Supporting Information

Phosphine catalyzed dearomative [3+2] cycloaddition of benzoxazoles with a cyclopropenone

Xingben Wang, Congjun Yu, Iuliana L. Atodiresei, and Frederic W. Patureau *

Institute of Organic Chemistry, RWTH Aachen University, Landoltweg 1, 52074 Aachen, Germany.
E-mail: Frederic.Patureau@rwth-aachen.de

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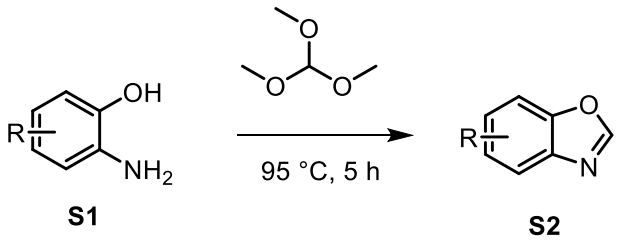
1. General information

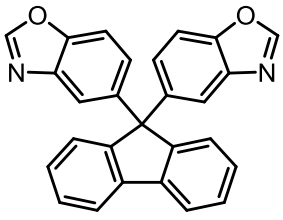
NMR spectra were obtained on an Agilent VNMRS 400 or a Bruker Av 600 using $CDCl_3$ as solvents. Chemical shifts are given in ppm and coupling constants (*J*) in Hz. ^1H spectra were calibrated in relation to the reference measurement of TMS (0.00 ppm). ^{13}C spectra were calibrated in relation to the deuterated solvent, namely $CDCl_3$ (77.16 ppm). The following abbreviations were used for ^1H NMR spectra to indicate the signal multiplicity: s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet) as well as combinations of them. Flash chromatography was performed on silica gel (60 M, 0.04-0.063 mm) by standard technique. All the chemicals used for synthesis were purchased from Sigma Aldrich, abcr, Alfa Aesar, TCI, Fisher, or chemPUR. High resolution mass spectra (HRMS) were obtained on a Thermo Scientific LTQ Orbitrap XL spectrometer. Crystallographic data were collected on a Bruker Kappa APEX II CCD-diffractometer with monochromatic Mo–Kα radiation (λ=0.71073 Å) and a CCD detector.

Heating: Aluminum blocks equipped with slots that accommodate the glass vial reactors were utilized for all herein described experiments requiring heating.

2. Preparation of some starting materials



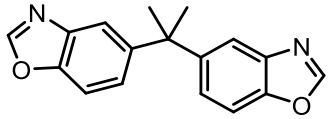
According to a known procedure,[1-2] a Schlenk-tube (50 mL) was charged with **S1** (5 mmol) and Trimethyl orthoformate (3 mL). The mixture was heated up to 95 °C. the reaction was stirred (5 h) and simultaneously allowed to acclimatize to room temperature. The reaction was quenched with water (20 mL), extracted with ethyl acetate (3x 10 mL), dried over $MgSO_4$ and concentrated under reduced pressure. The crude was purified by SiO_2 gel column chromatography to afford **S2**.



S2 = 1x: ^1H NMR (600 MHz, Chloroform-*d*) δ 8.03 (s, 2H), 7.80 (d, J = 7.8 Hz, 2H), 7.66 (d, J = 1.8 Hz, 2H), 7.47 - 7.42 (m, 4H), 7.40 - 7.35 (m, 2H), 7.32 (dd, J = 8.4, 1.8 Hz, 2H), 7.31 - 7.26 (m, 2H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 152.9, 151.0, 149.0, 143.0, 140.1, 140.0, 128.0, 127.8, 126.2, 120.4, 120.0, 110.6, 65.3.

ESI-HRMS: mass spectrometry: m/z calc. 401.1285 $[C_{27}H_{17}O_2N_2]^+$, measured 401.1273.

IR (neat, cm^{-1}): ṽ: 3850, 3116, 2677, 1731, 1606, 1506, 1470, 1447, 1243, 1115, 1063, 982, 919, 873, 812, 747.



S2 = 1y: ^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.06 (s, 2H), 7.76 (d, *J* = 1.8 Hz, 2H), 7.41 (d, *J* = 9.0 Hz, 2H), 7.15 (dd, *J* = 9.0, 1.8 Hz, 2H), 1.79 (s, 6H).

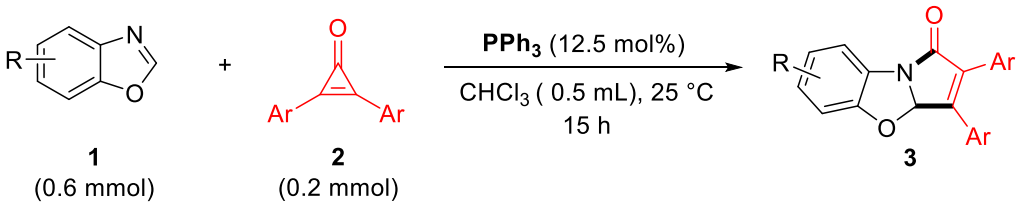
^{13}C NMR (150 MHz, Chloroform-*d*) δ 152.8, 148.1, 147.6, 139.9, 125.4, 118.1, 110.3, 43.3, 31.5.

ESI-HRMS: mass spectrometry: m/z calc. 301.0948 $[C_{17}H_{14}O_2N_2Na]^+$, measured 301.0944.

IR (neat, cm^{-1}): ṽ: 3137, 2964, 2869, 1757, 1612, 1513, 1467, 1361, 1288, 1246, 1110, 1060, 888, 812, 762, 662.

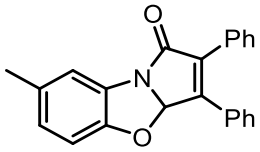
Cyclopropenone substrate **2a** was purchased from BLDpharm. Cyclopropenone **2b** was prepared according to a known literature procedure.[3]

3. General procedure



Triphenylphosphine (6.55 mg, 0.025 mmol, 0.125 equiv.), cyclopropenone **2** (0.2 mmol, 1 equiv.) and Benzoxazole **1** (0.6 mmol, 3 equiv.) were added sequentially, then the mixture was stirred at 25 ^{o}C for about 15 h (the consumption can be monitored by TLC). The mixture was filtered through celite and the filtrate was concentrated to dryness. The crude was purified by column chromatography to give the products **3**.

4. Product characterization



7-methyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

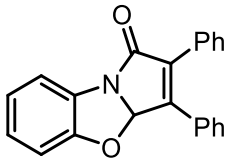
3aa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 65 mg product was obtained by 96% isolated yield as yellow solid. mp 190.0 – 191.5 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 - 7.54 (m, 2H), 7.46 - 7.42 (m, 2H), 7.41 - 7.34 (m, 7H), 6.87 - 6.84 (m, 2H), 6.78 (d, *J* = 7.8 Hz, 1H), 2.36 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.9, 153.2, 150.9, 134.9, 131.8, 131.3, 130.5, 130.5, 130.3, 129.6, 129.2, 129.0, 128.8, 128.7, 125.9, 117.8, 109.2, 97.2, 21.2.

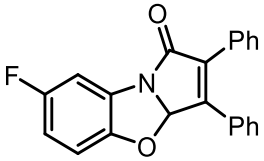
ESI-HRMS: mass spectrometry: m/z calc. 362.1152 $[C_{23}H_{17}O_2NNa]^+$, measured 362.1147.

IR (neat, cm^{-1}): ṽ: 3426, 3054, 2915, 1722, 1601, 1485, 1346, 1250, 1192, 1128, 1081, 1030, 959, 898, 776, 690.



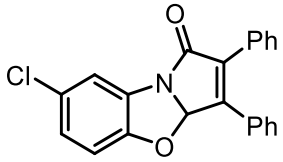
2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3ba: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 57 mg product was obtained by 88% isolated yield as yellow solid. mp 189.8 – 191.0 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.60 - 7.56 (m, 2H), 7.55 - 7.51 (m, 1H), 7.47 - 7.43 (m, 2H), 7.42 - 7.35 (m, 6H), 7.10 - 7.05 (m, 1H), 7.02 - 6.97 (m, 1H), 6.93 - 6.89 (m, 1H), 6.88 (s, 1H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.0, 155.3, 150.8, 134.8, 131.3, 130.5, 130.5, 130.4, 129.6, 129.2, 129.0, 128.8, 128.7, 125.8, 122.0, 117.1, 109.8, 97.1.
ESI-HRMS: mass spectrometry: m/z calc. 348.0995 $[C_{22}H_{15}O_2NNa]^+$, measured 348.0994.
IR (neat, cm^{-1}): ṽ: 3429, 3062, 2920, 1724, 1599, 1473, 1364, 1243, 1192, 1141, 1105, 1001, 948, 848, 752, 688.



7-fluoro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3ca: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 41 mg product was obtained by 60% isolated yield as yellow solid. mp 170.6 – 171.9 °C.
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.56 - 7.50 (m, 2H), 7.44 - 7.32 (m, 8H), 7.27 - 7.22 (m, 1H), 6.89 (s, 1H), 6.80 - 6.75 (m, 1H), 6.75 - 6.70 (m, 1H).
^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.65, 158.0 (d, J = 239.6 Hz), 151.3 (d, J = 2.3 Hz), 151.0, 134.7, 131. 1 (d, J = 12.4 Hz), 131.1, 130.7, 130.3, 129.6, 129.4, 129.1, 128.9, 128.7, 111.4 (d, J = 24.2 Hz), 109.4 (d, J = 9.2 Hz), 105.8 (d, J = 28.6 Hz), 97.9.
^{19}F NMR (564 MHz, Chloroform-*d*) δ -120.59 to -120.70 (m).
ESI-HRMS: mass spectrometry: m/z calc. 366.0901 $[C_{22}H_{14}O_2NFNa]^+$, measured 366.0899.
IR (neat, cm^{-1}): ṽ: 3425, 3062, 2922, 1716, 1617, 1480, 1351, 1252, 1172, 1122, 1075, 946, 804, 761, 692.



7-chloro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3da: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1).

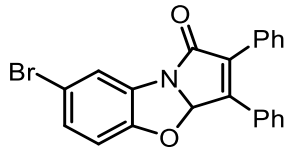
42 mg product was obtained by 58% isolated yield as yellow solid. mp 210.2– 211.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.56 - 7.52 (m, 2H), 7.49 (d, J = 2.4 Hz, 1H), 7.45 - 7.33 (m, 8H), 7.02 (dd, J = 8.4, 2.4 Hz, 1H), 6.89 (s, 1H), 6.79 (d, J = 9.0 Hz, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.7, 154.0, 151.0, 134.7, 131.5, 131.1, 130.7, 130.2, 129.6, 129.4, 129.1, 128.9, 128.7, 126.8, 125.5, 117.6, 110.3, 97.8.

ESI-HRMS: mass spectrometry: m/z calc. 382.0605 $[C_{22}H_{14}O_2NClNa]^+$, measured 382.0601.

IR (neat, cm^{-1}): ṽ: 3424, 2049, 2919, 1716, 1602, 1473, 1344, 1302, 1241, 1192, 1145, 1088, 958, 868, 776, 696.



7-bromo-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

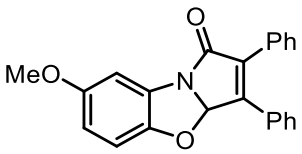
3ea: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 45 mg product was obtained by 56% isolated yield as yellow solid. mp 223.5 – 224.2 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.62 (d, J = 2.4 Hz, 1H), 7.56 - 7.51 (m, 2H), 7.44 - 7.33 (m, 8H), 7.17 (dd, J = 8.4, 1.8 Hz, 1H), 6.89 (s, 1H), 6.75 (d, J = 8.4 Hz, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.7, 154.5, 151.0, 134.7, 131.8, 131.1, 130.8, 130.2, 129.6, 129.4, 129.1, 128.9, 128.7, 128.5, 120.3, 113.7, 110.9, 97.7.

ESI-HRMS: mass spectrometry: m/z calc. 426.0100 $[C_{22}H_{14}O_2NBrNa]^+$, measured 426.0094.

IR (neat, cm^{-1}): ṽ: 3419, 3050, 2910, 1712, 1599, 1471, 1343, 1303, 1242, 1190, 1143, 1086, 956, 869, 774, 690.



7-methoxy-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

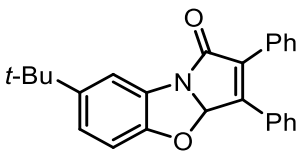
3fa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 65 mg product was obtained by 91% isolated yield as yellow solid. mp 159.4 – 160.7 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 - 7.54 (m, 2H), 7.46 - 7.34 (m, 8H), 7.16 (d, J = 2.5 Hz, 1H), 6.89 (s, 1H), 6.79 (d, J = 8.7 Hz, 1H), 6.58 (dd, J = 8.6 Hz, J = 2.7 Hz, 1H), 3.81 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.7, 155.2, 151.0, 149.2, 134.8, 131.3, 131.0, 130.5, 130.5, 129.6, 129.2, 129.0, 128.8, 128.7, 110.1, 109.5, 104.3, 97.4, 56.2.

ESI-HRMS: mass spectrometry: m/z calc. 378.1101 $[C_{23}H_{17}O_3NNa]^+$, measured 378.1096.

IR (neat, cm^{-1}): ṽ: 3425, 3062, 2920, 1720, 1619, 1481, 1369, 1308, 1256, 1185, 1028, 958, 871, 777, 690.



7-(*tert*-butyl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

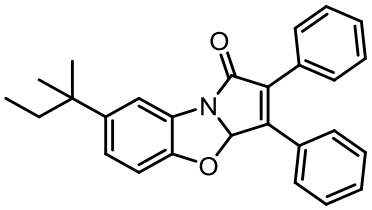
3ga: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 74 mg product was obtained by 97% isolated yield as yellow liquid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 - 7.56 (m, 3H), 7.47 -7.43 (m, 2H), 7.41 - 7.34 (m, 6H), 7.08 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.86 (s, 1H), 6.83 (d, *J* = 8.4 Hz, 1H), 1.36 (s, 9H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.0, 153.0, 150.8, 145.5, 134.8, 131.4, 130.5, 130.5, 130.2, 129.6, 129.2, 129.0, 128.8, 128.7, 122.2, 114.5, 108.8, 97.4, 34.8, 31.7.

ESI-HRMS: mass spectrometry: m/z calc. 382.1802 $[C_{26}H_{24}O_2N]^+$, measured 382.1802.

IR (neat, cm^{-1}): ṽ: 3434, 3058, 2961, 1720, 1608, 1485, 1341, 1233, 1196, 1140, 1060, 954, 779, 735, 693.



7-(*tert*-pentyl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

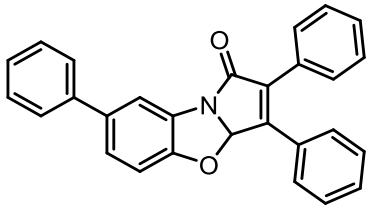
3ha: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 76 mg product was obtained by 96% isolated yield as yellow liquid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.61 - 7.57 (m, 2H), 7.53 (d, *J* = 1.8 Hz, 1H), 7.48 - 7.44 (m, 2H), 7.43 - 7.35 (m, 6H), 7.03 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.86 (s, 1H), 6.84 (d, *J* = 8.4 Hz, 1H), 1.68 (q, *J* = 7.2 Hz, 2H), 1.32 (s, 6H), 0.74 (t, *J* = 7.8 Hz, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.9, 152.9, 150.7, 143.7, 134.7, 131.3, 130.4, 130.4, 130.2, 129.5, 129.1, 128.9, 128.6, 122.9, 115.0, 108.6, 97.3, 37.9, 37.0, 28.9, 28.7, 9.2.

ESI-HRMS: mass spectrometry: m/z calc. 418.1778 $[C_{27}H_{25}O_2NNa]^+$, measured 418.1764.

IR (neat, cm^{-1}): ṽ: 3327, 3062, 2962, 1716, 1609, 1487, 1439, 1340, 1246, 1139, 1100, 1064, 959, 907, 807, 692.



2,3,7-triphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

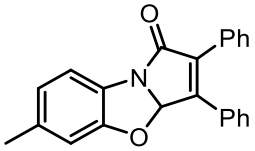
3ia: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 56 mg product was obtained by 70% isolated yield as yellow liquid. mp 235.6 – 236.2 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.77 (d, *J* = 1.8 Hz, 1H), 7.63 - 7.57 (m, 4H), 7.48 - 7.37 (m, 10H), 7.36 - 7.33 (m, 1H), 7.31 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 6.94 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 154.7, 150.8, 140.6, 135.7, 134.8, 131.2, 130.9, 130.5, 130.3, 129.5, 129.2, 128.9, 128.8, 128.7, 128.6, 127.0, 127.0, 124.6, 115.8, 109.7, 97.4.

ESI-HRMS: mass spectrometry: m/z calc. 424.1308 $[C_{28}H_{19}O_2NNa]^+$, measured 424.1294.

IR (neat, cm^{-1}): ṽ: 3438, 3065, 2908, 1721, 1600, 1475, 1434, 1347, 1233, 1141, 1079, 1029, 944, 807, 754, 686.



6-methyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

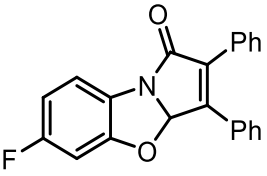
3ja: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 66 mg product was obtained by 97% isolated yield as yellow solid. mp 181.9 – 183.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 - 7.54 (m, 2H), 7.45 - 7.34 (m, 9H), 6.84 (s, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 6.73 (s, 1H), 2.33 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.1, 155.4, 150.7, 136.1, 134.9, 131.4, 130.5, 130.5, 129.6, 129.2, 129.0, 128.8, 128.7, 128.0, 122.2, 116.6, 110.6, 97.3, 21.7.

ESI-HRMS: mass spectrometry: m/z calc. 362.1152 $[C_{23}H_{17}O_2NNa]^+$, measured 362.1146.

IR (neat, cm^{-1}): ṽ: 3417, 1060, 2924, 1713, 1599, 1493, 1440, 1344, 1243, 1137, 1081, 954, 882, 809, 779, 692.



6-fluoro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3ka: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 36 mg product was obtained by 52% isolated yield as yellow solid. mp 192.6 – 194.0 °C.

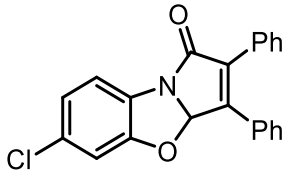
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.57 - 7.51 (m, 2H), 7.44 - 7.33 (m, 9H), 6.89 (s, 1H), 6.70 - 6.62 (m, 2H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.3, 161.0 (d, *J* = 243.9 Hz), 156.1 (d, *J* = 13.7 Hz), 150.6, 134.9, 131.2, 130.7, 130.3, 129.6, 129.4, 129.1, 128.9, 128.7, 126.7 (d, *J* = 3.0 Hz), 117.1 (d, *J* = 10.3 Hz), 107.9 (d, *J* = 23.7 Hz), 99.1 (d, *J* = 28.8 Hz), 98.3.

^{19}F NMR (564 MHz, Chloroform-*d*) δ -115.09 to -115.16 (m).

ESI-HRMS: mass spectrometry: m/z calc. 366.0901 $[C_{22}H_{14}O_2NFNa]^+$, measured 366.0903.

IR (neat, cm^{-1}): ṽ: 3274, 3083, 2920, 1724, 1617, 1481, 1445, 1345, 1314, 1233, 1118, 1080, 945, 844, 809, 690.



6-chloro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

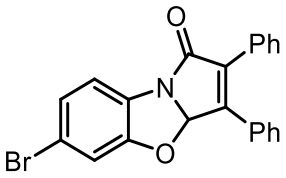
3la: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 30 mg product was obtained by 42% isolated yield as yellow solid. mp 169.5 – 172.2 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.56 - 7.52 (m, 2H), 7.44 - 7.34 (m, 9H), 6.96 (dd, *J* = 7.8, 1.8 Hz, 1H), 6.89 (d, *J* = 1.8 Hz, 1H), 6.89 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.9, 155.9, 150.7, 134.9, 131.1, 131.0, 130.7, 130.2, 129.6, 129.4, 129.4, 129.1, 128.9, 128.7, 121.9, 117.4, 110.7, 98.0.

ESI-HRMS: mass spectrometry: m/z calc. 382.0605 $[C_{22}H_{14}O_2NClNa]^+$, measured 382.0606.

IR (neat, cm^{-1}): ṽ: 3415, 1056, 2923, 1710, 1604, 1478, 1441, 1356, 1314, 1243, 1133, 1053, 940, 894, 801, 691.



6-bromo-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

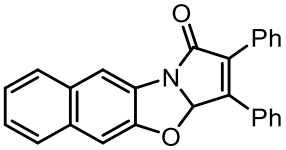
3ma: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 45 mg product was obtained by 56% isolated yield as yellow solid. mp 173.4 – 176.3 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.56 -7.52 (m, 2H), 7.44 - 7.34 (m, 9H), 7.11 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.04 (d, *J* = 1.8 Hz, 1H), 6.88 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 156.0, 150.7, 134.8, 131.1, 130.7, 130.2, 129.9, 129.6, 129.4, 129.1, 128.9, 128.7, 124.9, 118.2, 117.9, 113.4, 97.8.

ESI-HRMS: mass spectrometry: m/z calc. 426.0100 $[C_{22}H_{14}O_2BrNa]^+$, measured 426.0099.

IR (neat, cm^{-1}): ṽ: 3415, 3054, 2923, 1709, 1600, 1476, 1354, 1243, 1195, 1134, 1041, 942, 874, 799, 761, 690.



2,3-diphenylnaphtho[2,3-*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

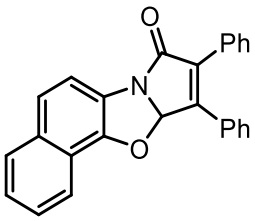
3na: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 55 mg product was obtained by 73% isolated yield as yellow solid. mp 247.3 – 247.9 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.88 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.61 - 7.57 (m, 2H), 7.48 - 7.36 (m, 10H), 7.19 (s, 1H), 6.93 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.1, 154.4, 150.8, 134.9, 132.4, 131.2, 130.7, 130.4, 130.4, 130.2, 129.6, 129.4, 129.1, 128.9, 128.8, 128.0, 127.2, 125.9, 124.6, 114.2, 105.0, 97.0.

ESI-HRMS: mass spectrometry: m/z calc. 398.1152 $[C_{26}H_{17}O_2NNa]^+$, measured 398.1152.

IR (neat, cm^{-1}): ṽ: 3447, 3055, 2921, 1723, 1607, 1464, 1347, 1312, 1253, 1146, 1068, 953, 898, 837, 747, 691.



9,10-diphenylnaphtho[2,1-*d*]pyrrolo[2,1-*b*]oxazol-8(10a*H*)-one

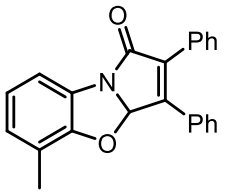
3oa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 65 mg product was obtained by 87% isolated yield as yellow solid. 224.9 – 227.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.97 - 7.93 (m, 1H), 7.86 - 7.82 (m, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.68-7.63 (m, 2H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.48 - 7.37 (m, 10H), 7.09 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.9, 150.9, 150.1, 135.1, 132.5, 131.5, 130.6, 130.6, 129.6, 129.3, 129.0, 128.9, 128.8, 128.5, 126.1, 125.7, 125.5, 121.9, 120.7, 120.3, 116.4, 98.4.

ESI-HRMS: mass spectrometry: m/z calc. 398.1152 $[C_{26}H_{17}O_2NNa]^+$, measured 398.1152.

IR (neat, cm^{-1}): ṽ: 3413, 3054, 2919, 1714, 1636, 1595, 1462, 1397, 1341, 1280, 1191, 1131, 1052, 962, 865, 747, 690.



5-methyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

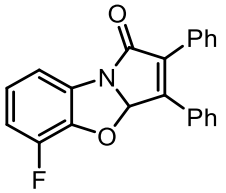
3pa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 65 mg product was obtained by 96% isolated yield as yellow solid. mp 203.2 – 204.8 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.61 - 7.57 (m, 2H), 7.46 - 7.34 (m, 9H), 6.93 - 6.88 (m, 2H), 6.85 (s, 1H), 2.28 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.9, 153.5, 150.6, 134.8, 131.4, 130.5, 130.3, 129.7, 129.5, 129.1, 128.8, 128.7, 128.7, 127.4, 121.6, 120.0, 114.4, 96.8, 14.8.

ESI-HRMS: mass spectrometry: m/z calc. 362.1152 $[C_{23}H_{17}O_2NNa]^+$, measured 362.1152.

IR (neat, cm^{-1}): ṽ: 3424, 3056, 2920, 1720, 1636, 1598, 1444, 1339, 1250, 1138, 1115, 1035, 966, 903, 776, 686.



5-fluoro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3qa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 23 mg product was obtained by 34% isolated yield as yellow solid. mp 163.9 – 165.6 °C.

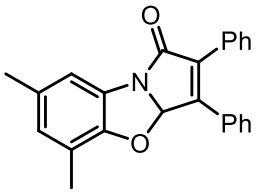
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.60 - 7.55 (m, 2H), 7.47 - 7.34 (m, 8H), 7.33 - 7.29 (m, 1H), 6.94 (s, 1H), 6.93 – 6.86 (m, 2H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.6, 150.4, 146.6 (d, *J* = 246.9 Hz), 141.6 (d, *J* = 12.3 Hz), 134.7, 133.0 (d, *J* = 4.3 Hz), 130.9, 130.6, 130.1, 129.5, 129.3, 128.9, 128.7, 128.7, 122.3 (d, *J* = 6.5 Hz), 113.9 (d, *J* = 17.4 Hz), 112.8 (d, *J* = 3.4 Hz), 98.4.

^{19}F NMR (564 MHz, Chloroform-*d*) δ -137.38 to -137.43 (m).

ESI-HRMS: mass spectrometry: m/z calc. 366.0901 $[C_{22}H_{14}O_2NFNa]^+$, measured 366.0897.

IR (neat, cm^{-1}): ṽ: 3433, 3058, 2922, 1722, 1624, 1465, 1335, 1250, 1170, 1136, 1070, 960, 880, 777.



5,7-dimethyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

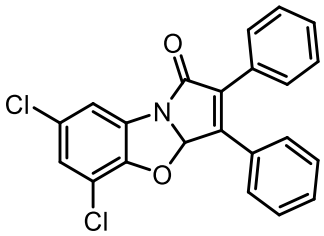
3ra: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 65 mg product was obtained by 92% isolated yield as yellow solid. mp 197.7 – 199.2 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.60- 7.56 (m, 2H), 7.46 - 7.34 (m, 8H), 7.20 - 7.17 (m, 1H), 6.83 (s, 1H), 6.73 - 6.69 (m, 1H), 2.33 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 151.5, 150.7, 134.8, 131.4, 131.2, 130.6, 130.3, 129.6, 129.5, 129.0, 128.8, 128.7, 128.6, 127.6, 119.4, 115.0, 96.9, 21.0, 14.8.

ESI-HRMS: mass spectrometry: m/z calc. 376.1308 $[C_{24}H_{19}O_2NNa]^+$, measured 376.1313.

IR (neat, cm^{-1}): $\tilde{\nu}$: 3416, 3058, 2917, 1717, 1630, 1482, 1361, 1306, 1197, 1130, 1030, 982, 905, 813, 774, 692.



5,7-dichloro-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

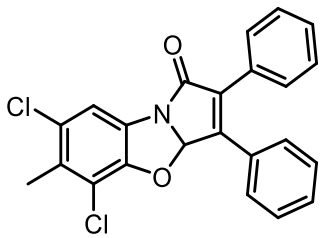
3sa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 100:1). 28 mg product was obtained by 36% isolated yield as yellow solid. mp 209.3 – 210.9 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 - 7.52 (m, 2H), 7.45 - 7.33 (m, 9H), 7.08 (d, J = 3.0 Hz, 1H), 6.94 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.4, 150.7, 150.4, 134.7, 132.2, 130.8, 130.7, 130.6, 129.9, 129.4, 129.0, 128.8, 128.7, 127.1, 125.8, 116.0, 115.0, 98.2.

ESI-HRMS: mass spectrometry: m/z calc. 416.0216 $[C_{22}H_{13}O_2NCl_2Na]^+$, measured 416.0213.

IR (neat, cm^{-1}): $\tilde{\nu}$: 3441, 1086, 2923, 1725, 1600, 1460, 1340, 1247, 1198, 1146, 1106, 1063, 961, 899, 770, 687.



5,7-dichloro-6-methyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

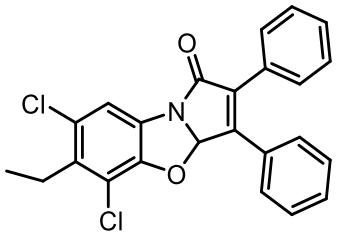
3ta: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 100:1). 28 mg product was obtained by 34% isolated yield as yellow solid. mp 243.3 – 244.3 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.58 - 7.54 (m, 2H), 7.44 (s, 1H), 7.43 - 7.35 (m, 8H), 6.91 (s, 1H), 2.42 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.6, 150.7, 150.6, 134.7, 131.5, 130.8, 130.7, 130.0, 129.4, 129.3, 129.2, 128.9, 128.7, 128.7, 127.0, 115.9, 115.8, 98.0, 17.0.

ESI-HRMS: mass spectrometry: m/z calc. 430.0372 $[C_{23}H_{15}O_2NCl_2Na]^+$, measured 430.0363.

IR (neat, cm^{-1}): ṽ: 3442, 3056, 2921, 1725, 1614, 1457, 1405, 1342, 1301, 1238, 1144, 1094, 962, 866, 784, 692.



5,7-dichloro-6-ethyl-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

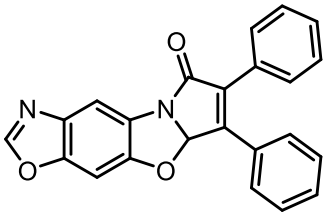
3ua: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 100:1). 34 mg product was obtained by 40% isolated yield as white solid. mp 206.5 – 208.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.59 - 7.53 (m, 2H), 7.46 - 7.33 (m, 9H), 6.91 (s, 1H), 2.96 - 2.86 (m, 2H), 1.16 (t, J = 7.8 Hz, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.6, 150.8, 150.6, 137.0, 134.7, 130.8, 130.7, 130.0, 129.4, 129.3, 129.2, 129.0, 128.8, 128.7, 126.6, 116.2, 115.4, 98.0, 24.4, 12.7.

ESI-HRMS: mass spectrometry: m/z calc. 444.0529 $[C_{24}H_{17}O_2NCl_2Na]^+$, measured 444.0522.

IR (neat, cm^{-1}): ṽ: 3470, 3086, 2927, 1740, 1608, 1457, 1404, 1331, 1224, 1141, 1065, 942, 870, 784, 748, 699.



6,7-oxazol-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

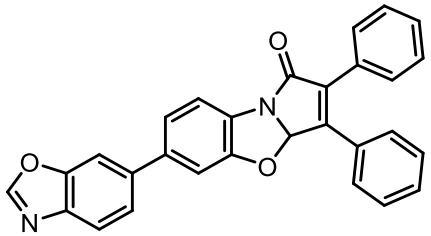
3va: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 20:1). 43 mg product was obtained by 59% isolated yield as yellow solid. mp 235.1 – 237.0 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 (s, 1H), 7.86 (s, 1H), 7.58 - 7.54 (m, 2H), 7.46 - 7.35 (m, 8H), 7.11 (s, 1H), 6.96 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.7, 154.2, 152.0, 150.4, 147.8, 134.8, 134.4, 131.0, 130.6, 130.1, 129.4, 129.3, 128.9, 128.7, 128.6, 128.3, 108.7, 98.1, 93.6.

ESI-HRMS: mass spectrometry: m/z calc. 367.1077 $[C_{23}H_{15}O_3N_2]^+$, measured 367.1077.

IR (neat, cm^{-1}): ṽ: 3445, 3112, 2922, 1726, 1619, 1457, 1373, 1347, 1208, 1163, 1122, 1066, 938, 838, 769, 687.



6-(benzo[*d*]oxazol-6-yl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

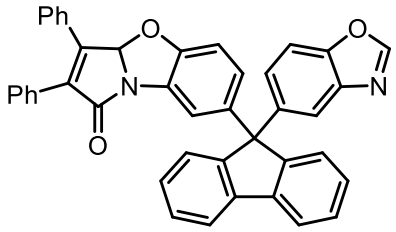
3wa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 20:1). 20 mg product was obtained by 22% isolated yield as yellow solid. mp 206.5 – 208.1 °C.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.12 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 1.8 Hz, 1H), 7.6 – 7.5 (m, 4H), 7.46 – 7.35 (m, 8H), 7.24 (dd, *J* = 7.9 Hz, *J* = 1.7 Hz, 1H), 7.15 (d, *J* = 1.8 Hz, 1H), 6.94 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.9, 155.9, 152.9, 150.8, 139.4, 139.1, 138.9, 134.8, 131.1, 130.5, 130.2, 130.0, 129.4, 129.2, 128.9, 128.7, 128.6, 124.2, 121.3, 120.6, 117.0, 109.4, 108.9, 97.5.

ESI-HRMS: mass spectrometry: m/z calc. 465.1210 $[C_{29}H_{18}O_3N_2Na]^+$, measured 465.1199.

IR (neat, cm^{-1}): ṽ: 3423, 3125, 2922, 1719, 1592, 1504, 1468, 1352, 1250, 1219, 1144, 1061, 948, 867, 811, 694.



7-(9-(benzo[*d*]oxazol-5-yl)-9*H*-fluoren-9-yl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

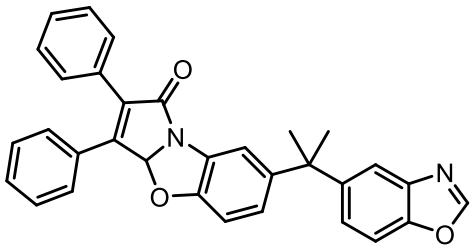
3xa: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 20:1). 67 mg product was obtained by 55% isolated yield as yellow oil.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 (s, 1H), 7.81 - 7.75 (m, 2H), 7.65 (d, *J* = 2.4 Hz, 1H), 7.57 - 7.54 (m, 2H), 7.52 - 7.50 (m, 1H), 7.50 - 7.46 (m, 2H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.42 - 7.39 (m, 2H), 7.39 - 7.32 (m, 9H), 7.32 - 7.28 (m, 2H), 6.87 (dd, *J* = 9.0, 2.4 Hz, 1H), 6.81 (s, 1H), 6.72 (d, *J* = 8.4 Hz, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 154.2, 152.8, 151.1, 150.9, 150.5, 148.9, 143.1, 140.0, 140.0, 139.9, 139.8, 134.7, 131.2, 130.5, 130.4, 130.3, 129.5, 129.2, 128.9, 128.7, 128.6, 128.0, 127.9, 127.7, 126.2, 126.1, 126.1, 125.0, 120.4, 120.3, 119.9, 117.4, 110.6, 108.9, 97.6, 65.1.

ESI-HRMS: mass spectrometry: m/z calc. 629.1836 $[C_{42}H_{26}O_3N_2Na]^+$, measured 629.1817.

IR (neat, cm^{-1}): ṽ: 3450, 3061, 2923, 1724, 1606, 1513, 1481, 1443, 1340, 1243, 1201, 1122, 1065, 907, 807, 727.



7-(2-(benzo[*d*]oxazol-5-yl)propan-2-yl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

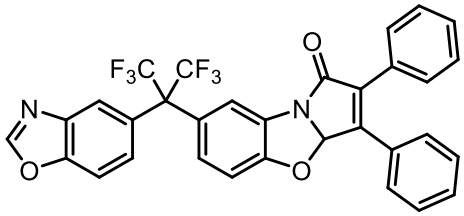
3ya: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 20:1). 58 mg product was obtained by 60% isolated yield as yellow liquid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.06 (s, 1H), 7.78 (d, J = 1.8 Hz, 1H), 7.58 - 7.53 (m, 2H), 7.46 - 7.41 (m, 4H), 7.40 - 7.33 (m, 6H), 7.23 (dd, J = 8.4, 1.8 Hz, 1H), 6.90 (dd, J = 8.4, 1.8 Hz, 1H), 6.84 (s, 1H), 6.78 (d, J = 8.4 Hz, 1H), 1.77 (s, 3H), 1.75 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 153.2, 152.7, 150.7, 148.1, 147.7, 144.8, 139.8, 134.7, 131.2, 130.4, 130.3, 130.2, 129.5, 129.1, 128.9, 128.6, 128.6, 125.4, 124.0, 118.0, 115.7, 110.3, 108.8, 97.3, 43.0, 31.4, 31.4.

ESI-HRMS: mass spectrometry: m/z calc. 507.1679 $[C_{32}H_{24}O_3N_2Na]^+$, measured 507.1676.

IR (neat, cm^{-1}): ṽ: 3650, 3059, 2926, 1719, 1609, 1513, 1484, 1438, 1340, 1250, 1138, 1065, 958, 878, 811, 692.



7-(2-(benzo[*d*]oxazol-5-yl)-1,1,1,3,3,3-hexafluoropropan-2-yl)-2,3-diphenylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3za: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 20:1). 48 mg product was obtained by 41% isolated yield as yellow solid. mp 196.1 – 197.3 °C.

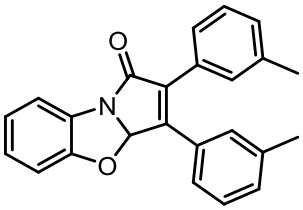
^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.14 (s, 1H), 8.00 (s, 1H), 7.60 -7.54 (m, 3H), 7.49 - 7.46 (m, 1H), 7.46 - 7.32 (m, 9H), 7.19 - 7.14 (m, 1H), 6.90 (d, J = 9.0 Hz, 1H), 6.89 (s, 1H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 174.8, 155.6, 153.5, 150.5, 149.9, 140.0, 134.6, 131.1, 130.6, 130.6, 130.1, 130.0, 129.5, 129.3, 128.9, 128.7, 128.6, 128.1, 127.9, 127.0, 125.1 (≈ broad d corresponding to the main lines of a q, $J \approx 285$ Hz), 123.1, 119.1, 110.7, 109.0, 97.9.

^{19}F NMR (564 MHz, Chloroform-*d*) δ -63.75.

ESI-HRMS: mass spectrometry: m/z calc. 615.1114 $[C_{32}H_{18}O_3N_2F_6Na]^+$, measured 615.1102.

IR (neat, cm^{-1}): ṽ: 3315, 3124, 2920, 1721, 1615, 1489, 1446, 1344, 1303, 1203, 1127, 1064, 961, 885, 811, 692.



2,3-di-*m*-tolylbenzo[*d*]pyrrolo[2,1-*b*]oxazol-1(3a*H*)-one

3bb: The crude mixture was purified by SiO_2 gel column chromatography with pentane/EA (from 60:1). 38 mg product was obtained by 54% isolated yield as yellow liquid.

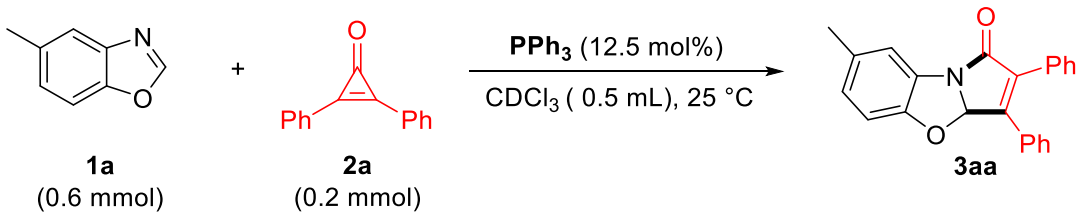
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.50 (dd, J = 7.8, 1.2 Hz, 1H), 7.40 (s, 1H), 7.34 - 7.30 (m, 1H), 7.28 (s, 1H), 7.25 - 7.17 (m, 6H), 7.08 - 7.03 (m, 1H), 7.00 - 6.96 (m, 1H), 6.86 (s, 1H), 2.34 (s, 3H), 2.33 (s, 3H).

^{13}C NMR (150 MHz, Chloroform-*d*) δ 175.1, 155.2, 150.7, 138.6, 138.3, 134.7, 131.2, 130.3, 130.3, 130.0, 129.8, 129.0, 128.7, 128.5, 126.4, 125.9, 125.6, 121.8, 117.0, 109.6, 97.0, 21.4, 21.4.

ESI-HRMS: mass spectrometry: m/z calc. 378.1308 $[C_{24}H_{19}O_2NNa]^+$, measured 376.1306.

IR (neat, cm^{-1}): $\tilde{\nu}$: 3432, 3035, 2920, 1720, 1596, 1474, 1344, 1305, 1238, 1131, 1102, 1009, 933, 825, 748, 693.

5. ^{31}P NMR study.



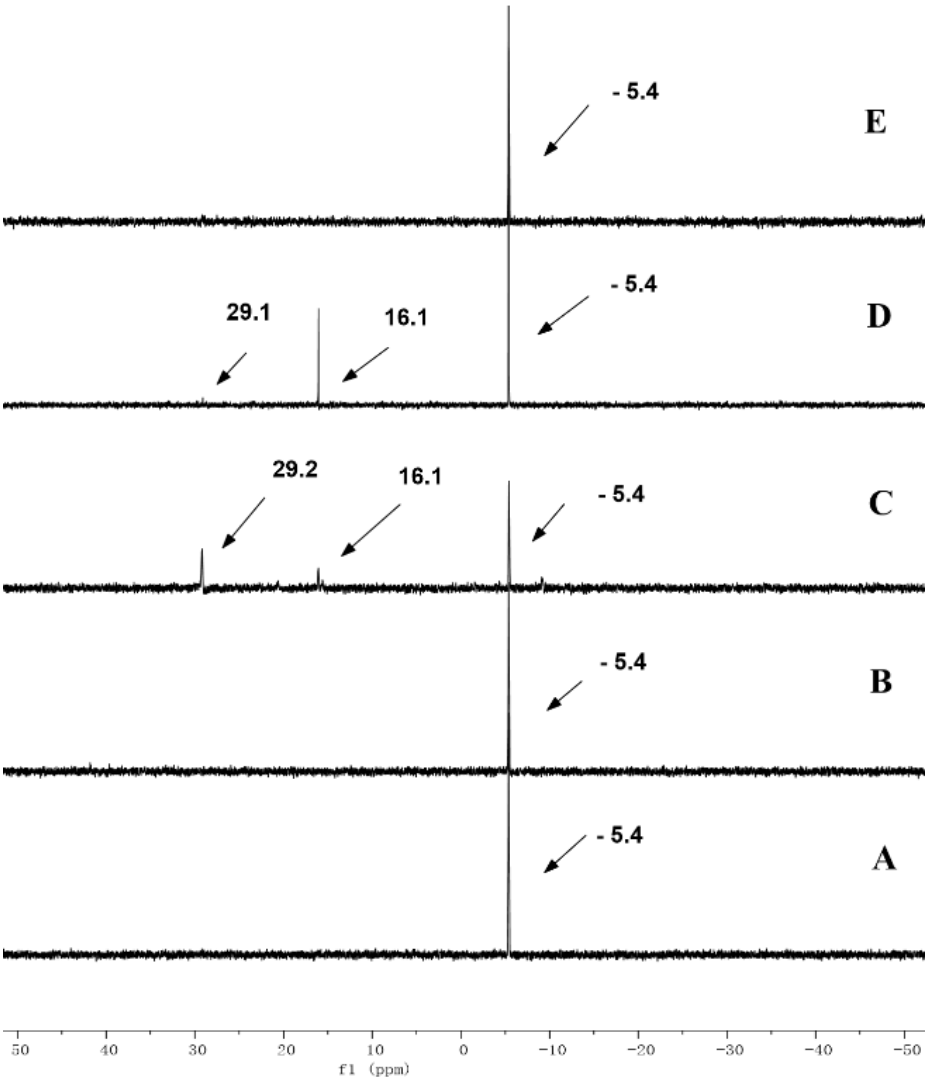
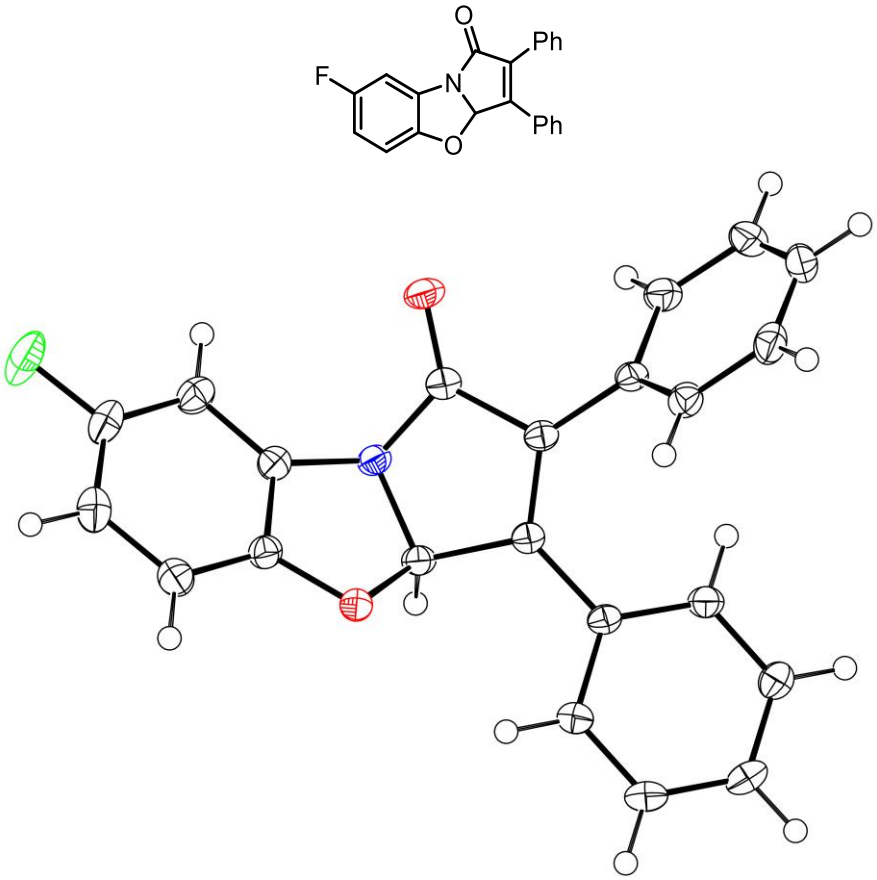


Figure S1. ^{31}P NMR experiments in $CDCl_3$: **A)**: only PPh_3 in $CDCl_3$; **B)**: PPh_3 and **1a** (1:24); **C)**: PPh_3 and **2a** (1:8); **D)**: PPh_3, **1a** and **2a** (1:24:8); **E)**: PPh_3, **1a** and **2a** (1:24:8); and the mixture was stirred for 15 h.

6. X-ray structure of 3ca (CCDC 2093753)

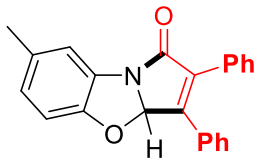


(ORTEP view, 50% probability level)

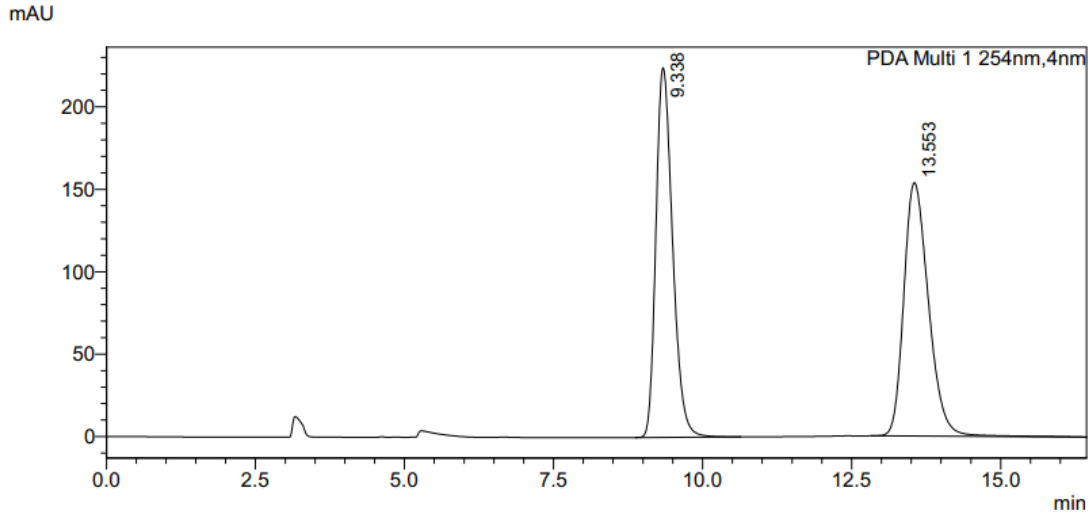
Crystallization of compound **3ca** ($C_{22}H_{14}F_1N_1O_2$) from pentane at room temperature gave monoclinic crystals of space group $P2_1/n$ (14) suitable for single crystal X-ray structure determination. Cell constants a = 6.2797(3), b = 22.8959(10), c = 11.1534(4) Å, $\alpha = \gamma = 90°$, β = 94.874(2), Z = 4, and a molecular weight of M_r = 343.34 result in a density of 1.427 gcm^{-3} and a linear absorption coefficient of μ = 0.1 mm^{-1} for MoK$_\alpha$ radiation (λ = 0.71073 Å).

24983 reflections covering the range $-8 \le h \le 8$, $-29 \le k \le 30$, and $-14 \le l \le 13$ (Θ_{max} = 28.4°) were collected (ϕ and ω scans) at 150 K on an Bruker APEX-II CCD diffractometer equipped with a graphite-monochomator and merged to give 4008 independent diffraction data (Rint = 0.0223) of which 3627 with I > 2σ(I). The data set was corrected for absorption effects using the multi-scan absorption correction method SADABS[4] (T_{min} = 0.6878, T_{max} = 0.7457). The structure was solved by intrinsic phasing using the ShelXT 2018/2 structure solution program[5] and refined against F^2 on all data by full-matrix least-squares methods using ShelXL-2018/3[6] and ShelXle GUI.[7] 3627 reflexions were used in the final full-matrix least squares refinement including 235 parameters. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed at idealised positions and refined isotropically using the riding model. Refinement converged at $R1$ = 0.0386 for the observed data and $wR2$ = 0.1020 for all data ($w = 1/[\sigma^2(Fo^2)+(0.0494P)^2+0.6360P]$ where $P=(Fo^2+2Fc^2)/3$), a residual electron density of –0.215/+0.329 eÅ^{-3}, and a final goodness of fit of 1.045.

7. Chiral analytical HPLC profile for product 3aa



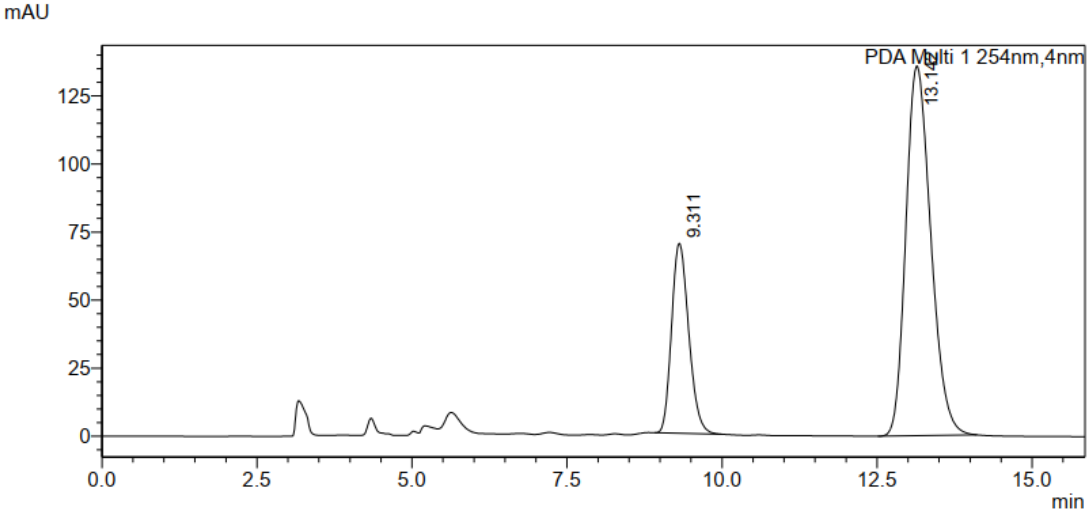
The enantiomeric excess was determined by chiral analytical HPLC with a chiralcel OD column (hexanes: 2-propanol= 95:5, 1.0 mL/min, 245 nm, 74:26 *er* for chiral ligand **P4**, see main text); major enantiomer t_r = 13.14 min, minor enantiomer t_r = 9.31 min.



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.338	4359947	224135	49.534			
2	13.553	4441915	153685	50.466			
Total		8801862	377821				



<Peak Table>

PDA Ch1 254nm

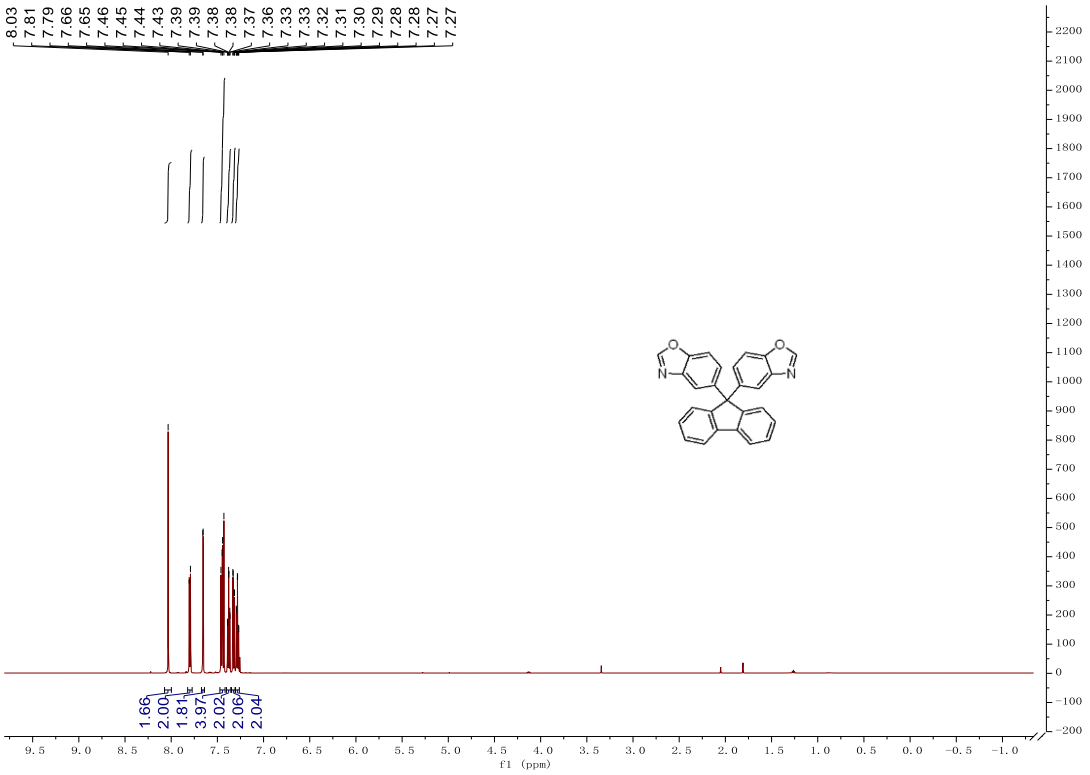
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.311	1346270	69821	26.127			
2	13.142	3806495	135811	73.873			
Total		5152765	205632				

8. References

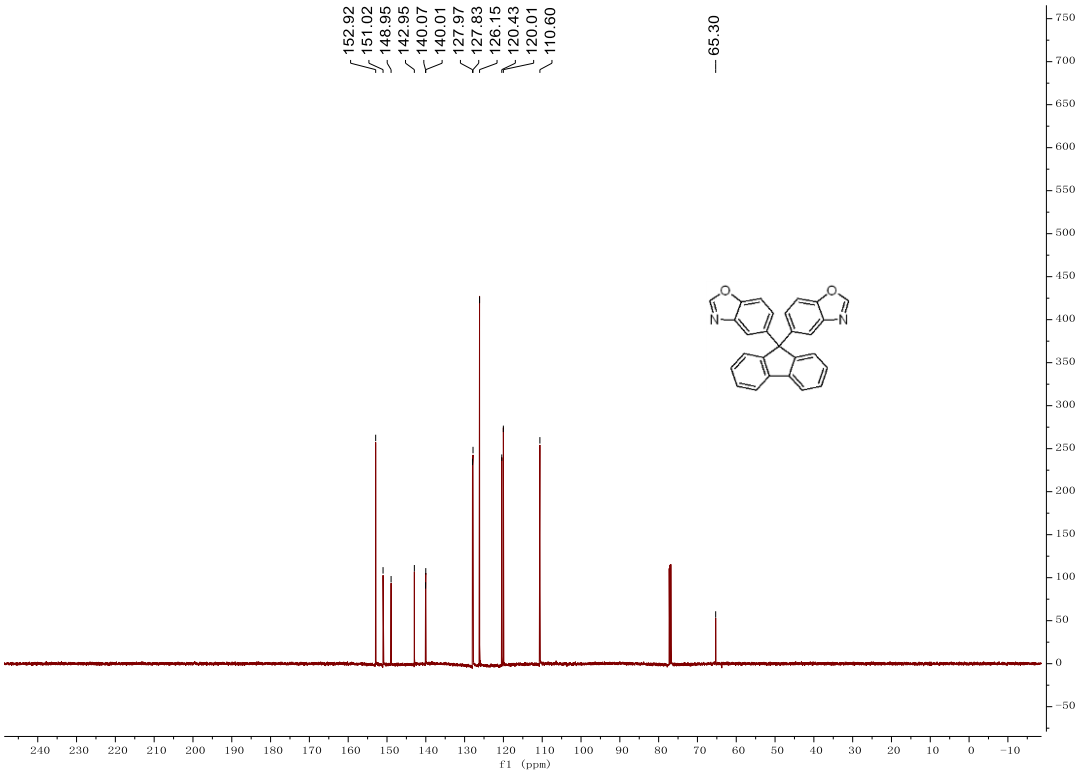
[1] X. D. Ma, G. Zhang, *ACS Catal.* **2021**, *11*, 5108.
[2] Q. Xiong, G. Li, S. Dong, X. Liu, X. Feng, *Org. Lett.* **2019**, *21*, 8771.
[3] P. Zhou, W. T. Yang, A. U. Rahman, G. Li, B. Jiang, *J. Org. Chem.* **2020**, *85*, 360.
[4] a) SADABS-2016/2 - Bruker AXS area detector scaling and absorption correction. b) L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst*. **2015**, *48*, 3.
[5] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3.
[6] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3.
[7] C. B. Hübschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Cryst.* **2011**, *44*, 1281.

9. Copies of ^{1}H and ^{13}C Spectra

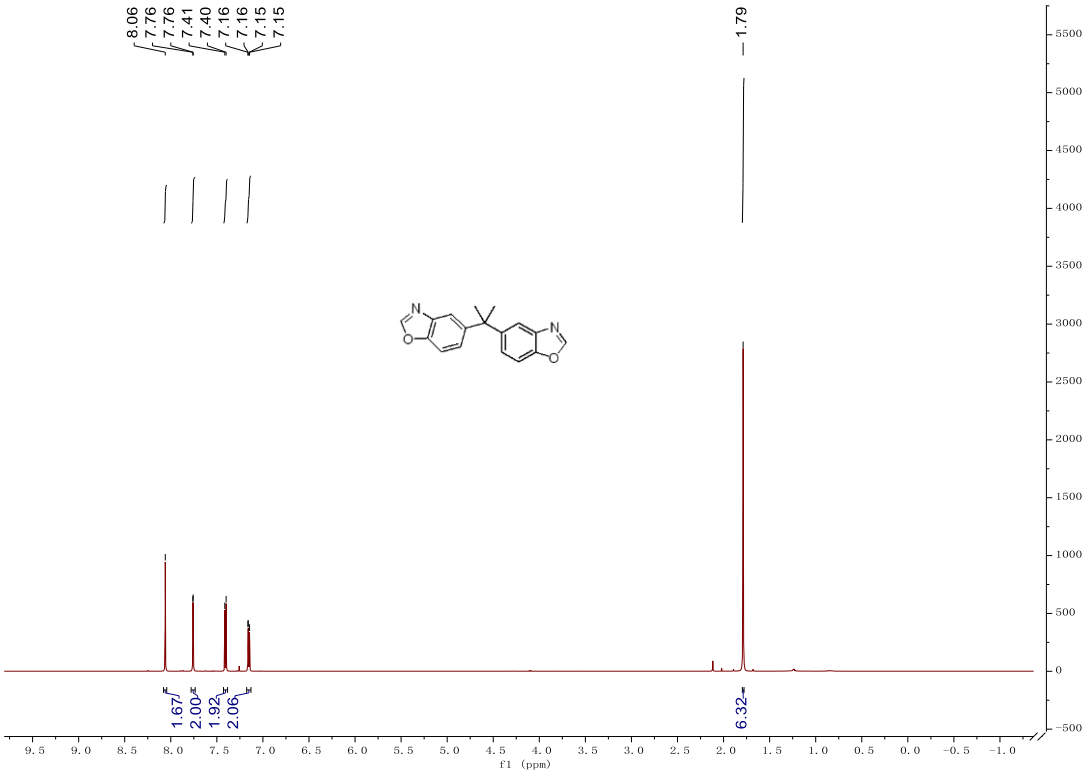
^{1}H NMR (**1x**) (600 MHz, Chloroform-*d*)



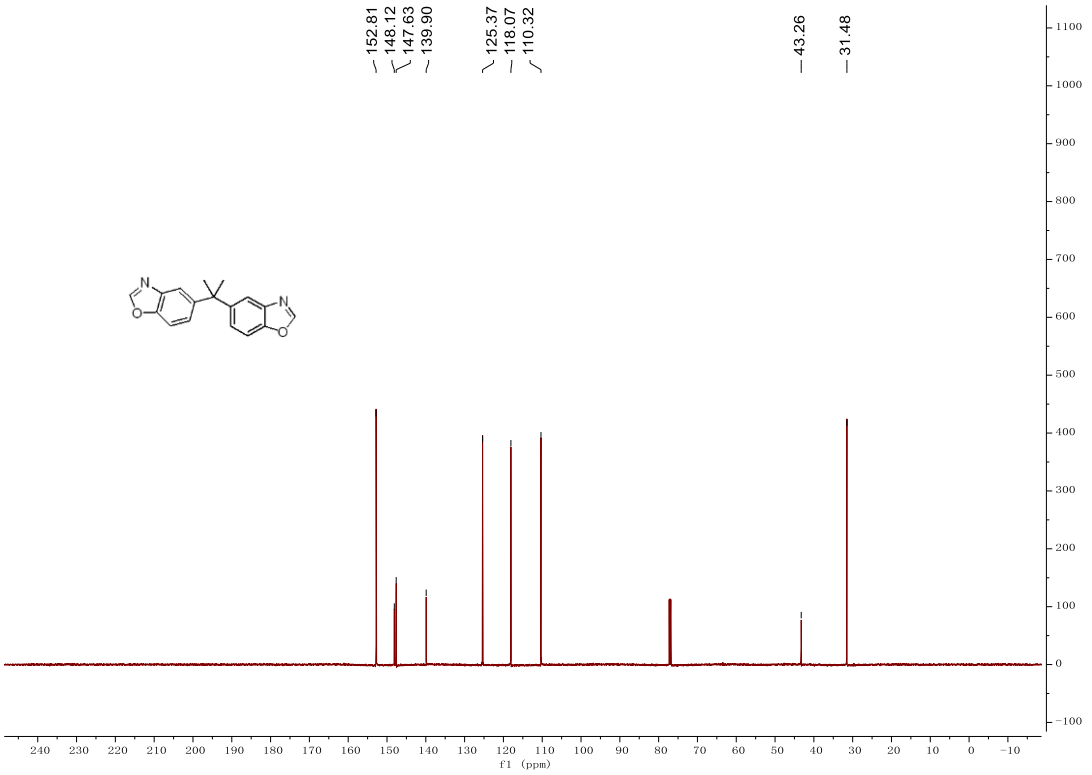
^{13}C NMR (**1x**) (150 MHz, Chloroform-*d*)



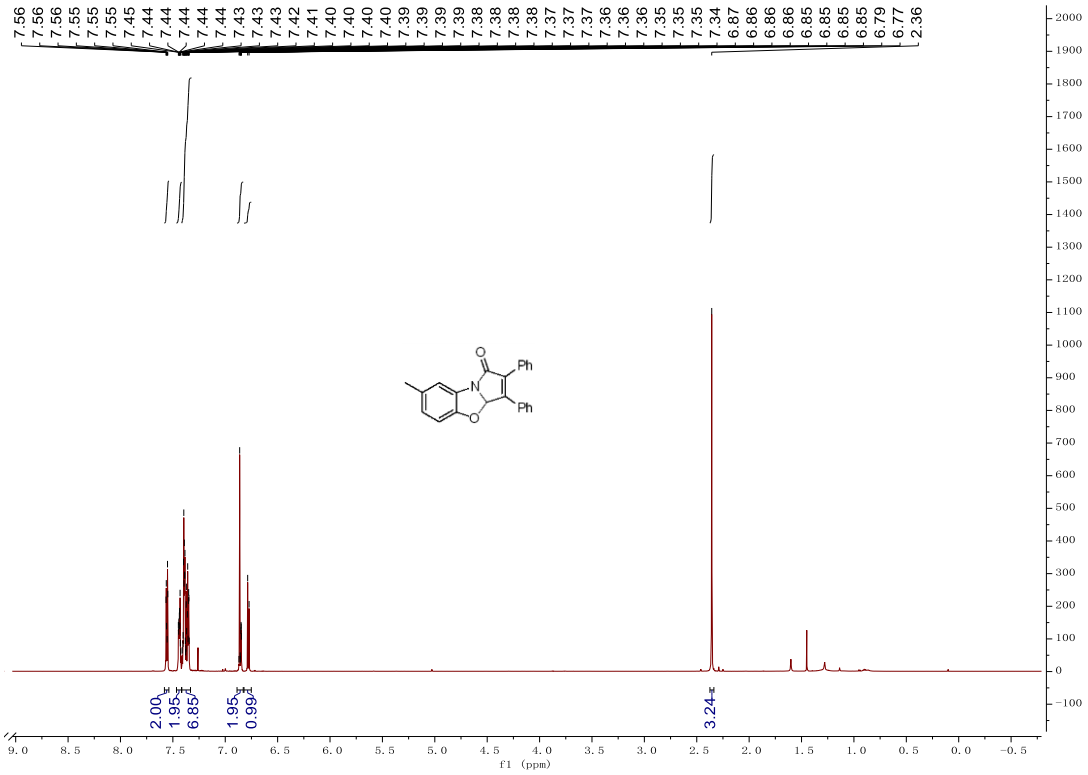
^{1}H NMR (**1y**) (600 MHz, Chloroform-*d*)



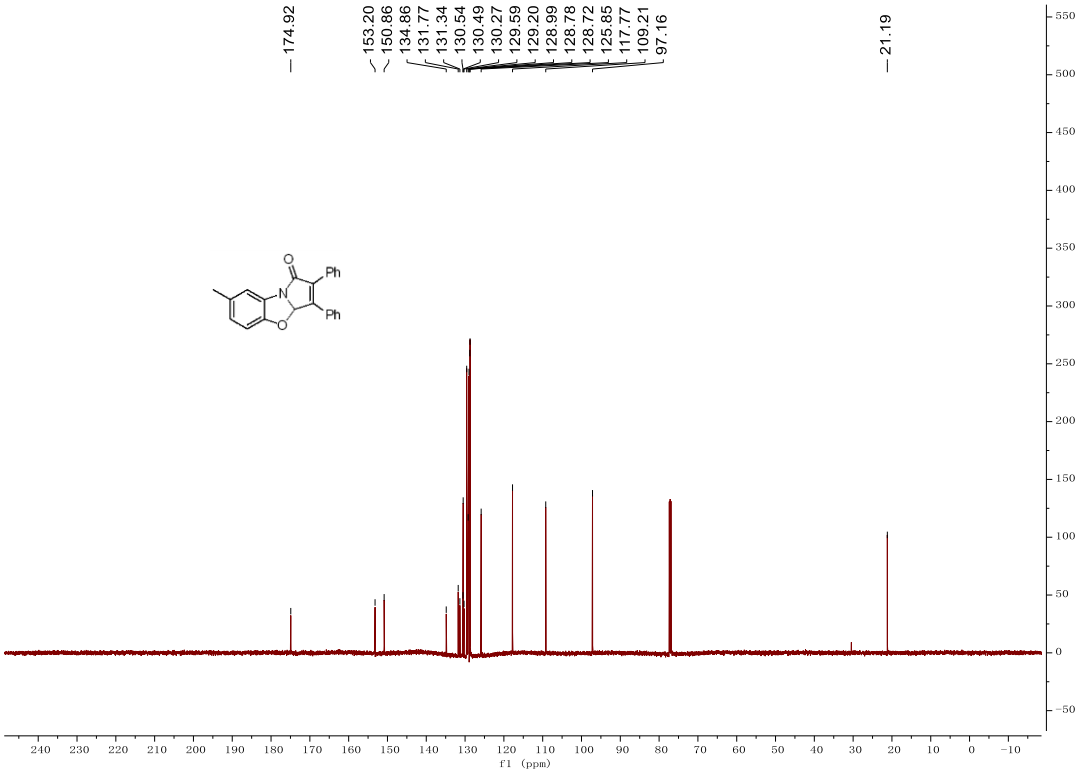
^{13}C NMR (**1y**) (150 MHz, Chloroform-*d*)



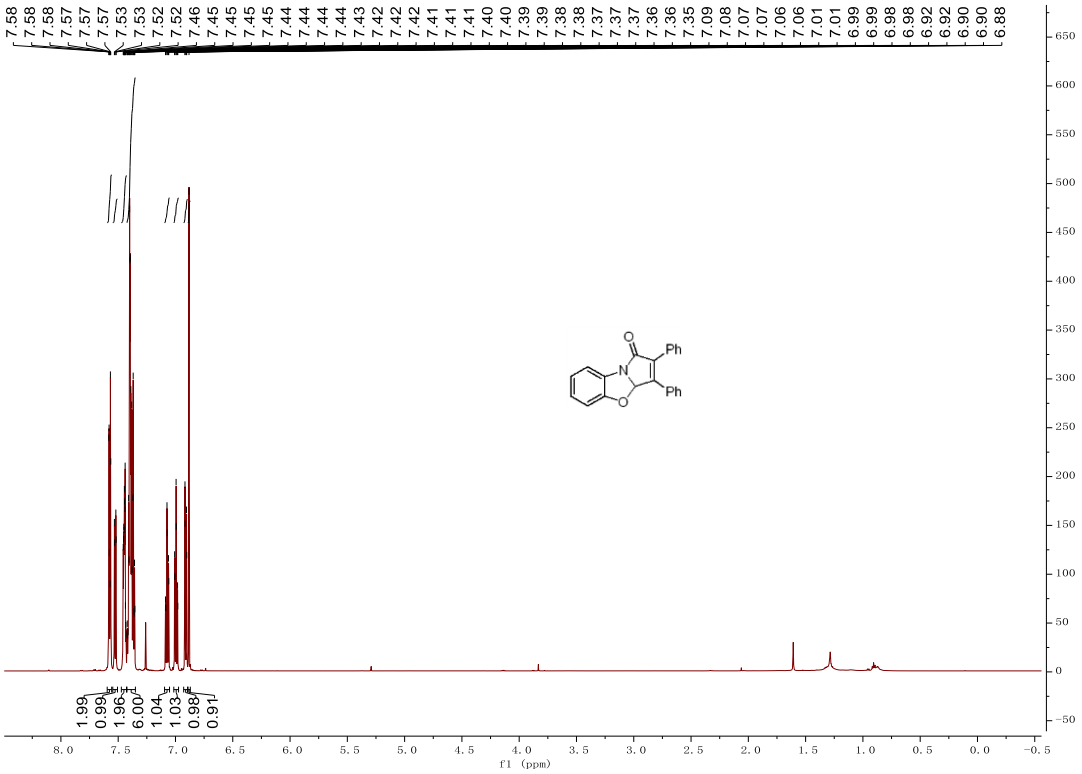
^{1}H NMR (**3aa**) (600 MHz, Chloroform-*d*)



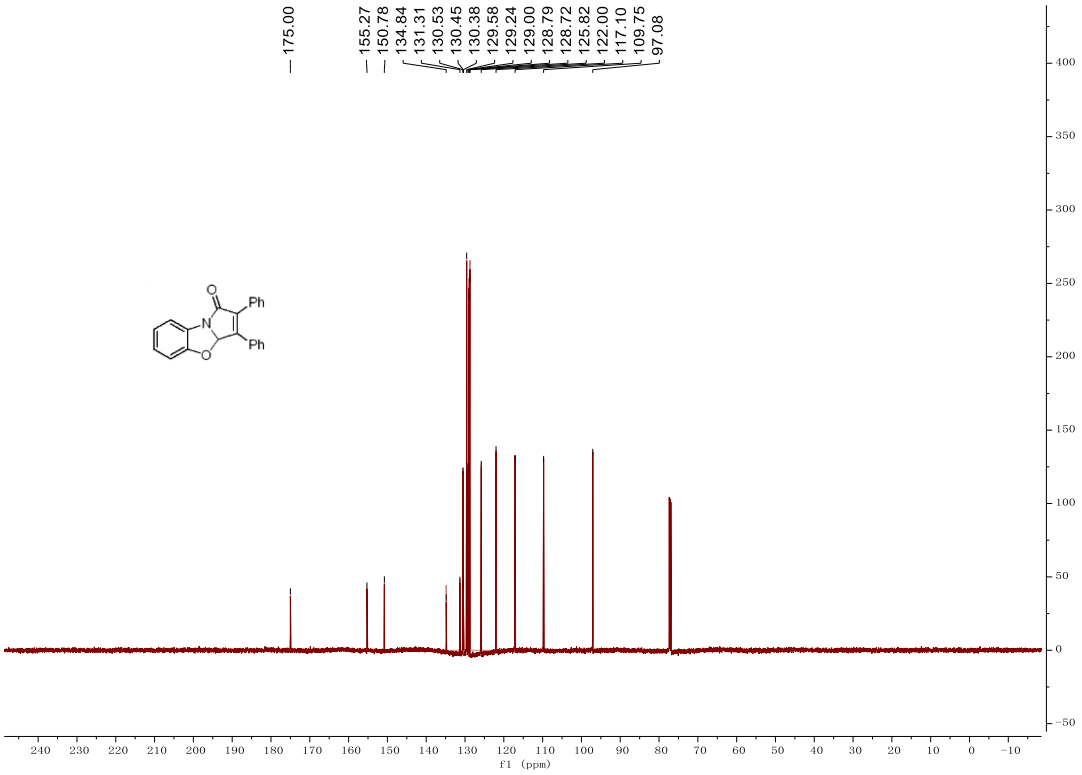
^{13}C NMR (**3aa**) (150 MHz, Chloroform-*d*)



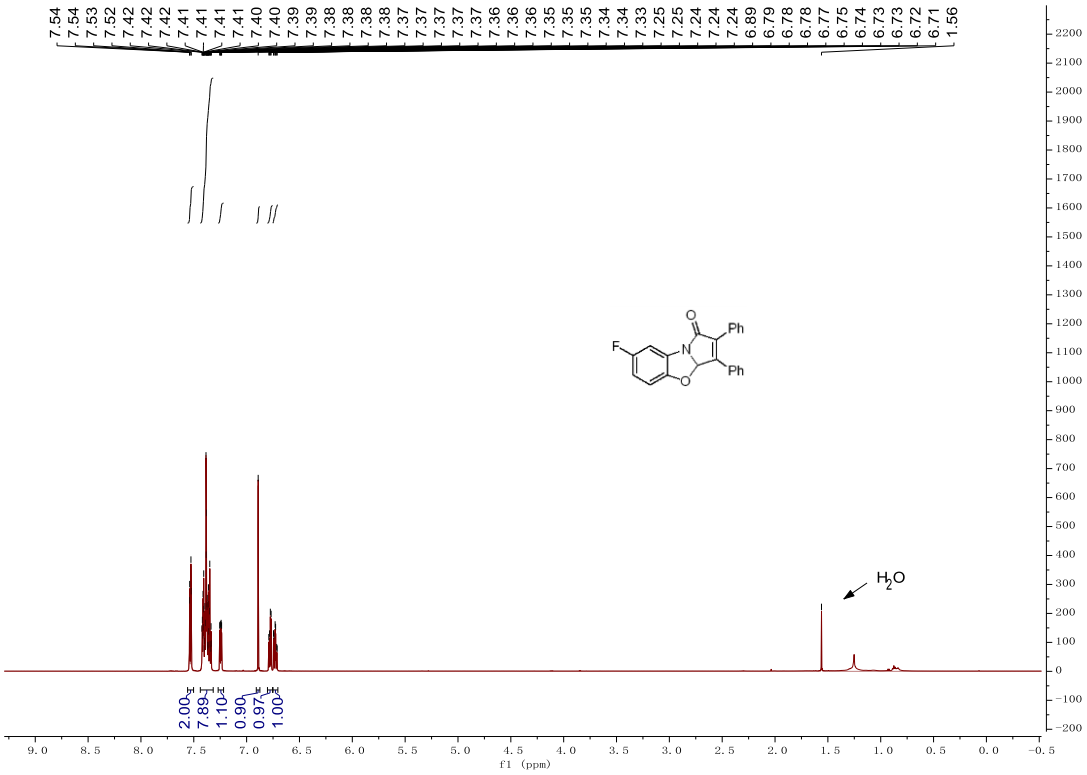
^{1}H NMR (**3ba**) (600 MHz, Chloroform-*d*)



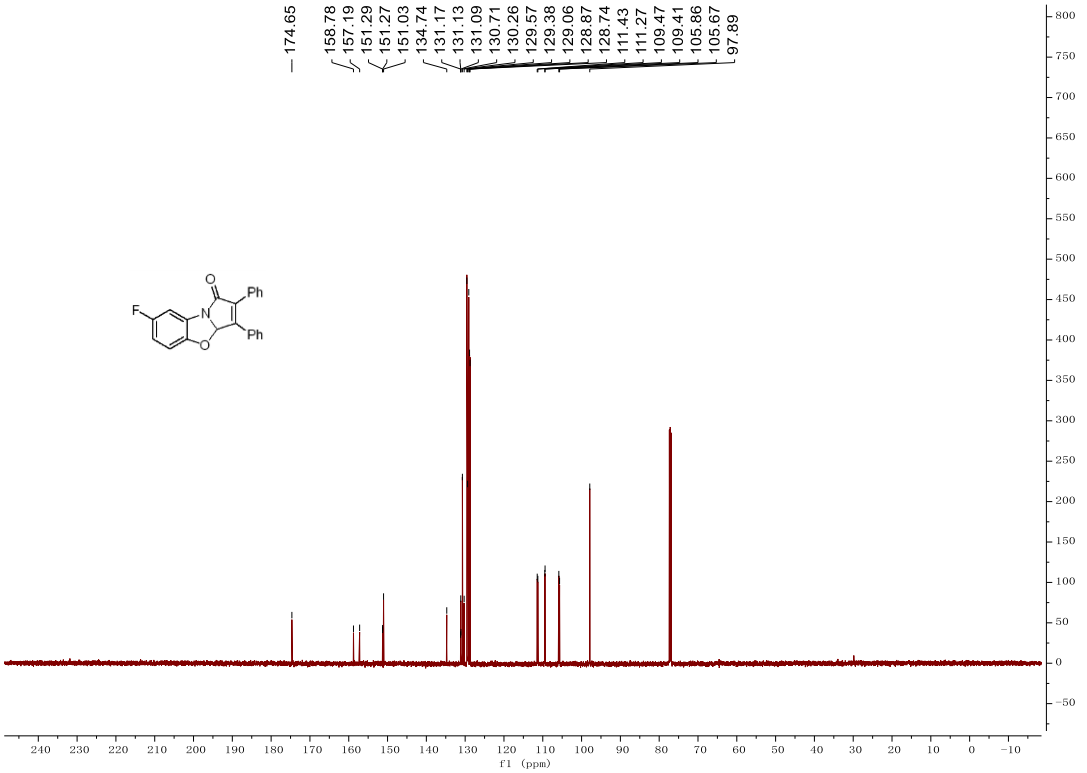
^{13}C NMR (**3ba**) (150 MHz, Chloroform-*d*)



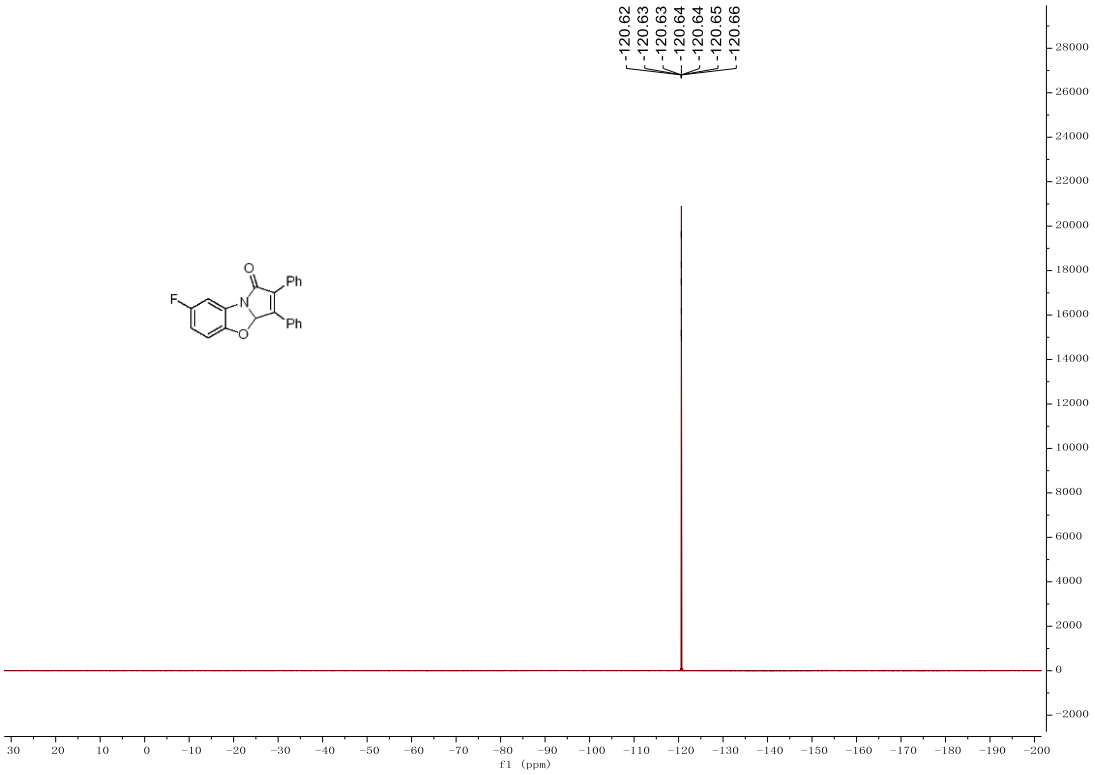
^{1}H NMR (**3ca**) (600 MHz, Chloroform-*d*)



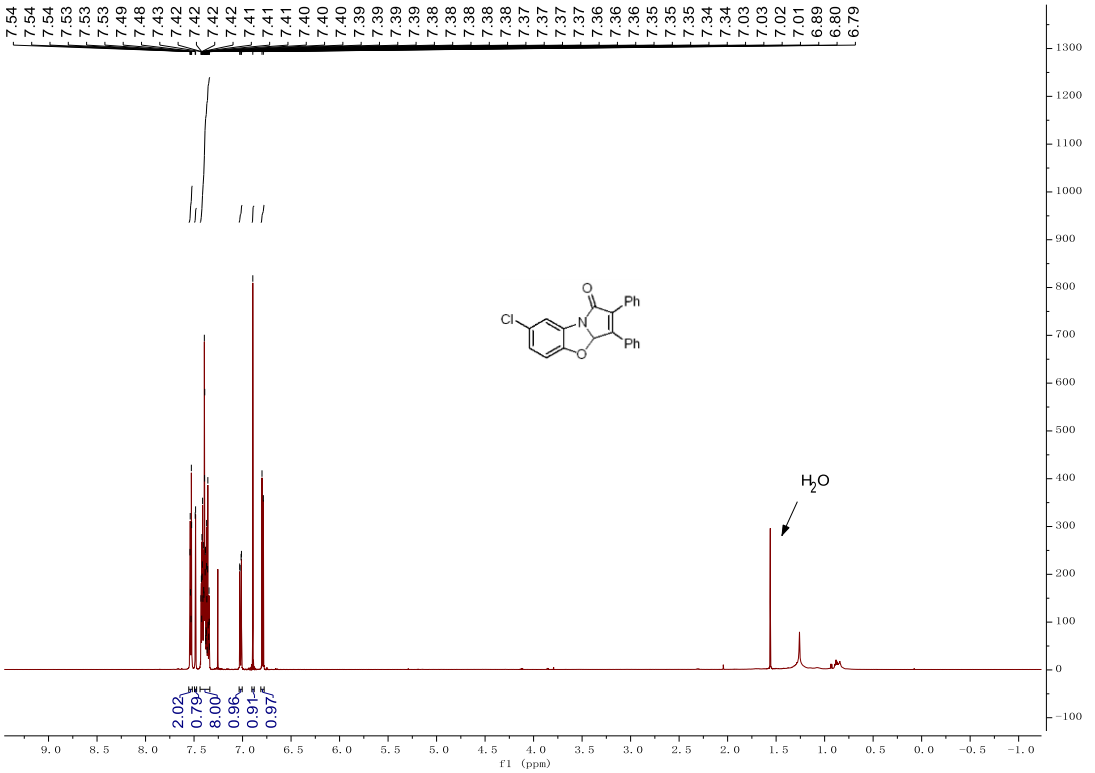
^{13}C NMR (**3ca**) (150 MHz, Chloroform-*d*)



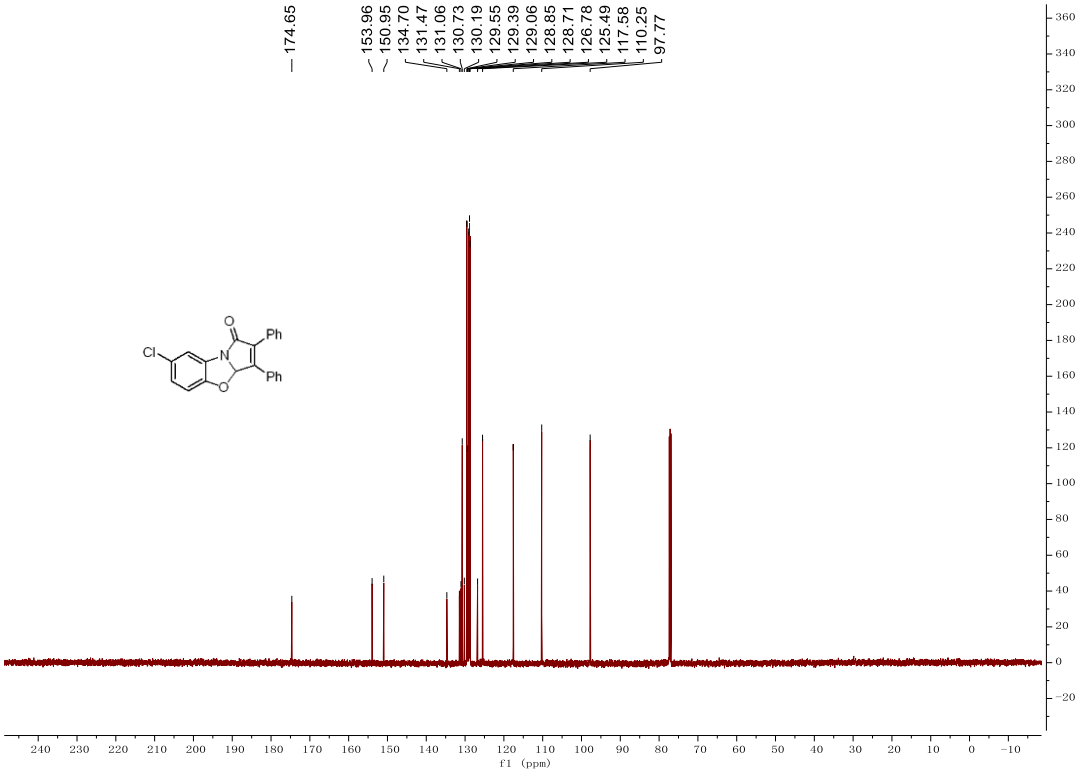
^{19}F NMR (**3ca**) (564 MHz, Chloroform-*d*)



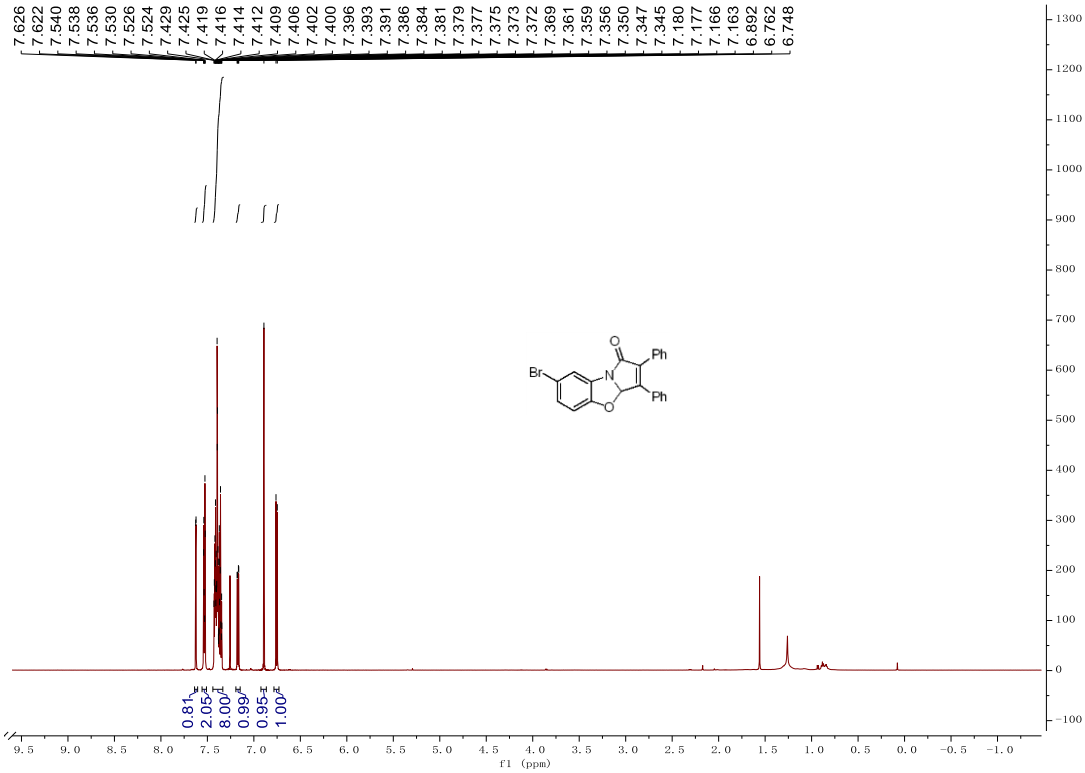
^{1}H NMR (**3da**) 600 MHz, Chloroform-*d*)



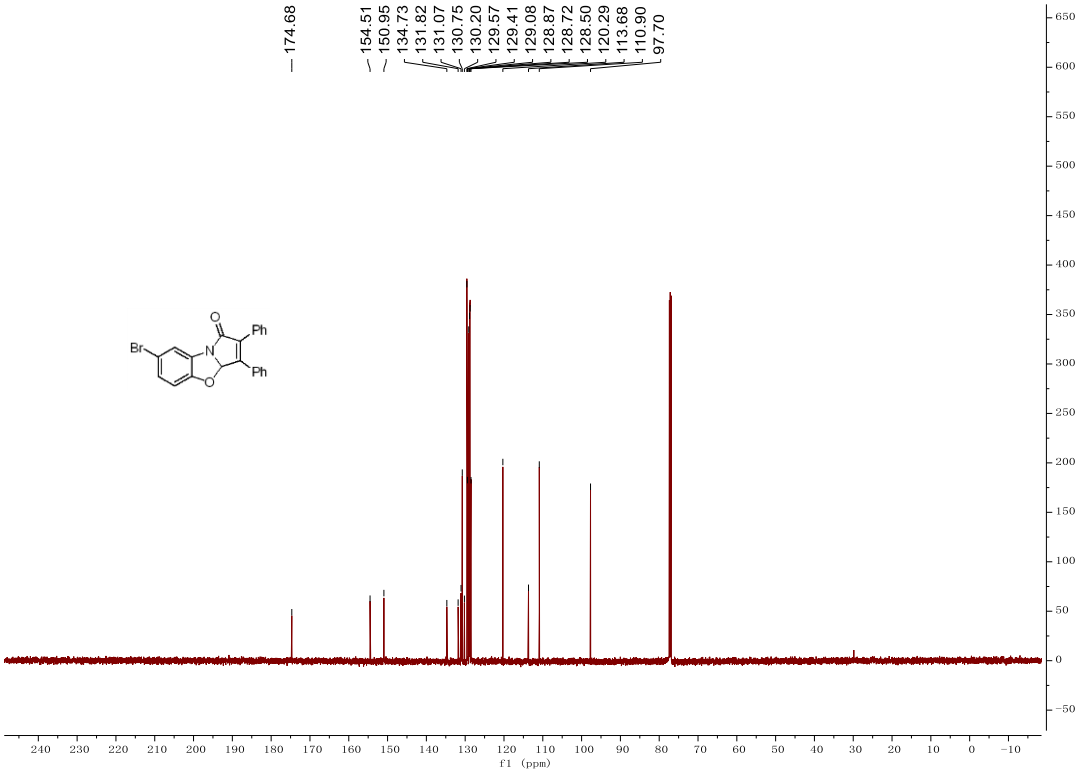
^{13}C NMR (**3da**) (150 MHz, Chloroform-*d*)



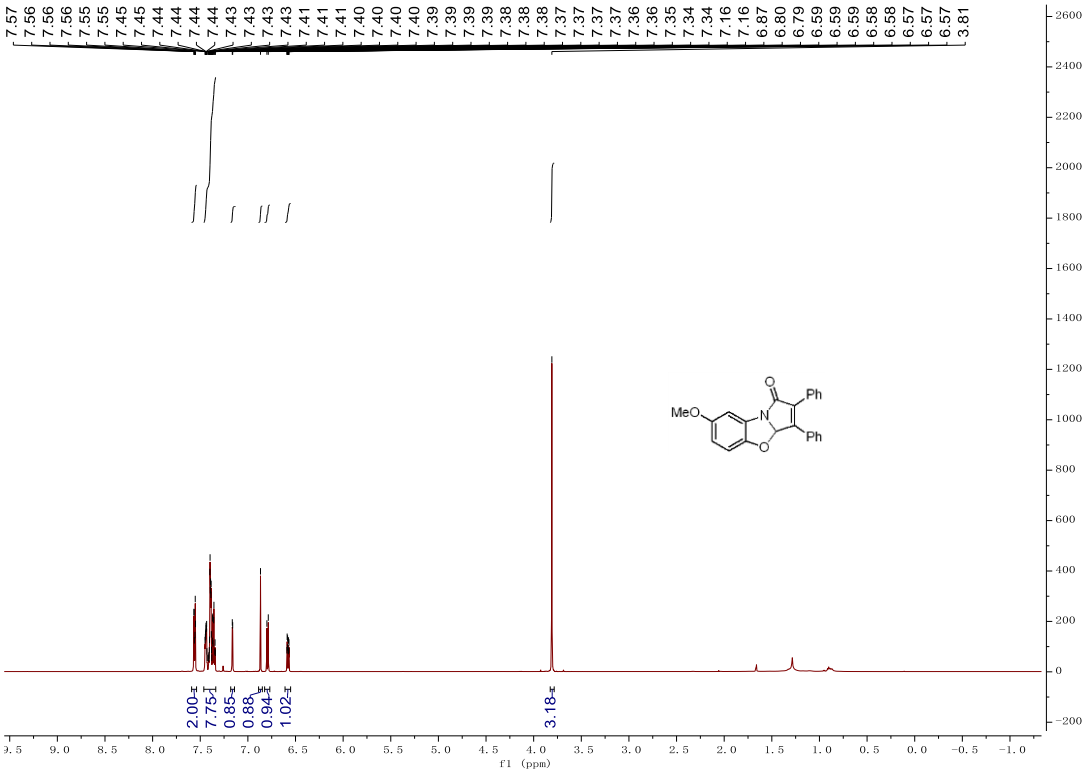
^{1}H NMR (**3ea**) (600 MHz, Chloroform-*d*)



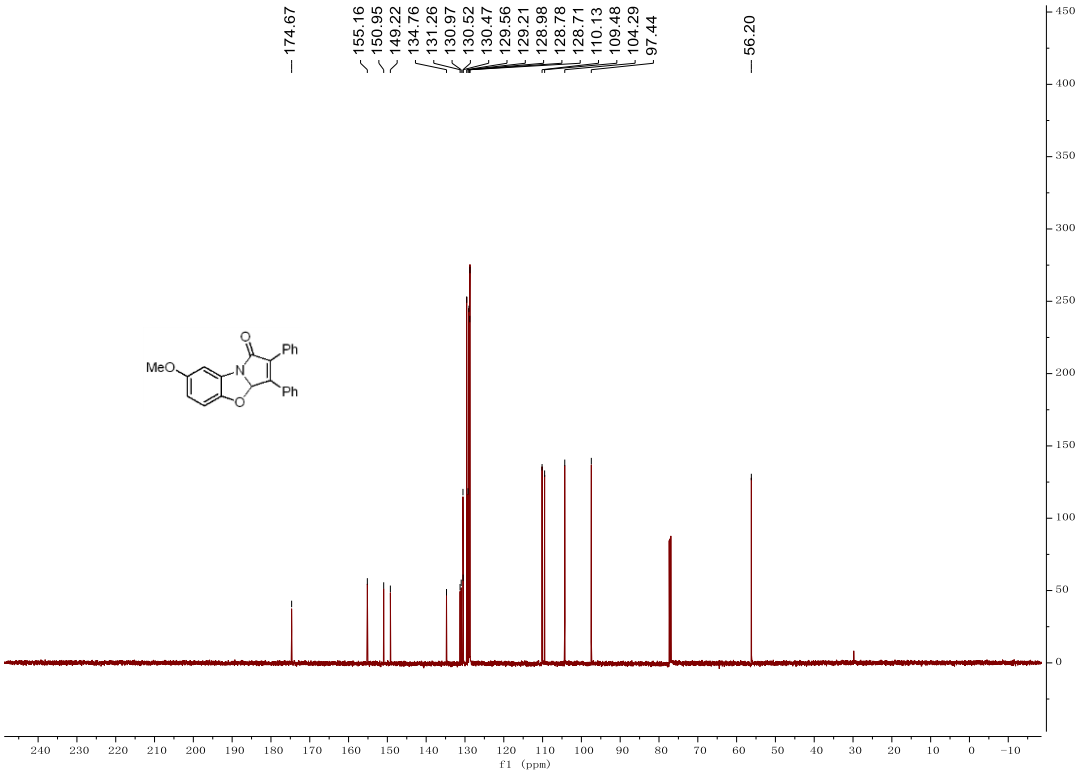
^{13}C NMR (**3ea**) (150 MHz, Chloroform-*d*)



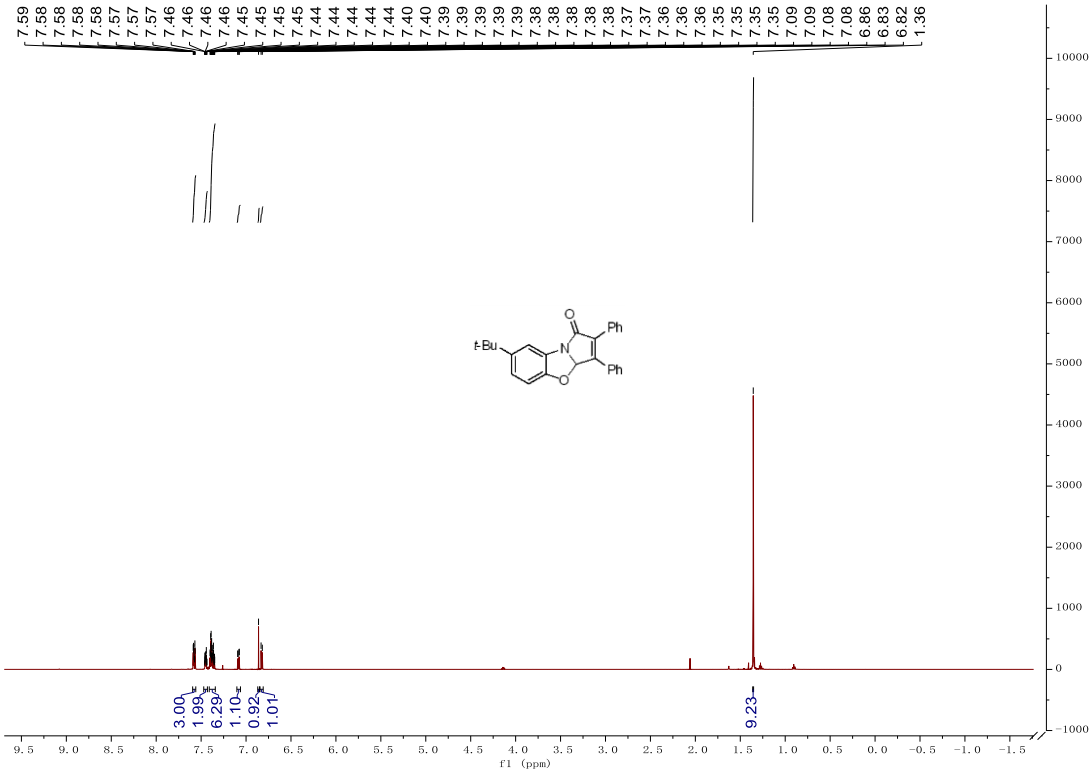
^{1}H NMR (**3fa**) (600 MHz, Chloroform-*d*)



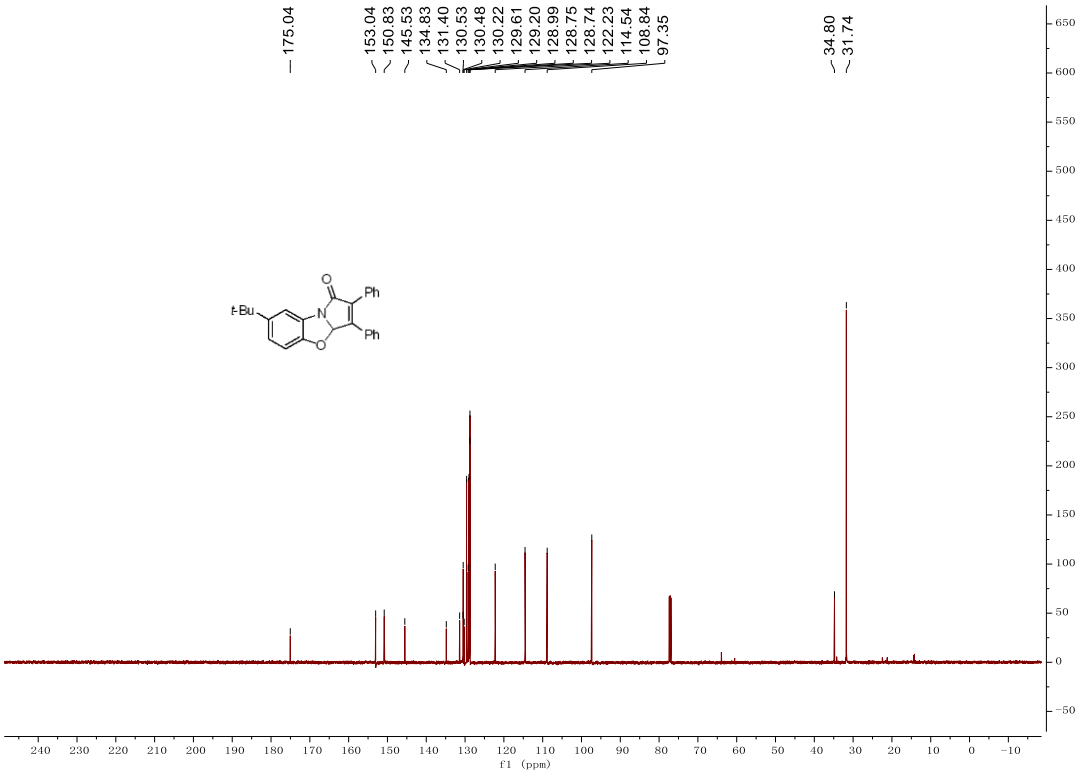
^{13}C NMR (**3fa**) (150 MHz, Chloroform-*d*)



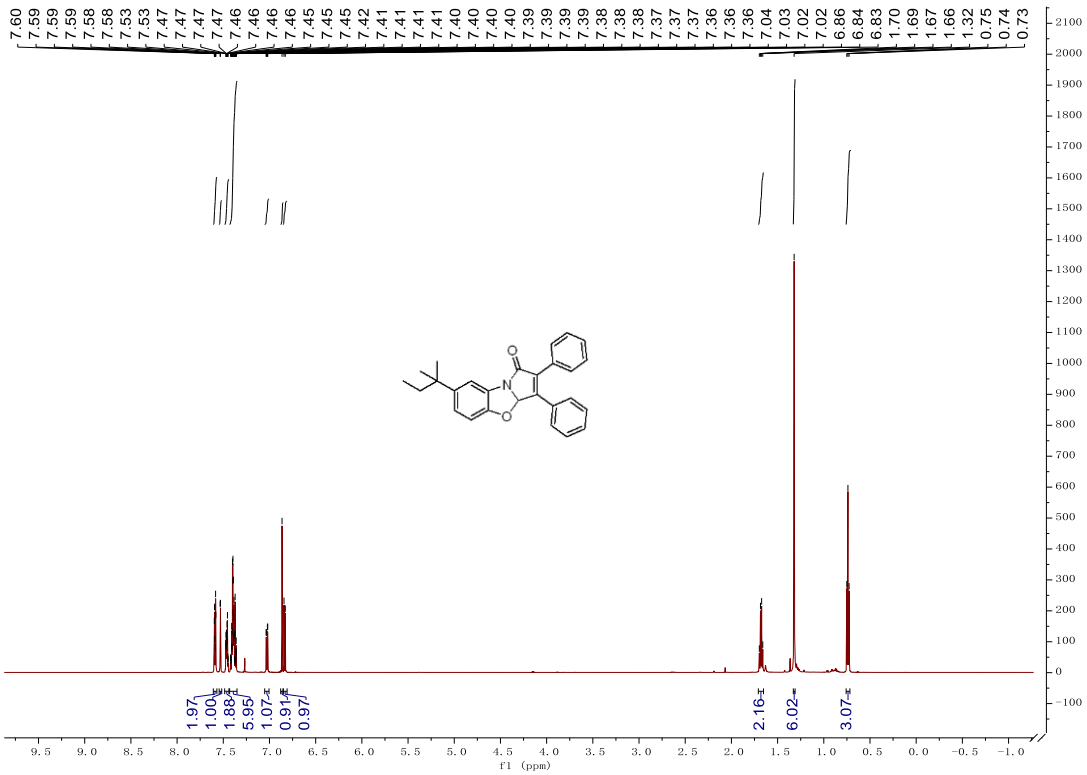
^{1}H NMR (**3ga**) (600 MHz, Chloroform-*d*)



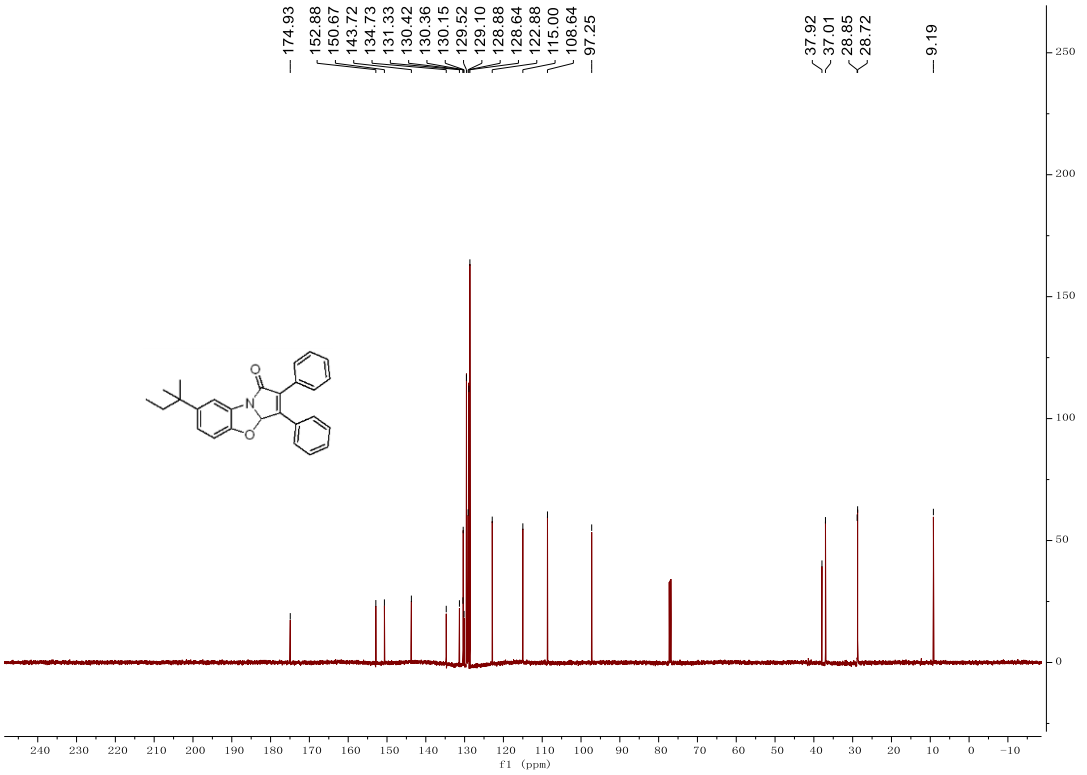
^{13}C NMR (**3ga**) (150 MHz, Chloroform-*d*)



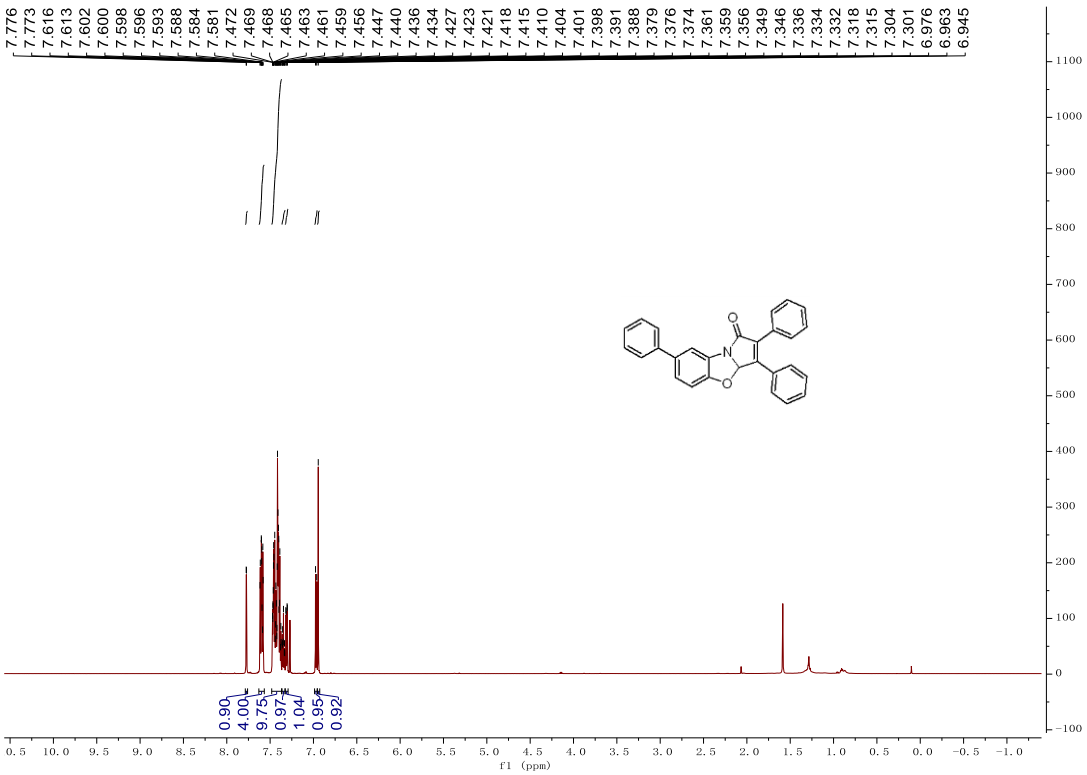
^{1}H NMR (**3ha**) (600 MHz, Chloroform-*d*)



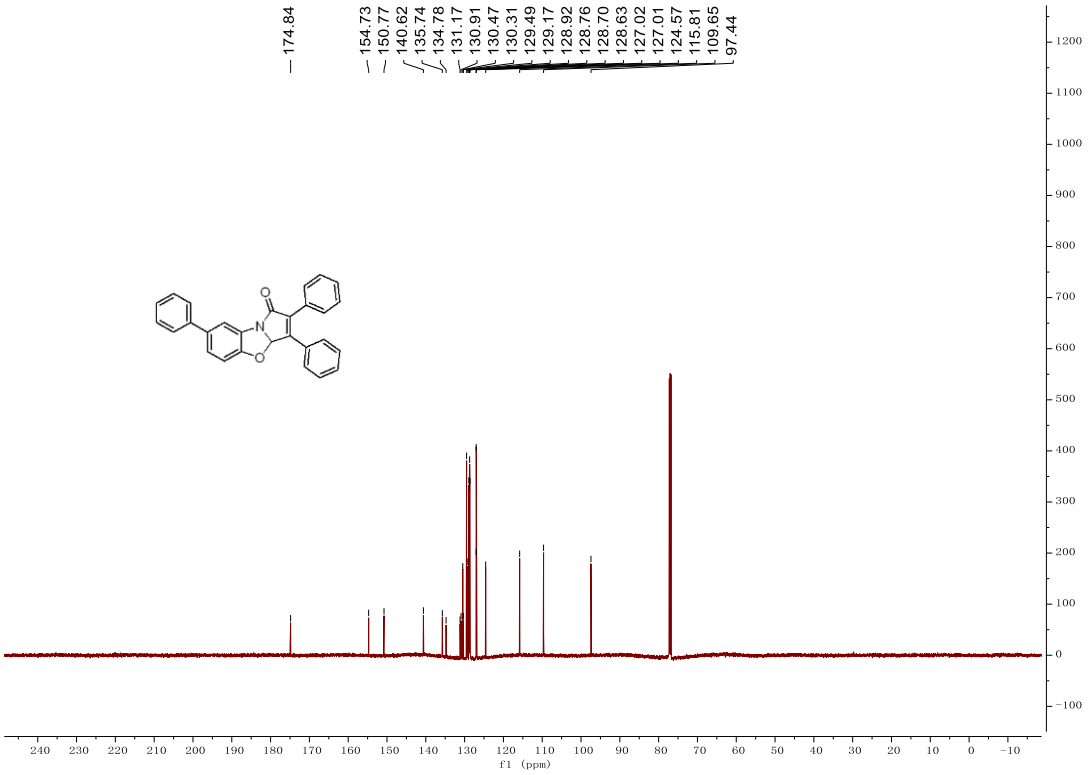
^{13}C NMR (**3ha**) (150 MHz, Chloroform-*d*)



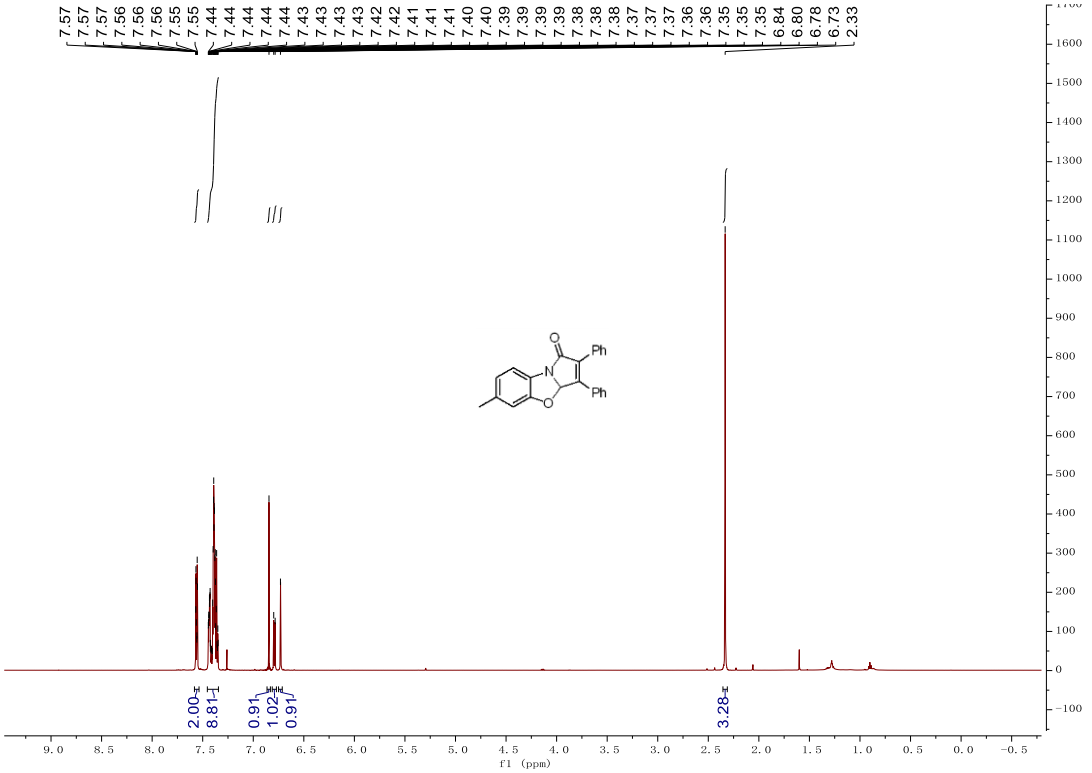
^{1}H NMR (**3ia**) (600 MHz, Chloroform-*d*)



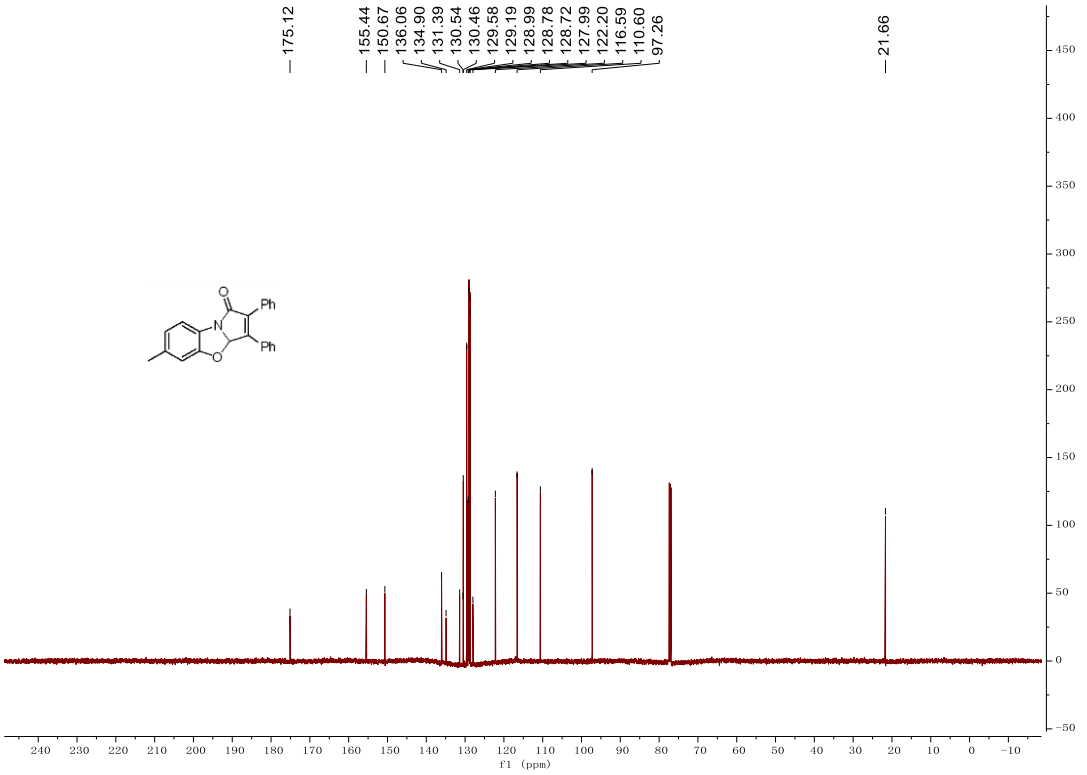
^{13}C NMR (**3ia**) (150 MHz, Chloroform-*d*)



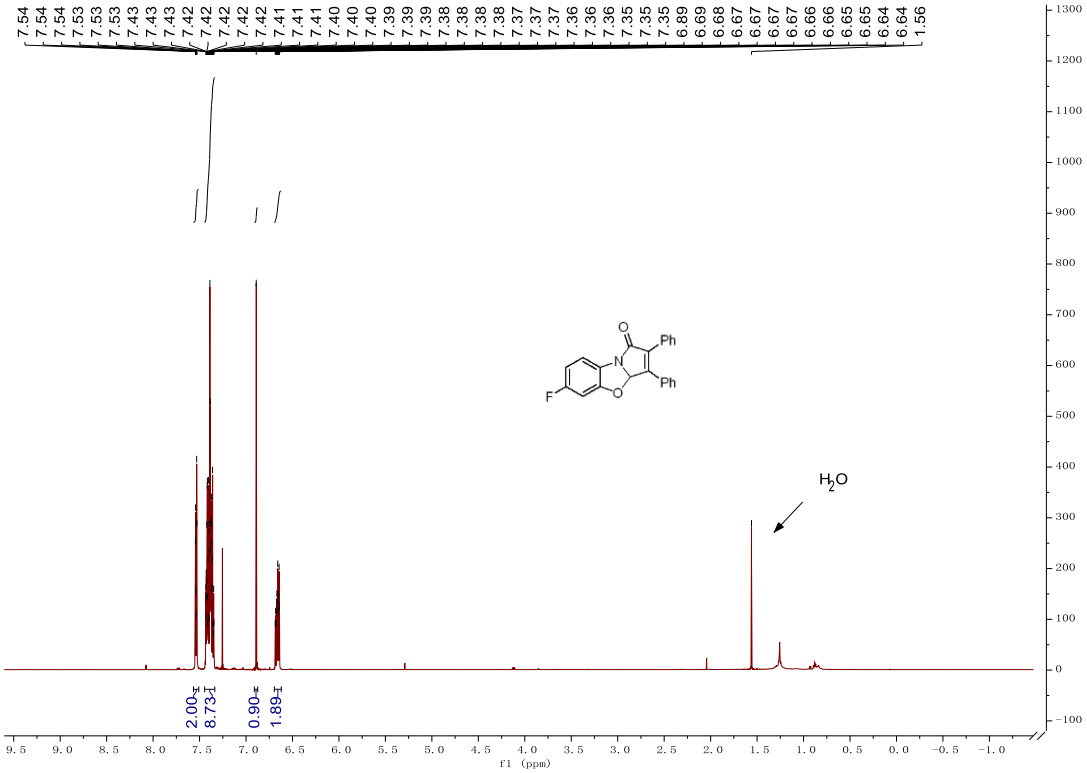
^{1}H NMR (**3ja**) (600 MHz, Chloroform-*d*)



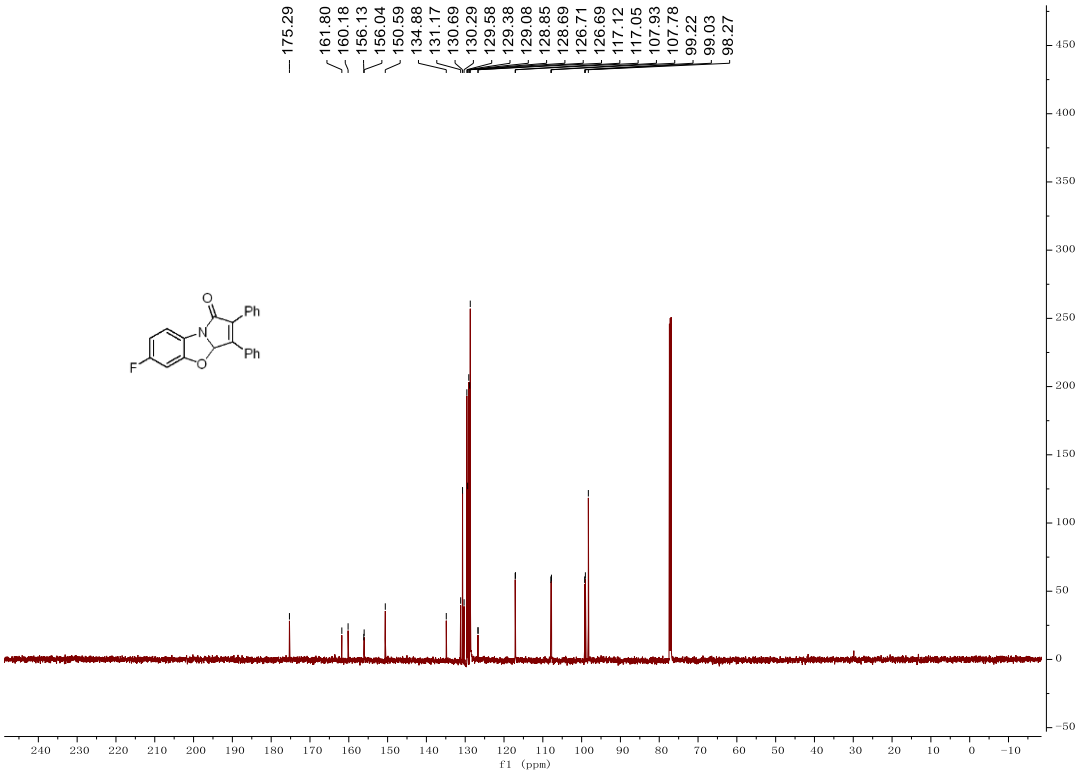
^{13}C NMR (**3ja**) (150 MHz, Chloroform-*d*)



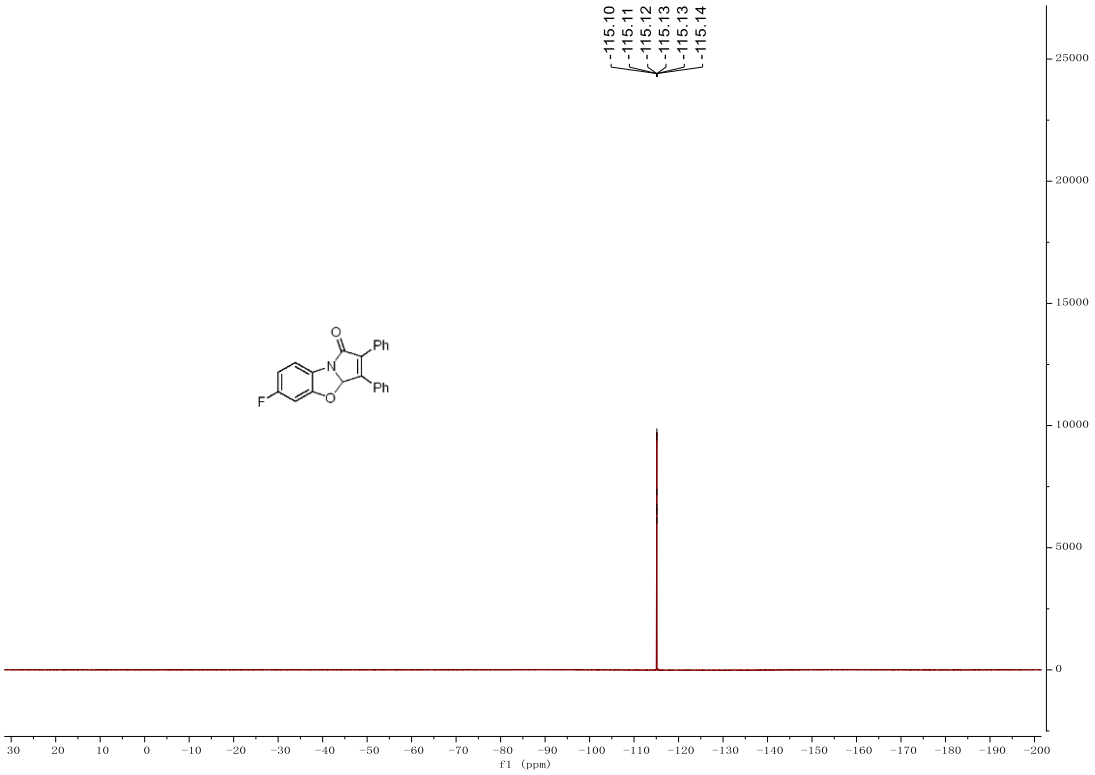
^{1}H NMR (**3ka**) (600 MHz, Chloroform-*d*)



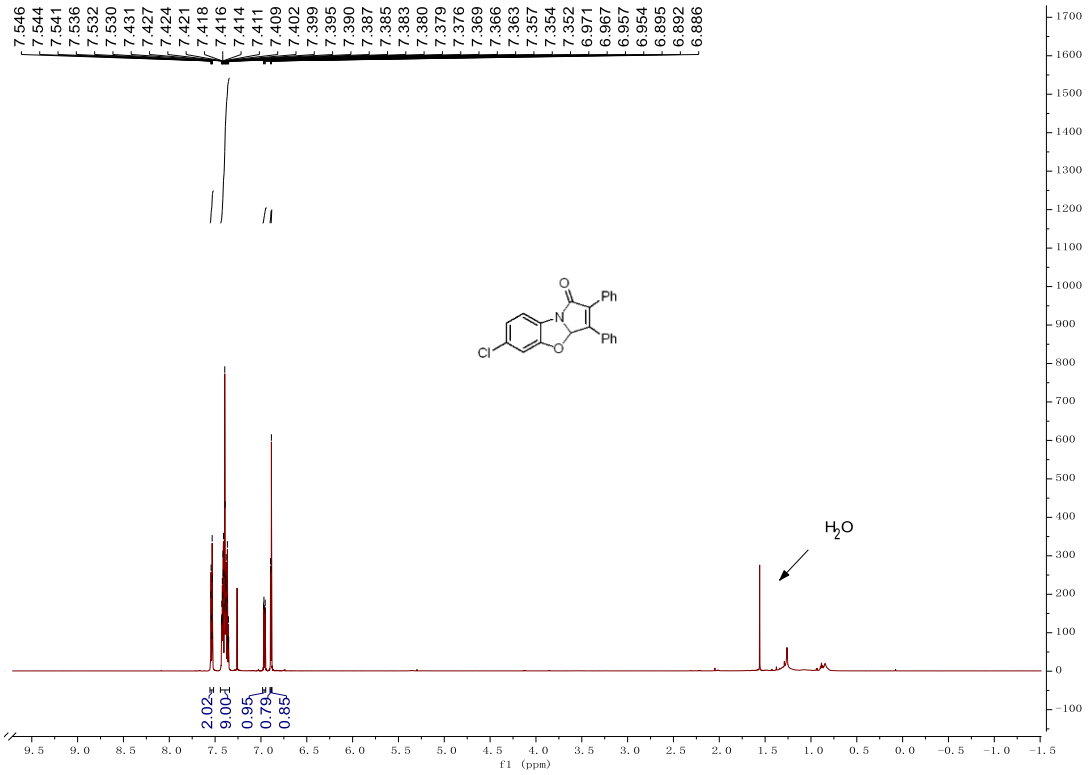
^{13}C NMR (**3ka**) (150 MHz, Chloroform-*d*)



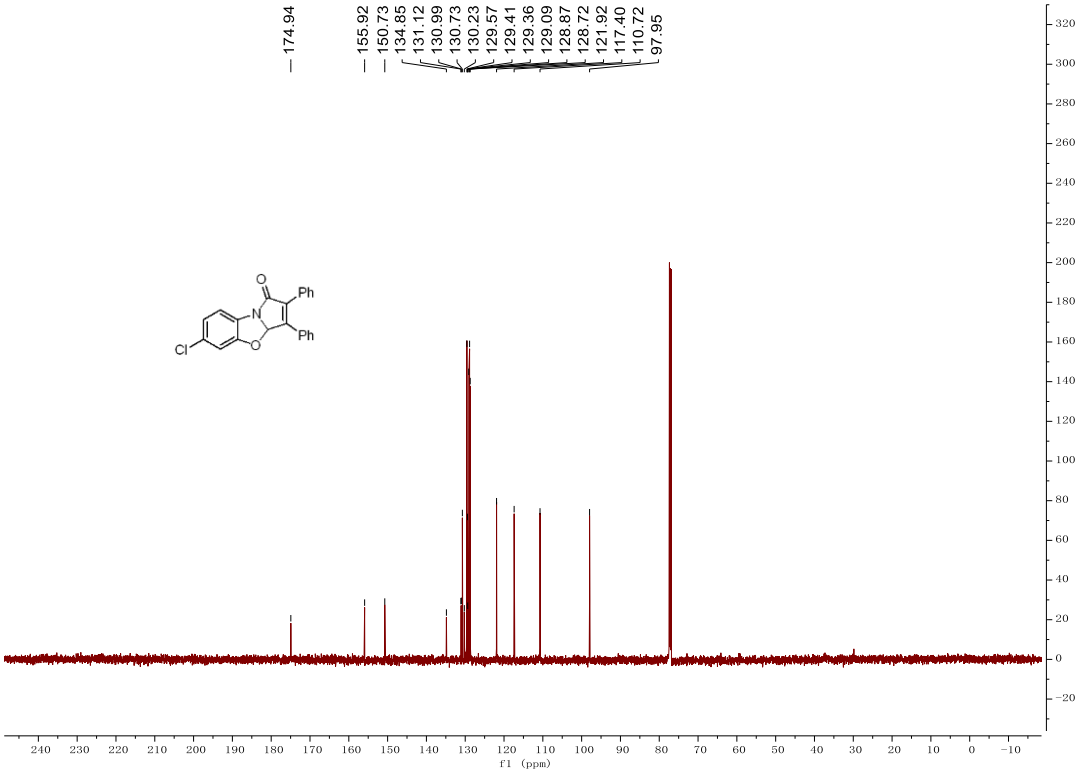
^{19}F NMR (**3ka**) (564 MHz, Chloroform-*d*)



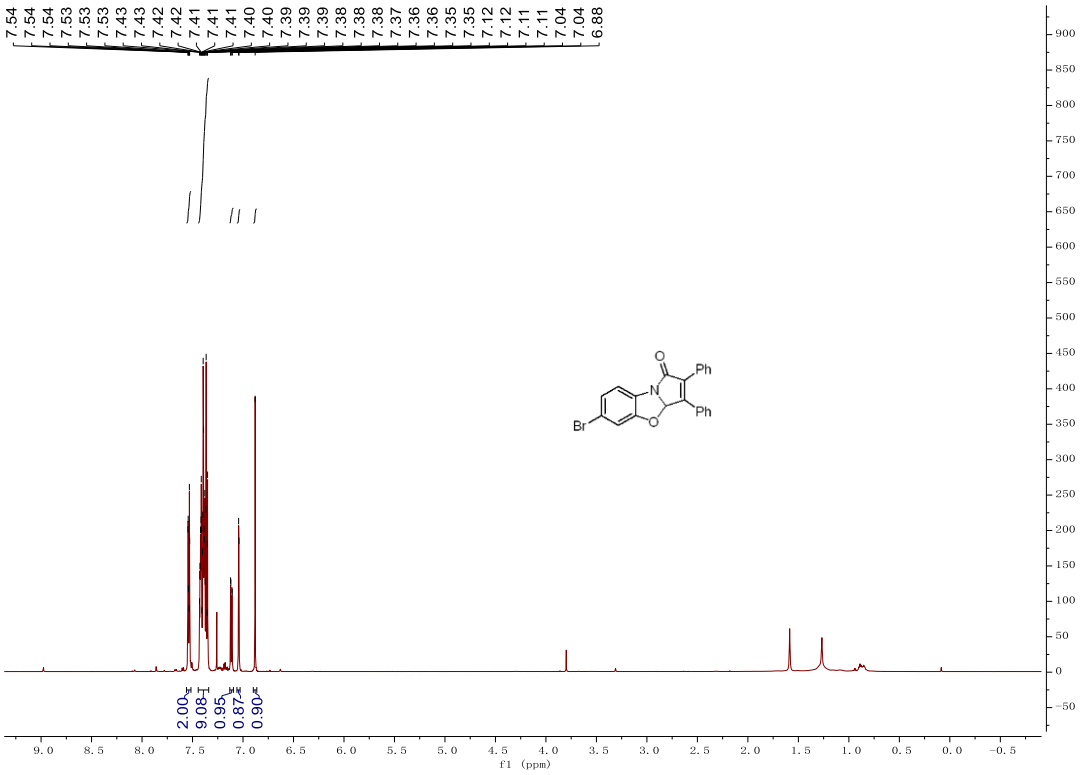
^{1}H NMR (**3la**) (600 MHz, Chloroform-*d*)



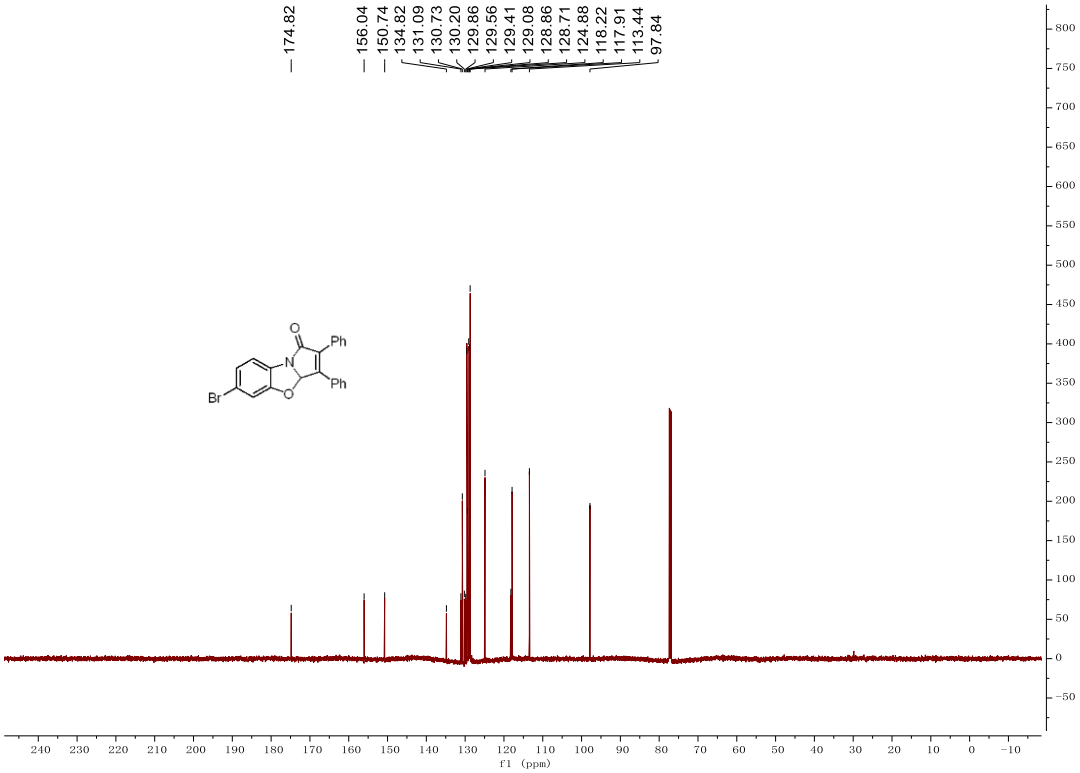
^{13}C NMR (**3la**) (150 MHz, Chloroform-*d*)



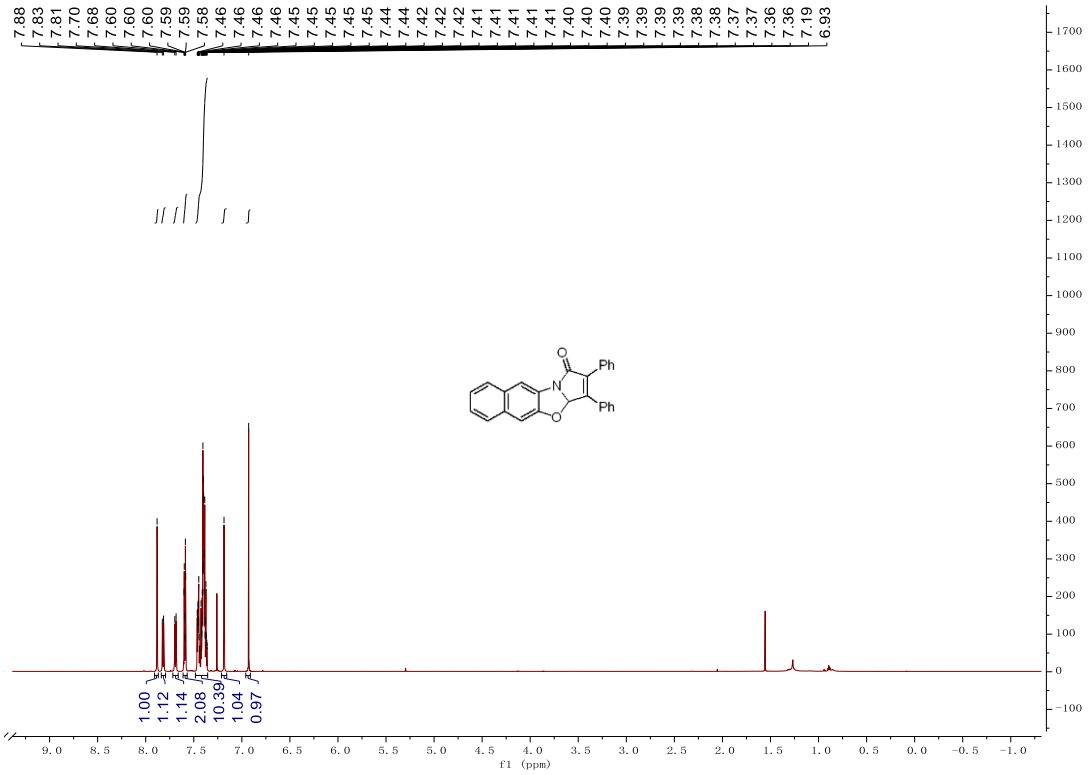
^{1}H NMR (**3ma**) (600 MHz, Chloroform-*d*)



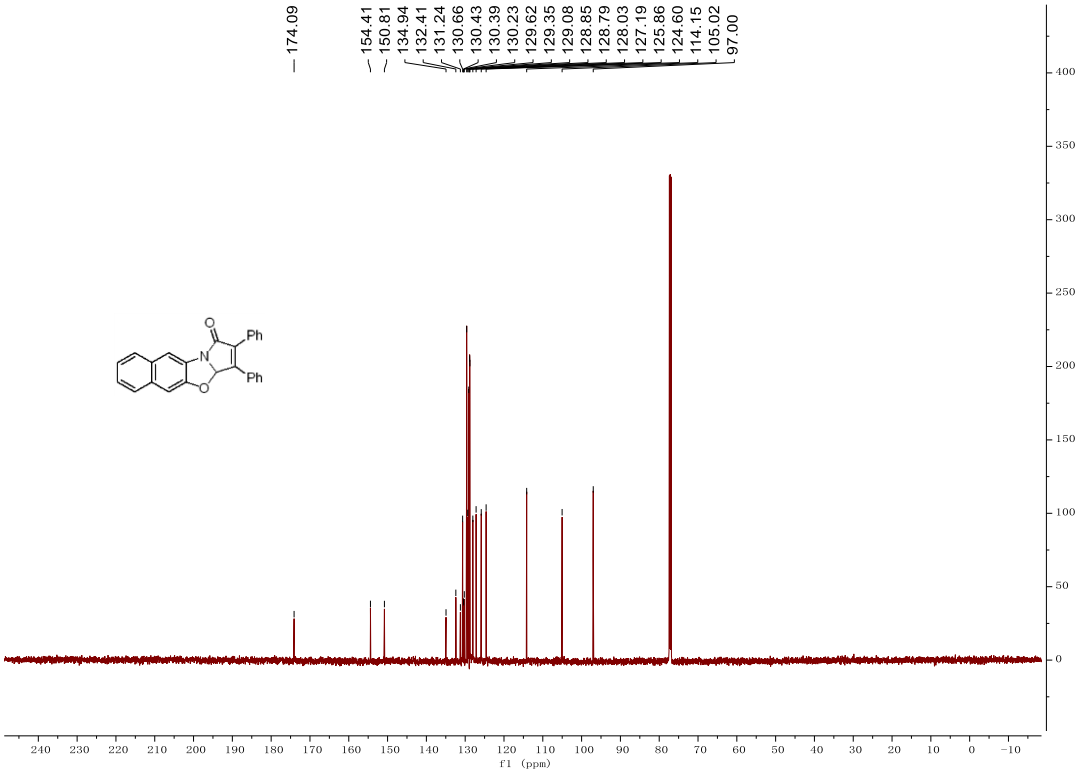
^{13}C NMR (**3ma**) (150 MHz, Chloroform-*d*)



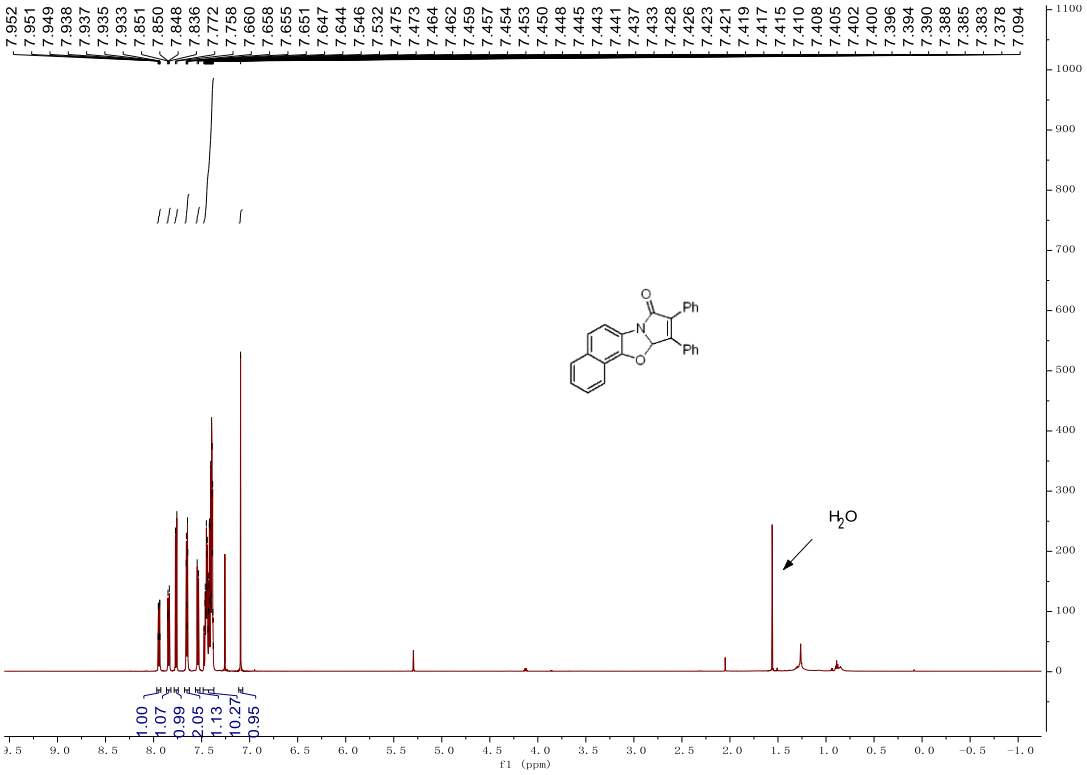
^{1}H NMR (**3na**) (600 MHz, Chloroform-*d*)



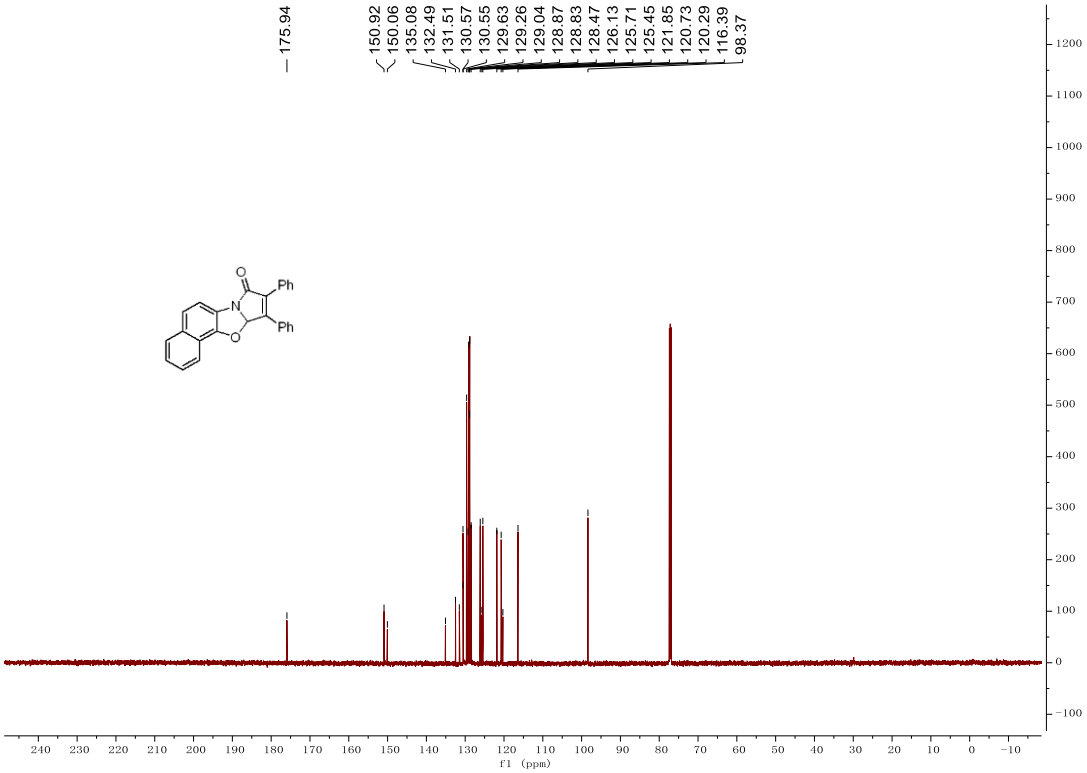
^{13}C NMR (**3na**) (150 MHz, Chloroform-*d*)



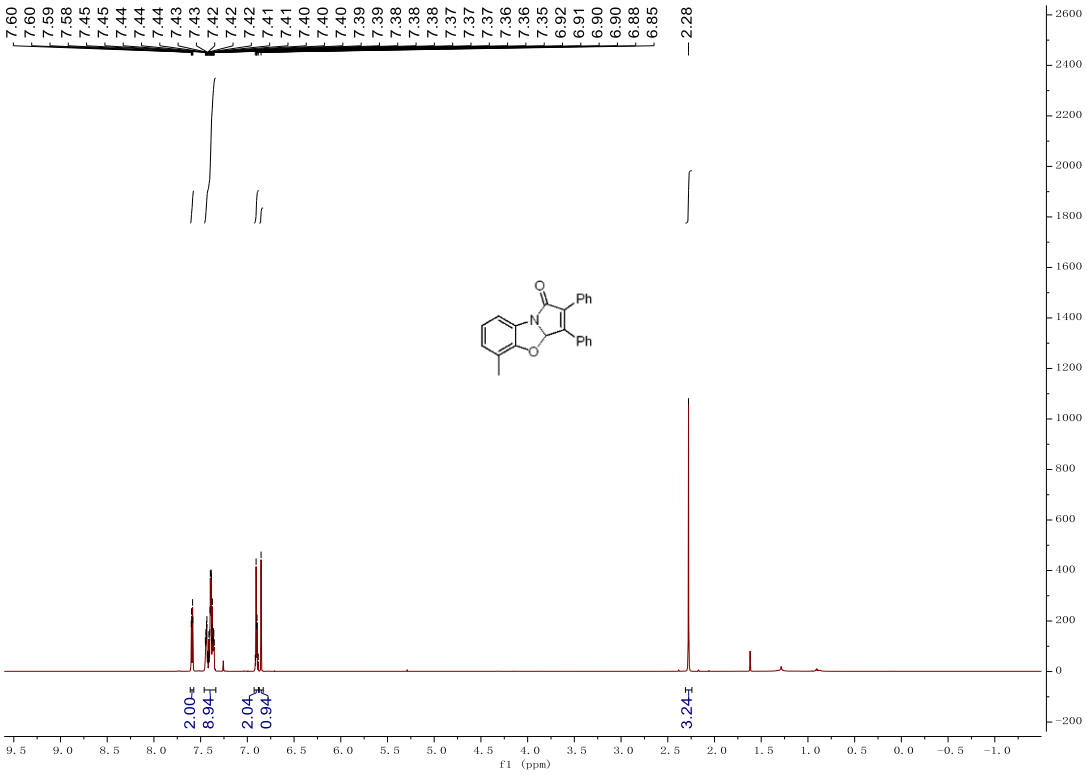
^{1}H NMR (**3oa**) (600 MHz, Chloroform-*d*)



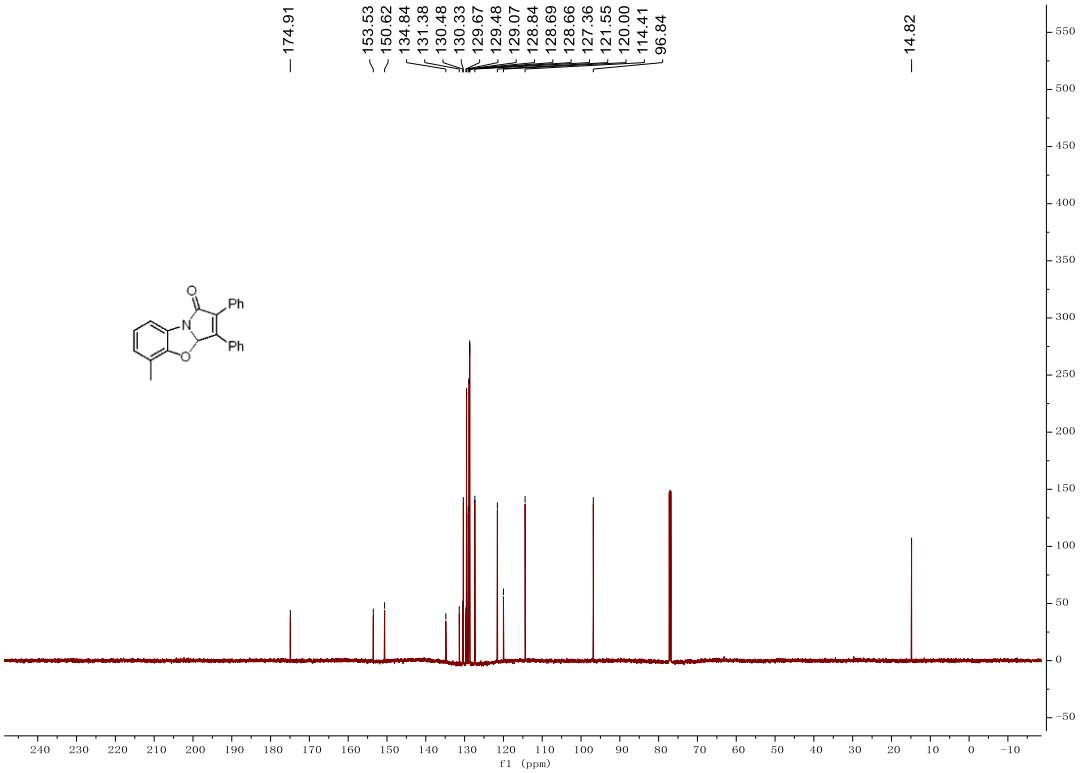
^{13}C NMR (**3oa**) (150 MHz, Chloroform-*d*)



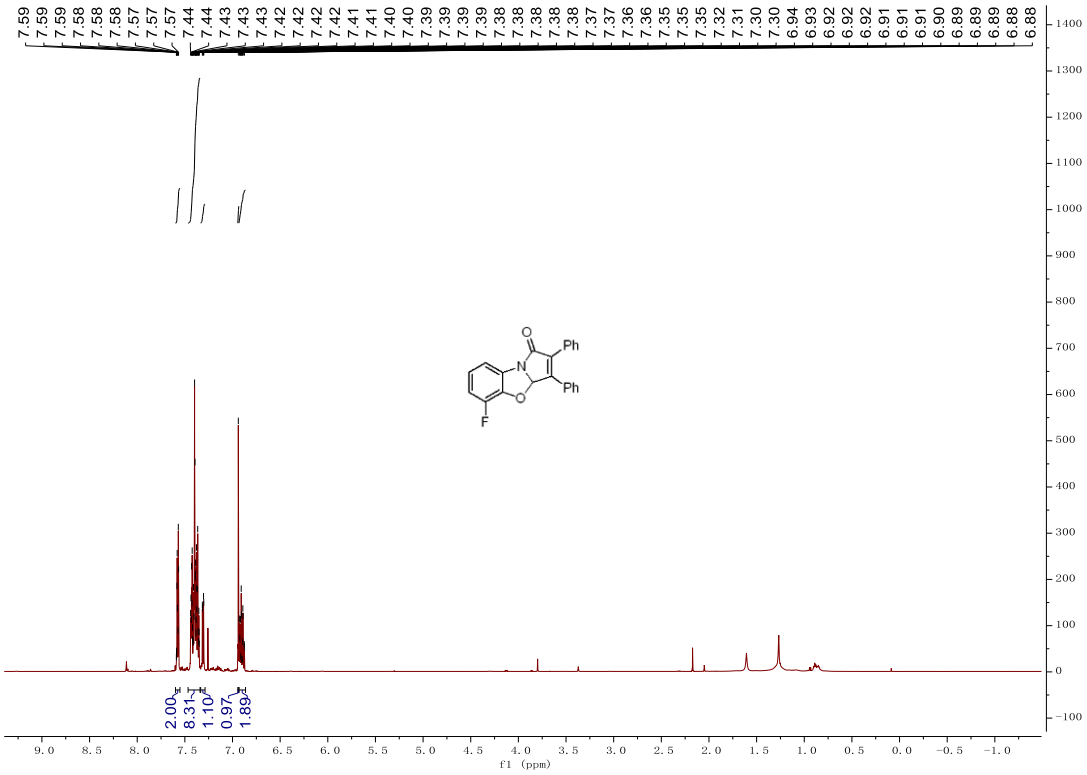
^{1}H NMR (**3pa**) (600 MHz, Chloroform-*d*)



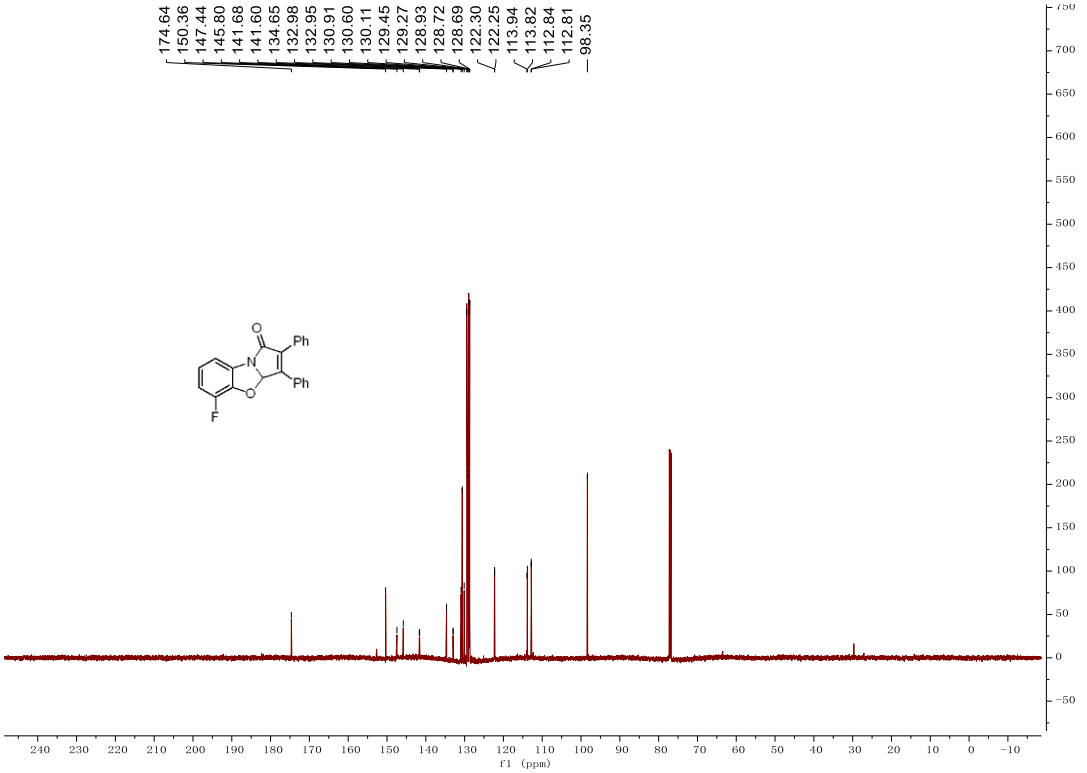
^{13}C NMR (**3pa**) (150 MHz, Chloroform-*d*)



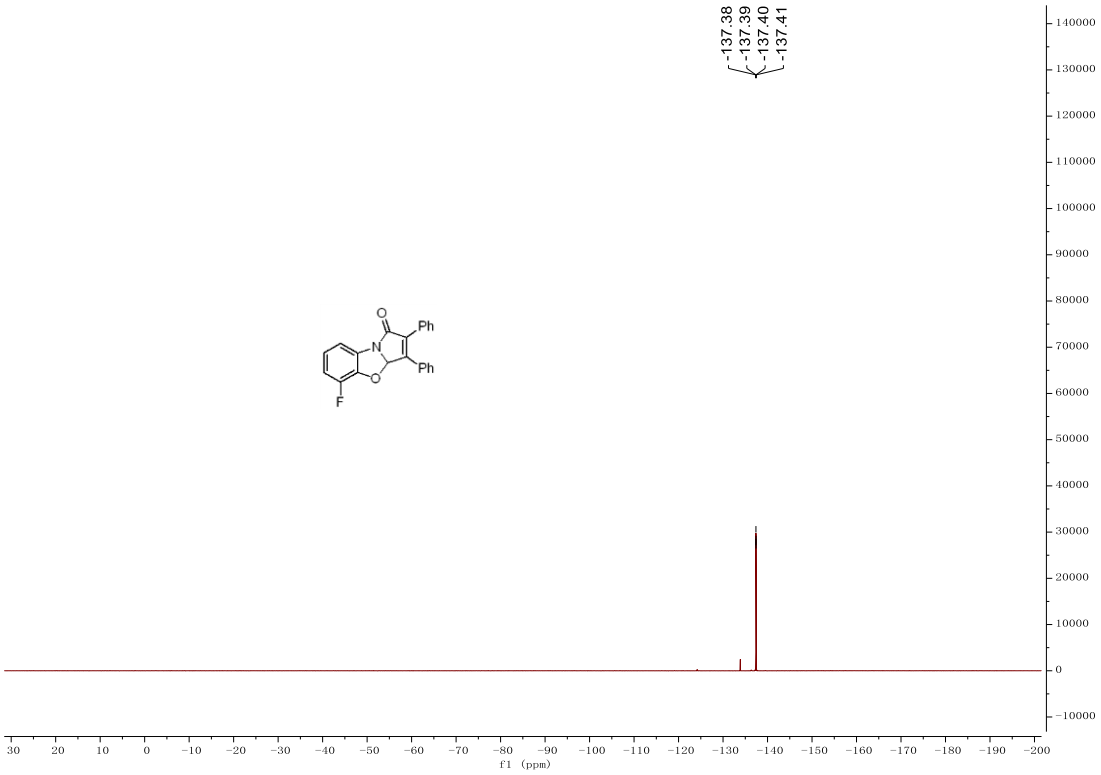
^{1}H NMR (**3qa**) (600 MHz, Chloroform-*d*)



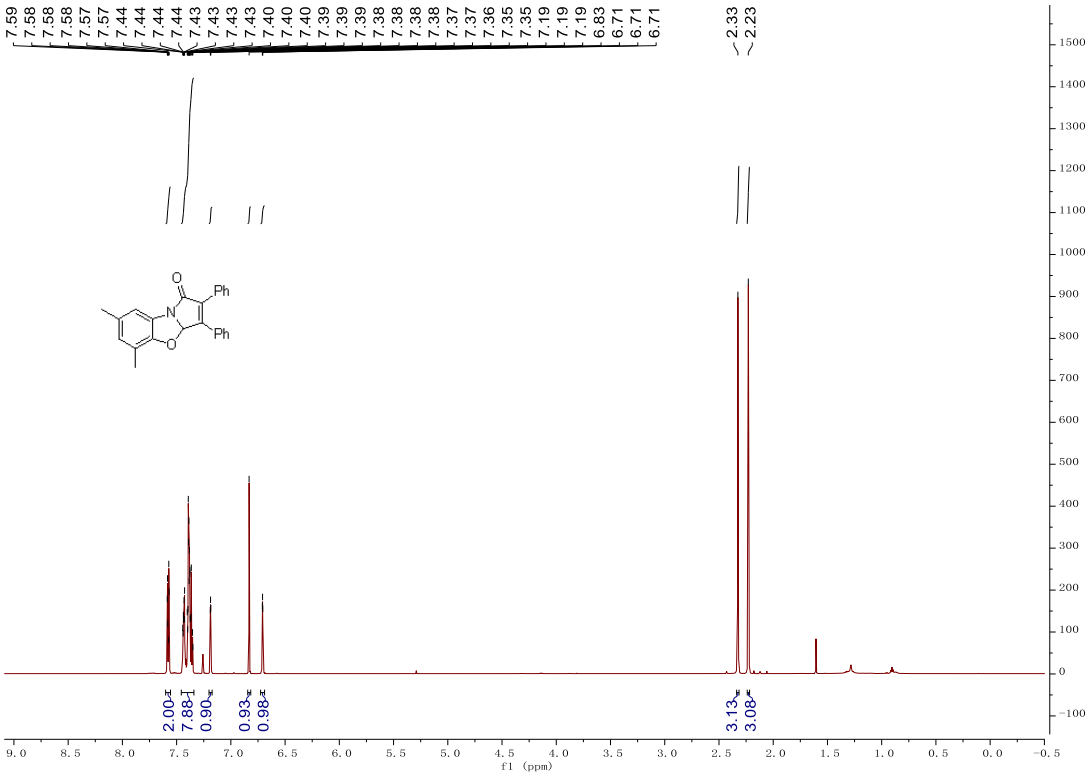
^{13}C NMR (**3qa**) (150 MHz, Chloroform-*d*)



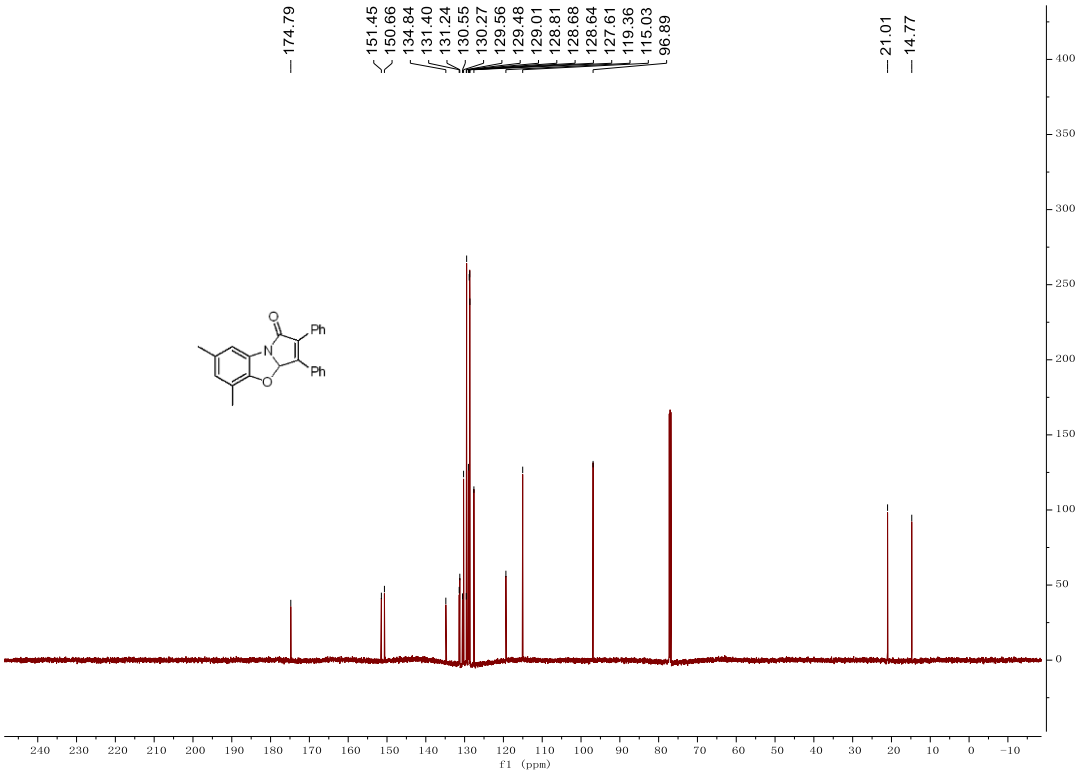
^{19}F NMR (**3qa**) (564 MHz, Chloroform-*d*)



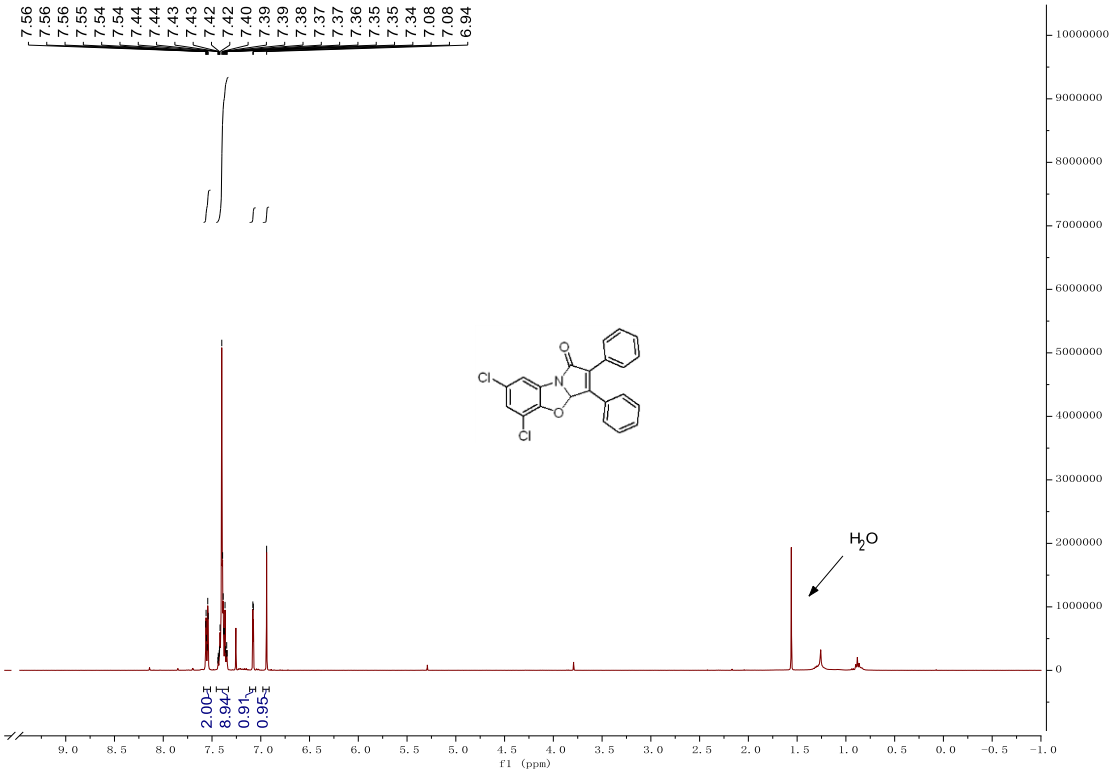
^{1}H NMR (**3ra**) (600 MHz, Chloroform-*d*)



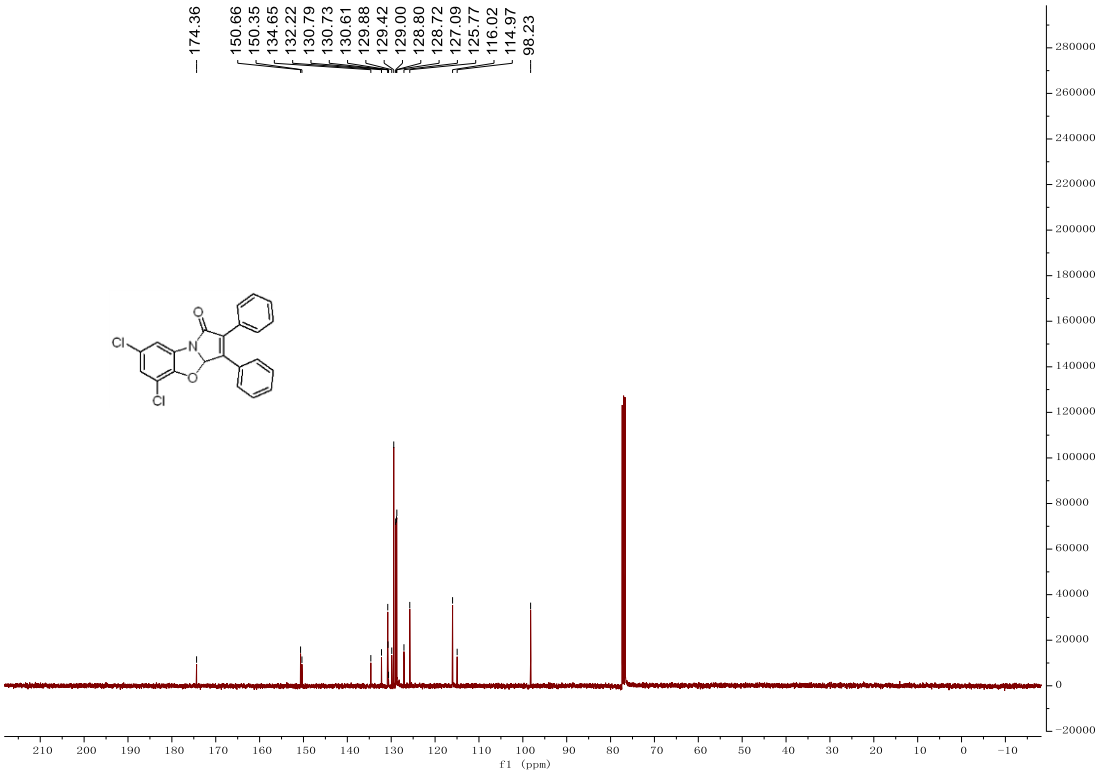
^{13}C NMR (**3ra**) (150 MHz, Chloroform-*d*)



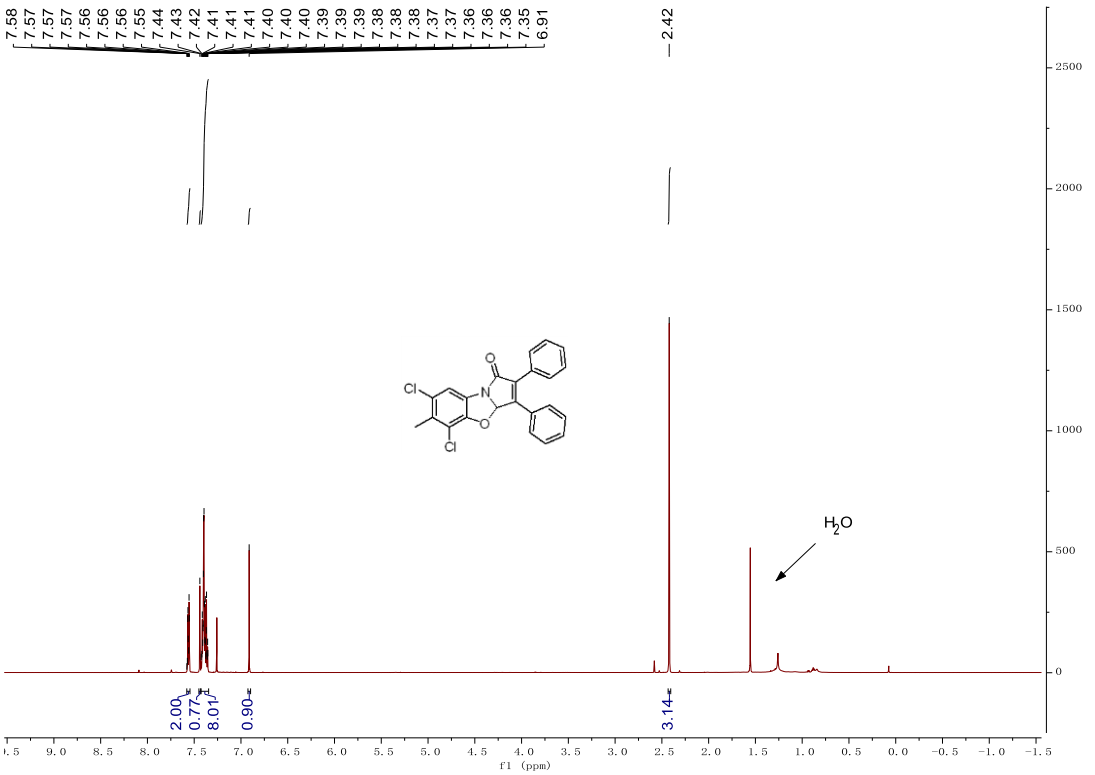
^{1}H NMR (**3sa**) (600 MHz, Chloroform-*d*)



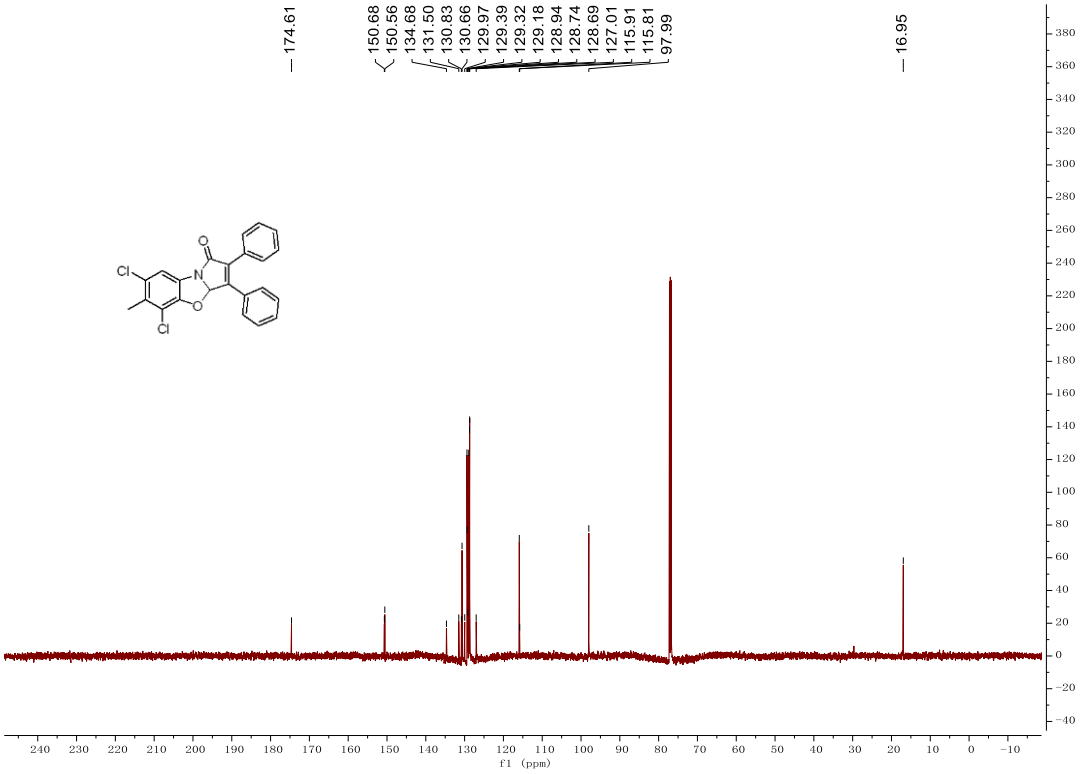
^{13}C NMR (**3sa**) (150 MHz, Chloroform-*d*)



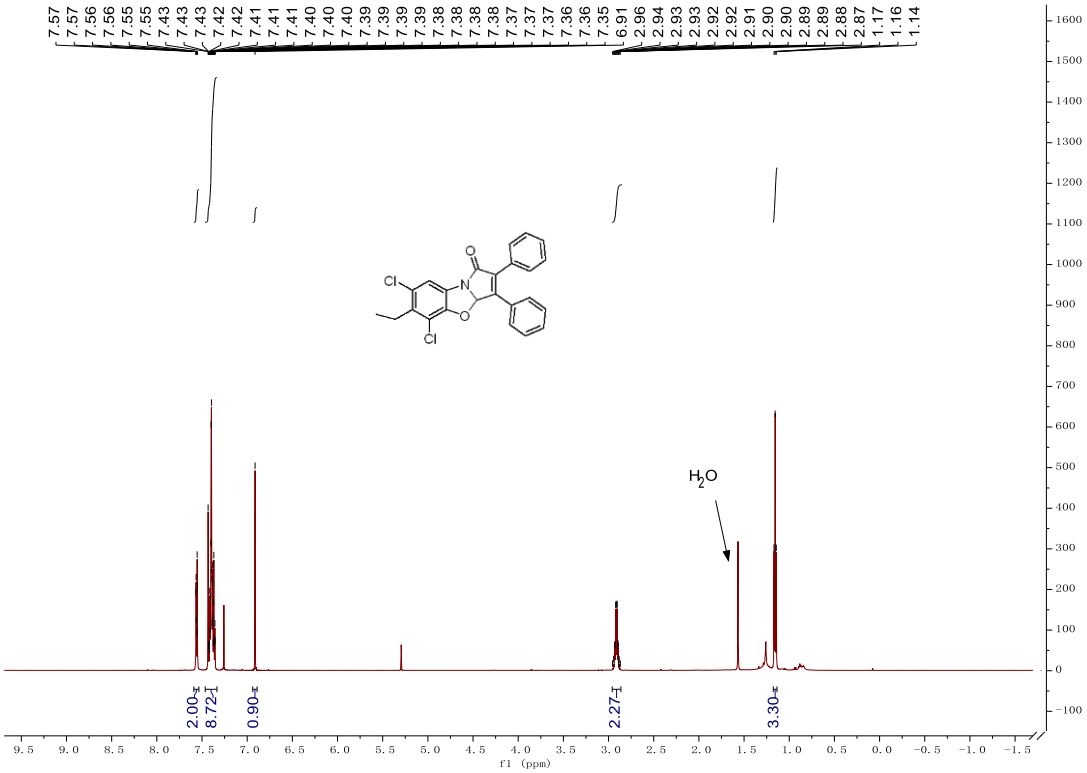
^{1}H NMR (**3ta**) (600 MHz, Chloroform-*d*)



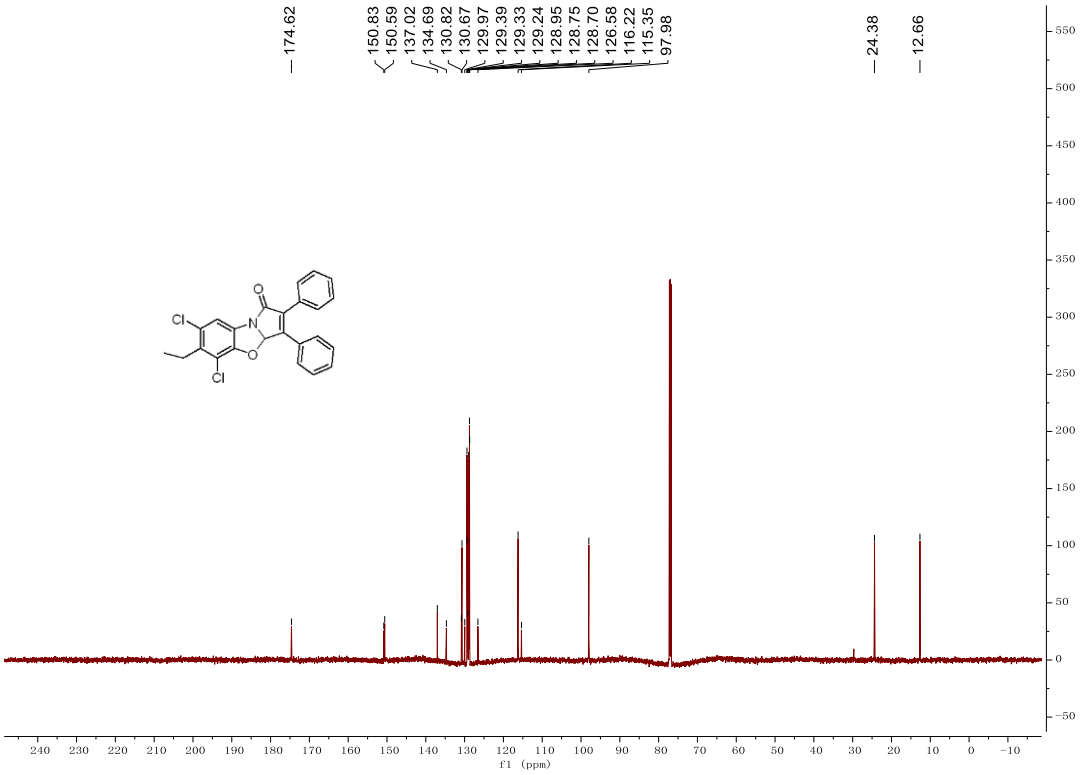
^{13}C NMR (**3ta**) (150 MHz, Chloroform-*d*)



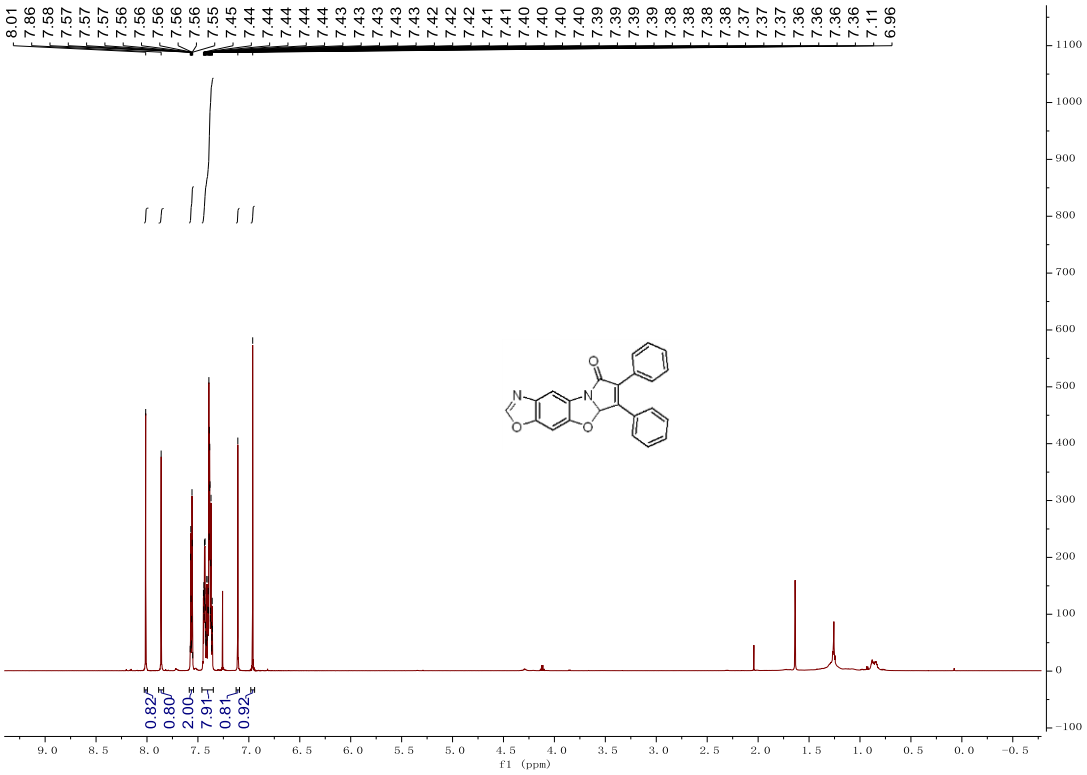
^{1}H NMR (**3ua**) (600 MHz, Chloroform-*d*)



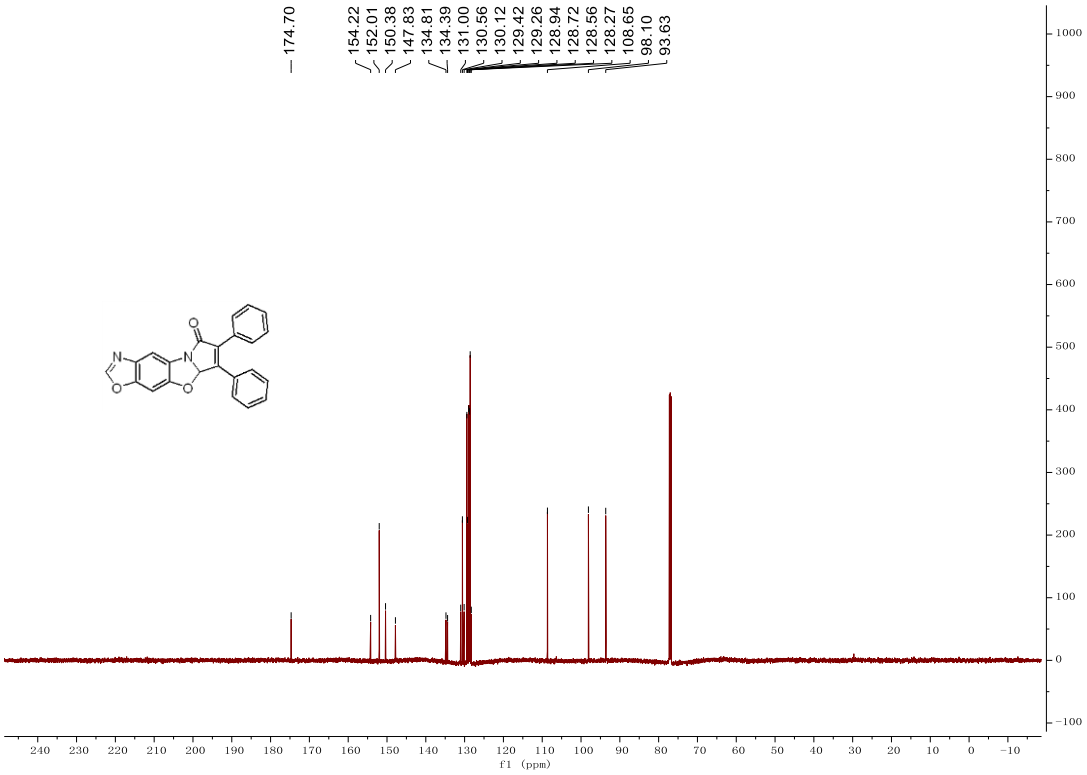
^{13}C NMR (**3ua**) (150 MHz, Chloroform-*d*)



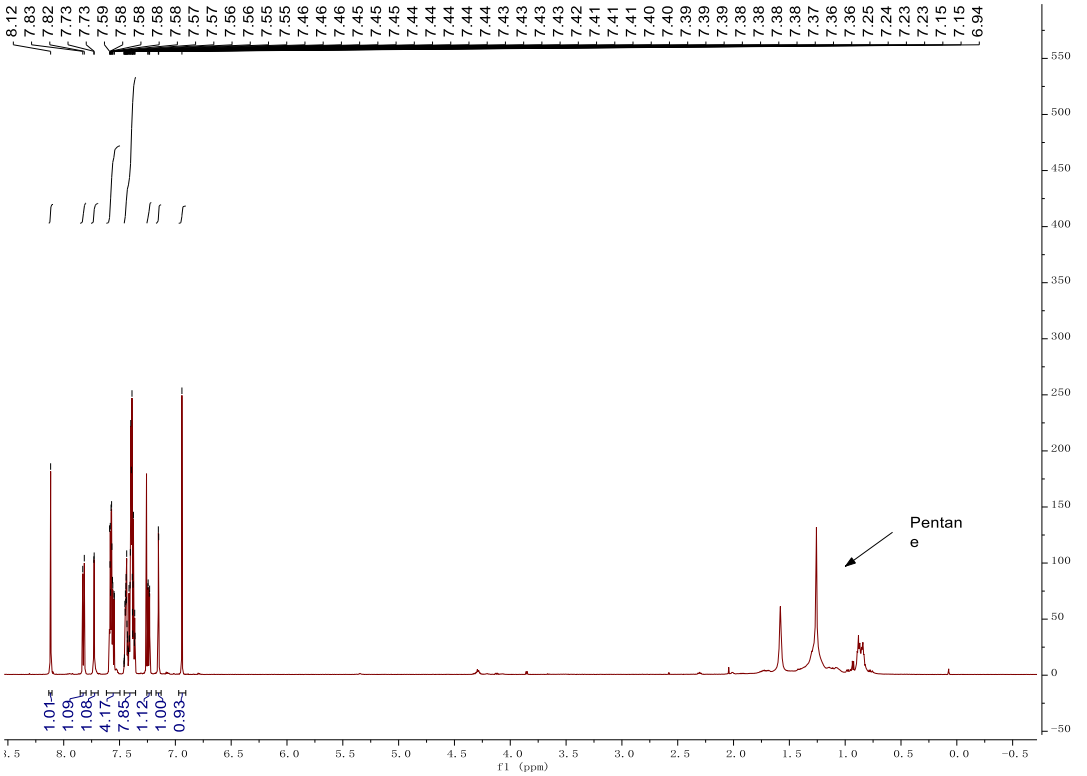
^{1}H NMR (**3va**) (600 MHz, Chloroform-*d*)



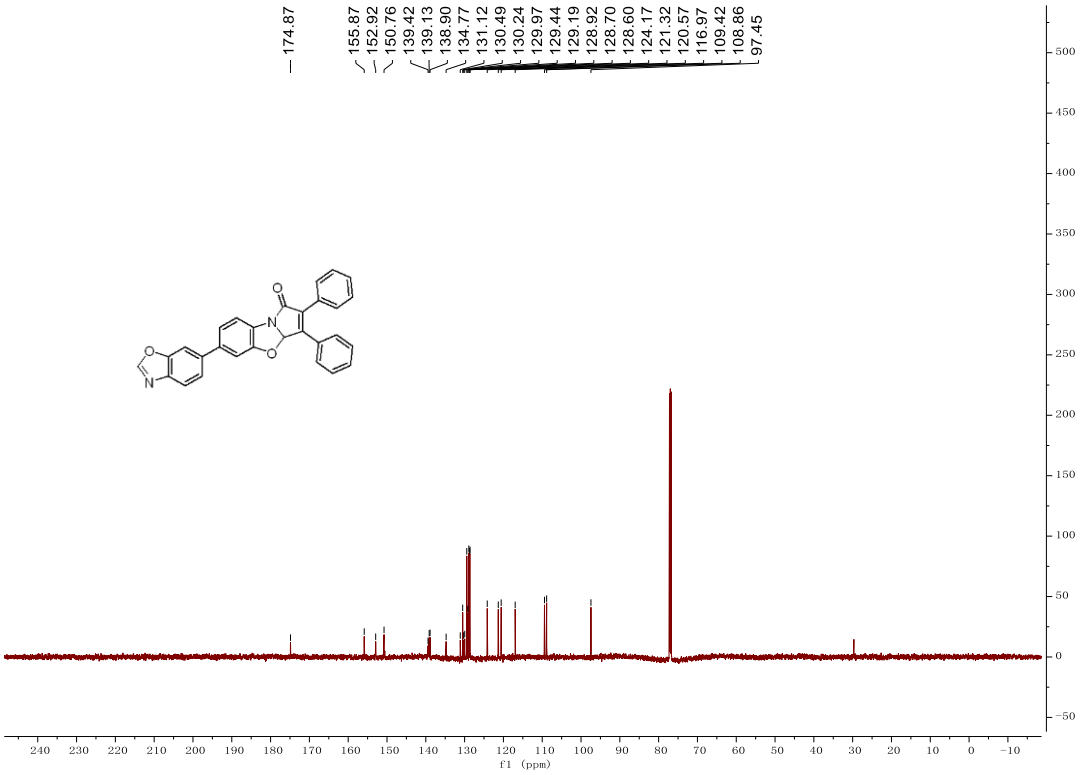
^{13}C NMR (**3va**) (150 MHz, Chloroform-*d*)



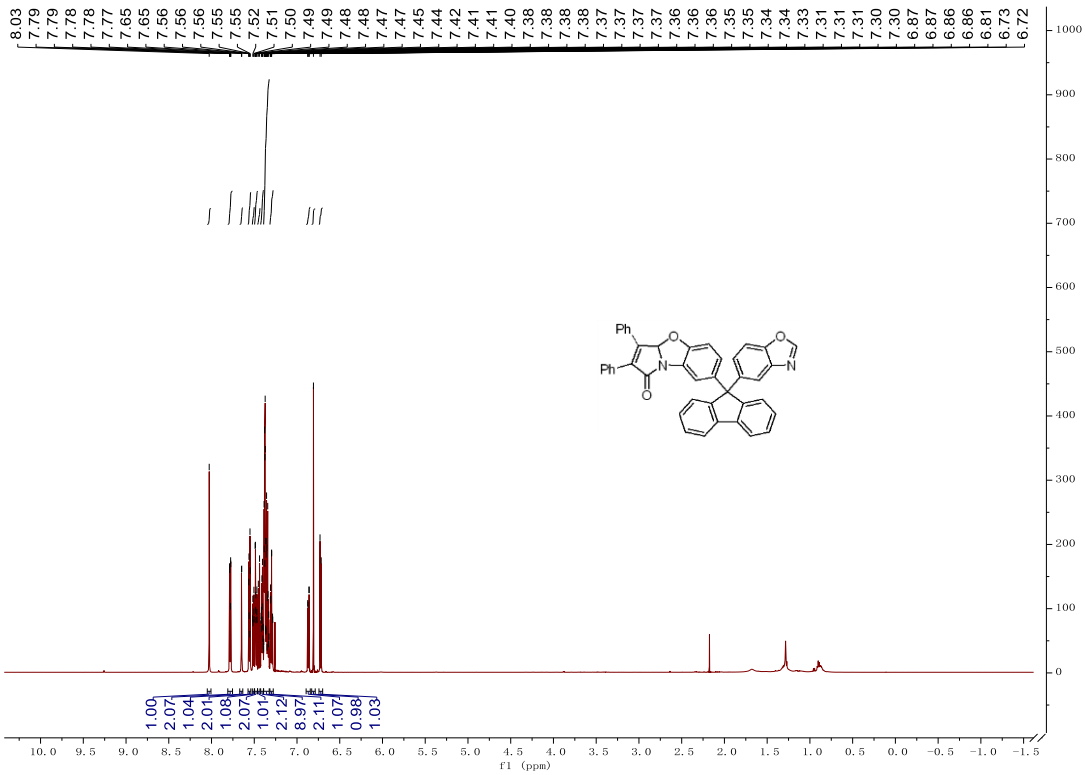
^{1}H NMR (**3wa**) (600 MHz, Chloroform-*d*)



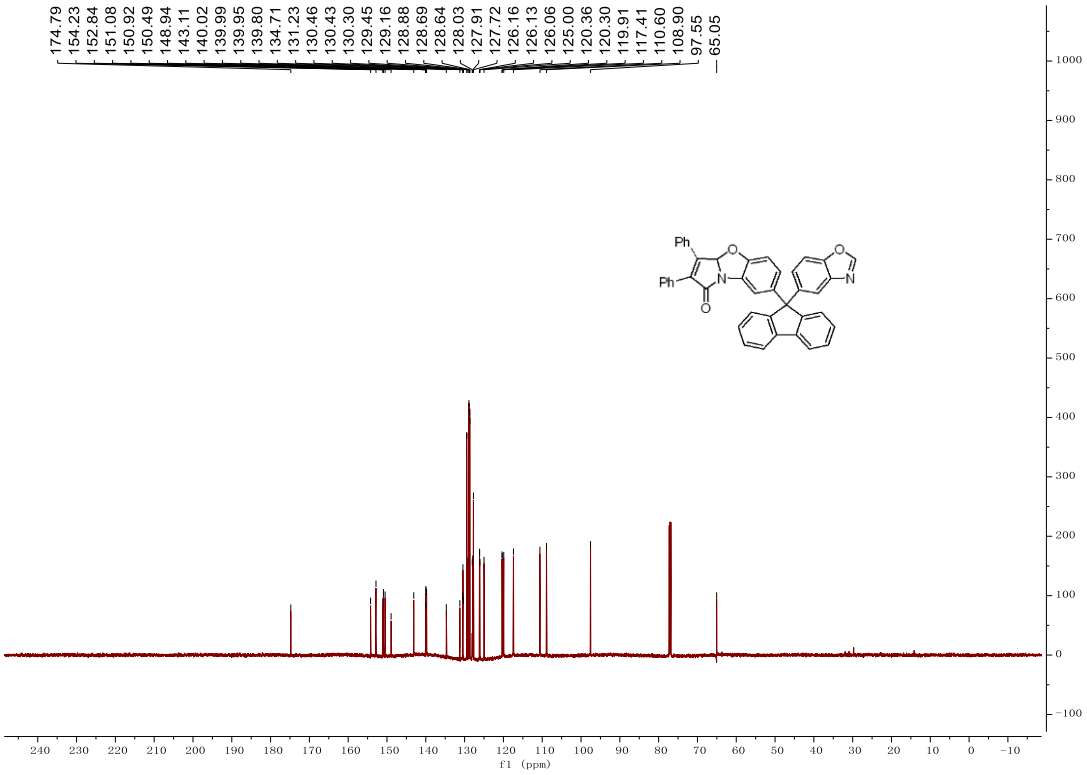
^{13}C NMR (**3wa**) (150 MHz, Chloroform-*d*)



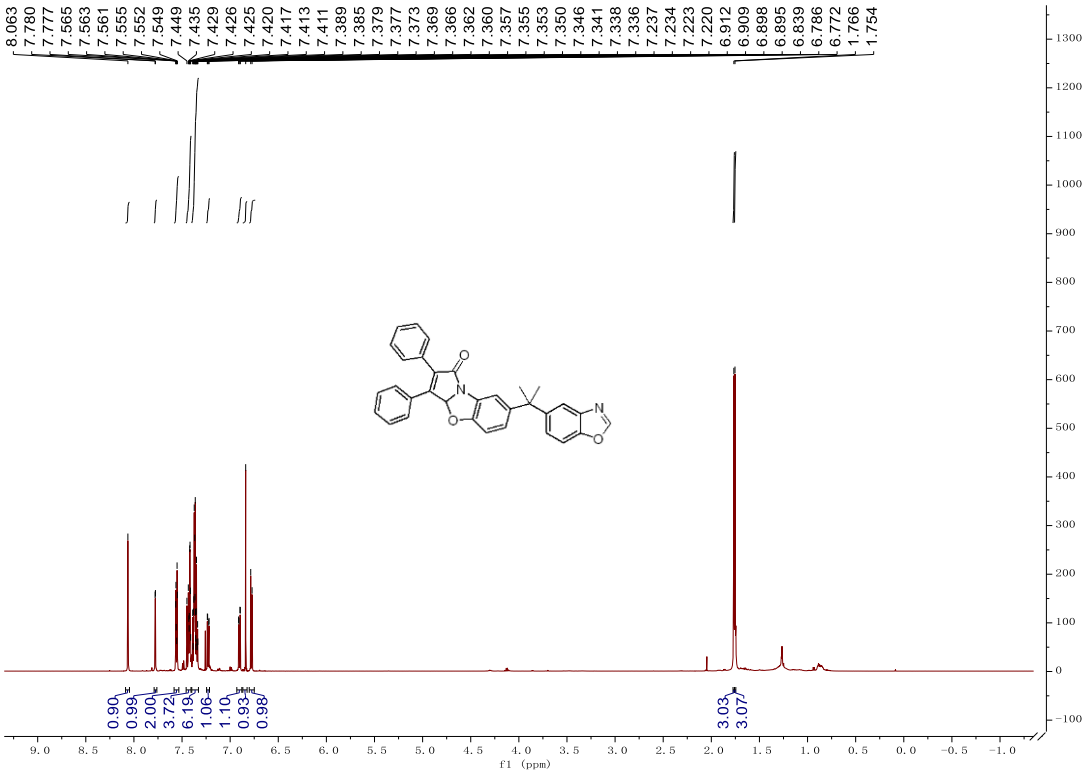
^{1}H NMR (**3xa**) (600 MHz, Chloroform-*d*)



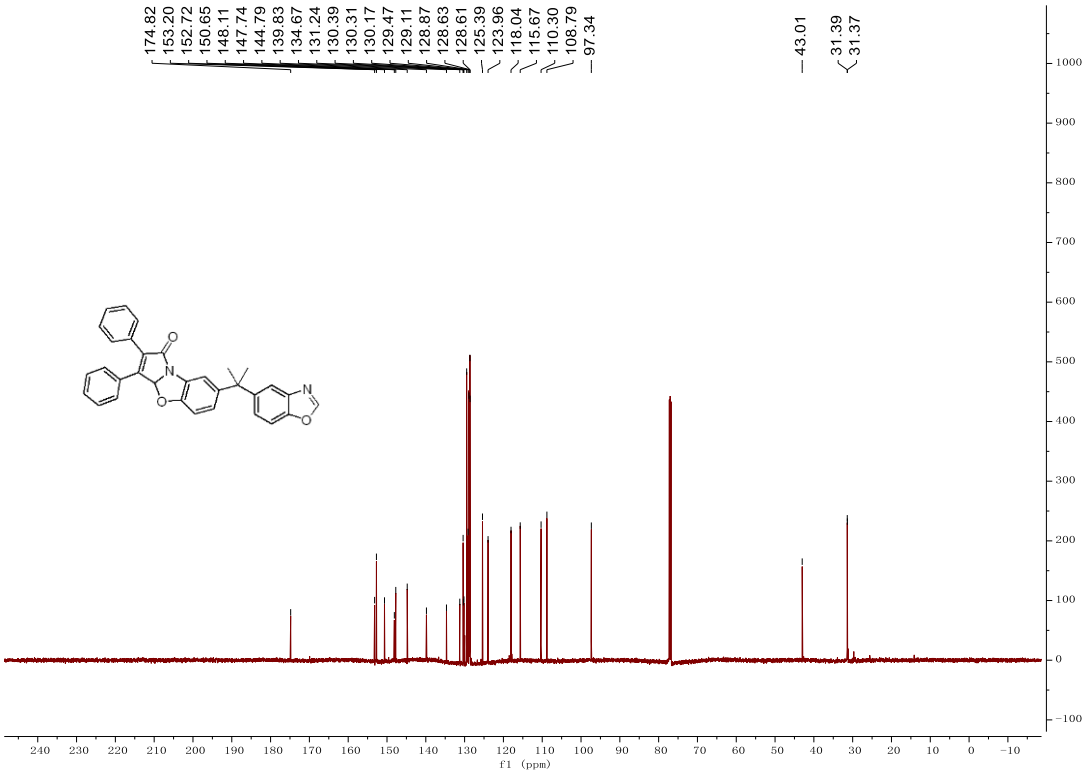
^{13}C NMR (**3xa**) (150 MHz, Chloroform-*d*)



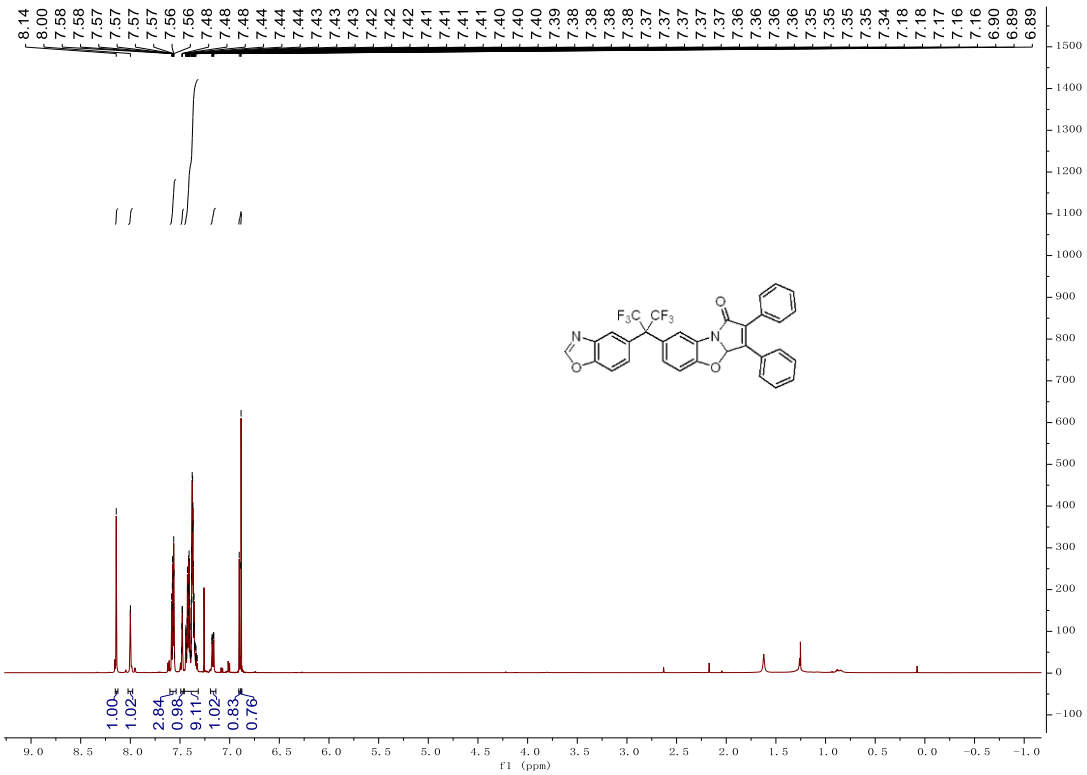
^{1}H NMR (**3ya**) (600 MHz, Chloroform-*d*)



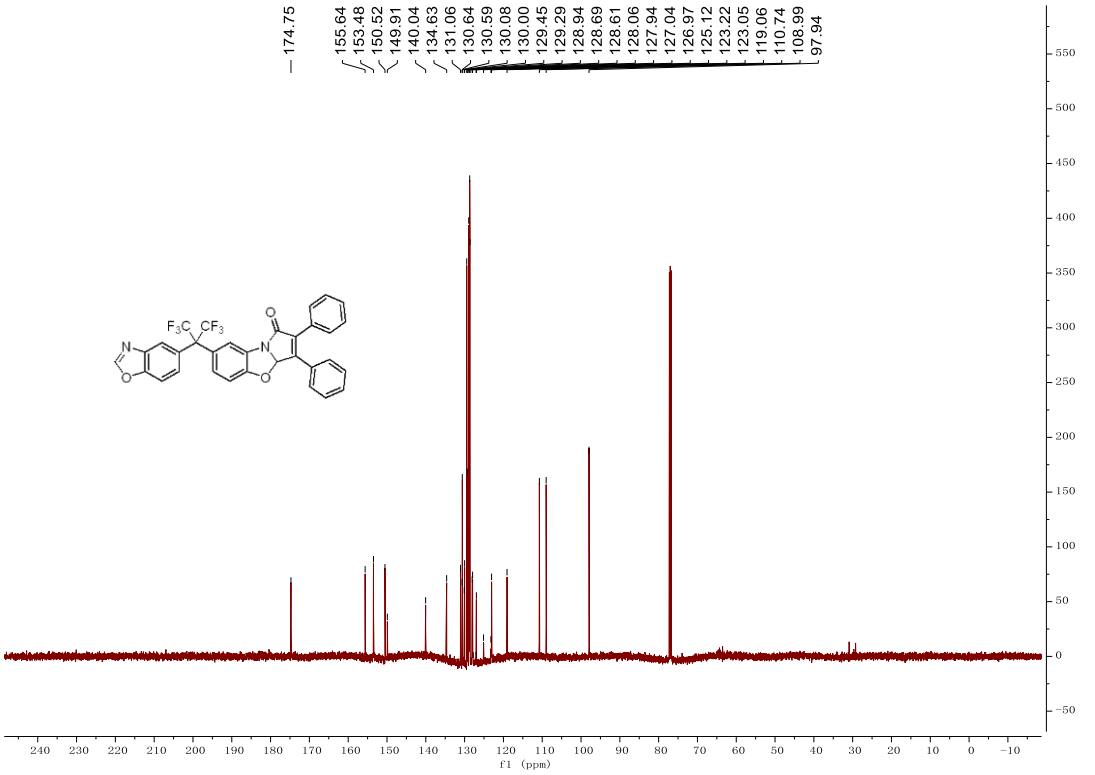
^{13}C NMR (**3ya**) (150 MHz, Chloroform-*d*)



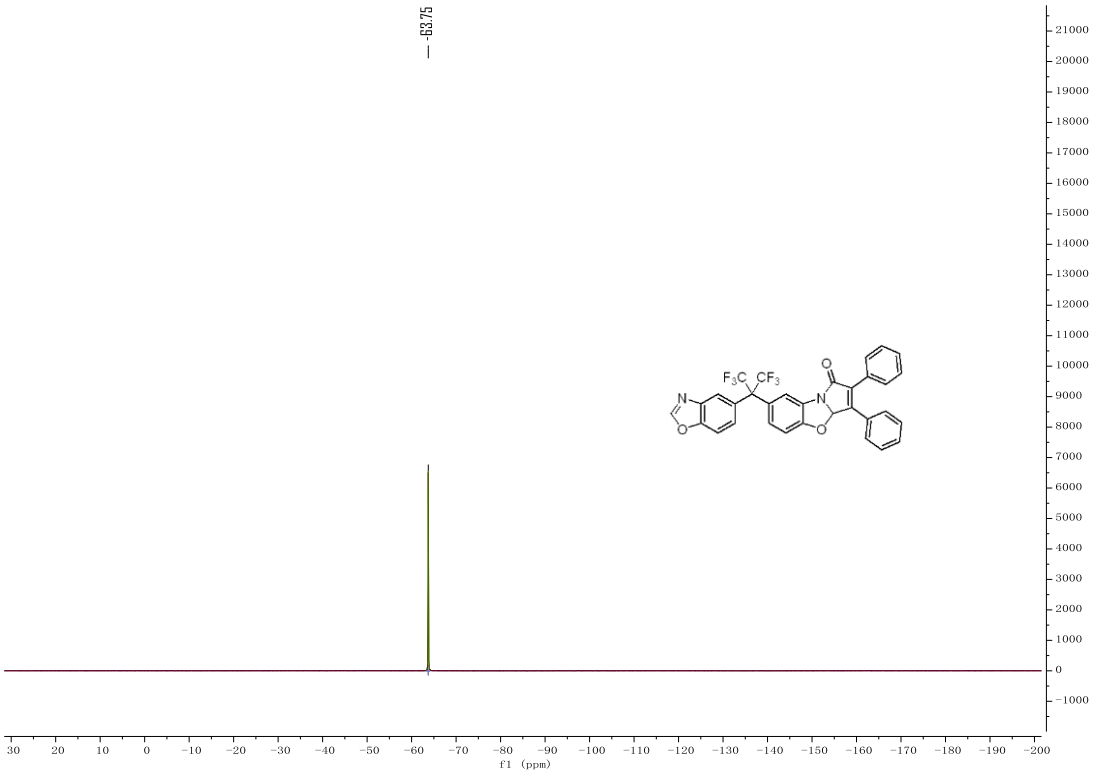
^{1}H NMR (**3za**) (600 MHz, Chloroform-*d*)



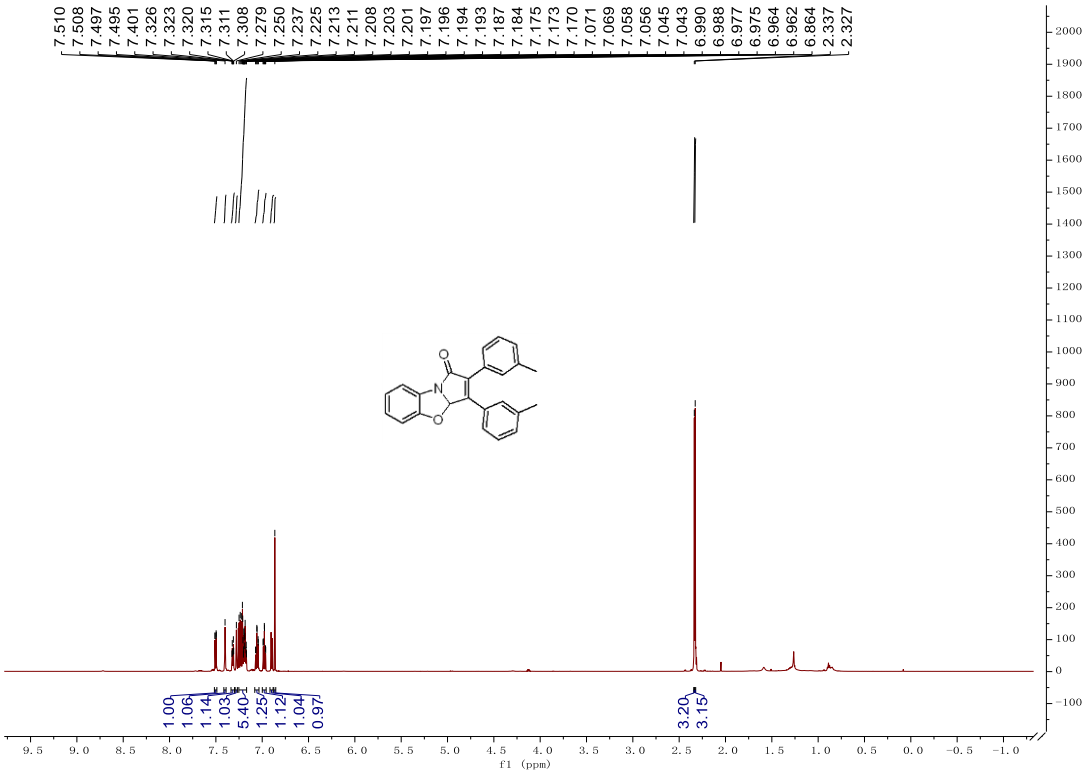
^{13}C NMR (**3za**) (150 MHz, Chloroform-*d*)



^{19}F NMR (**3za**) (564 MHz, Chloroform-*d*)



^{1}H NMR (**3bb**) (600 MHz, Chloroform-*d*)



^{13}C NMR (**3bb**) (150 MHz, Chloroform-*d*)