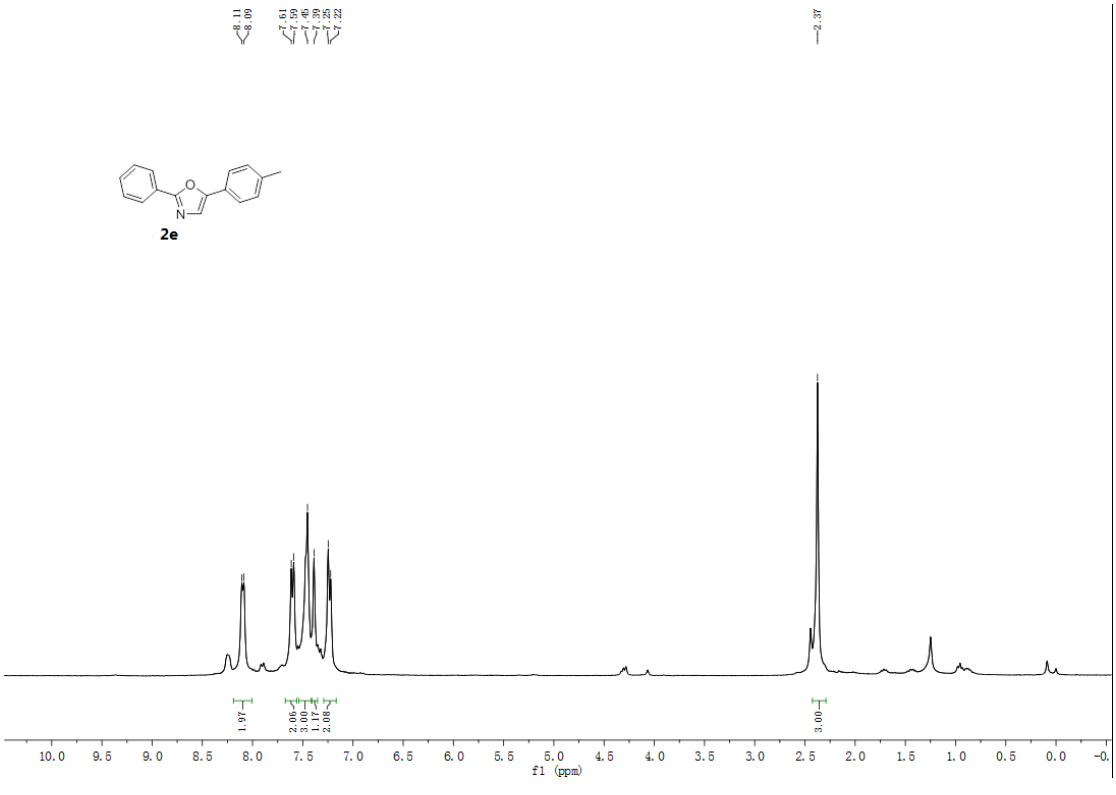
131.96
130.38
128.72
127.03
126.71
126.17
125.42
123.80
122.13
77.42
77.00
76.58
Br
O
N
2d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.09
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7.59
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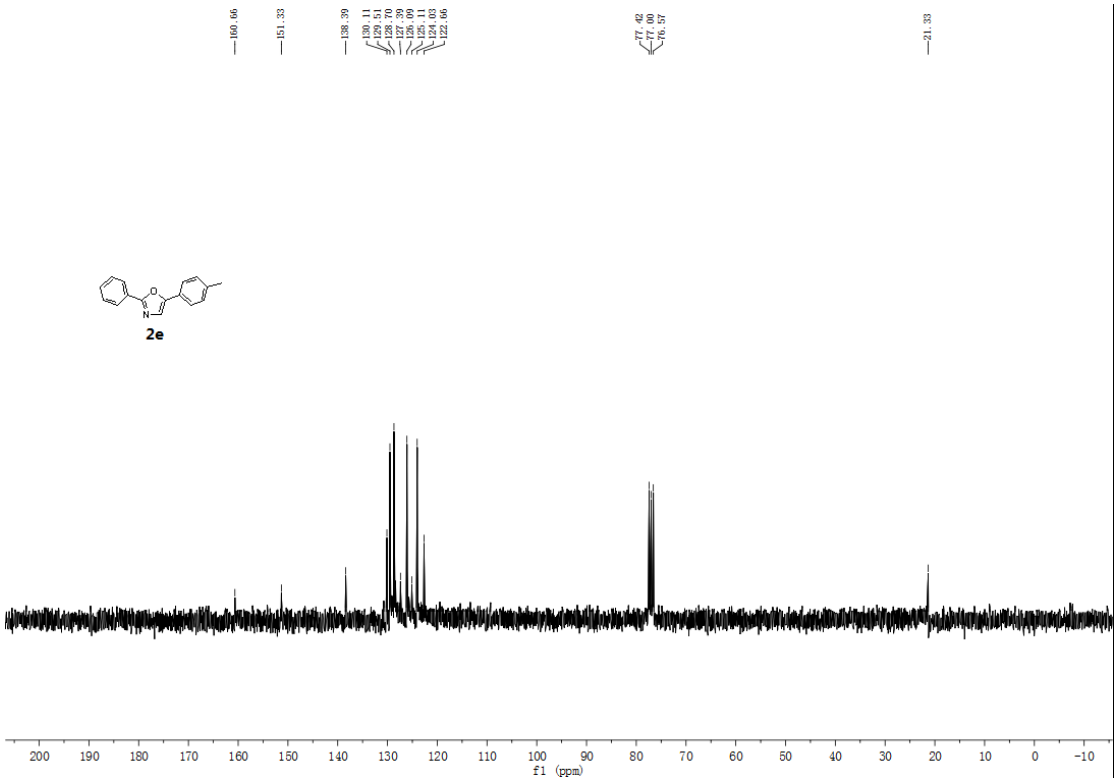
7.39
7.25
7.22
2.37
O
N
2e
1.07
2.06
3.00
1.17
2.08
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.39
126.09
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124.03
122.66
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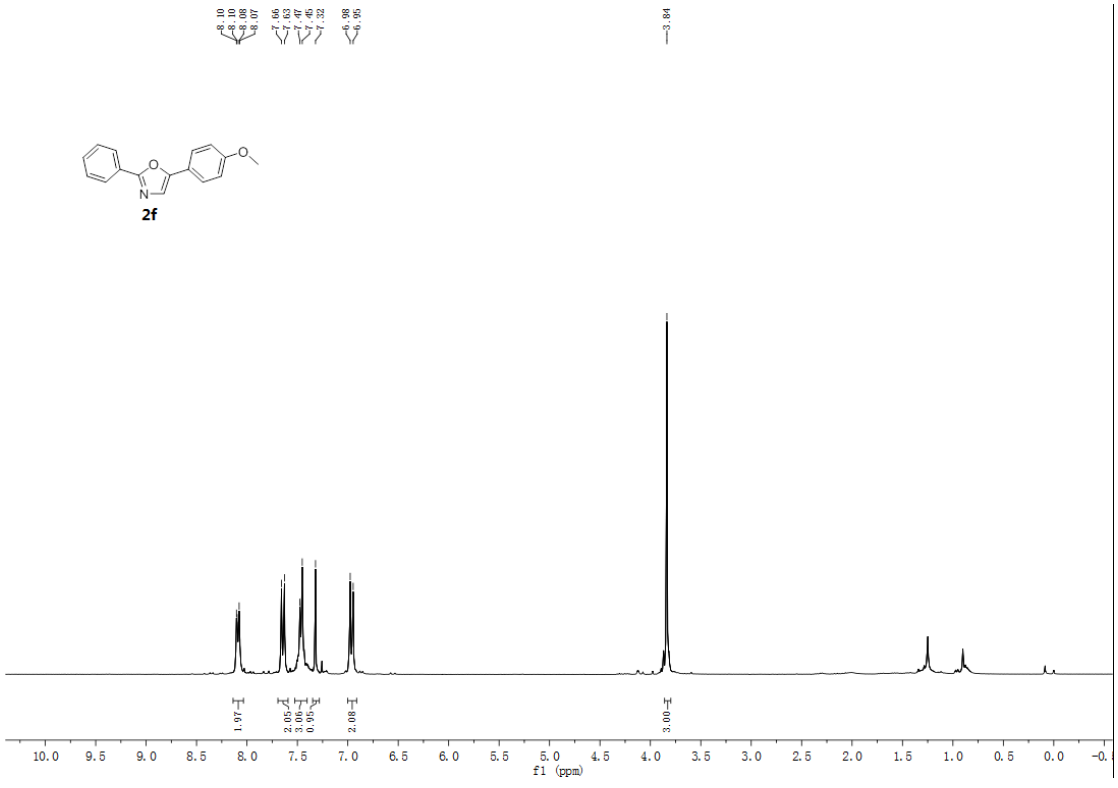
77.00
76.57
21.33
2e
f1 (ppm)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8.10
8.08
8.07
7.66
7.63
7.47
7.46
7.32
6.98
6.95
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2f
1.97
2.05
3.06
0.95
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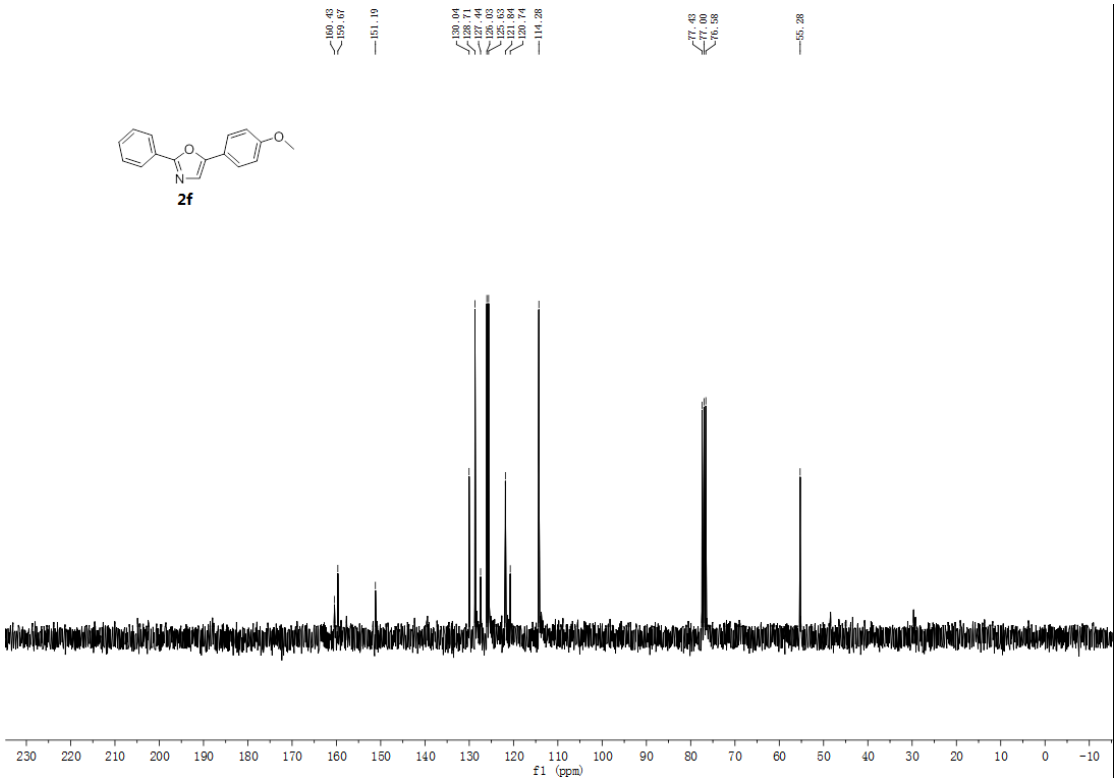
3.00
f1 (ppm)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120.74
114.28
77.43
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55.28
O
N
O
2f
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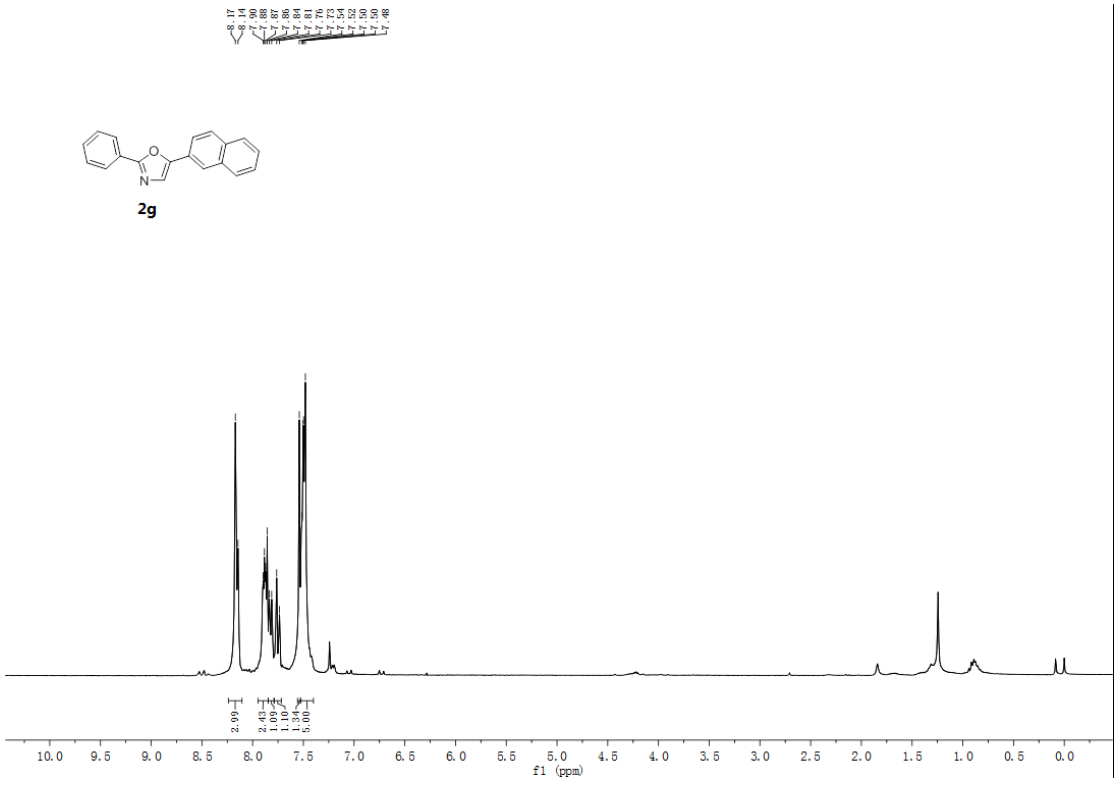
f1 (ppm)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7.88
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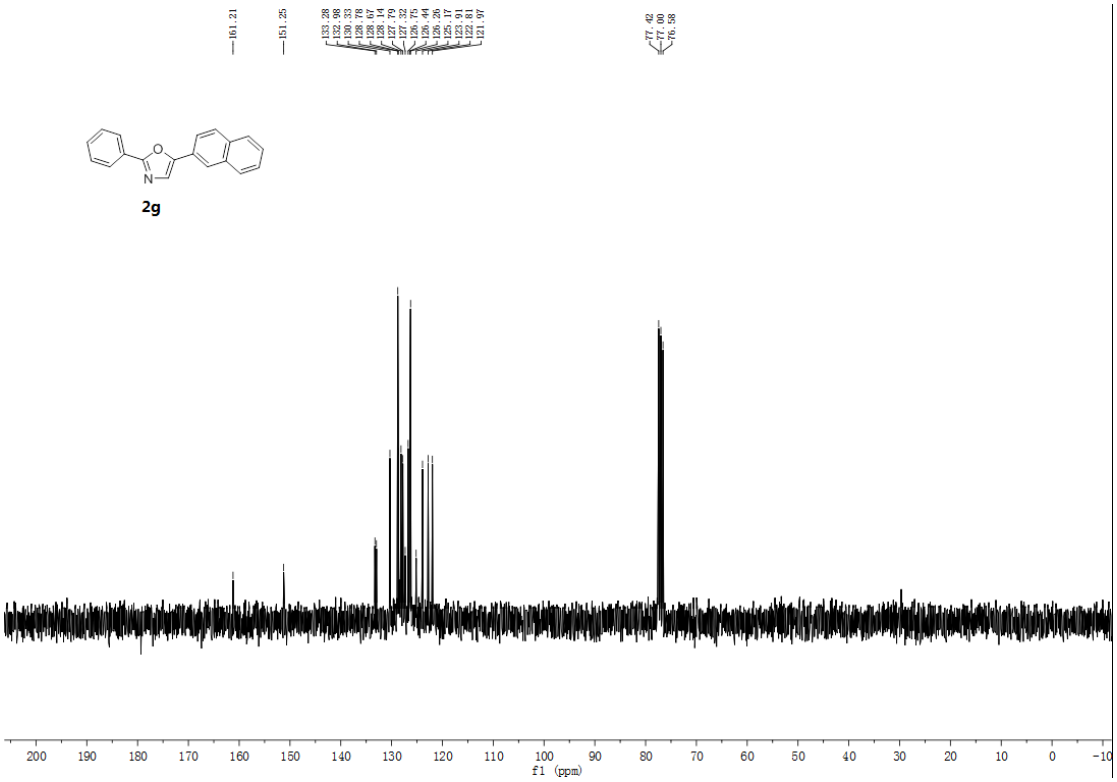
7.81
7.76
7.73
7.54
7.52
7.50
7.48
O
N
2g
2.99
2.43
1.09
1.10
1.94
5.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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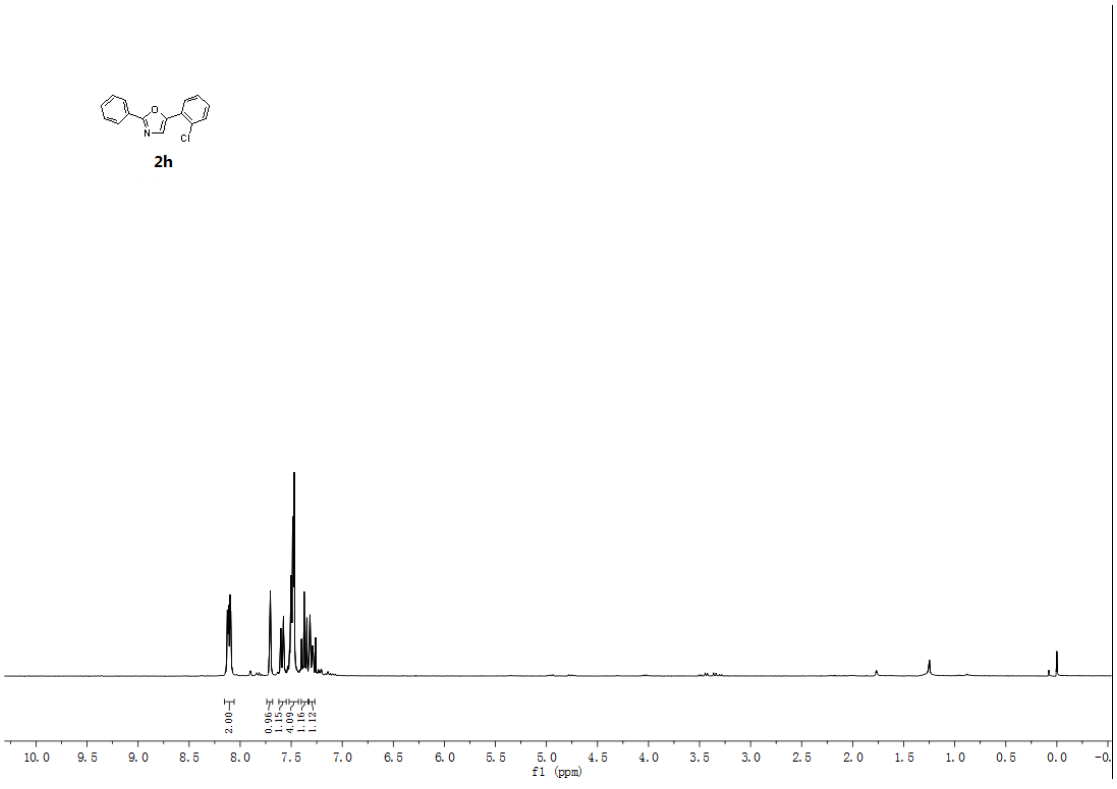
127.32
126.75
126.04
125.26
125.17
123.91
122.81
121.97
77.42
77.00
76.58
O
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

**2g**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Cl
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9.5
9.0
8.5
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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0.5
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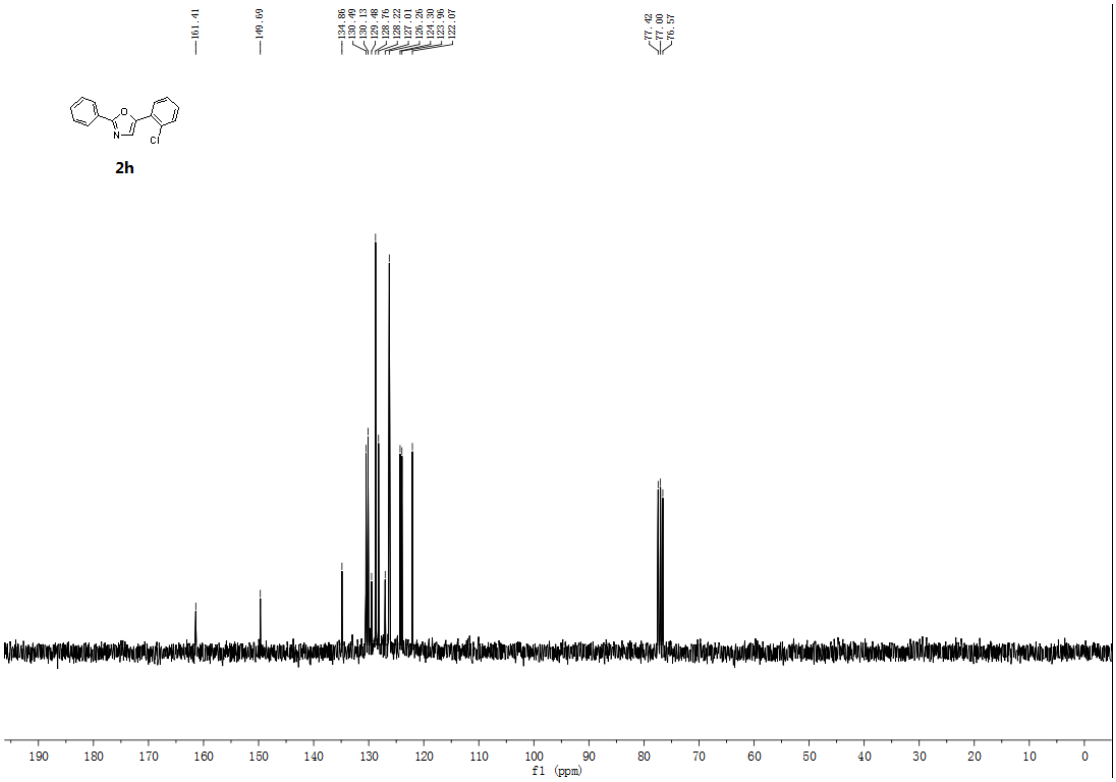
f1 (ppm)

**2h**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124.30
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122.07
77.42
77.00
76.57
O
N
Cl
2h
190
180
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130
120
110
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90
80
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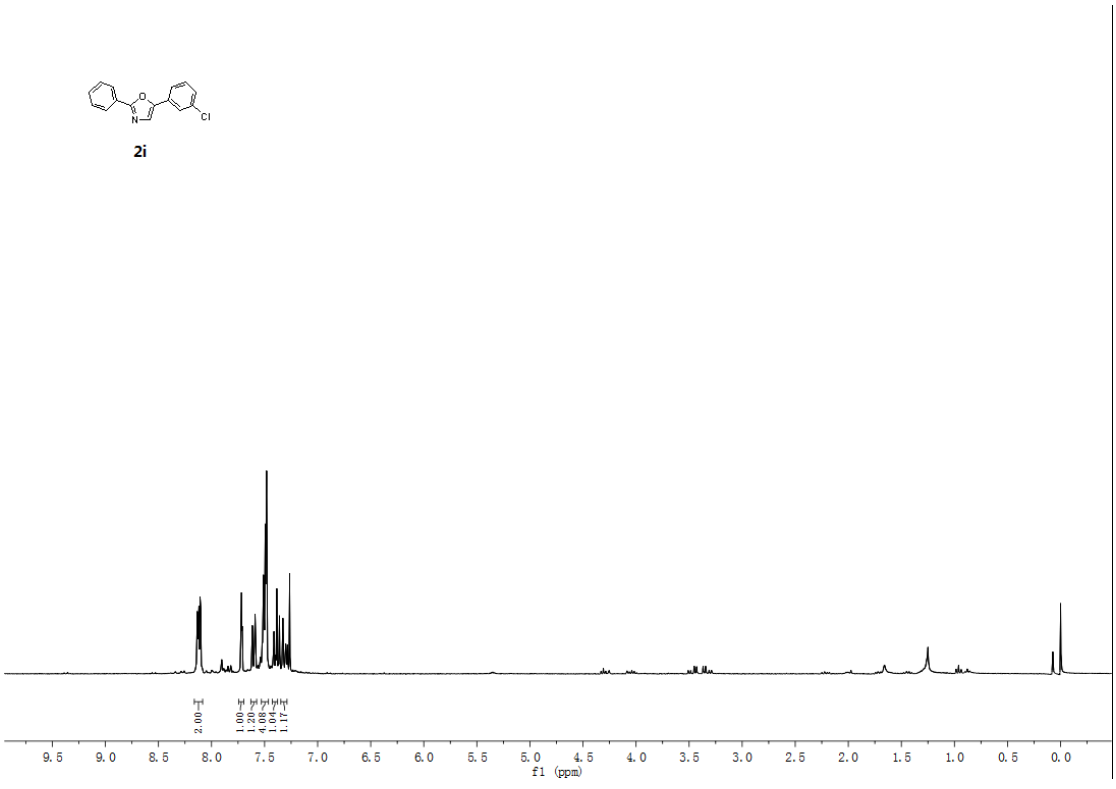
50
40
30
20
10
0
f1 (ppm)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Cl
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8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
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1.0
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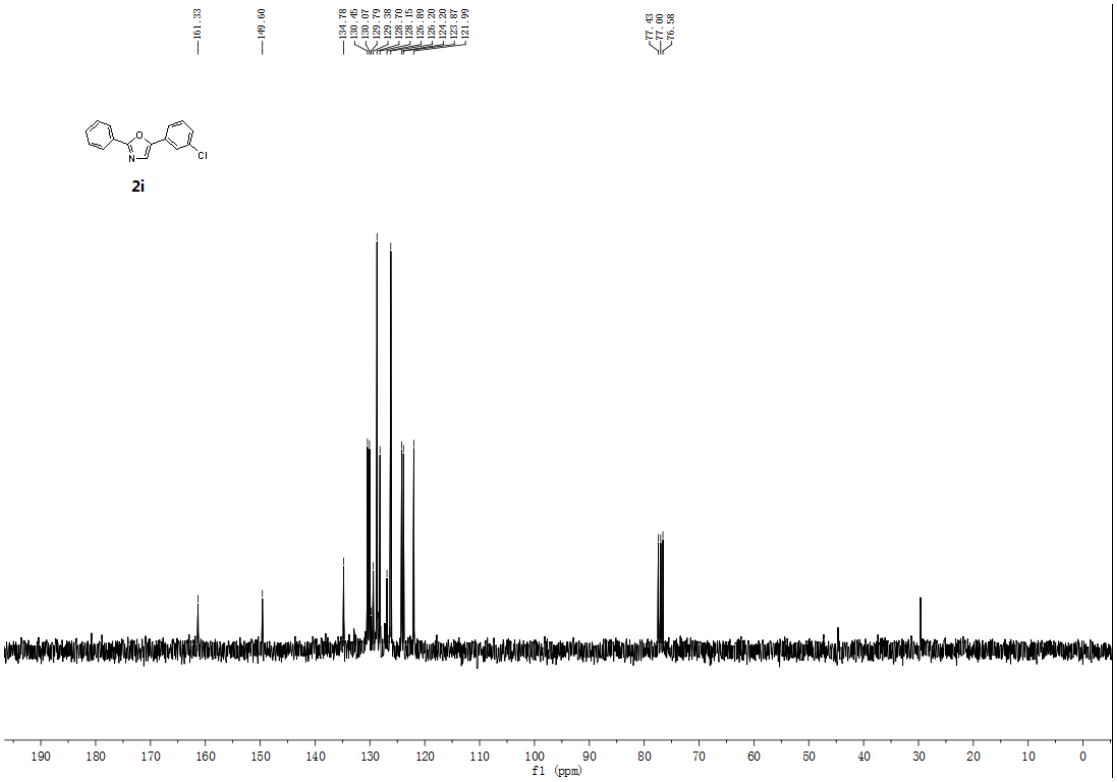
f1 (ppm)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124.20
123.87
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76.58
Cl
N
O
2i
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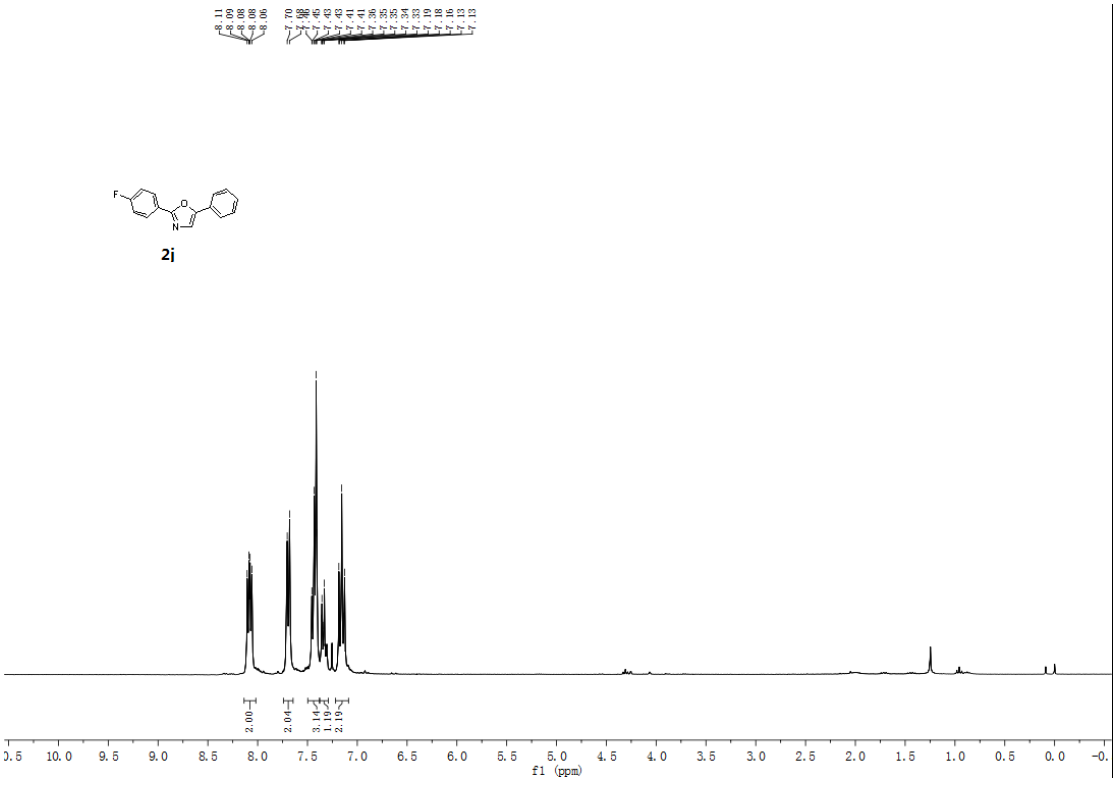
f1 (ppm)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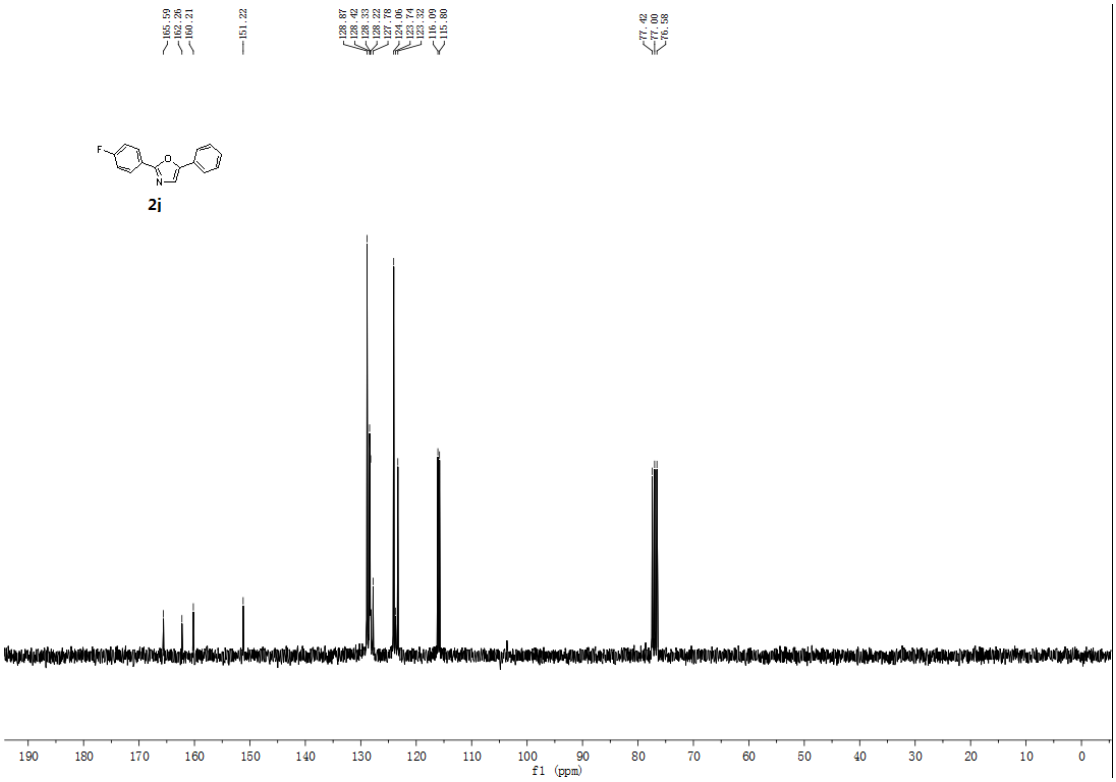
7.33
7.19
7.18
7.16
7.13
7.13
F
N
O
2j
2.00
2.04
3.14
1.19
2.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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124.06
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77.00
76.58
F
O
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2j
190
180
170
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130
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90
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50
40
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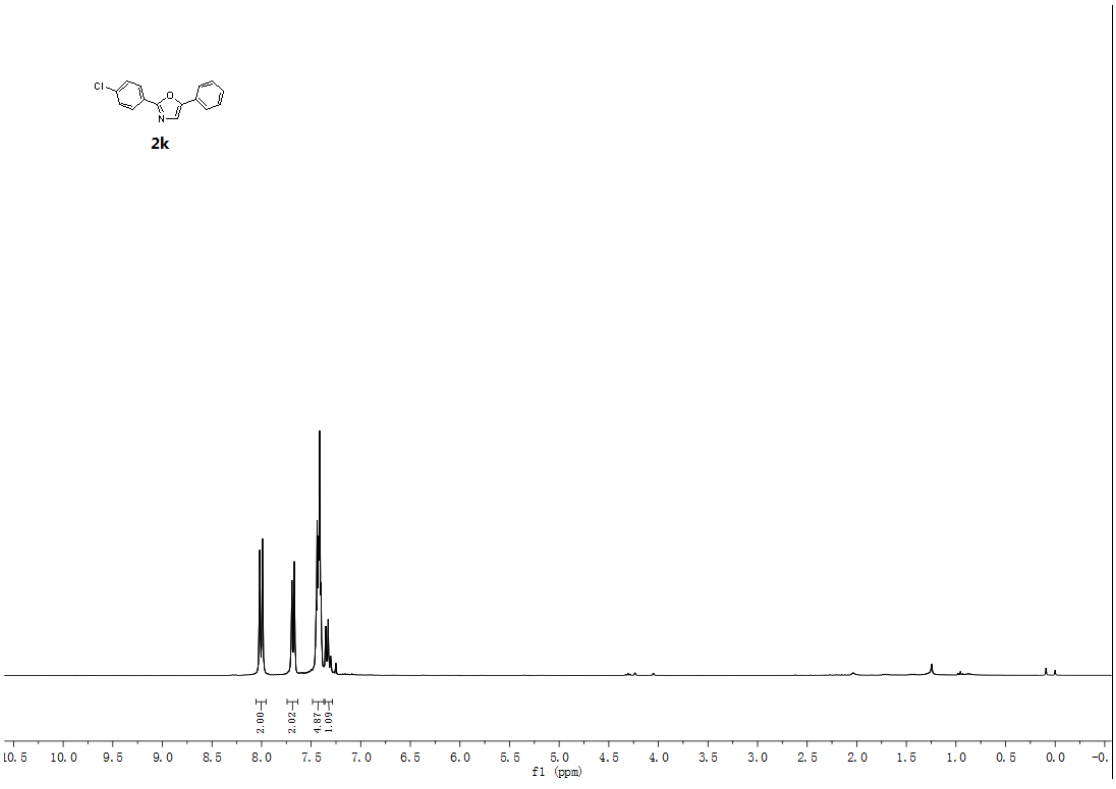
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7.5
7.0
6.5
6.0
5.5
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3.5
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2.0
1.5
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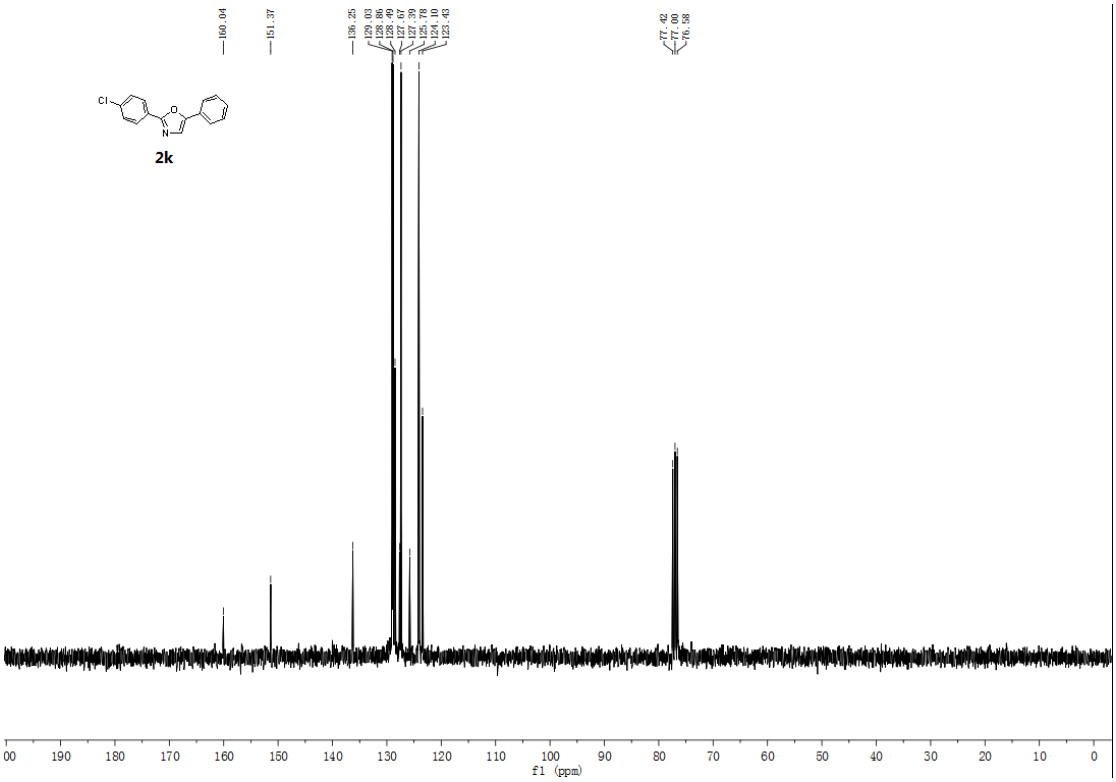
f1 (ppm)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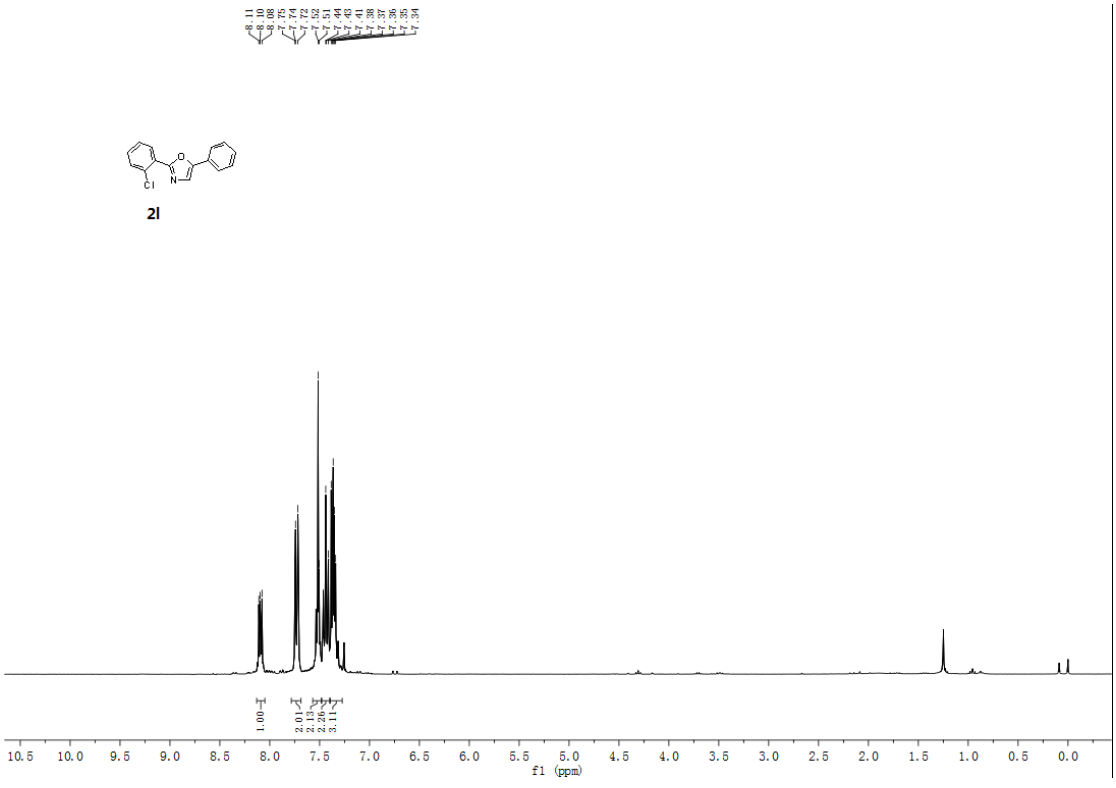
77.00
76.58
Cl
O
N
2k
f1 (ppm)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7.51
7.44
7.43
7.41
7.38
7.37
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Cl
O
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2l
1.00
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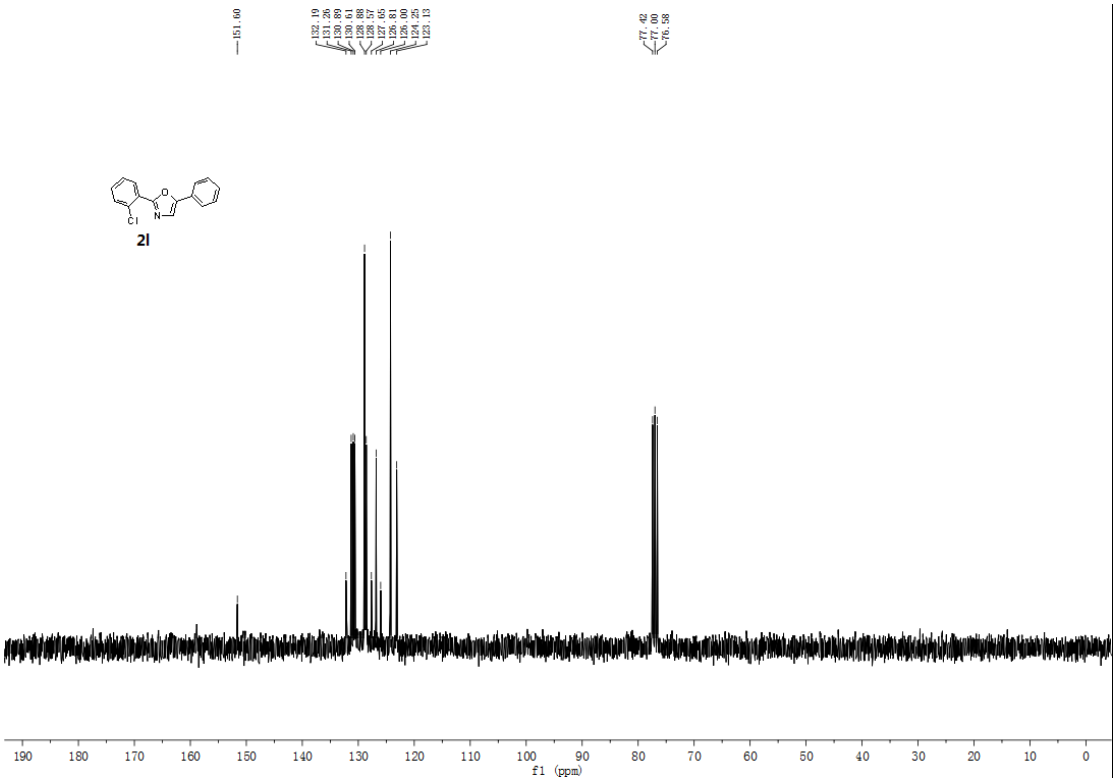
2.15
2.26
3.11
f1 (ppm)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126.00
124.25
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77.00
76.58
Cl
O
N
2l
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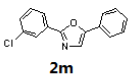
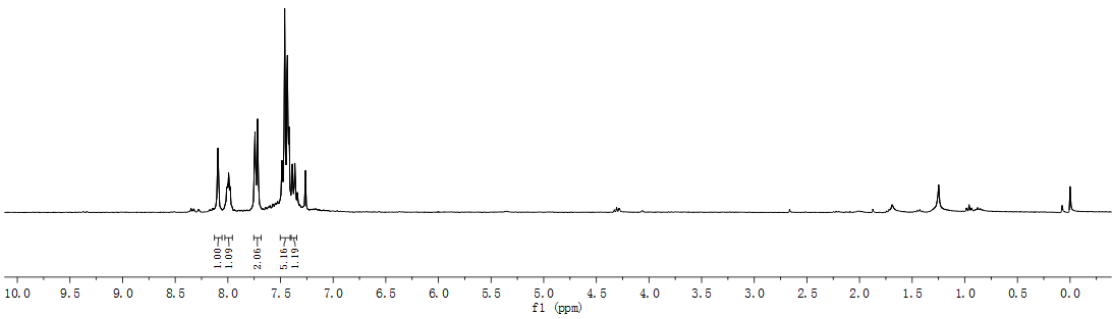
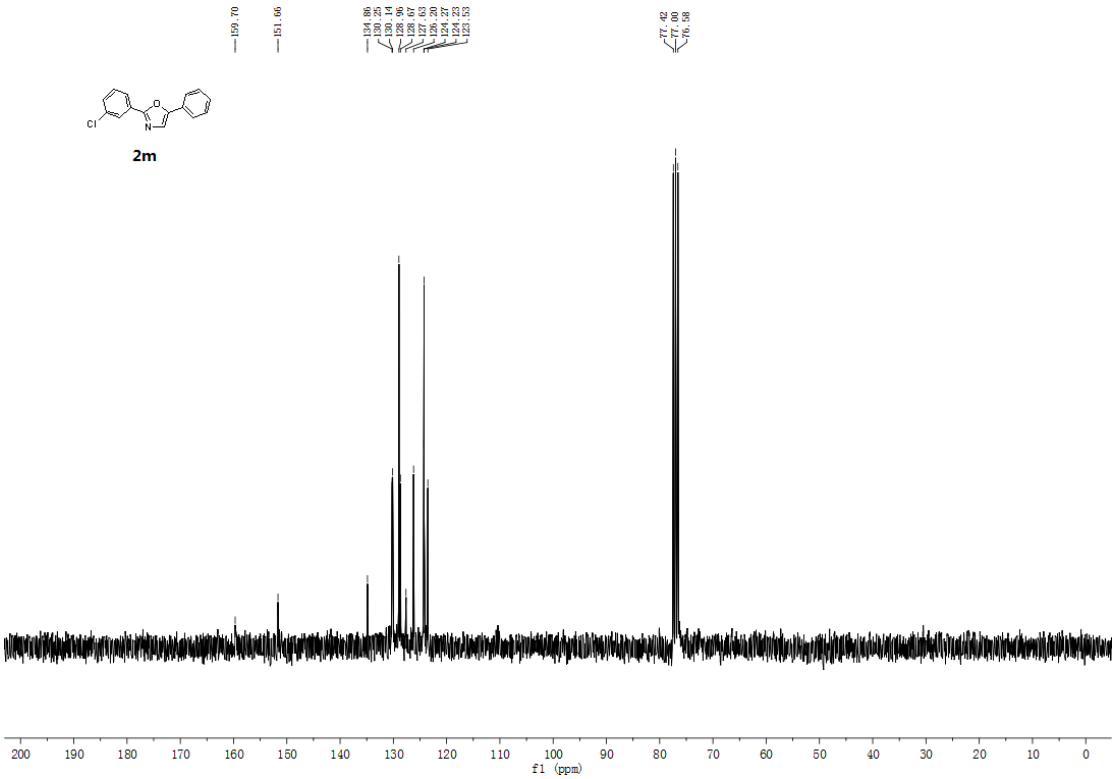
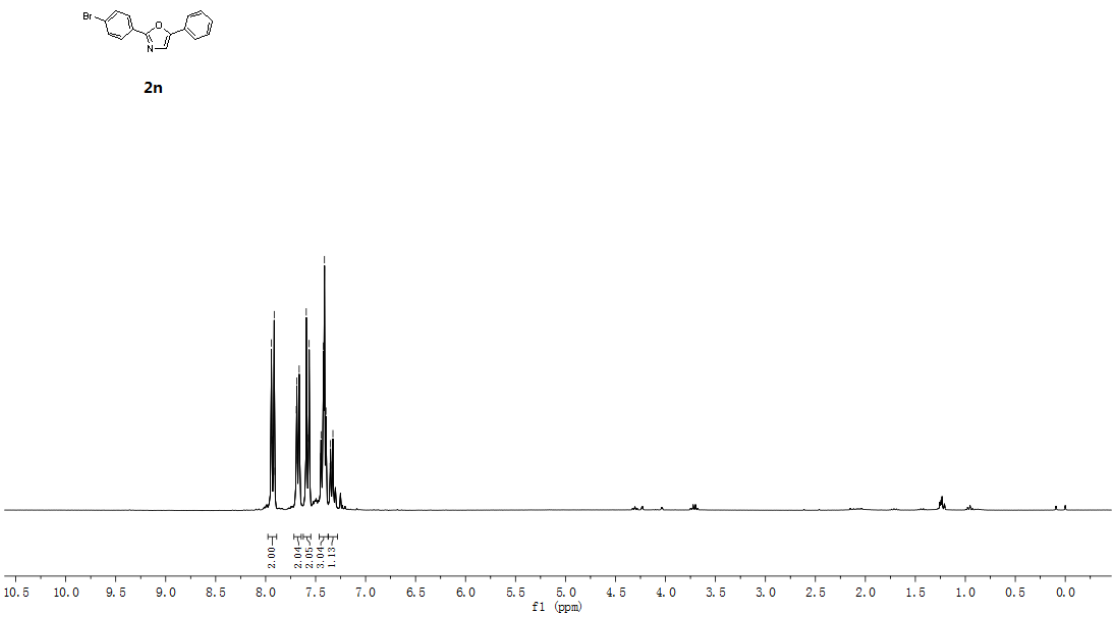
f1 (ppm)

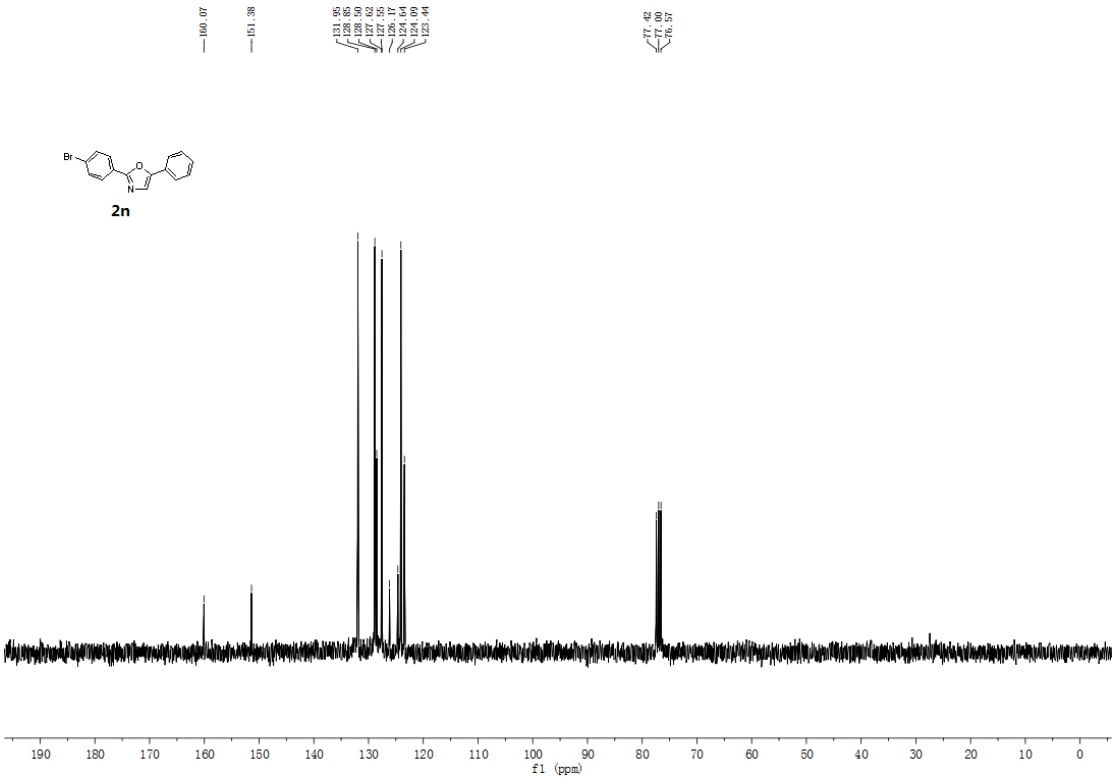

Cl
O
N

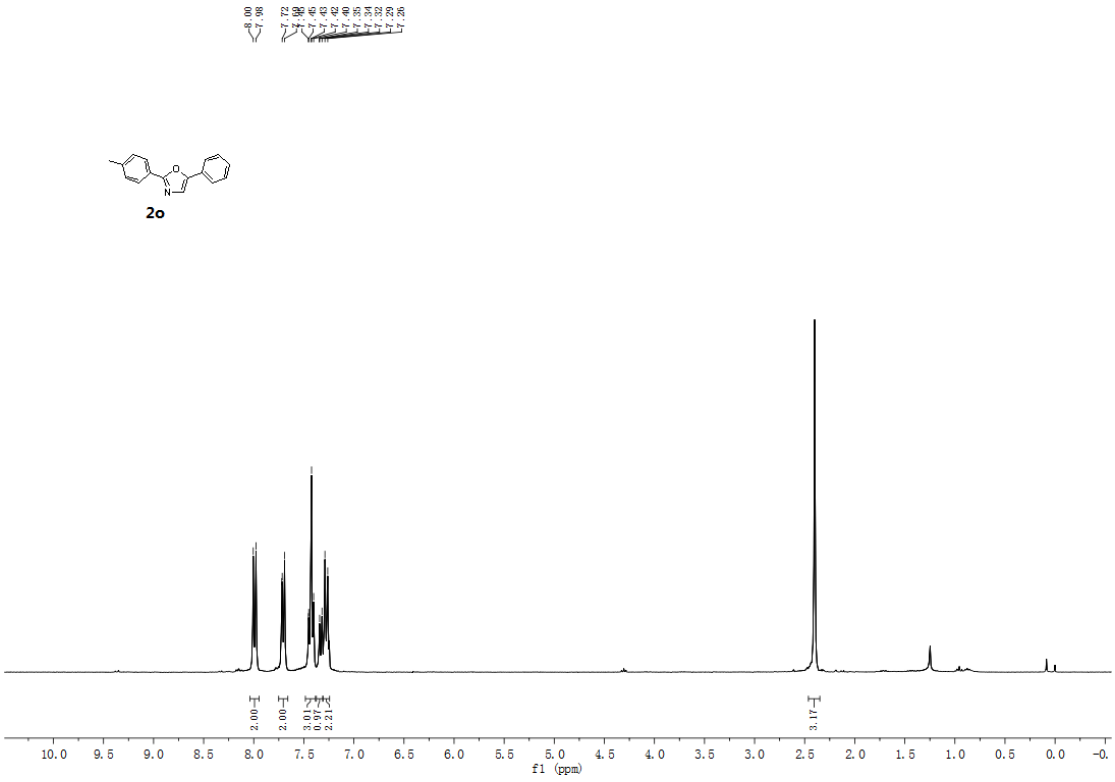
2m

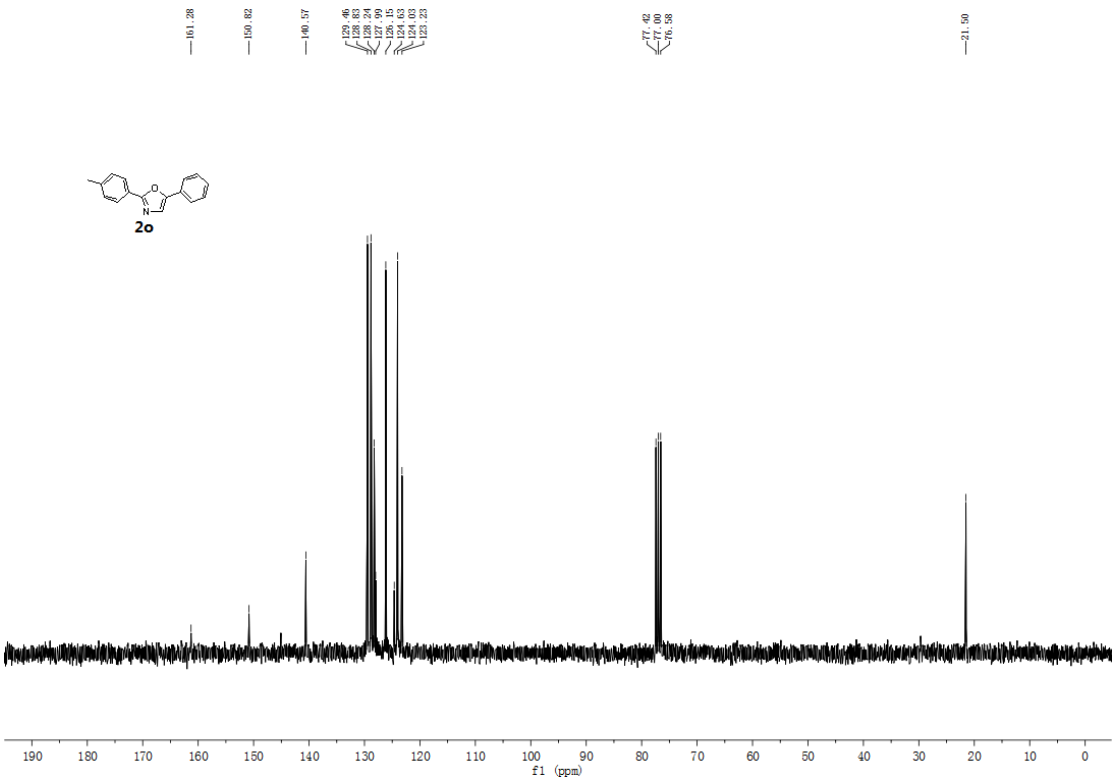

1.00
1.09
2.06
5.16
1.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

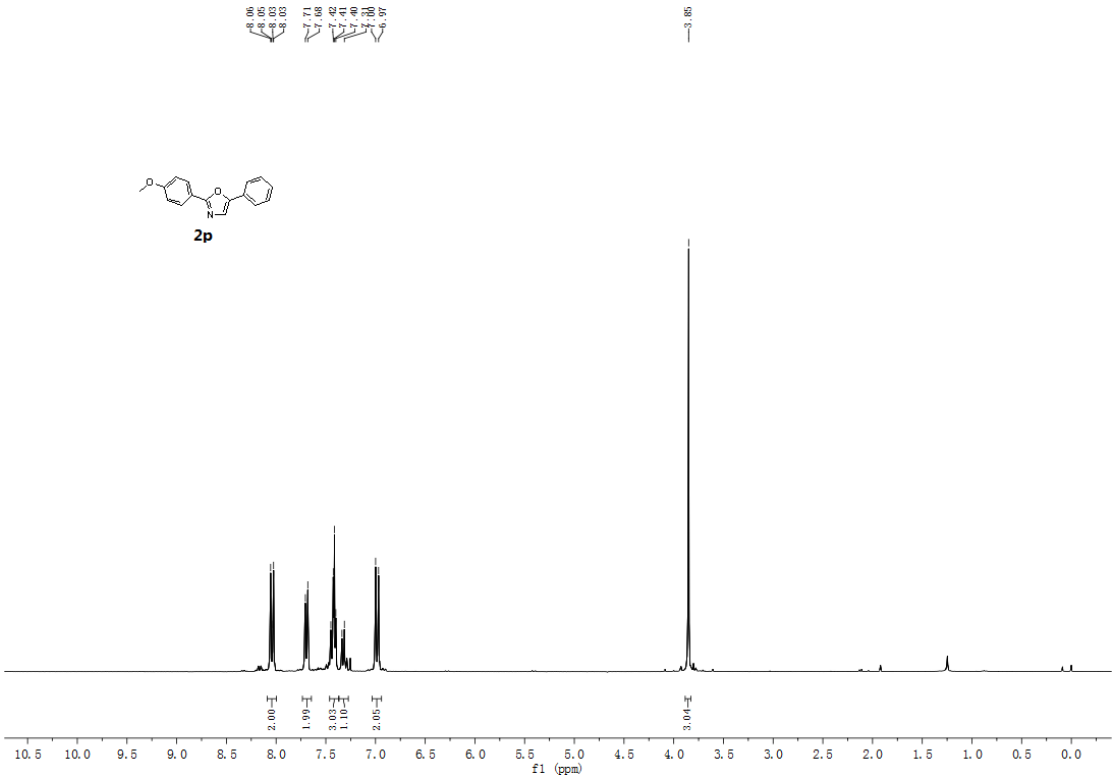

159.70
151.66
134.86
130.25
130.14
128.96
128.67
127.63
126.30
124.27
124.23
123.53
77.42
77.00
76.58
Cl
O
N
2m
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
7.94
7.94
7.92
7.91
7.91
7.69
7.68
7.66
7.59
7.59
7.57
7.56
7.45
7.45
7.44
7.42
7.41
7.40
7.36
7.35
7.35
7.33

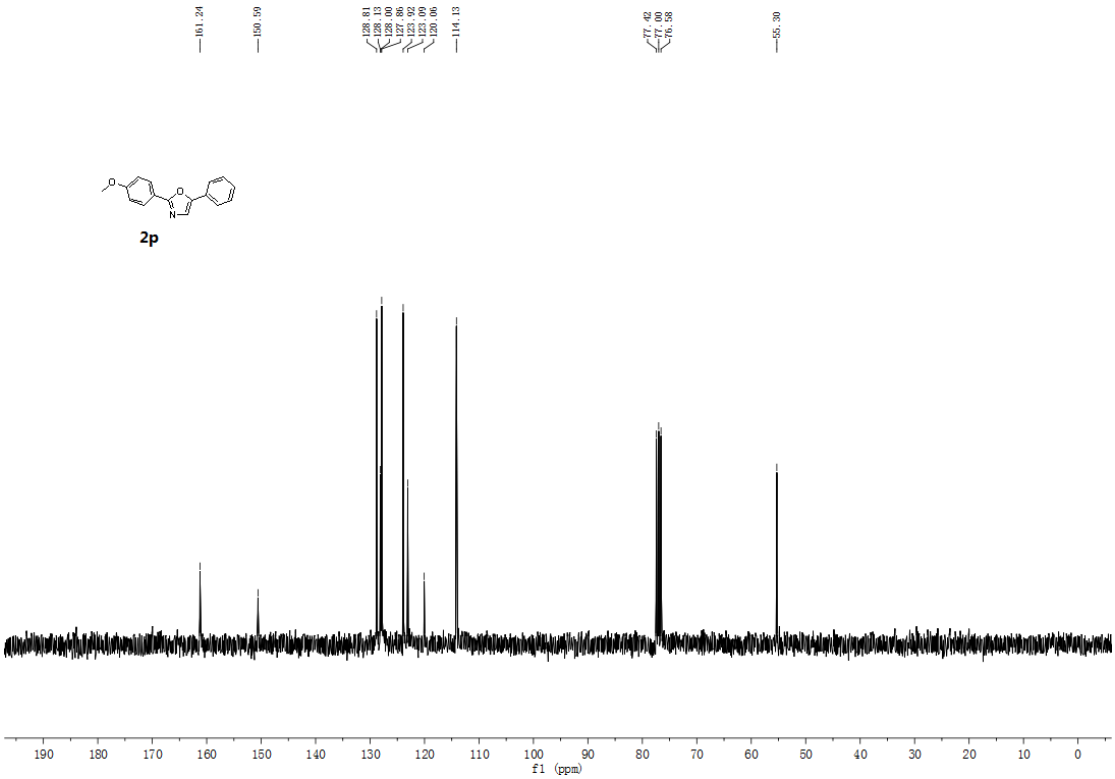

Br
O
N
2n
2.00
2.04
2.05
3.04
1.13
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

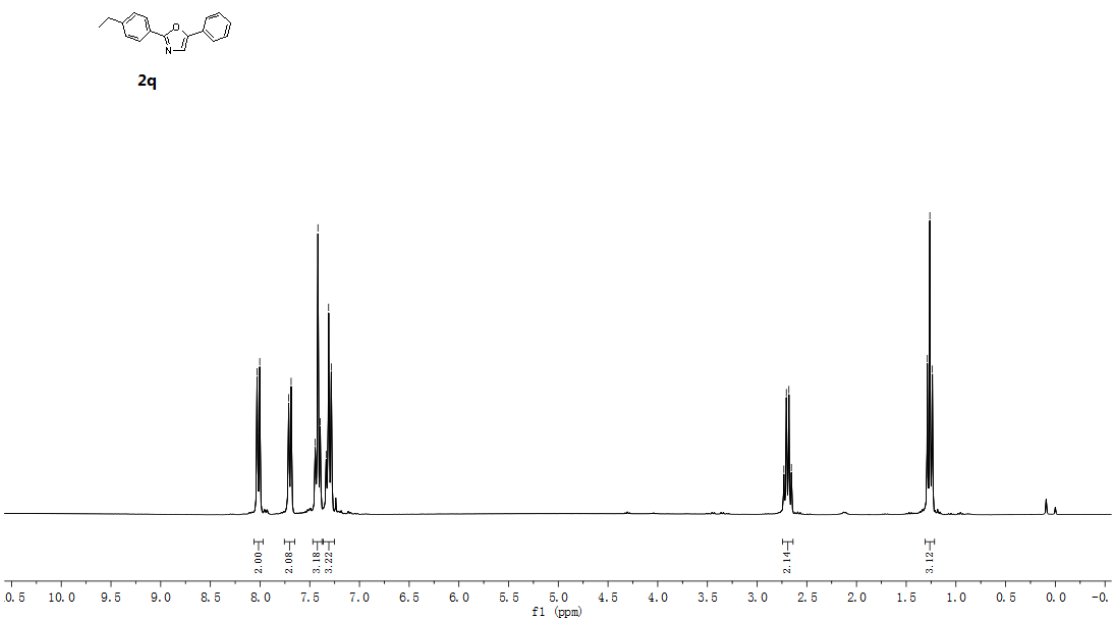

160.07
151.38
131.95
128.85
128.50
127.62
127.55
126.17
124.64
124.09
123.44
77.42
77.00
76.57
Br
O
N
2n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

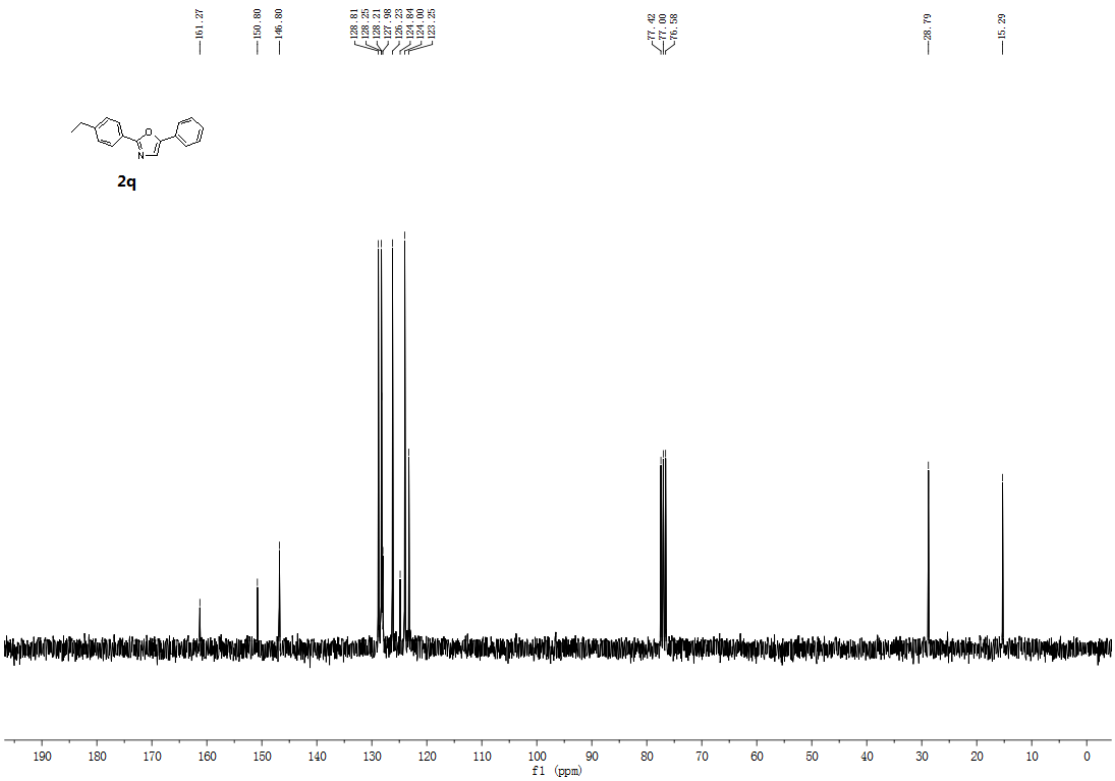

8.00
7.98
7.72
7.70
7.46
7.45
7.42
7.40
7.35
7.34
7.32
7.29
7.26
O
N
2o
2.00
2.00
3.01
0.97
2.21
3.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

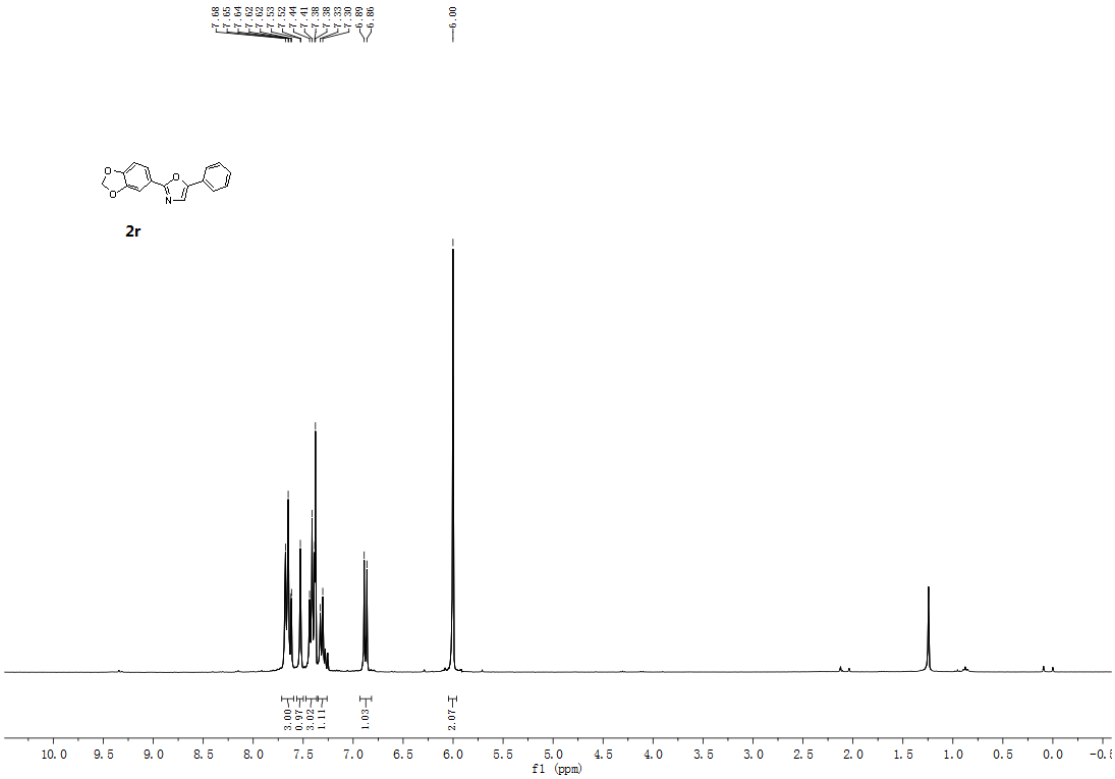

161.28
150.82
140.57
129.46
128.83
128.24
127.99
126.15
124.63
124.03
123.23
77.42
77.00
76.58
21.59
2o
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

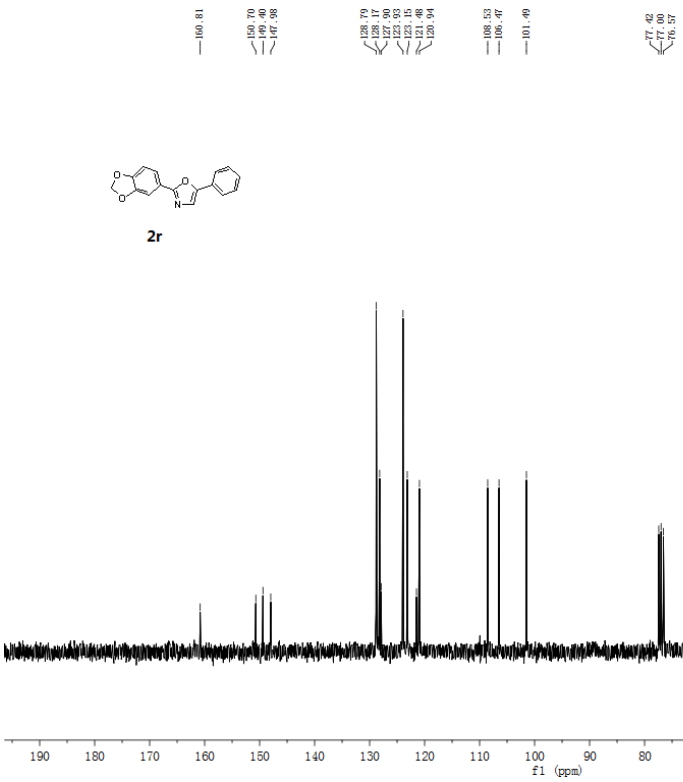

8.06
8.05
8.03
8.03
7.71
7.68
7.42
7.41
7.40
7.39
7.00
6.97
3.85
2p
2.00
1.99
3.03
1.10
2.05
3.04
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

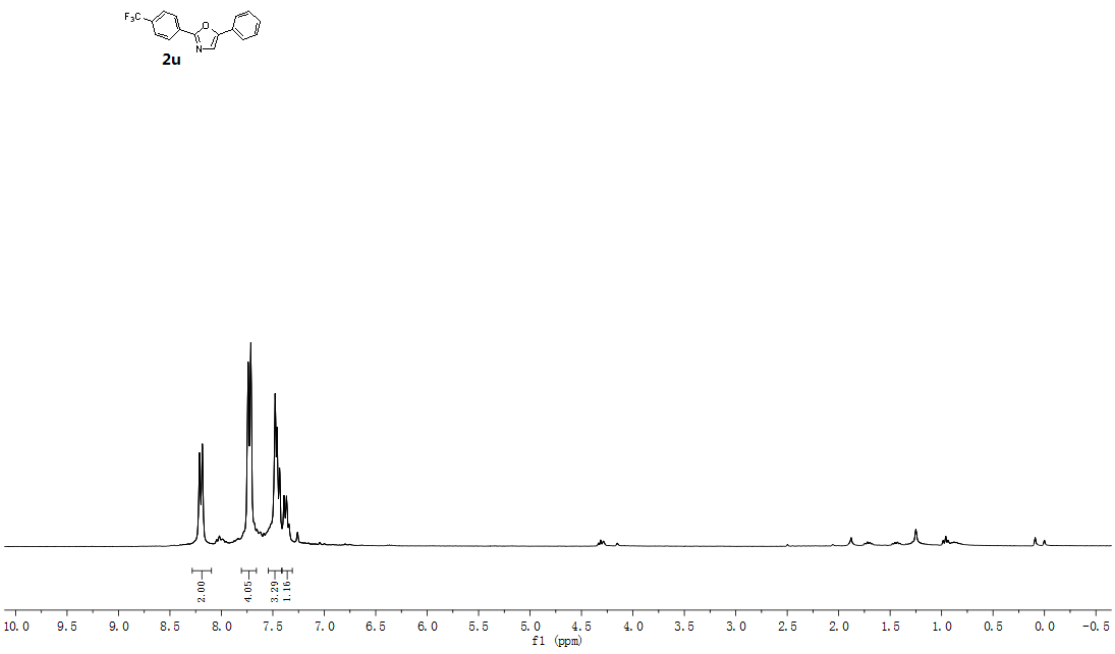

161.24
150.59
128.81
128.13
128.00
127.86
123.92
123.09
120.06
114.13
77.42
77.00
76.58
55.30
2p
f1 (ppm)
8.03
8.00
7.71
7.69
7.45
7.42
7.40
7.34
7.31
7.28
2.73
2.71
2.68
2.66
1.29
1.26
1.24

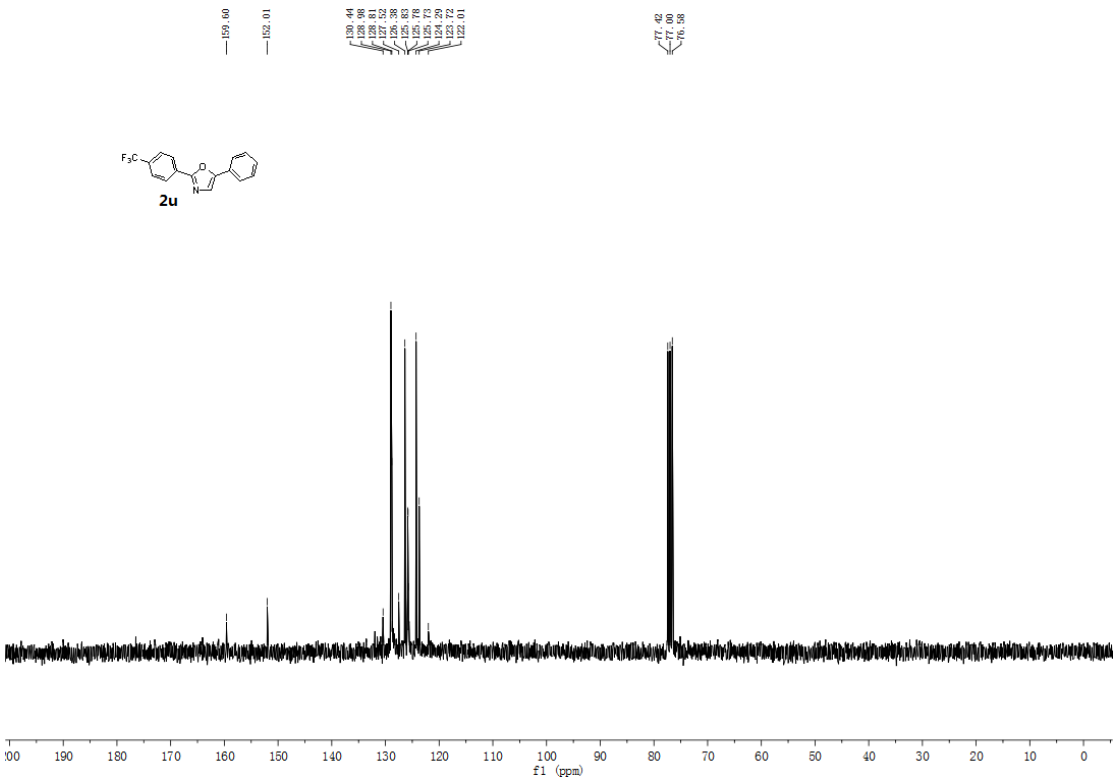

2q
f1 (ppm)
2.00
2.08
3.18
3.22
2.14
3.12

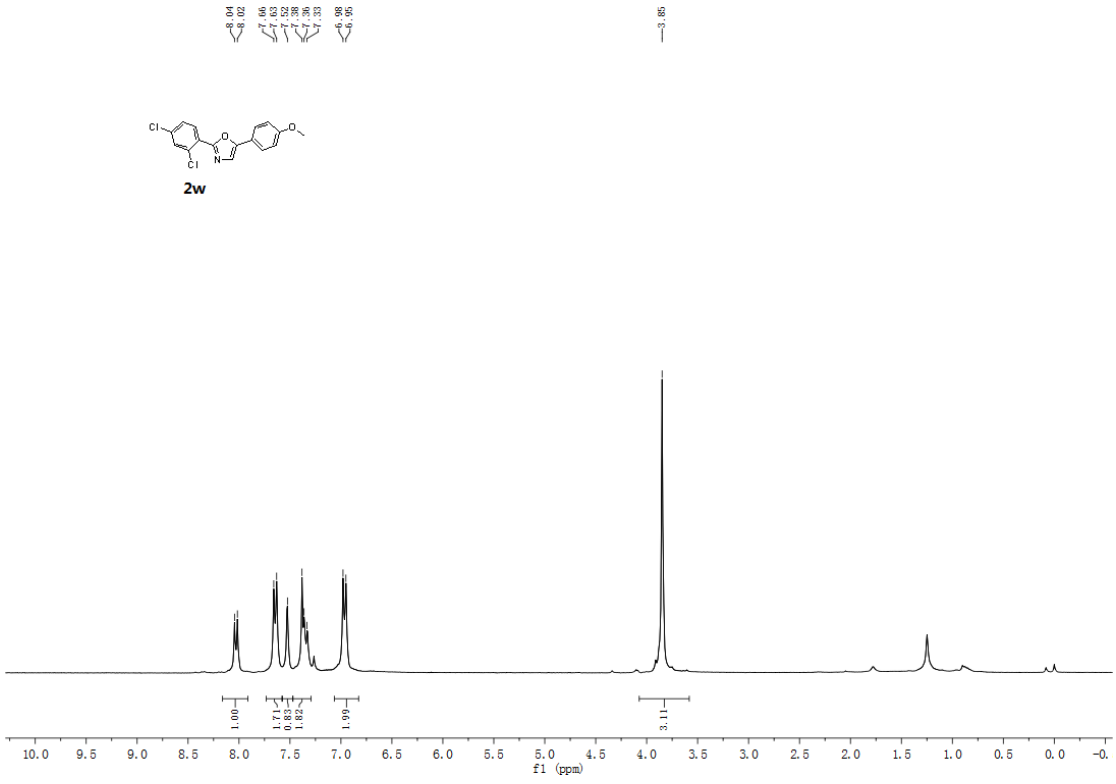

161.27
150.80
146.80
128.81
128.25
128.21
127.98
126.23
124.84
124.00
123.25
77.42
77.00
76.58
28.79
15.29
2q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

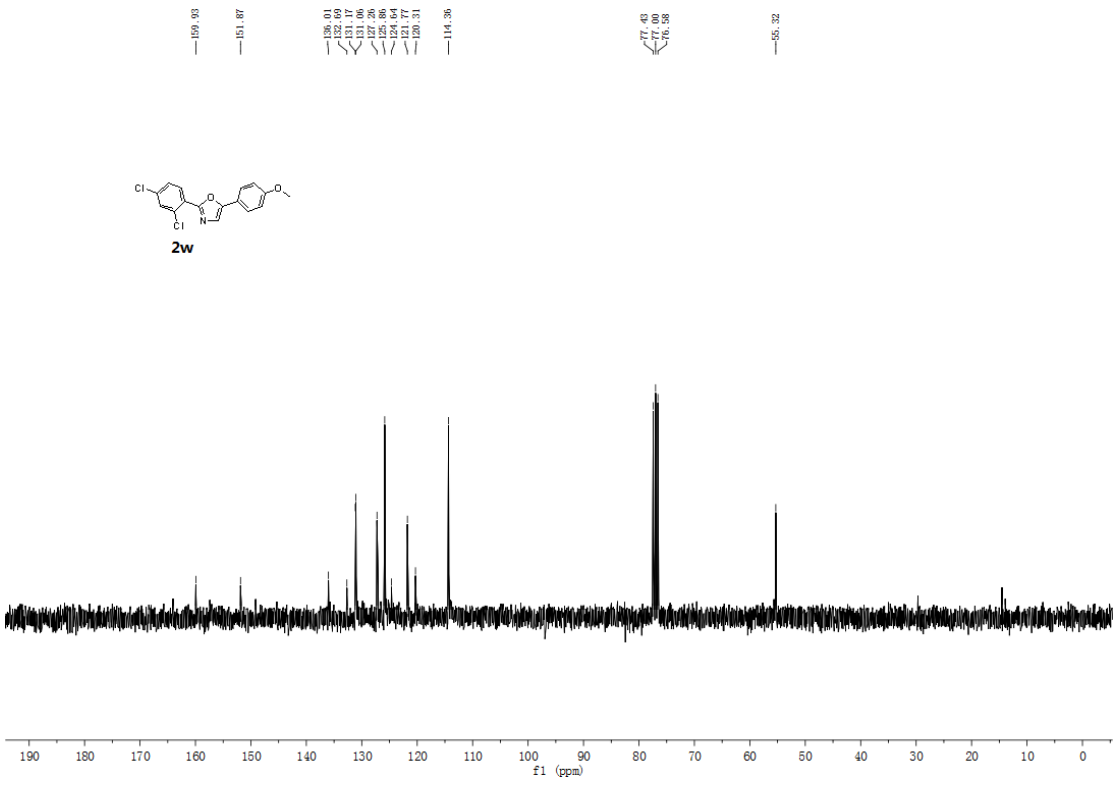

7.68
7.65
7.64
7.62
7.62
7.53
7.52
7.44
7.41
7.38
7.38
7.33
7.30
6.89
6.86
6.00
2r
3.00
0.97
3.02
1.11
1.03
2.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

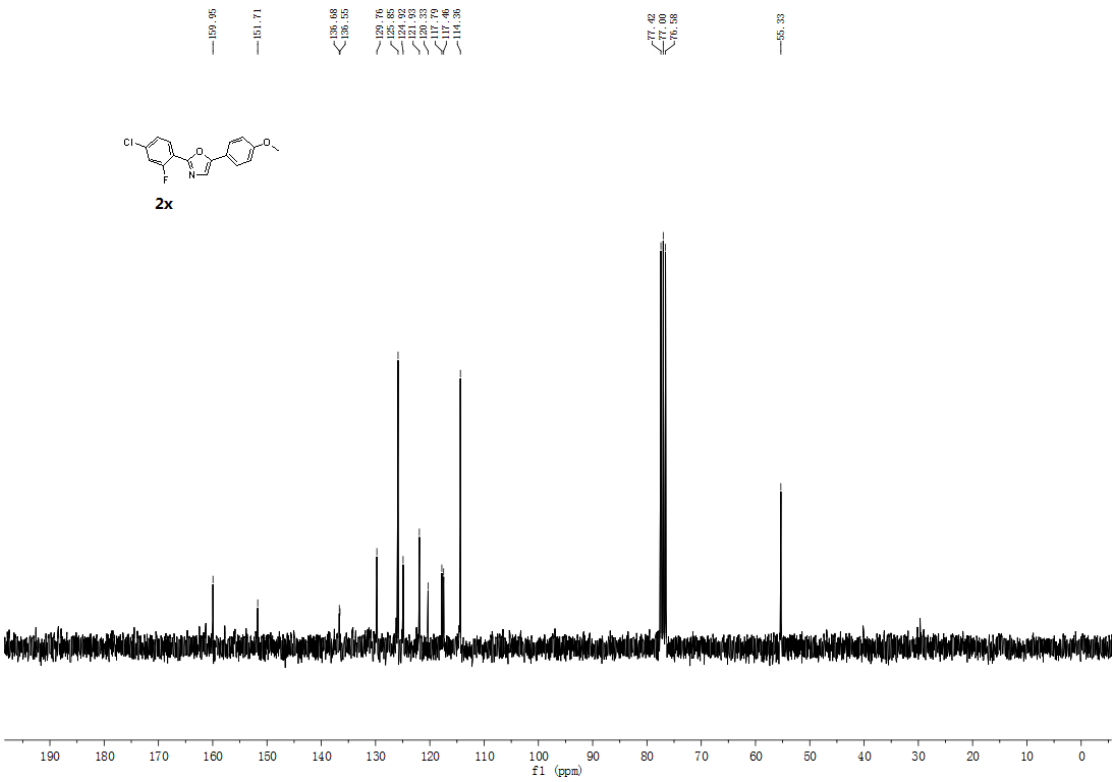

160.81
150.70
149.40
147.98
128.79
128.17
127.90
123.93
121.15
121.46
120.94
108.53
106.47
101.49
77.42
77.00
76.57
2r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


F3C
2u
2.00
4.05
3.29
1.16
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
-0.5
f1 (ppm)


159.60
152.01
130.44
128.98
128.81
127.52
126.38
125.83
125.78
125.73
124.29
123.72
122.01
77.42
77.00
76.58
F3C
O
N
2u
f1 (ppm)


8.04
8.02
7.66
7.63
7.52
7.38
7.36
7.33
6.98
6.95
3.85
Cl
Cl
O
N
O
2w
1.00
1.71
0.83
1.02
1.99
3.11
f1 (ppm)


159.93
151.87
138.01
132.69
131.17
131.06
127.26
125.86
124.64
121.77
120.31
114.36
77.43
77.00
76.58
55.32
Cl
O
N
Cl
O
2w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)
8.05
8.02
8.00
7.66
7.63
7.38
7.27
7.24
6.98
6.95
3.85
Cl
O
N
F
O
2x
1.00
1.71
0.89
1.83
1.99
3.05
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
-0.
f1 (ppm)


159.95
151.71
136.68
136.55
129.76
125.85
124.92
121.93
120.33
117.79
117.46
114.36
77.42
77.00
76.58
55.33
Cl
F
O
N
O
2x
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)