Supporting Information for

A Copper-Catalyzed Tandem Reaction for the Construction of Coumarin Fused 9*H*-Pyrrolo[1,2-*a*]indoles

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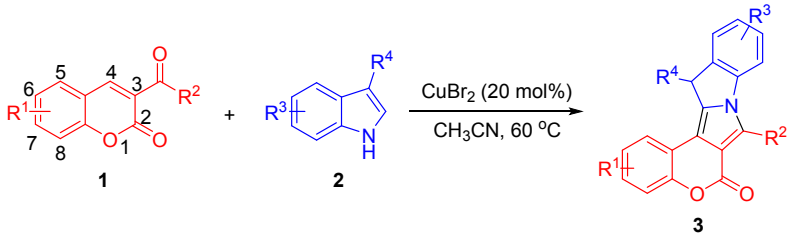
Table of Contents

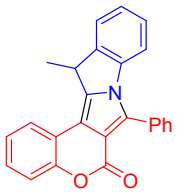
1. General methods

NMR spectra were recorded with tetramethylsilane as the internal standard. ^{1}H NMR spectra were recorded at 400 MHz, and ^{13}C NMR spectra were recorded at 100 MHz (Bruker Avance). ^{1}H NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm). ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.00 ppm). Data are given as: s (singlet), d (doublet), t (triplet), q (quartet), dd (double of doublet), br (broad) or m (multiplets), coupling constants (Hz) and integration. Flash column chromatography was carried out using silica gel eluting with ethyl acetate and petroleum ether. High resolution mass spectra were obtained with the Q-TOF-Premier mass spectrometer. Reactions were monitored by TLC and visualized with ultraviolet light. IR spectra were recorded on a ThermoFisherNicolet Avatar 360 FTIR spectrometer on a KBr beamsplitter. All the solvents were used directly without any purification.

2. Experimental data for products 3

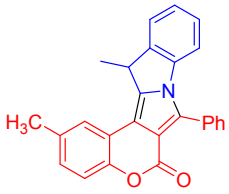


General procedure： To a 5.0 mL vial were successively added 3-arylcarbonyl coumarin **1** (0.16 mmol), 3-alkyl indole **2** (0.24 mmol), $CuBr_2$ (7.1 mg, 0.032 mmol) and 1.0 mL CH_3CN. The resulting mixture was stirred at 60 °C till almost full consumption of **1** monitored by thin layer chromatography, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding products **3**. For products **3e**, **3g** and **3k-n**, the precipitate was generated, and only a simple filtration was needed to purify the product.



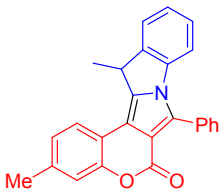
13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3a**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 52.9 mg, 91% yield; reaction time = 17 h; mp 201.0-202.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (t, *J* = 8.0 Hz, 1H), 7.55 (s, 2H), 7.44 (d, *J* = 4.0 Hz, 3H), 7.36 (d, *J* = 4.0 Hz, 1H), 7.22-7.09 (m, 4H), 7.01 (t, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 4.29 (q, *J* = 8.0 Hz, 1H), 1.63 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 150.2, 140.7, 137.7, 133.1, 129.8, 129.5, 128.4, 128.3, 127.3, 126.7, 126.1, 124.8, 124.1, 122.9, 122.7, 116.4, 116.0, 113.2, 112.4, 109.0, 34.5, 16.9. IR (KBr) *v* 3441, 3058, 2982, 2931, 1732, 1609, 1469, 1402, 1300, 1154, 1082, 970, 743 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}NNaO_2$ $[M+Na]^+$ 386.1151, found 386.1144.



2,13-dimethyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3b**)

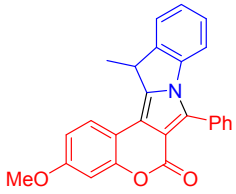
Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 40.0 mg, 66% yield; reaction time = 23 h; mp 208.1-209.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 2H), 7.56-7.54 (m, 4H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.24-7.21 (m, 2H), 7.14-7.09 (m, 2H), 6.86 (d, *J* = 8.0 Hz, 1H), 4.45 (q, *J* = 8.0 Hz, 1H), 2.46 (s, 3H), 1.76 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.4, 141.8, 138.9, 134.0, 133.4, 131.0, 130.6, 129.6, 129.5, 128.4, 128.1, 127.8, 125.8, 125.2, 123.9, 117.3, 116.8, 114.4, 113.5, 110.2, 35.6, 21.2, 18.1. IR (KBr) *v* 3432, 3058, 3030, 2982, 2926, 1726, 1610, 1472, 1404, 1374, 1291, 1184, 1098, 995, 919, 805, 745, 696 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{20}NO_2$ $[M+H]^+$ 378.1489, found 378.1486.



3,13-dimethyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3c**)

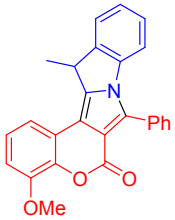
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 37.8 mg, 63% yield; reaction time = 40 h; mp 145.4-146.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.57 (d, *J* = 8.0 Hz, 3H), 7.46 (d, *J* = 4.0 Hz, 3H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.15 (dd, $J_1 = J_2 = 8.0$ Hz, 1H), 7.03 (dd, $J_1 = J_2 = 8.0$ Hz, 3H), 6.79 (d, *J* = 8.0 Hz, 1H), 4.33 (q, *J* = 8.0 Hz, 1H), 2.34 (s, 3H), 1.66 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 151.3, 141.9, 138.9, 137.6,

133.6, 130.9, 130.6, 130.5, 129.6, 129.4, 128.4, 127.7, 125.8, 125.2, 124.9, 123.5, 117.8, 114.4, 113.5, 110.0, 35.6, 21.4, 18.0. IR (KBr) *v* 3053, 2958, 2922, 2853, 1726, 1618, 1577, 1468, 1445, 1406, 1088, 1071, 975, 857, 773, 695 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{20}NO_2$ $[M+H]^+$ 378.1489, found 378.1471.



3-methoxy-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3d**)

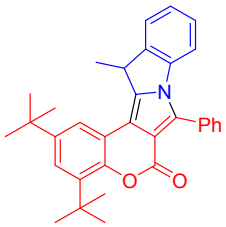
Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 40:1 to 10:1); 40.3 mg, 64% yield; reaction time = 64 h; mp 164.8-165.6 °C; ^1H NMR (400 MHz, $CDCl_3$), δ 7.65 (d, *J* = 8.0 Hz, 3H), 7.54 (t, *J* = 4.0 Hz, 3H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 3H), 4.39 (q, *J* = 8.0 Hz, 1H), 3.84 (s, 3H), 1.73 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.4, 141.9, 138.9, 132.8, 130.9, 130.6, 130.5, 129.6, 129.4, 128.3, 127.7, 125.7, 125.2, 124.5, 114.5, 113.5, 111.5, 110.1, 109.4, 102.1, 55.6, 35.5, 18.1. IR (KBr) *v* 3352, 3059, 2971, 2931, 1732, 1615, 1500, 1471, 1412, 1239, 1157, 1099, 1034, 752 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{20}NO_3$ $[M+H]^+$ 394.1438, found 394.1422.



4-methoxy-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3e**)

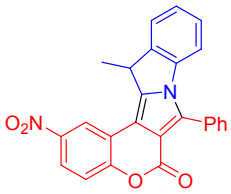
Light pink solid obtained by filtration of the precipitate; 40.9 mg, 65% yield; reaction time = 38 h; mp 248.5-249.3 °C; ^1H NMR (400 MHz, $CDCl_3$), δ 7.64 (d, *J* = 4.0 Hz, 2H), 7.52 (t, *J* = 4.0 Hz, 3H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.35 (d, *J* = 4.0 Hz, 1H), 7.20 (q, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 8.0 Hz, 1H), 6.87 (t, *J* = 8.0 Hz, 2H), 4.40 (q, *J* = 8.0 Hz, 1H), 3.93 (s, 3H), 1.73 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 148.1, 141.9, 140.9, 138.9, 134.4, 131.0, 130.6, 129.5, 129.4, 128.3, 127.7, 125.8, 125.2, 123.8, 117.9, 115.6, 114.5, 113.5, 110.0, 109.8, 56.2, 35.6, 18.2. IR (KBr) *v* 3435, 3063, 2971, 2936, 2837, 1729, 1609, 1475, 1409, 1295, 1270, 1210, 1179, 1162,

1110, 1055, 995, 767 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{20}NO_3$ $[M+H]^+$ 394.1438, found 394.1427.



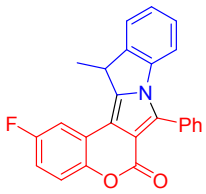
2,4-di-*tert*-butyl-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3f**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 53.3 mg, 70% yield; reaction time = 22 h; mp 222.4-223.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.61 (dd, $J_1 = J_2 = 4.0$ Hz, 3H), 7.48-7.41 (m, 4H), 7.31 (d, $J = 4.0$ Hz, 1H), 7.15 (t, $J = 8.0$ Hz, 1H), 7.06 (t, $J = 8.0$ Hz, 1H), 6.87 (d, $J = 8.0$ Hz, 1H), 4.39 (q, $J = 8.0$ Hz, 1H), 1.71 (d, $J = 4.0$ Hz, 3H), 1.46 (s, 9H), 1.36 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5, 146.7, 144.7, 140.9, 138.0, 136.7, 132.7, 129.7, 129.1, 128.6, 128.2, 127.2, 126.7, 124.7, 124.1, 121.3, 117.6, 115.6, 114.5, 112.5, 109.1, 34.7, 34.3, 33.7, 30.6, 29.1, 16.9. IR (KBr) *v* 3443, 3055, 2958, 2871, 1735, 1607, 1474, 1394, 1361, 1268, 1182, 1158, 1096, 1042, 997, 870, 748 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{34}NO_2$ $[M+H]^+$ 476.2584, found 476.2569.



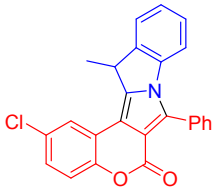
13-methyl-2-nitro-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3g**)

Yellow solid obtained by filtration of the precipitate; 59.5 mg, 91% yield; reaction time = 23 h; mp 245.5-246.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.67 (d, $J = 4.0$ Hz, 1H), 8.19 (dd, $J_1 = J_2 = 4.0$ Hz, 1H), 7.66 (s, 2H), 7.60-7.55 (m, 4H), 7.43 (d, $J = 8.0$ Hz, 1H), 7.30 (t, $J = 8.0$ Hz, 1H), 7.18 (t, $J = 8.0$ Hz, 1H), 6.90 (d, $J = 8.0$ Hz, 1H), 4.56 (q, $J = 8.0$ Hz, 1H), 1.83 (d, $J = 8.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.2, 155.2, 143.9, 141.5, 138.6, 135.5, 131.7, 130.8, 129.9, 128.8, 128.6, 128.0, 126.5, 125.4, 122.5, 119.5, 118.3, 118.0, 113.8, 112.7. 109.1, 35.7, 18.5. IR (KBr) *v* 3465, 3064, 2976, 1744, 1586, 1517, 1474, 1409, 1381, 1336, 1245, 1186, 1153, 1081, 978, 903, 809, 745, 700 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{16}N_2NaO_4$ $[M+Na]^+$ 431.1002, found 431.0995.



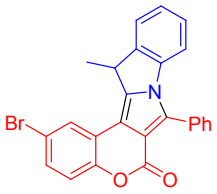
2-fluoro-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3h**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 60.4 mg, 99% yield; reaction time = 11 h; mp 191.7-192.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.57 (s, 2H), 7.49-7.46 (m, 3H), 7.43 (d, J = 8.0 Hz, 1H), 7.35 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 7.23-7.15 (m, 2H), 7.06 (t, J = 8.0 Hz, 1H), 6.95-6.90 (m, 1H), 6.79 (d, J = 8.0 Hz, 1H), 4.35 (q, J = 8.0 Hz, 1H), 1.68 (d, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 157.1 (d, J = 73.0 Hz, 1C), 146.3, 140.6, 137.7, 133.6, 129.9, 129.8, 129.5, 128.5, 128.2, 127.4, 126.8, 125.0, 124.2, 117.8 (d, J = 11.0 Hz, 1C), 117.1 (d, J = 9.0 Hz, 1C), 113.0 (d, J = 24.0 Hz, 1C), 112.6, 108.7, 108.5, 34.5, 17.0. IR (KBr) v 3451, 3063, 2980, 2929, 1735, 1609, 1474, 1404, 1375, 1288, 1246, 1189, 1142, 1101, 993, 805, 748, 698 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{16}FNNaO_2$ $[M+Na]^+$ 404.1057, found 404.1045.



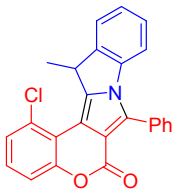
2-chloro-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3i**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 44.0 mg, 69% yield; reaction time = 10 h; mp 197.2-198.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.60 (s, 1H), 7.55 (s, 2H), 7.47-7.44 (m, 3H), 7.40 (d, J = 8.0 Hz, 1H), 7.17-7.13 (m, 3H), 7.04 (t, J = 8.0 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H), 4.33 (q, J = 8.0 Hz, 1H), 1.66 (d, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 149.7, 141.7, 138.7, 134.7, 131.0, 130.6, 129.7, 129.2, 129.0, 128.5, 127.9, 127.1, 126.1, 125.3, 123.3, 118.9, 118.6, 113.6, 113.3, 109.7, 35.6, 18.0. IR (KBr) v 3447, 3069, 2972, 2930, 1736, 1607, 1471, 1406, 1368, 1282, 1255, 1185, 1086, 983, 743 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{16}ClNNaO_2$ $[M+Na]^+$ 420.0762, found 420.0754.



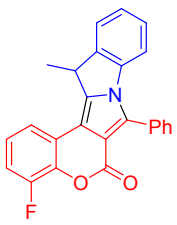
2-bromo-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3j**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 54.1 mg, 76% yield; reaction time = 10 h; mp 199.3-200.5 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.77 (d, J = 4.0 Hz, 1H), 7.56 (s, 2H), 7.48-7.46 (m, 3H), 7.42 (d, J = 8.0 Hz, 1H), 7.30 (dd, J_1 = J_2 = 4.0 Hz, 1H), 7.19-7.15 (m, 1H), 7.11 (d, J = 8.0 Hz, 1H), 7.06 (t, J = 8.0 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 4.36 (q, J = 8.0 Hz, 1H), 1.68 (d, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.1, 149.1, 140.6, 137.7, 133.6, 130.0, 129.5, 128.9, 128.6, 128.1, 127.4, 126.8, 125.2, 125.0, 124.2, 118.2, 118.0, 115.5, 112.6, 112.1, 108.7, 34.5, 17.0. IR (KBr) v 3444, 2967, 2928, 1734, 1605, 1468, 1394, 1365, 1257, 1216, 1184, 1152, 1095, 975, 811 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{16}BrNNaO_2$ $[M+Na]^+$ 464.0257, found 464.0244.



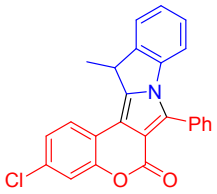
1-chloro-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3k**)

White solid obtained by filtration of the precipitate; 62.3 mg, 98% yield; reaction time = 37 h; mp 247.9-248.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.56-7.48 (m, 5H), 7.38 (d, J = 8.0 Hz, 1H), 7.22-7.14 (m, 4H), 7.01 (t, J = 8.0 Hz, 1H), 6.65 (d, J = 8.0 Hz, 1H), 4.68 (q, J = 8.0 Hz, 1H), 1.53 (d, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 152.2, 142.3, 138.4, 136.5, 131.4, 131.2, 130.3, 129.7, 128.8, 128.6, 128.4, 127.5, 127.4, 126.0, 125.9, 124.7, 117.3, 116.5, 113.6, 111.0, 40.0, 21.9. IR (KBr) v 3452, 3053, 2968, 2929, 1739, 1566, 1476, 1442, 1287, 1229, 1186, 1156, 1101, 979, 945, 756, 742 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}ClNO_2$ $[M+H]^+$ 398.0942, found 398.0938.



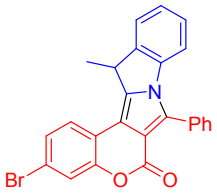
4-fluoro-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3l**)

White solid obtained by filtration of the precipitate; 53.2 mg, 87% yield; reaction time = 26 h; mp 239.3-240.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.63 (s, 2H), 7.54-7.50 (m, 5H), 7.23-7.05 (m, 4H), 6.86 (d, *J* = 8.0 Hz, 1H), 4.41 (q, *J* = 8.0 Hz, 1H), 1.73 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 150.5 (d, *J* = 248.0 Hz, 1C), 141.7, 139.5 (d, *J* = 11.0 Hz, 1C), 138.7, 134.7, 131.2, 130.7 (d, *J* = 28.0 Hz, 1C), 129.6, 129.2, 128.4, 127.8, 126.1, 125.2, 123.7 (d, *J* = 7.0 Hz, 1C), 119.3, 118.8 (d, *J* = 4.0 Hz, 1C), 113.9, 113.8, 113.6, 109.6, 35.6, 18.0. IR (KBr) *v* 3442, 3059, 2970, 1729, 1621, 1476, 1398, 1302, 1260, 1183, 1158, 1098, 1066, 1043, 1001, 745 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}FNO_2$ $[M+H]^+$ 382.1238, found 381.1240.



3-chloro-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3m**)

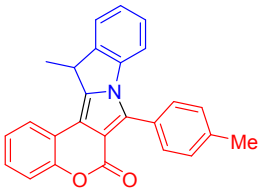
White solid obtained by filtration of the precipitate; 49.1 mg, 77% yield; reaction time = 22 h; mp 244.7-245.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.63 (s, 2H), 7.55-7.51 (m, 3H), 7.48 (d, *J* = 4.0 Hz, 1H), 7.30 (d, *J* = 4.0 Hz, 1H), 7.25-7.22 (m, 2H), 7.13 (t, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 4.40 (q, *J* = 8.0 Hz, 1H), 1.73 (d, *J* = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 151.6, 141.7, 138.7, 134.3, 132.4, 131.0, 130.9, 130.6, 129.6, 129.2, 128.4, 127.9, 126.0, 125.2, 124.5, 124.2, 117.8, 115.8, 113.6, 109.5, 35.6, 18.0. IR (KBr) *v* 3442, 3065, 2980, 2935, 1740, 1608, 1472, 1407, 1376, 1294, 1156, 1100, 1021, 973, 747 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}ClNO_2$ $[M+H]^+$ 398.0942, found 398.0933.



3-bromo-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3n**)

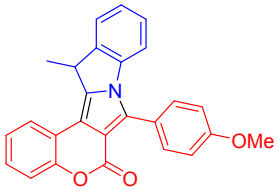
White solid obtained by filtration of the precipitate; 55.6 mg, 79% yield; reaction time = 22 h; mp 260.5-261.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.63 (s, 2H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.54-7.53 (m, 3H), 7.47 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 2H), 7.37 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 8.0 Hz, 1H), 4.39 (q, *J* = 8.0 Hz, 1H), 1.73 (d, *J* =

4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 151.6, 141.7, 138.7, 134.4, 131.1, 130.9, 130.6, 129.6, 129.2, 128.4, 127.9, 127.1, 126.1, 125.2, 124.8, 120.7, 119.9, 116.3, 113.6, 109.6, 35.6, 17.9. IR (KBr) *v* 3449, 3064, 2980, 1740, 1606, 1470, 1407, 1372, 1293, 1156, 1099, 1061, 972, 748 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}BrNO_2$ $[M+H]^+$ 442.0437, found 442.0424.



13-methyl-7-(p-tolyl)-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3o**)

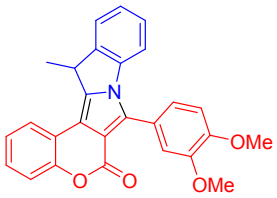
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 90:1 to 60:1); 39.4 mg, 65% yield; reaction time = 70 h; mp 202.8-203.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.74 (dd, $J_1 = J_2 = 4.0$ Hz, 1H), 7.52 (d, $J = 4.0$ Hz, 2H), 7.46 (d, $J = 8.0$ Hz, 1H), 7.34-7.23 (m, 5H), 7.20 (t, $J = 8.0$ Hz, 1H), 7.11 (t, $J = 8.0$ Hz, 1H), 6.92 (d, $J = 8.0$ Hz, 1H), 4.38 (q, $J = 8.0$ Hz, 1H), 2.47 (s, 3H), 1.72 (d, $J = 8.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 151.3, 141.8, 139.5, 138.9, 134.0, 130.9, 130.5, 129.2, 127.7, 127.2, 126.5, 125.8, 125.2, 123.9, 123.8, 117.5, 117.2, 114.3, 113.6, 110.0, 35.6, 21.6, 18.1. IR (KBr) *v* 3050, 2964, 2924, 1733, 1608, 1539, 1461, 1409, 1388, 1294, 1259, 1211, 1080, 970, 830, 759, 742 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{20}NO_2$ $[M+H]^+$ 378.1489, found 378.1488.



7-(4-methoxyphenyl)-13-methyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3p**)

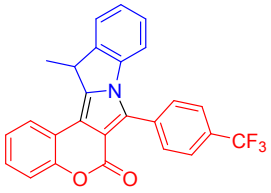
White solid obtained by column chromatography (petroleum ether/ethyl acetate = 40:1 to 25:1); 46.5 mg, 74% yield; reaction time = 63 h; mp 202.8-203.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.75 (dd, $J_1 = J_2 = 4.0$ Hz, 1H), 7.56 (d, $J = 8.0$ Hz, 2H), 7.46 (d, $J = 8.0$ Hz, 1H), 7.31-7.24 (m, 3H), 7.21 (t, $J = 8.0$ Hz, 1H), 7.12 (t, $J = 8.0$ Hz, 1H), 7.05 (d, $J = 8.0$ Hz, 2H), 6.93 (d, $J = 8.0$ Hz, 1H), 4.38 (q, $J = 8.0$ Hz, 1H), 3.90 (s, 3H), 1.72 (d, $J = 4.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 158.9, 151.3, 141.8, 138.9, 133.9, 132.3, 130.7, 127.8, 127.2, 125.8, 125.2, 123.9, 123.8, 121.5, 117.5, 117.2, 114.2, 113.9, 113.6, 109.9, 55.4, 35.6, 18.1. IR (KBr) *v* 3435, 2933, 2834, 1724, 1608, 1469, 1397, 1290, 1248, 1174, 1112, 1086, 970, 843, 753 cm^{-1}. HRMS (ESI) calcd

for $C_{26}H_{20}NO_3$ $[M+H]^+$ 394.1438, found 394.1429.



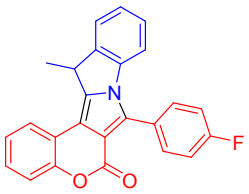
7-(3,4-dimethoxyphenyl)-13-methyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3q**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 30:1 to 5:1); 33.8 mg, 50% yield; reaction time = 36 h; mp 142.7-143.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.77 (t, *J* = 4.0 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.34-7.22 (m, 5H), 7.17-7.13 (m, 2H), 7.04 (d, *J* = 8.0 Hz, 1H), 6.98 (s, 1H), 4.43 (q, *J* = 8.0 Hz, 1H), 3.99 (s, 3H), 3.90 (s, 3H), 1.76 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 151.3, 150.0, 148.6, 141.8, 138.9, 133.9, 130.7, 127.8, 127.2, 125.8, 125.2, 123.9, 123.8, 123.3, 121.7, 117.6, 117.2, 114.2, 114.0, 113.6, 111.0, 109.9, 56.1, 55.9, 35.6, 18.0. IR (KBr) *v* 3423, 3064, 2962, 2931, 1733, 1608, 1501, 1470, 1414, 1303, 1260, 1151, 1093, 1028, 756 cm^{-1}. HRMS (ESI) calcd for $C_{27}H_{22}NO_4$ $[M+H]^+$ 424.1543, found 424.1539.



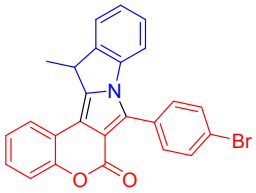
13-methyl-7-(4-(trifluoromethyl)phenyl)-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3r**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 90:1 to 60:1); 26.1 mg, 38% yield; reaction time = 40 h; mp 230.2-231.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.81-7.78 (m, 5H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.34-7.25 (m, 4H), 7.18 (t, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 4.45 (q, *J* = 8.0 Hz, 1H), 1.77 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 151.3, 141.8, 138.6, 135.0, 133.1, 131.4, 131.1, 128.6, 127.9, 127.5, 126.2, 125.4, 125.3, 124.1, 123.8, 122.7, 117.6, 116.9, 114.8, 113.4, 110.7, 35.7, 18.0. IR (KBr) *v* 3438, 3068, 2931, 1730, 1613, 1473, 1415, 1326, 1160, 1122, 1062, 974, 855, 757 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{16}F_3NO_2$ $[M+H]^+$ 432.1206, found 432.1197.



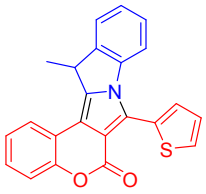
7-(4-fluorophenyl)-13-methyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3s**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 90:1 to 65:1); 42.2 mg, 69% yield; reaction time = 12 h; mp 201.5-202.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.78 (dd, $J_1 = J_2 = 4.0$ Hz, 1H), 7.64 (s, 2H), 7.51 (d, $J = 8.0$ Hz, 1H), 7.33-7.22 (m, 6H), 7.16 (t, $J = 8.0$ Hz, 1H), 6.88 (d, $J = 8.0$ Hz, 1H), 4.44 (q, $J = 8.0$ Hz, 1H), 1.76 (d, $J = 8.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.4 (d, $J = 248.0$ Hz, 1C), 158.9, 151.3, 141.8, 138.8, 134.3, 132.9, 129.4, 127.8, 127.3, 126.0, 125.5, 125.3, 124.0, 123.8, 117.6, 117.1, 115.6 (d, $J = 18.0$ Hz, 1C), 114.4, 113.4, 110.3, 35.7, 18.0. IR (KBr) *v* 3429, 3065, 2928, 1724, 1607, 1539, 1468, 1392, 1296, 1217, 1157, 1103, 1082, 971, 848, 752 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}FNO_2$ $[M+H]^+$ 382.1238, found 382.1234.



7-(4-bromophenyl)-13-methyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3t**)

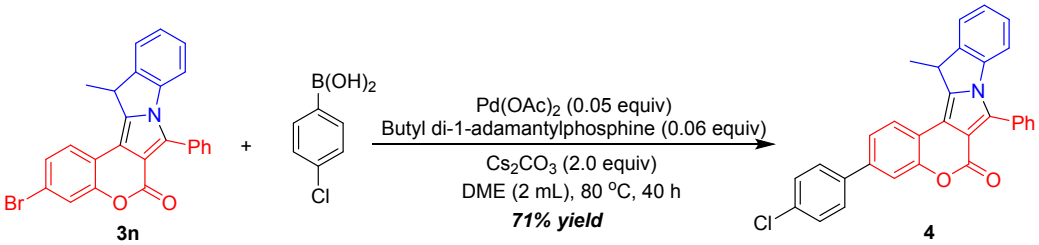
Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 90:1 to 60:1); 23.9 mg, 34% yield; reaction time = 12 h; mp 222.0-223.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.70 (d, $J = 8.0$ Hz, 1H), 7.61 (d, $J = 8.0$ Hz, 2H), 7.48-7.42 (m, 3H), 7.25-7.17 (m, 4H), 7.10 (t, $J = 8.0$ Hz, 1H), 6.85 (d, $J = 8.0$ Hz, 1H), 4.36 (q, $J = 8.0$ Hz, 1H), 1.68 (d, $J = 8.0$ Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 150.2, 140.8, 137.7, 133.5, 131.5, 130.6, 128.1, 127.3, 126.8, 126.4, 125.0, 124.3, 123.0, 122.9, 122.8, 116.6, 115.9, 113.5, 112.4, 109.3, 34.6, 17.0. IR (KBr) *v* 3445, 3070, 2973, 2927, 1733, 1609, 1469, 1409, 1298, 1261, 1184, 1154, 1107, 1061, 971, 758 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{17}BrNO_2$ $[M+H]^+$ 442.0437, found 442.0442.



13-methyl-7-(thiophen-2-yl)-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**3u**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 60:1); 23.5 mg, 40% yield; reaction time = 72 h; mp 214.8-215.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.68 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 4.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.29-7.15 (m, 6H), 7.10 (t, *J* = 8.0 Hz, 1H), 6.82 (d, *J* = 8.0 Hz, 1H), 4.34 (q, *J* = 8.0 Hz, 1H), 1.67 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 151.4, 141.6, 138.7, 134.9, 130.7, 129.3, 128.8, 128.0, 127.4, 127.3, 126.0, 125.2, 124.0, 123.8, 121.9, 117.6, 117.0, 114.8, 113.5, 112.3, 35.8, 17.9. IR (KBr) *v* 3087, 2956, 2920, 1726, 1650, 1555, 1375, 1295, 1209, 860, 757 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{16}NO_2S$ $[M+H]^+$ 370.0896, found 370.0882.

3. Experimental data for products 4

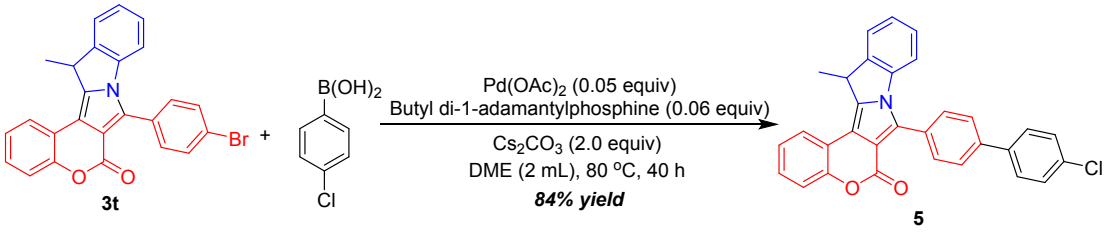


General procedure: Under nitrogen atmosphere, compound **3n** (100.0 mg, 0.33 mmol), 4-chlorophenylboronic acid (1.5 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 40 h till almost full consumption of **3n** monitored by thin layer chromatography, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding products **4**.

3-(4-chlorophenyl)-13-methyl-7-phenyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**4**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 80:1 to 55:1); 77.1 mg, 71% yield; reaction time = 40 h; mp 224.6-225.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.80 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 2H), 7.55-7.40 (m, 10H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 6.88 (d, *J* = 8.0 Hz, 1H), 4.43 (q, *J* = 8.0 Hz, 1H), 1.76 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 151.7, 141.8, 138.9, 138.8, 138.4, 134.3, 133.8, 130.9, 130.6, 129.5, 129.4, 129.1, 128.4, 128.1, 127.8, 125.9, 125.2, 124.2, 122.5, 116.4, 115.6, 114.0, 113.6, 110.0, 35.6, 18.0. IR (KBr) *v* 3055, 2923, 2851, 1728, 1612, 1468, 1394, 1378, 1298, 1261, 1180, 1087, 1059, 1008, 974, 885, 741 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{21}ClNO_2$ $[M+H]^+$ 474.1255, found 474.1238.

4. Experimental data for products 5

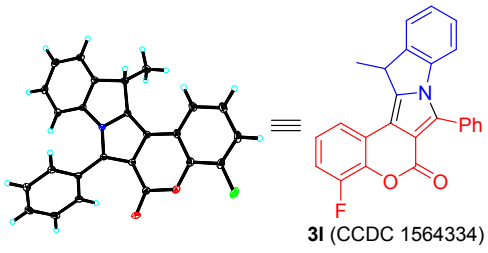


General procedure: Under nitrogen atmosphere, compound **3t** (81.2 mg, 0.18 mmol), 4-chlorophenylboronic acid (1.5 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 40 h till almost full consumption of **3n** monitored by thin layer chromatography, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding products **5**.

7-(4'-chloro-[1,1'-biphenyl]-4-yl)-13-methyl-6*H*,13*H*-chromeno[4',3':3,4]pyrrolo[1,2-*a*]indol-6-one (**5**)

Light yellow solid obtained by column chromatography (petroleum ether/ethyl acetate = 65:1 to 35:1); 71.2 mg, 84% yield; reaction time = 40 h; mp 236.8-237.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.65 (s, 4H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.43 (d, *J* = 4.0 Hz, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.27-7.15 (m, 4H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 4.36 (q, *J* = 8.0 Hz, 1H), 1.69 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 151.3, 141.9, 140.8, 138.9, 138.8, 134.5, 133.9, 131.5, 130.2, 129.1, 128.7, 128.5, 127.8, 127.3, 126.8, 126.0, 125.3, 124.0, 123.8, 117.6, 117.1, 114.5, 113.6, 110.3, 35.7, 18.0. IR (KBr) *v* 2926, 1725, 1608, 1550, 1464, 1413, 1391, 1350, 1080, 855, 752 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{21}ClNO_2$ $[M+H]^+$ 474.1255, found 474.1258.

5. Crystal data for 3l

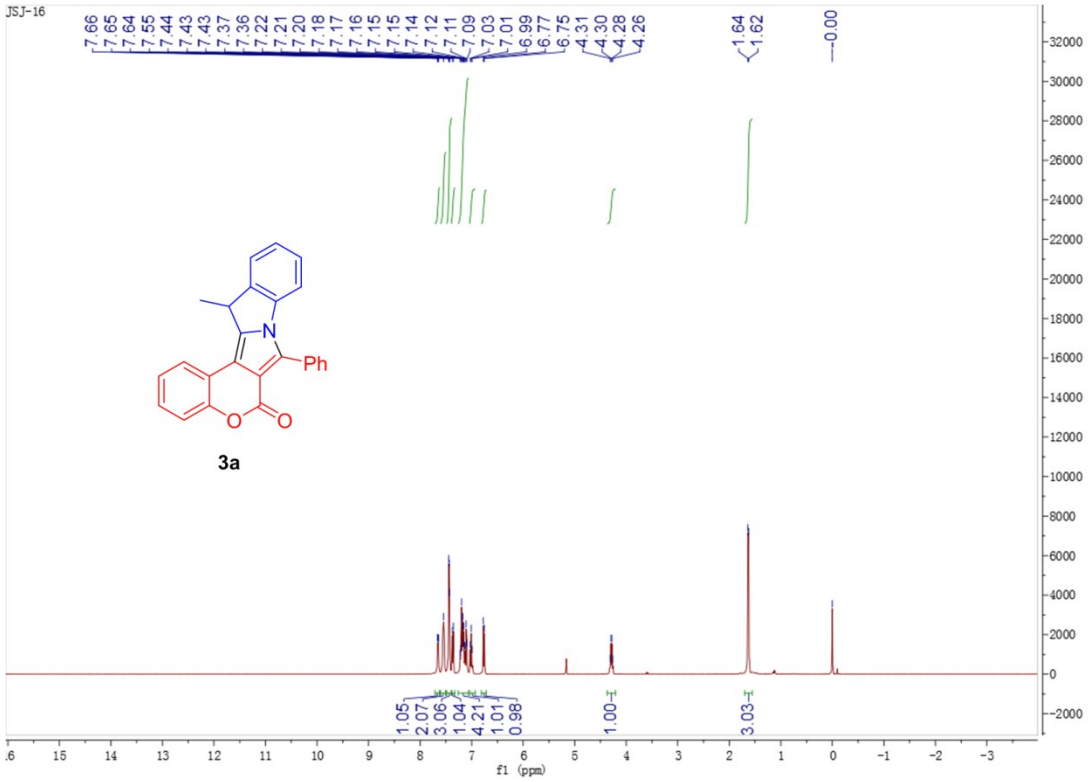


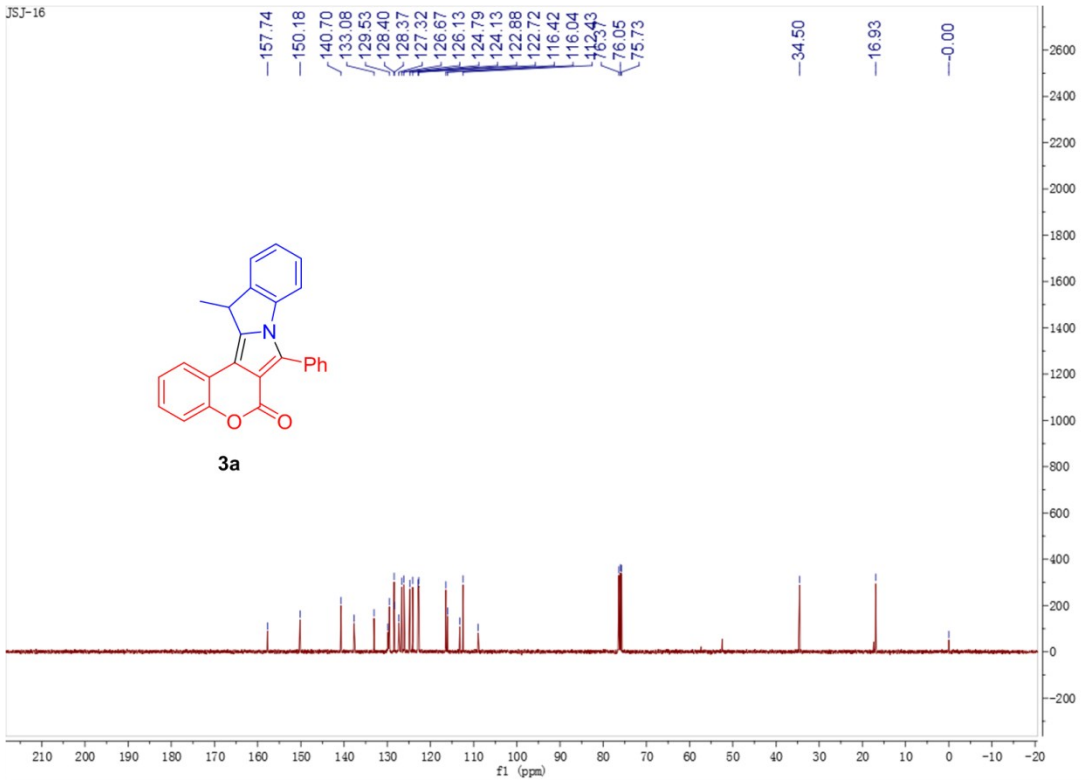
Displacement ellipsoids are drawn at the 30% probability level.

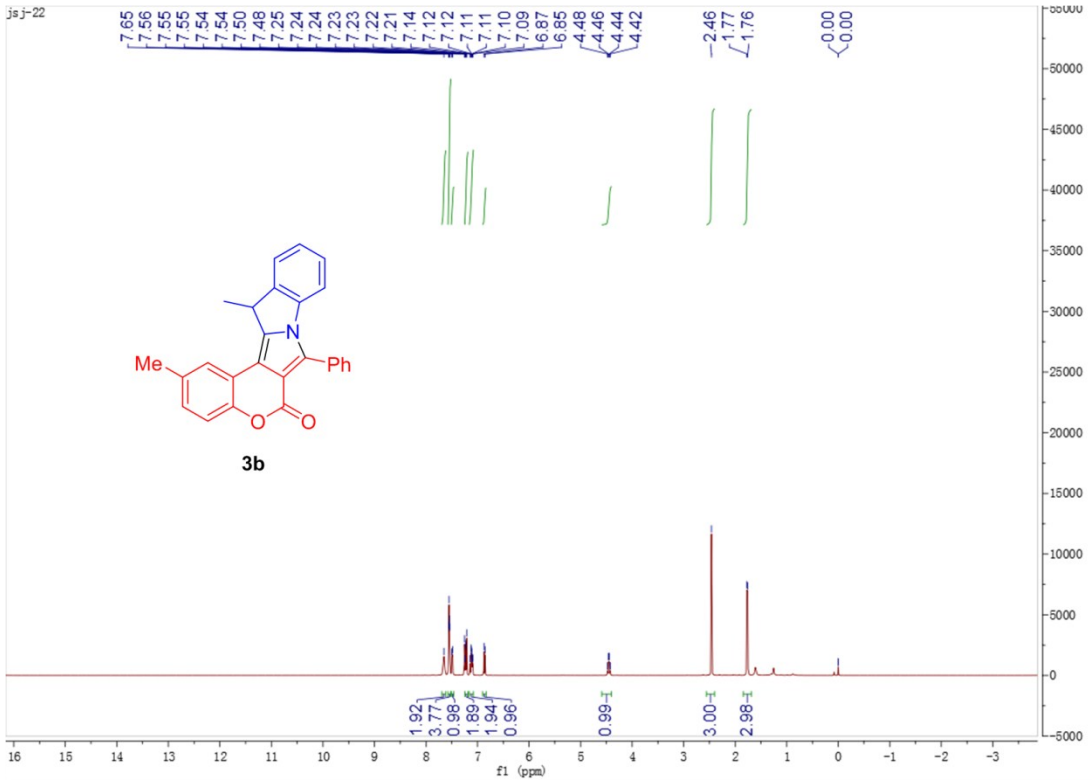
Table S1. Crystal data and structure refinement for **3l**.

Identification code	**3l**	
Empirical formula	$C_{25}H_{16}FNO_2$	
Formula weight	381.39	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.9398(17) Å	α= 90°.
	b = 10.9448(10) Å	β= 95.219(2)°.
	c = 16.3541(14) Å	γ= 90°.
Volume	3554.3(5) $Å^3$	
Z	8	
Density (calculated)	1.425 Mg/m^3	
Absorption coefficient	0.098 mm^{-1}	
F(000)	1584	
Crystal size	0.450 x 0.380 x 0.320 mm^3	
Theta range for data collection	2.051 to 31.131°.	
Index ranges	-27<=h<=27, -15<=k<=15, -23<=l<=23	
Reflections collected	19608	
Independent reflections	5309 [R(int) = 0.0365]	
Completeness to theta = 25.242°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5309 / 0 / 263	
Goodness-of-fit on F^2	0.982	
Final R indices [I>2sigma(I)]	R1 = 0.0535, wR2 = 0.1276	
R indices (all data)	R1 = 0.0715, wR2 = 0.1380	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.448 and -0.359 $e.Å^{-3}$	

6. Copies of ^{1}H NMR and ^{13}C NMR spectra



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7.50
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7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.14
7.12
7.12
7.11
7.11
7.10
7.09
6.87
6.85
4.48
4.46
4.44
4.42
2.46
1.77
1.76
0.00
0.00
Me
Ph
N
O
O
3b
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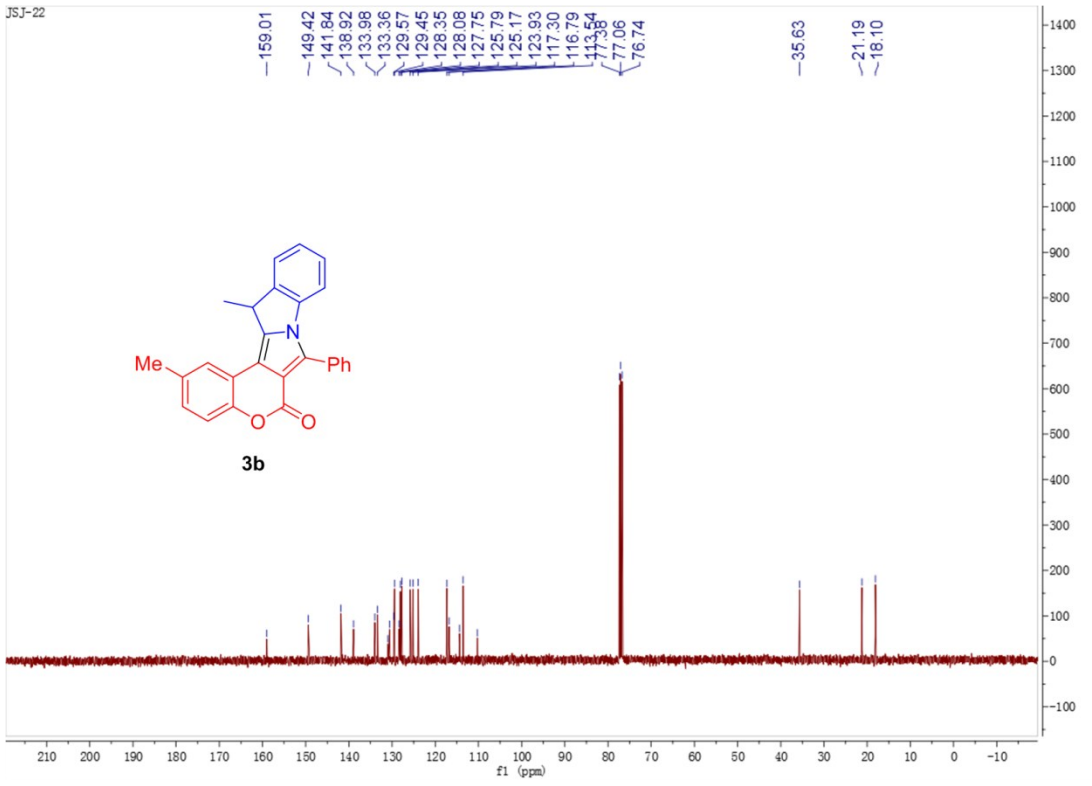
3.77
0.98
1.89
1.94
0.96
0.99
3.00
2.98
f1 (ppm)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128.08
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125.79
125.17
123.93
117.30
116.79
113.54
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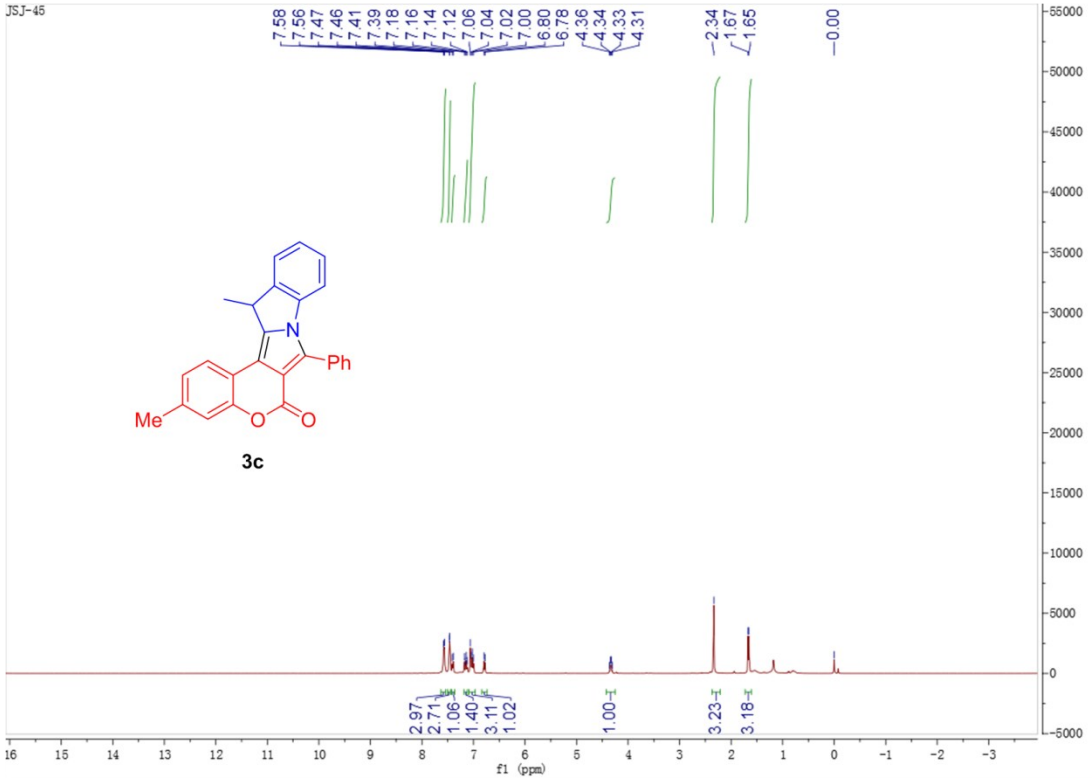
77.06
76.74
35.63
21.19
18.10
Me
Ph
N
O
O
3b
f1 (ppm)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7.12
7.06
7.04
7.02
7.00
6.80
6.78
4.36
4.34
4.33
4.31
2.34
1.67
1.65
0.00
N
Ph
Me
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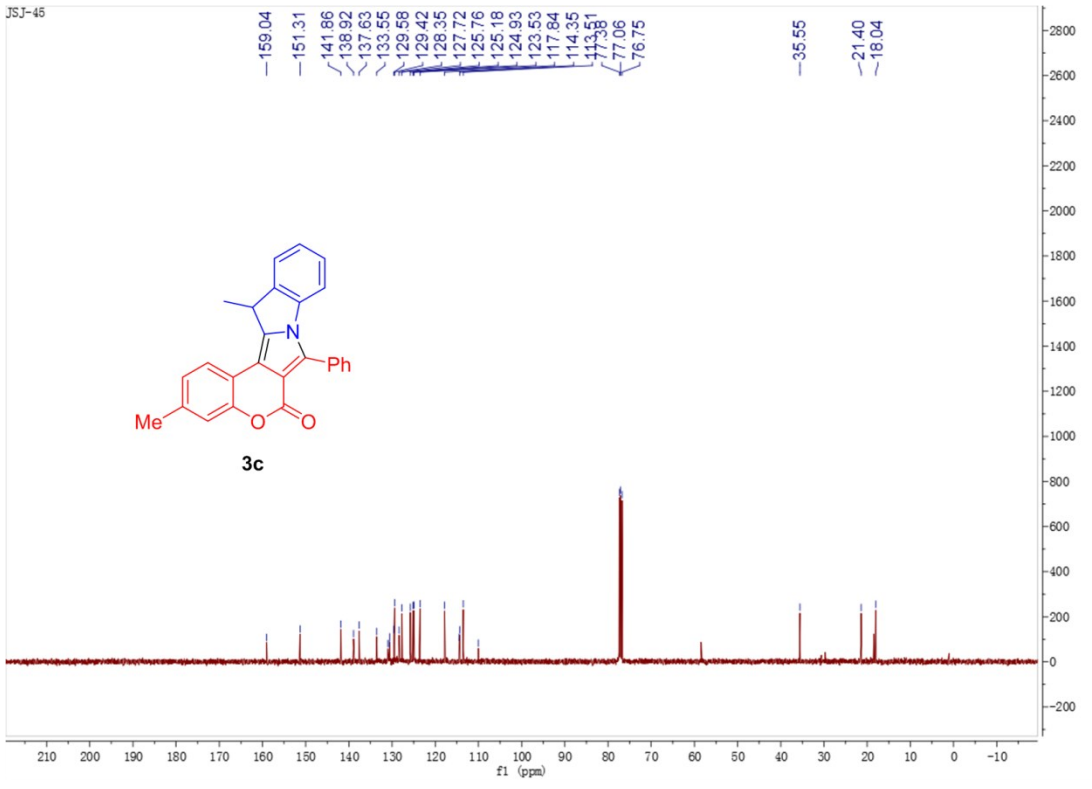
1.40
3.11
1.02
1.00
3.23
3.18
f1 (ppm)

3c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125.18
124.93
123.53
117.84
114.35
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76.75
35.55
21.40
18.04
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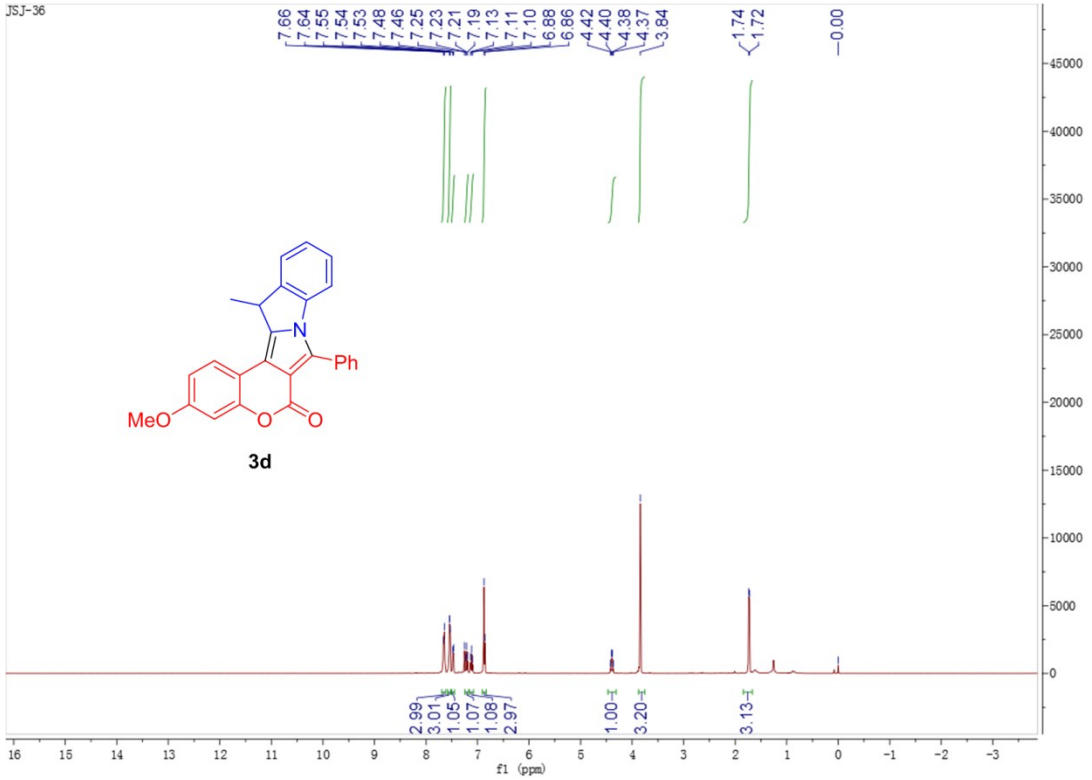
Ph
Me
O
O
f1 (ppm)

3c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7.19
7.13
7.11
7.10
6.88
6.86
4.42
4.40
4.38
4.37
3.84
1.74
1.72
0.00
N
Ph
MeO
O
O
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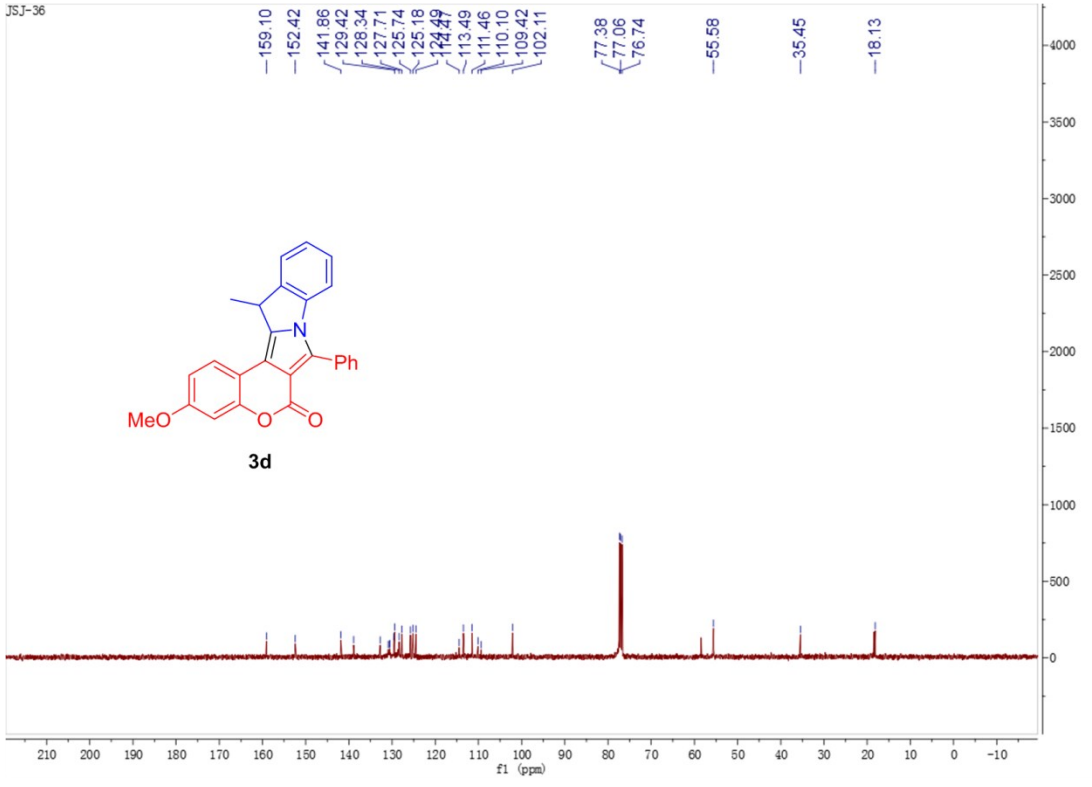
1.05
1.07
1.08
2.97
1.00
3.20
3.13
f1 (ppm)

3d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110.10
109.42
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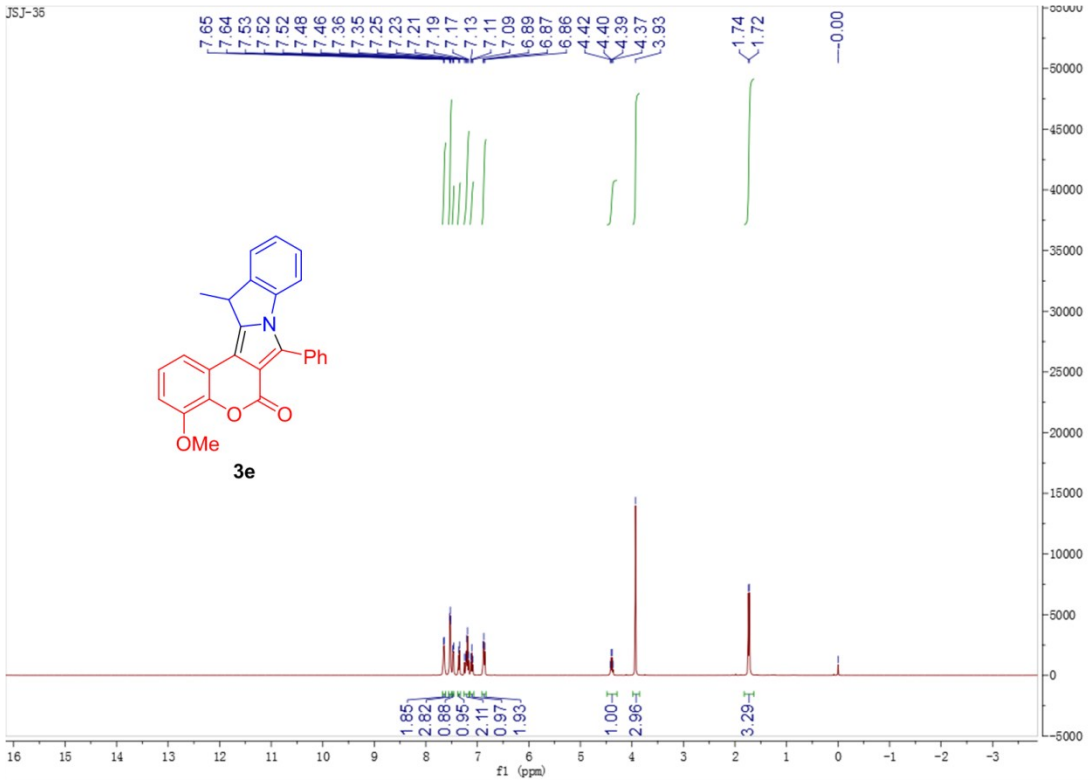
77.06
76.74
55.58
35.45
18.13
N
Ph
MeO
O
O
f1 (ppm)

3d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7.35
7.25
7.23
7.21
7.19
7.17
7.13
7.11
7.09
6.89
6.87
6.86
4.42
4.40
4.39
4.37
3.93
1.74
1.72
0.00
Ph
O
O
OMe
3e
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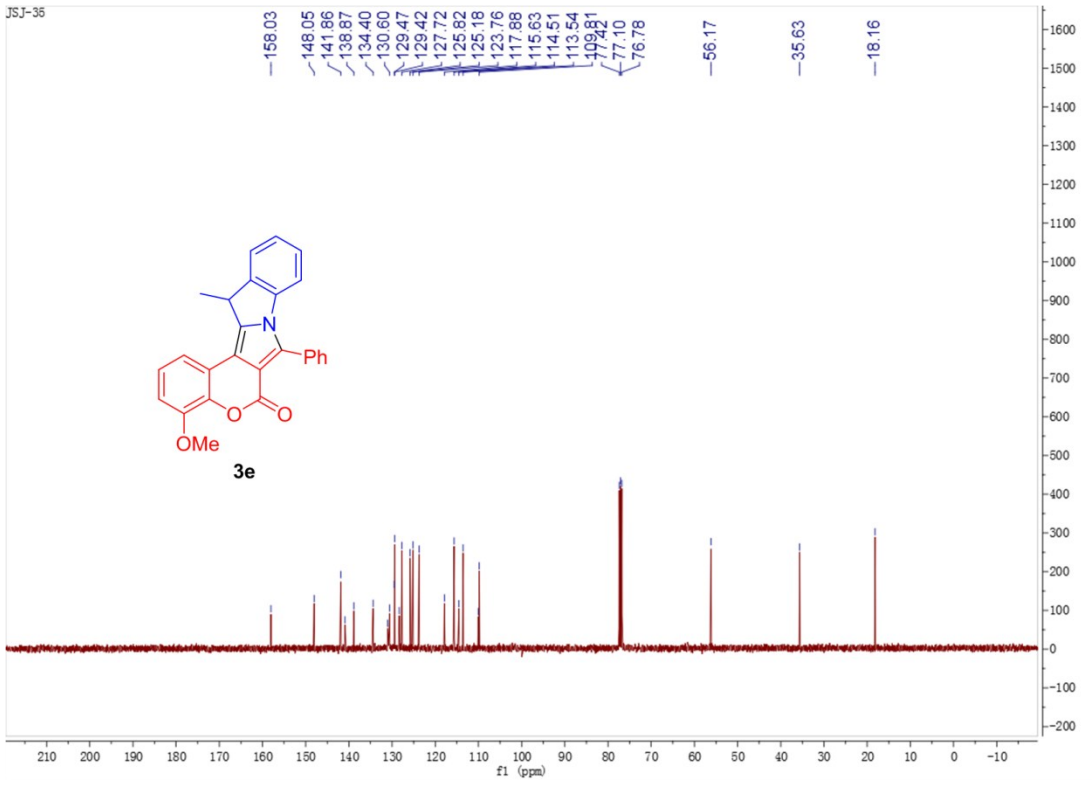
0.88
0.95
2.11
0.97
1.93
1.00
2.96
3.29
f1 (ppm)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129.47
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127.72
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117.88
115.63
114.51
113.54
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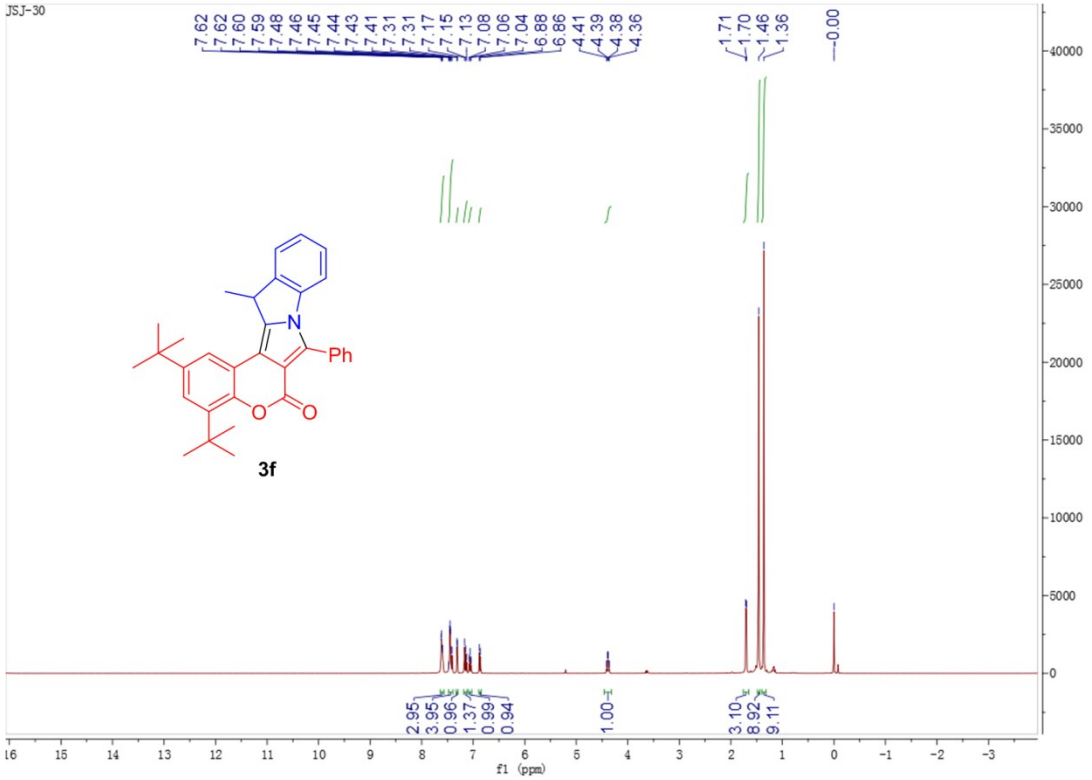
77.10
76.78
56.17
35.63
18.16
Ph
O
O
OMe
3e
f1 (ppm)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7.31
7.17
7.15
7.13
7.08
7.06
7.04
6.88
6.86
4.41
4.39
4.38
4.36
1.71
1.70
1.46
1.36
0.00
Ph
O
O
N
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0.96
1.37
0.99
0.94
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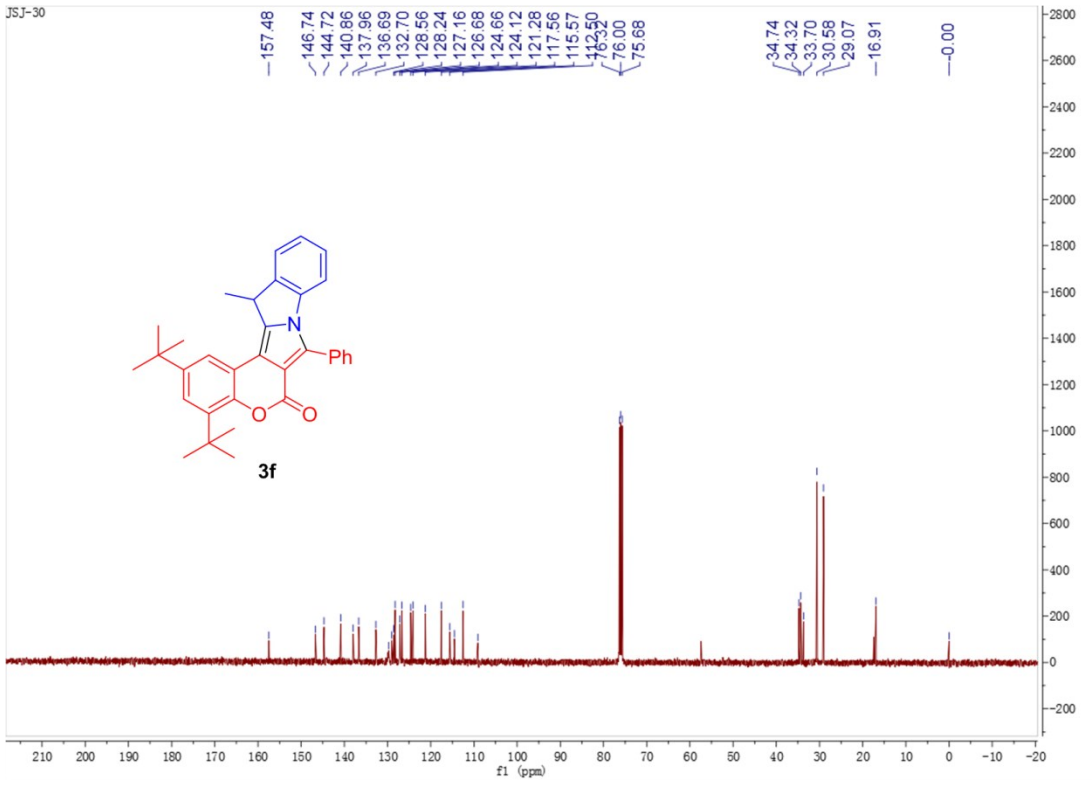
3.10
8.92
9.11
f1 (ppm)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132.70
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127.16
126.68
124.66
124.12
121.28
117.56
115.57
112.50
76.32
76.00
75.68
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33.70
30.58
29.07
16.91
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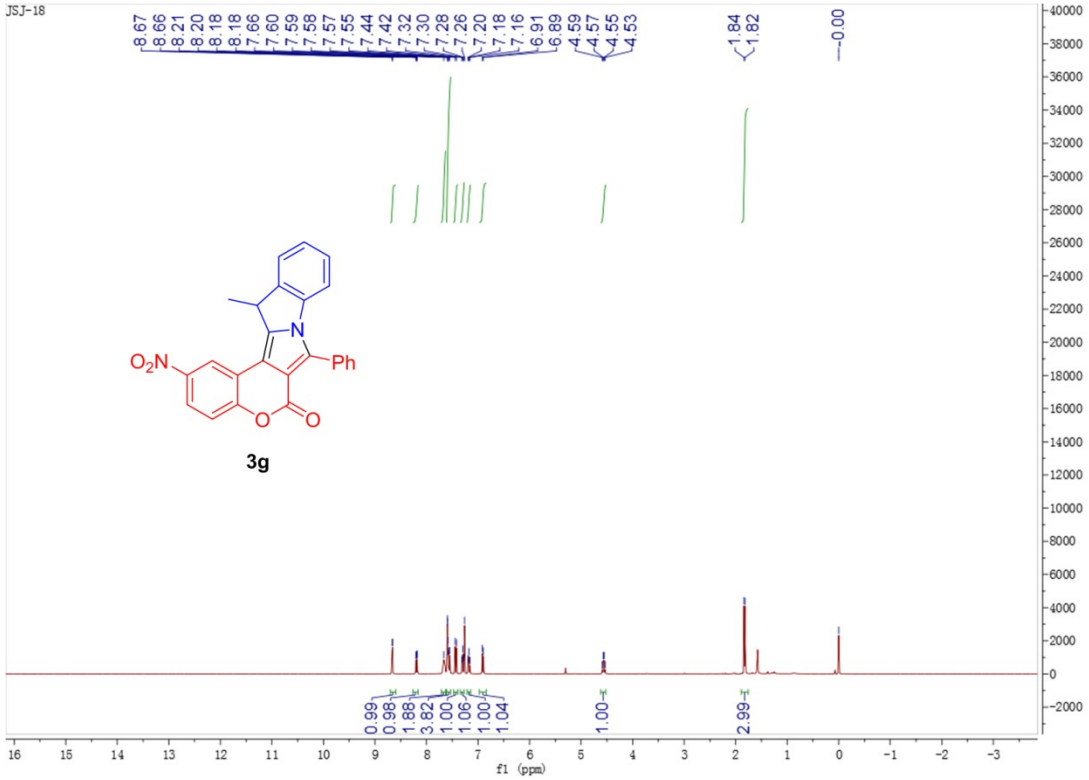
Ph
O
O
N
3f
f1 (ppm)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7.57
7.55
7.44
7.42
7.32
7.30
7.28
7.26
7.20
7.18
7.16
6.91
6.89
4.59
4.57
4.55
4.53
1.84
1.82
0.00
O2N
N
Ph
O
O
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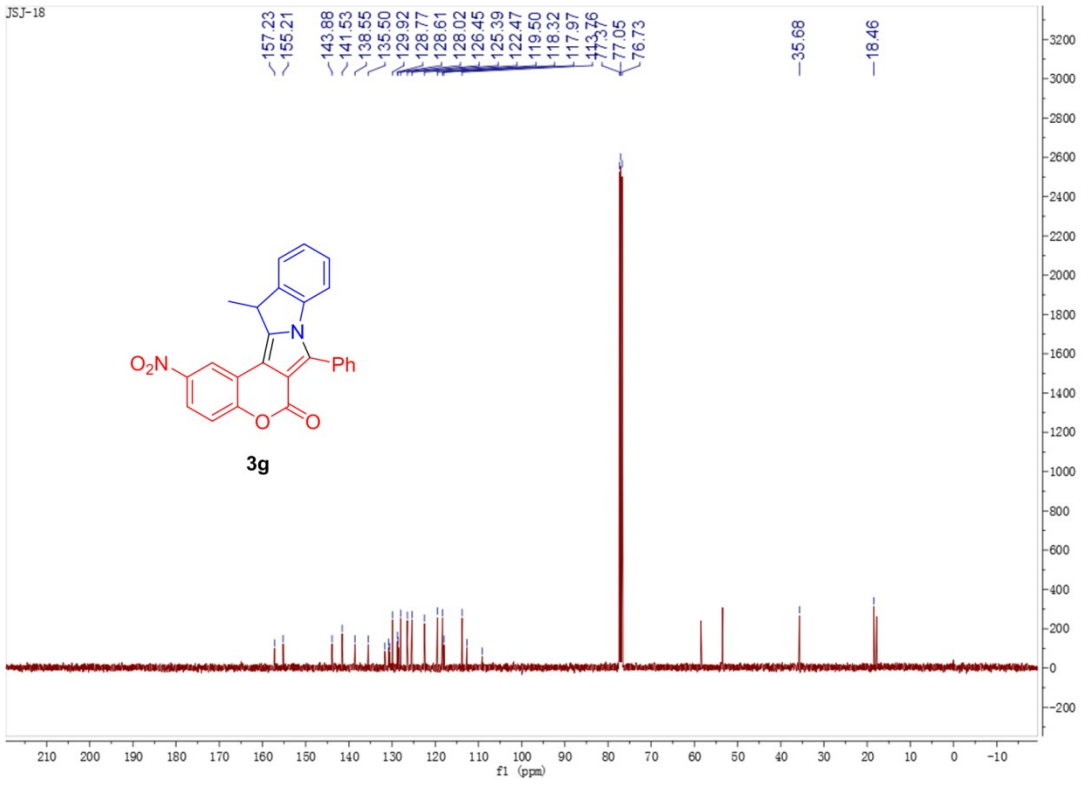
3.82
1.00
1.06
1.00
1.04
1.00
2.99
f1 (ppm)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125.39
122.47
119.50
118.32
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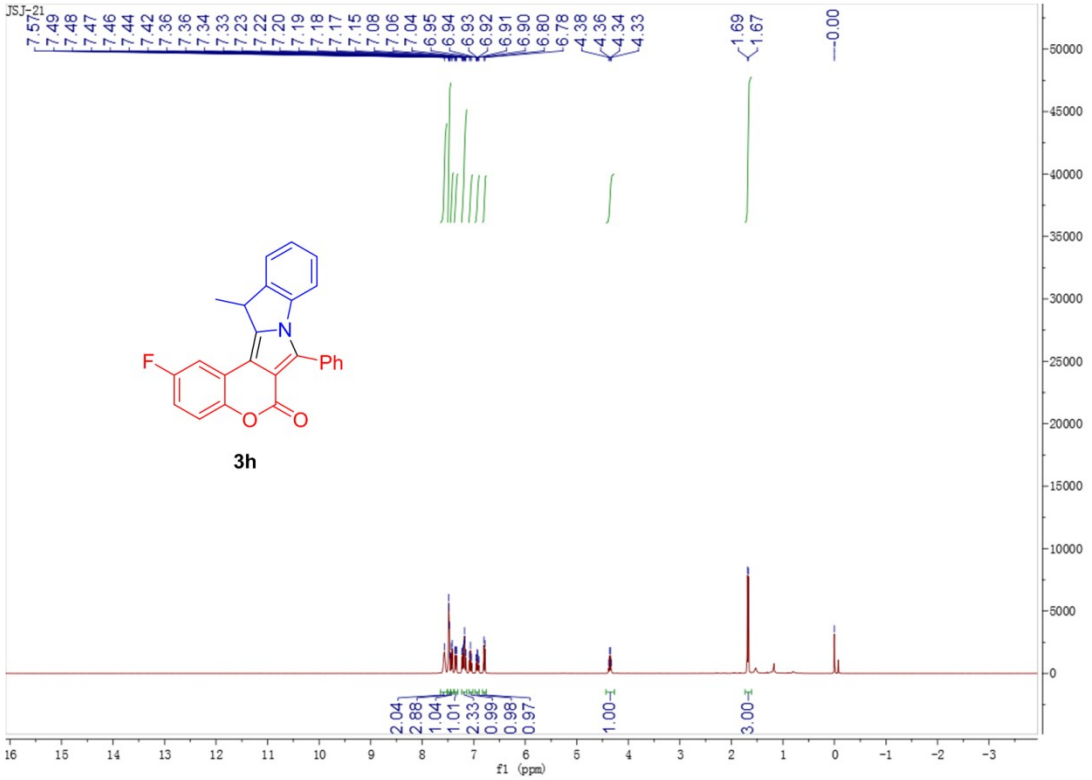
76.73
35.68
18.46
O2N
N
Ph
O
O
3g
f1 (ppm)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7.23
7.22
7.20
7.19
7.18
7.17
7.15
7.08
7.06
7.04
6.95
6.94
6.93
6.92
6.91
6.90
6.80
6.78
4.38
4.36
4.34
4.33
1.69
1.67
0.00
F
Ph
O
O
N
3h
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2.88
1.04
1.01
2.33
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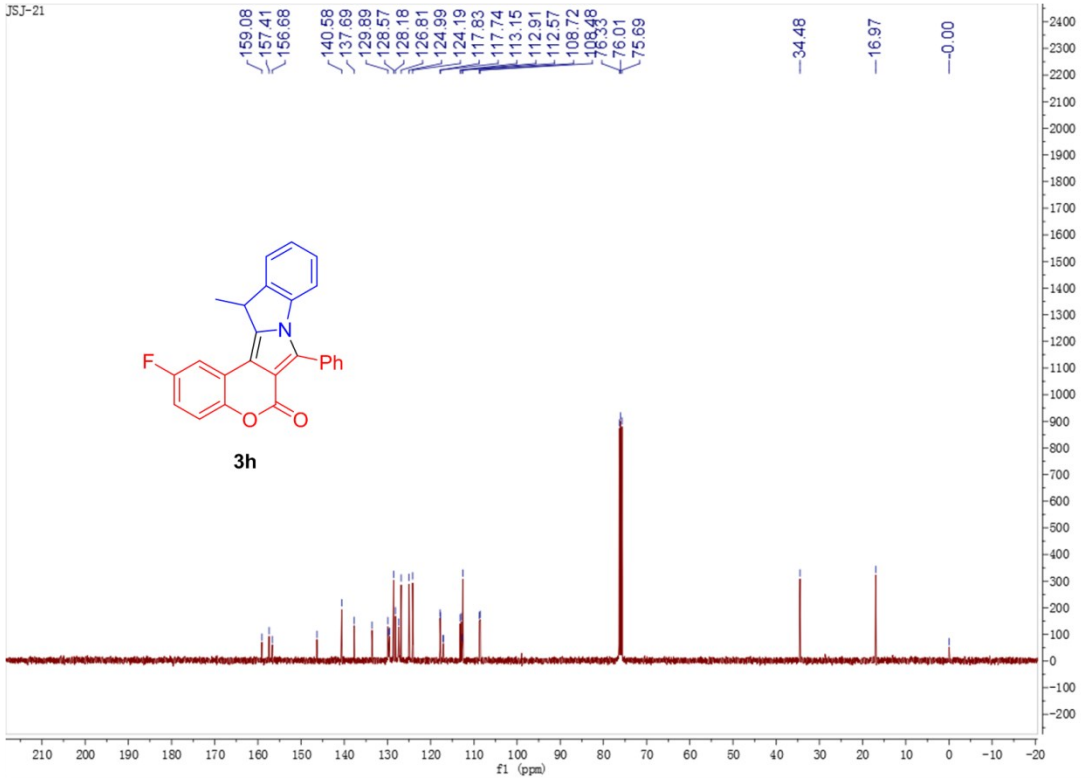
0.98
0.97
1.00
3.00
f1 (ppm)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124.19
117.83
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113.15
112.91
112.57
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75.69
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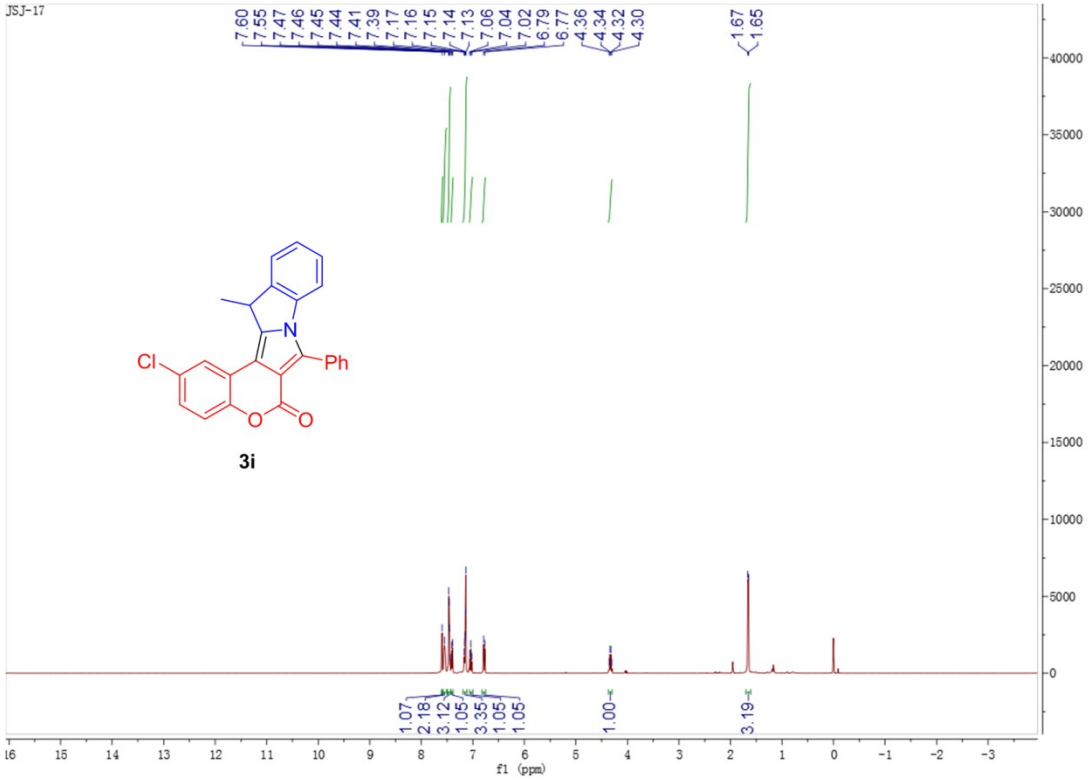
16.97
0.00
F
Ph
O
O
N
3h
f1 (ppm)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7.14
7.13
7.06
7.04
7.02
6.79
6.77
4.36
4.34
4.32
4.30
1.67
1.65
Cl
Ph
O
O
N
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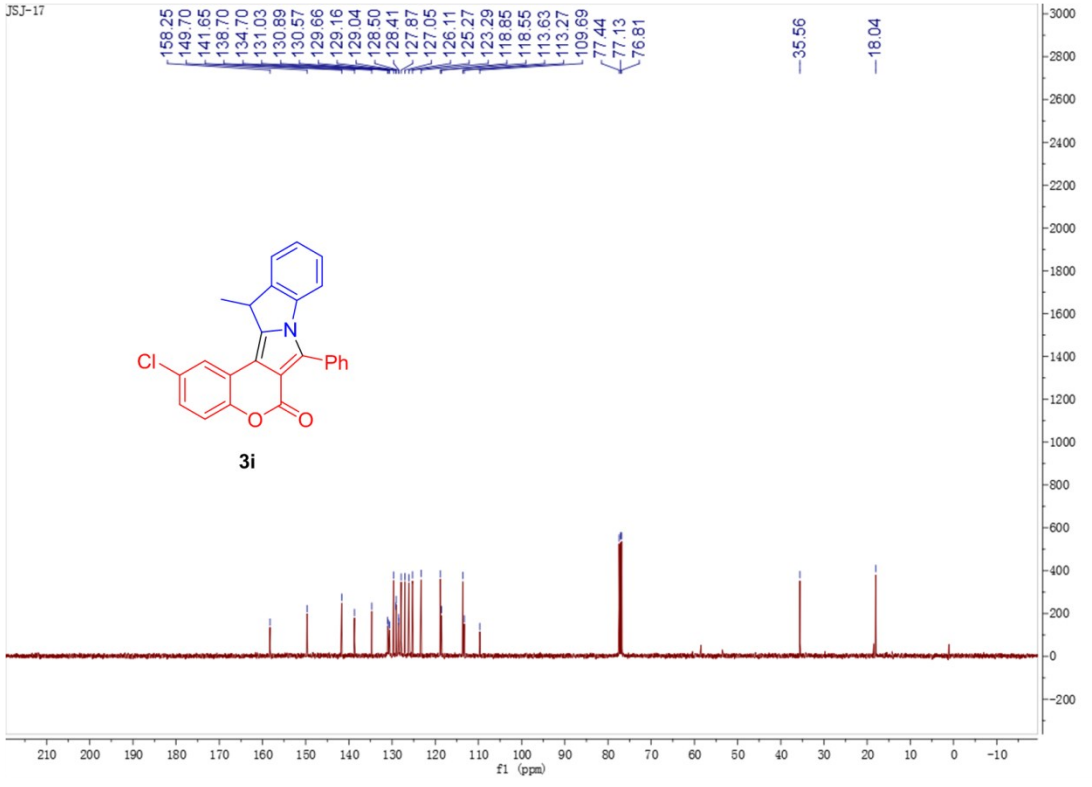
3.12
1.05
3.35
1.05
1.05
1.00
3.19
f1 (ppm)

3i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Ph
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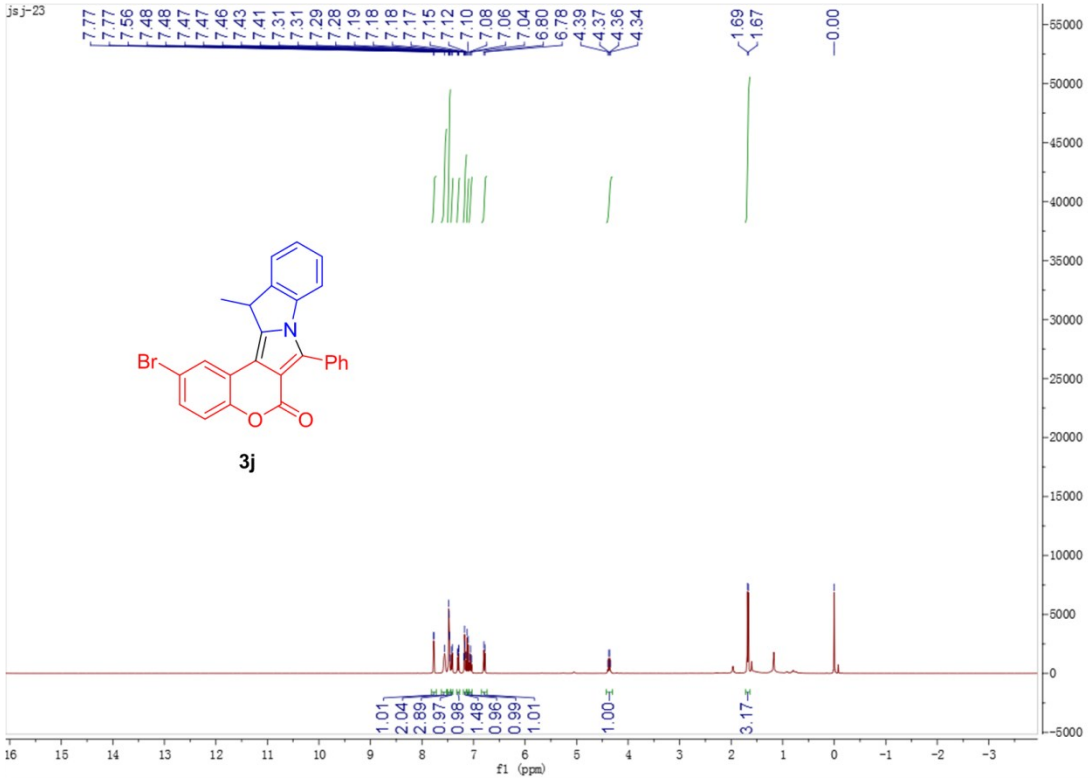
O
N
f1 (ppm)

3i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7.29
7.28
7.19
7.18
7.18
7.17
7.15
7.12
7.10
7.08
7.06
7.04
6.80
6.78
4.39
4.37
4.36
4.34
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1.67
0.00
Br
Ph
O
O
N
1.01
2.04
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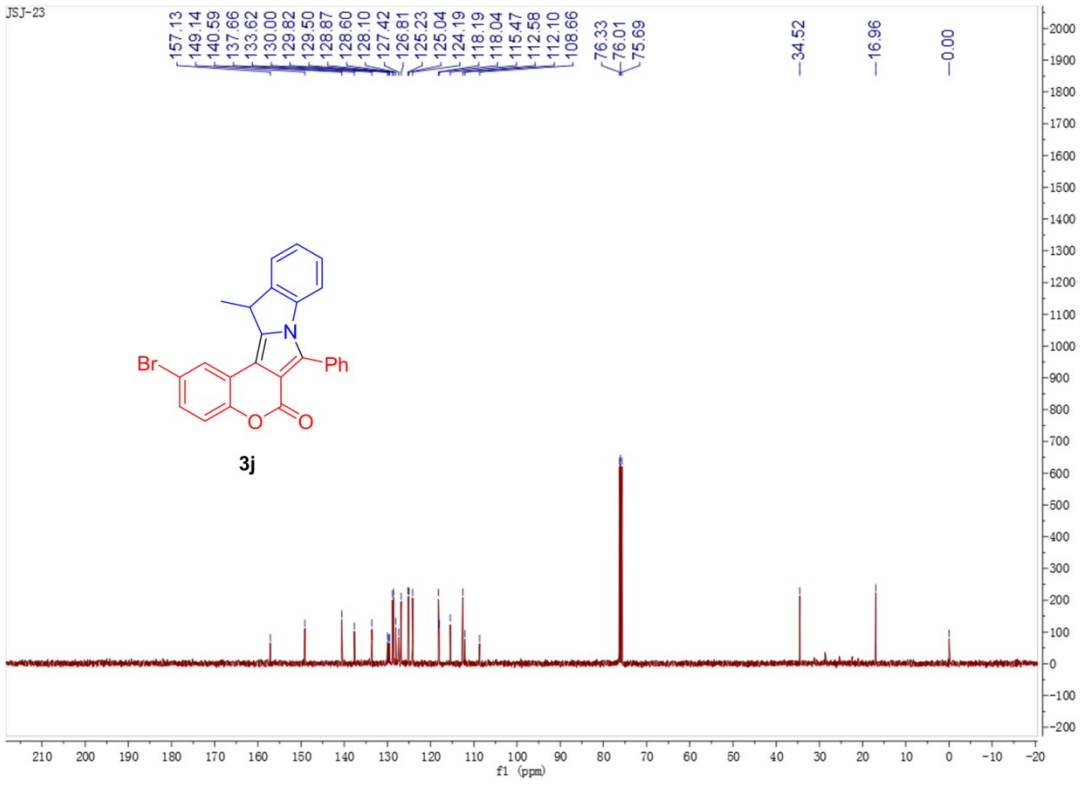
0.98
1.48
0.96
0.99
1.01
1.00
3.17
f1 (ppm)

3j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127.42
126.81
125.23
125.04
124.19
118.19
118.04
115.47
112.58
112.10
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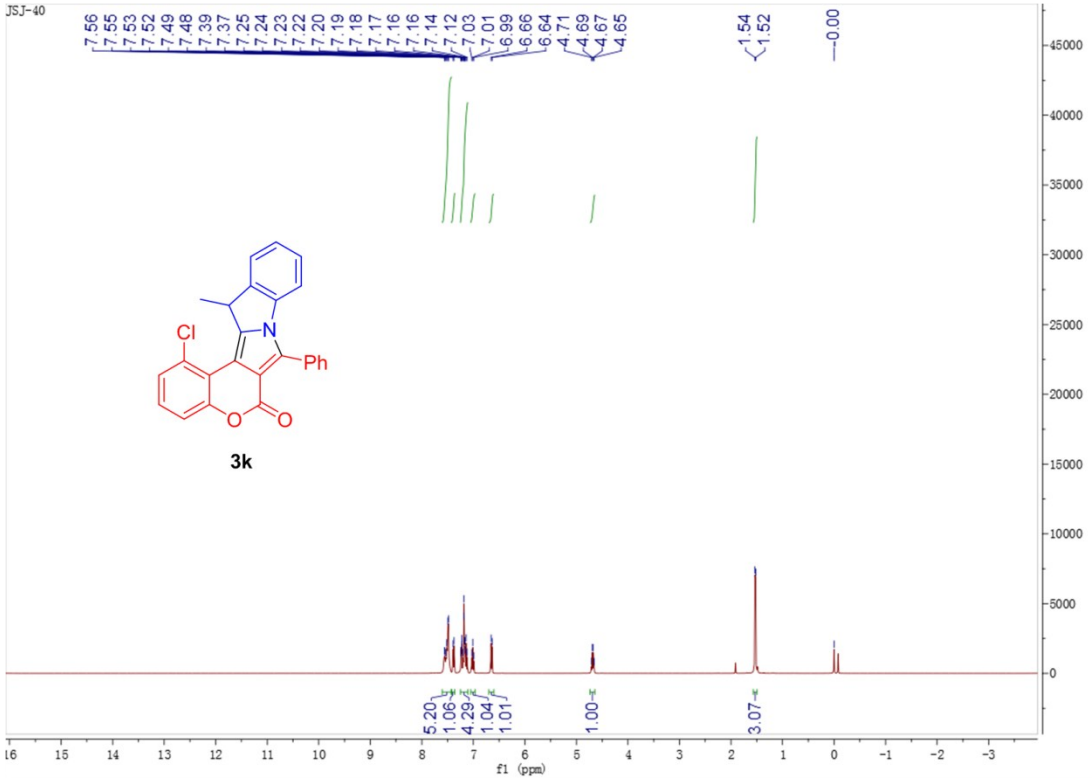
75.69
34.52
16.96
0.00
Br
Ph
O
O
N
f1 (ppm)

3j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7.19
7.18
7.17
7.16
7.16
7.14
7.12
7.03
7.01
6.99
6.66
6.64
4.71
4.69
4.67
4.65
1.54
1.52
0.00
Cl
N
Ph
O
O
3k
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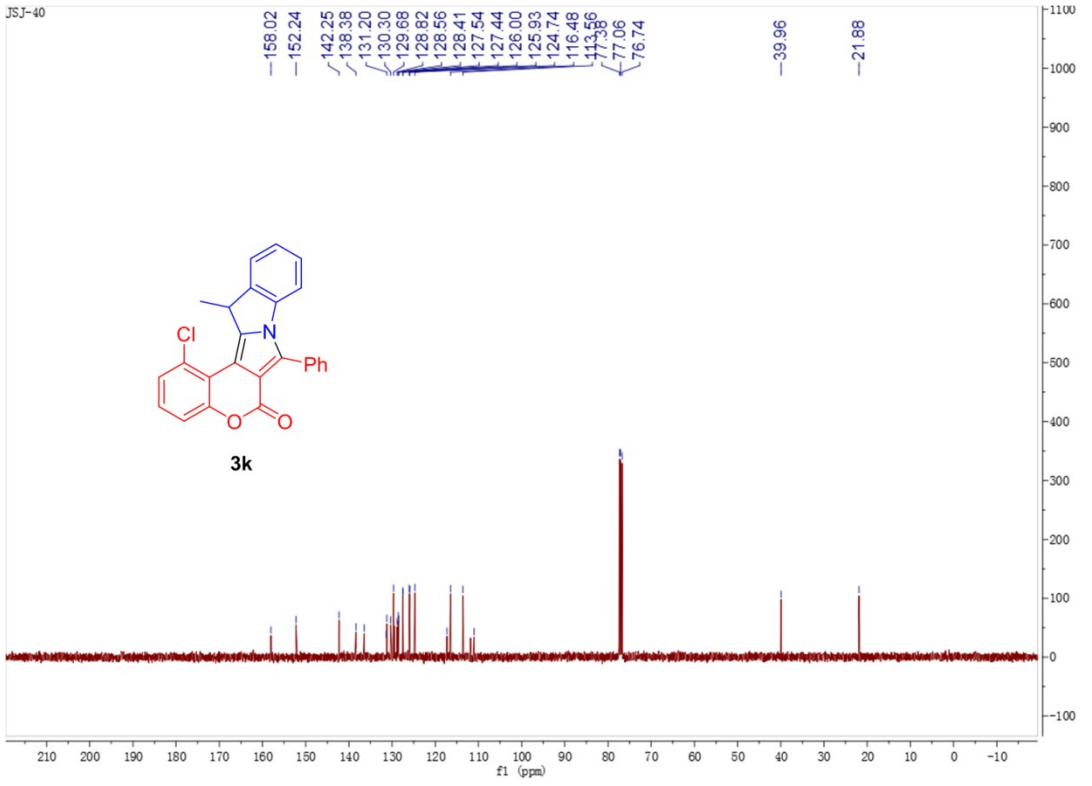
1.06
4.29
1.04
1.01
1.00
3.07
f1 (ppm)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127.44
126.00
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124.74
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21.88
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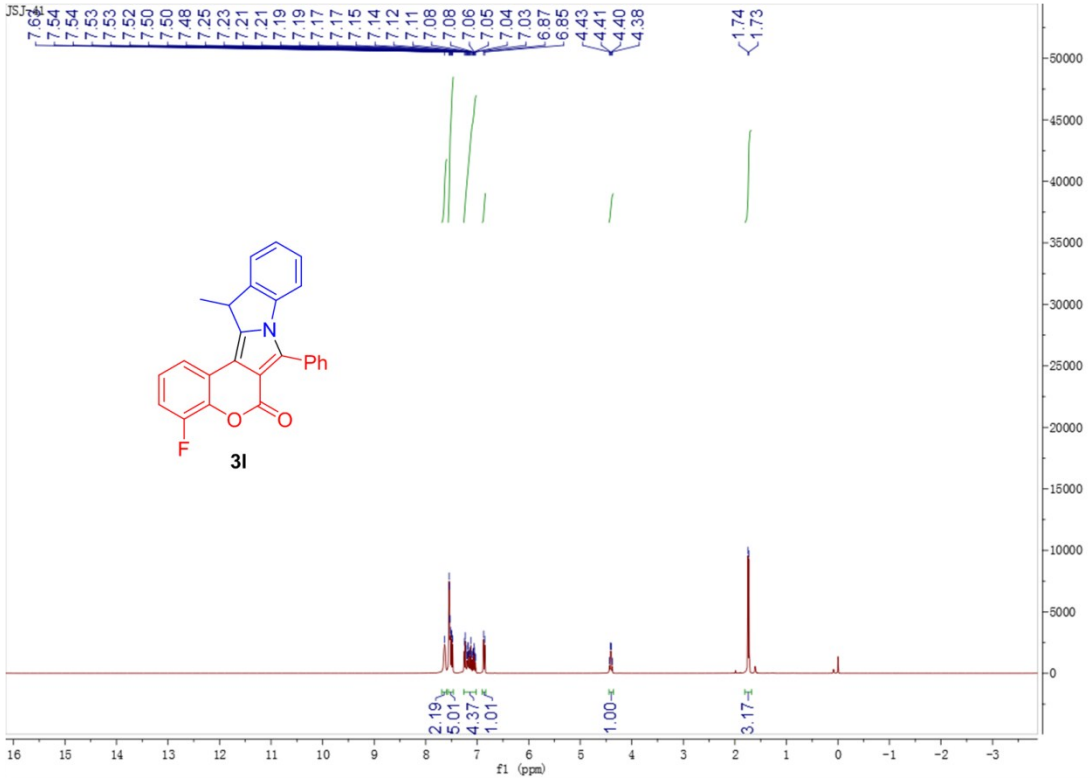
N
Ph
O
O
3k
f1 (ppm)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7.19
7.19
7.17
7.17
7.15
7.14
7.12
7.11
7.08
7.08
7.06
7.05
7.04
7.03
6.87
6.85
4.43
4.41
4.40
4.38
1.74
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Ph
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O
F
3l
2.19
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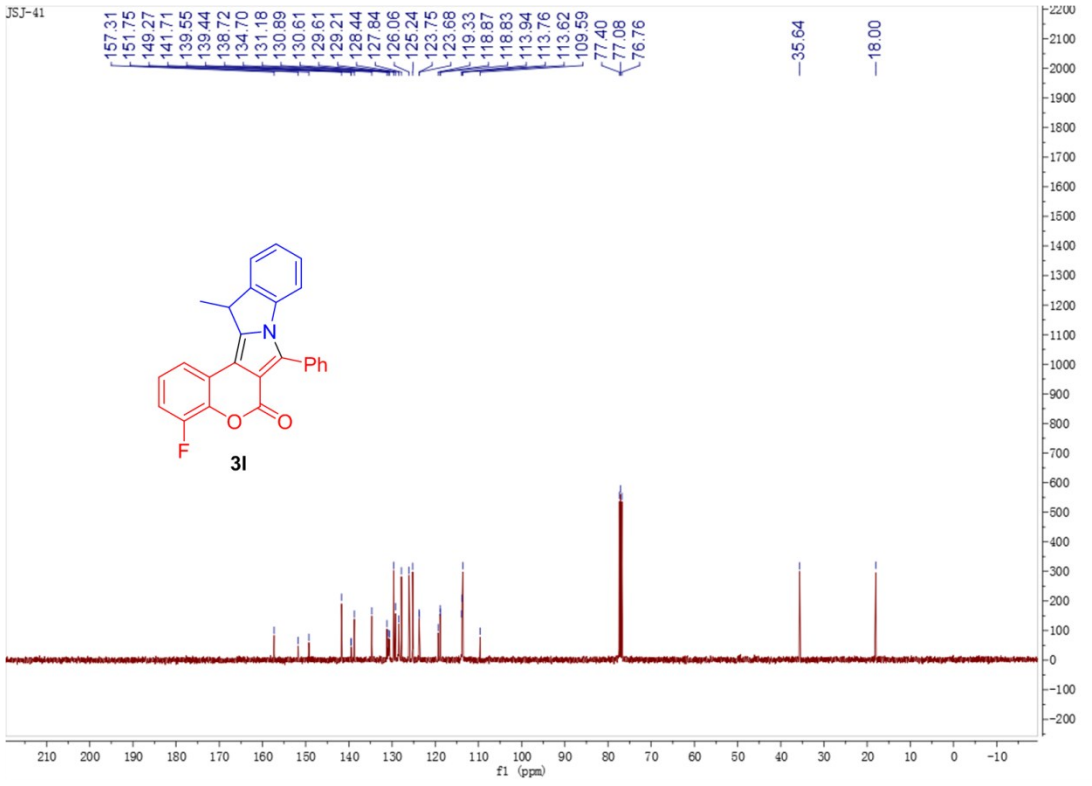
1.01
1.00
3.17
f1 (ppm)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129.61
129.21
128.44
127.84
126.06
125.24
123.75
123.68
119.33
118.87
118.83
113.94
113.76
113.62
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77.08
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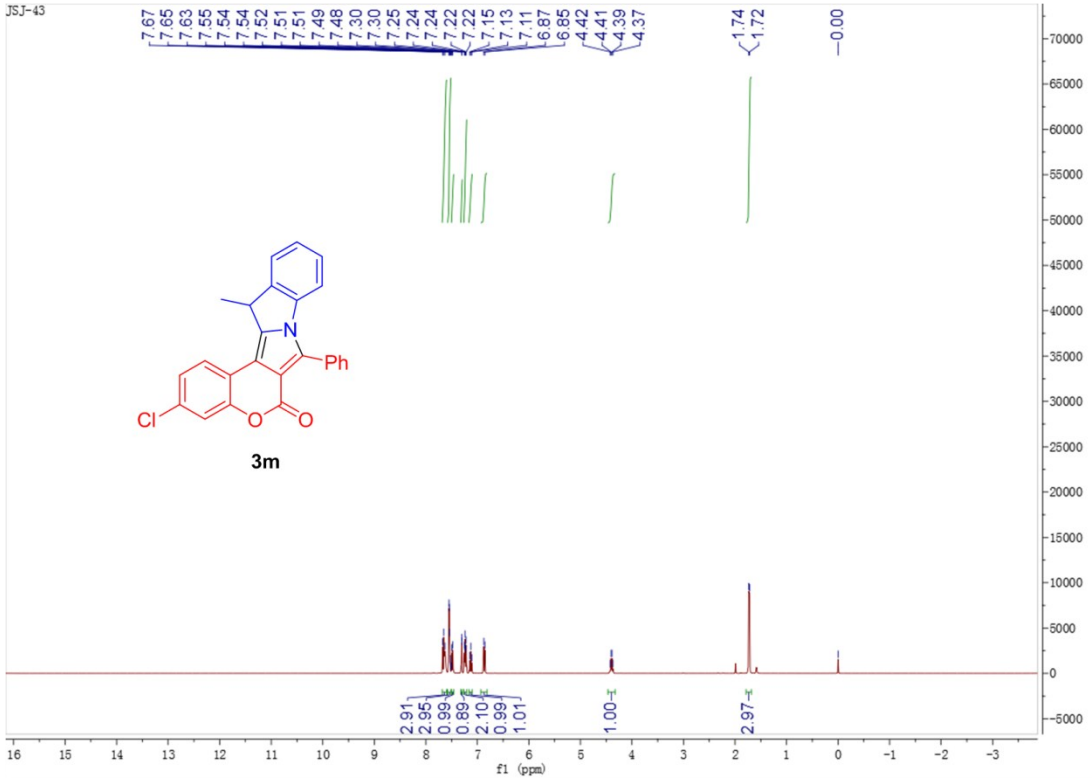
35.64
18.00
N
Ph
O
O
F
3l
f1 (ppm)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7.25
7.24
7.24
7.22
7.22
7.15
7.13
7.11
6.87
6.85
4.42
4.41
4.39
4.37
1.74
1.72
0.00
Ph
Cl
O
O
N
3m
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2.10
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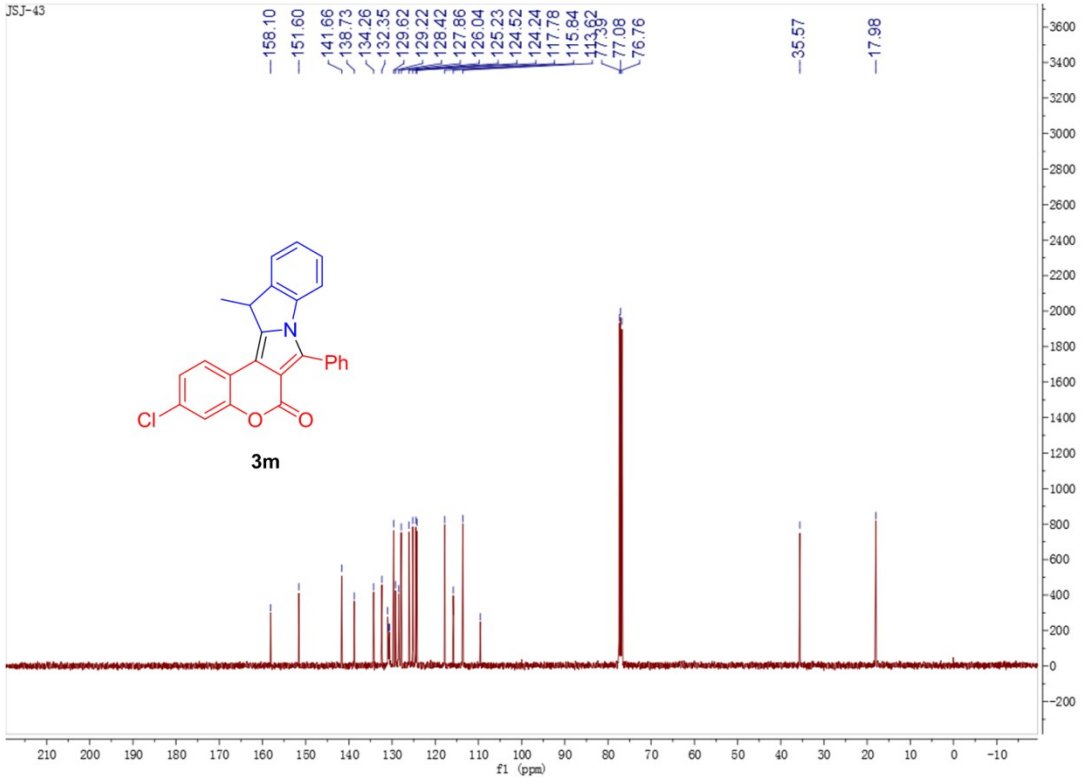
1.01
1.00
2.97
f1 (ppm)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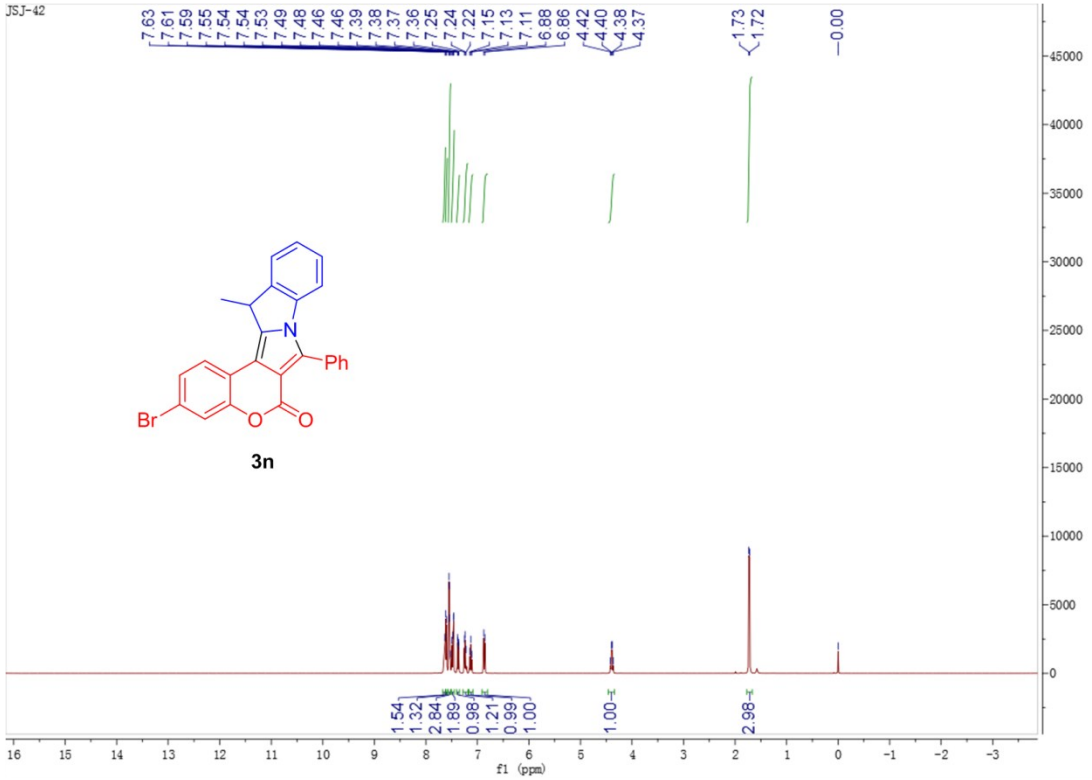
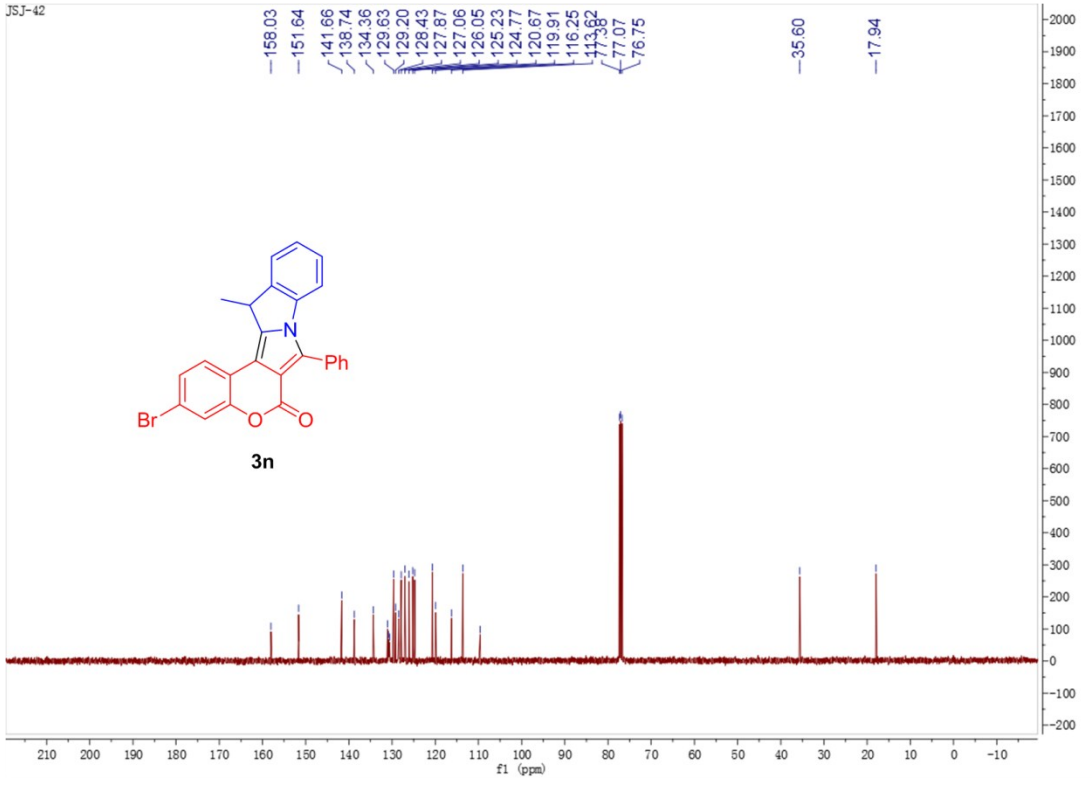
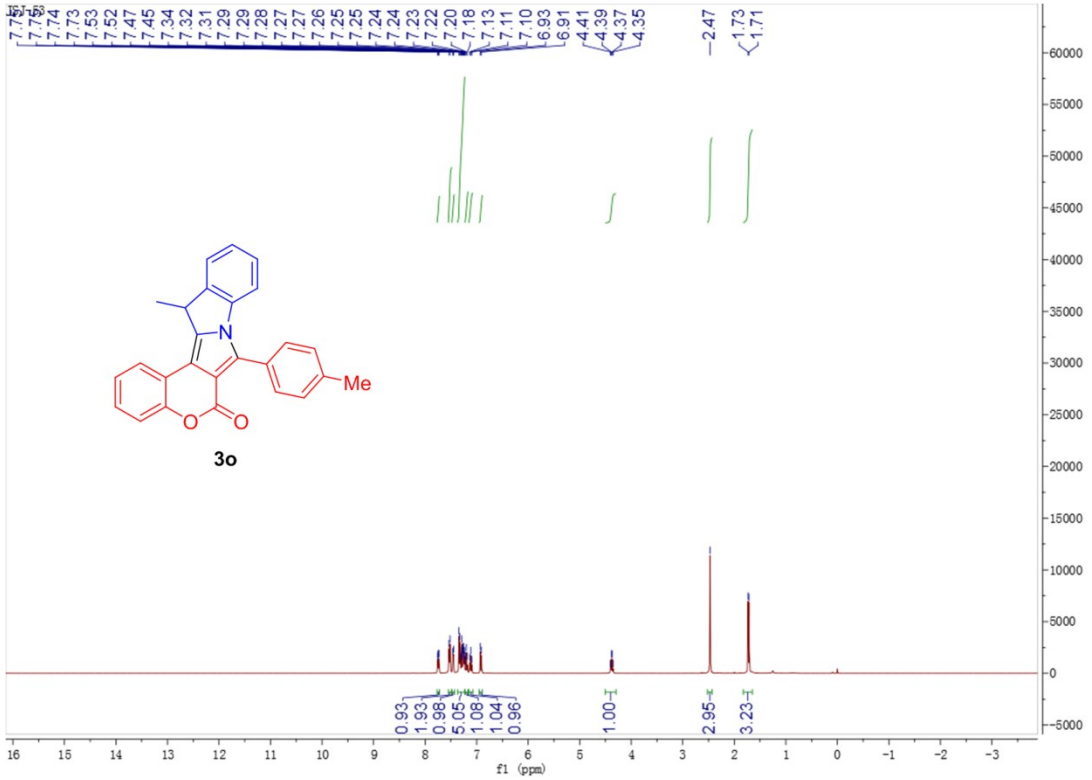
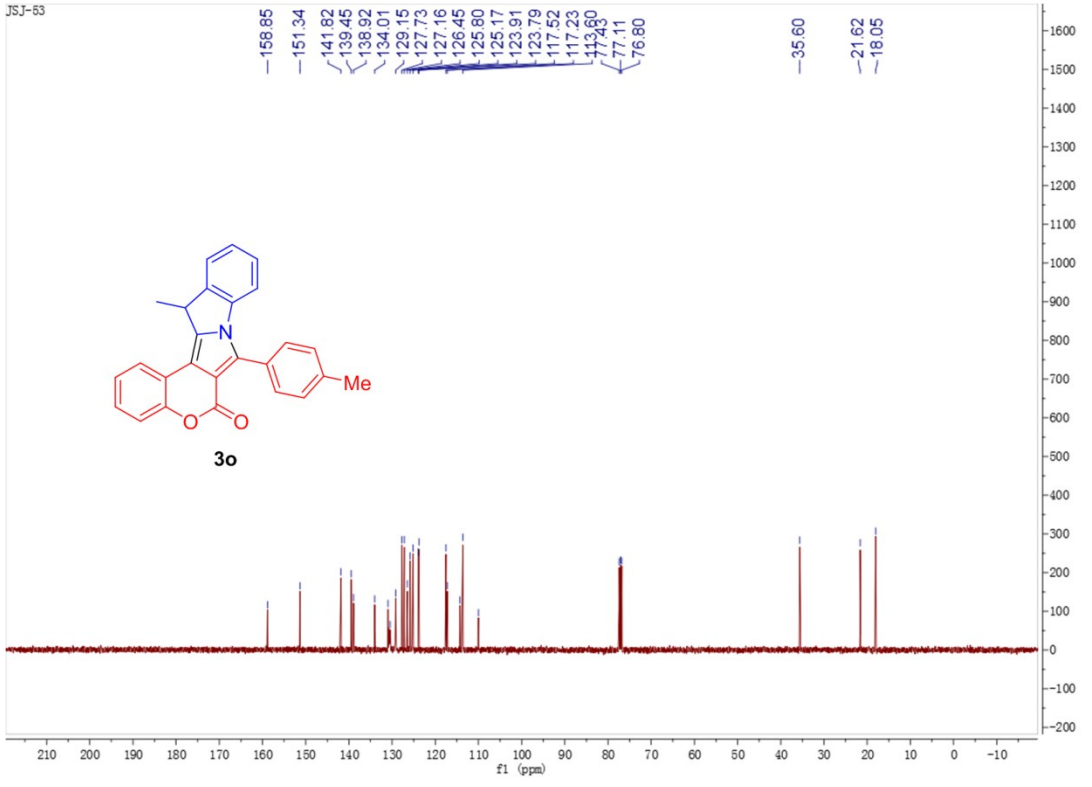
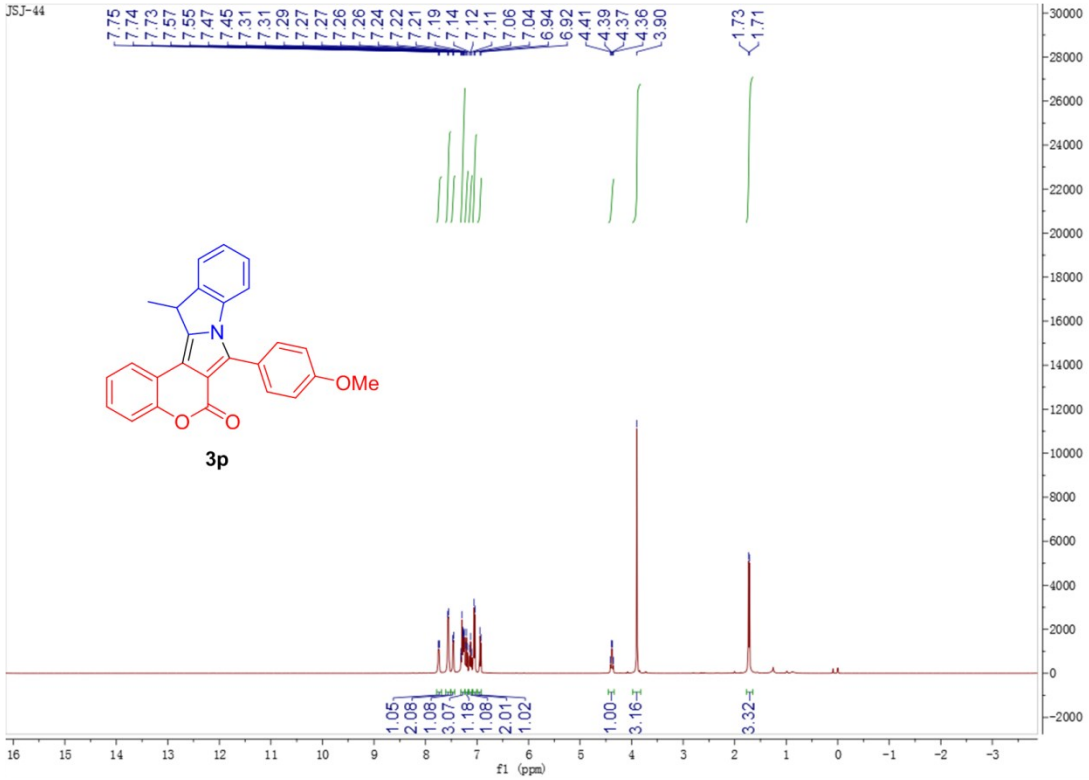
125.23
124.52
124.24
117.78
115.84
77.08
76.76
35.57
17.98
Ph
Cl
O
O
N
3m
f1 (ppm)

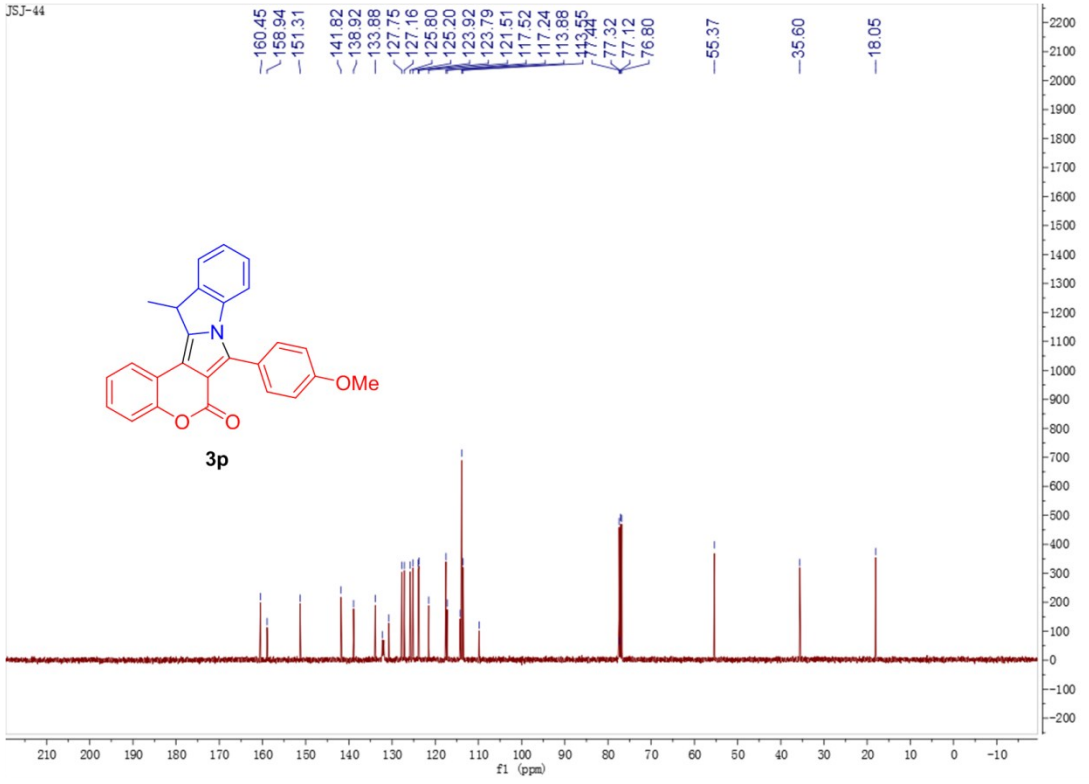

JSJ-42
7.63
7.61
7.59
7.55
7.54
7.54
7.53
7.49
7.48
7.46
7.46
7.39
7.38
7.37
7.36
7.25
7.24
7.22
7.15
7.13
7.11
6.88
6.86
4.42
4.40
4.38
4.37
1.73
1.72
0.00
Ph
Br
O
O
N
3n
1.54
1.32
2.84
1.89
0.98
1.21
0.99
1.00
1.00
2.98
f1 (ppm)

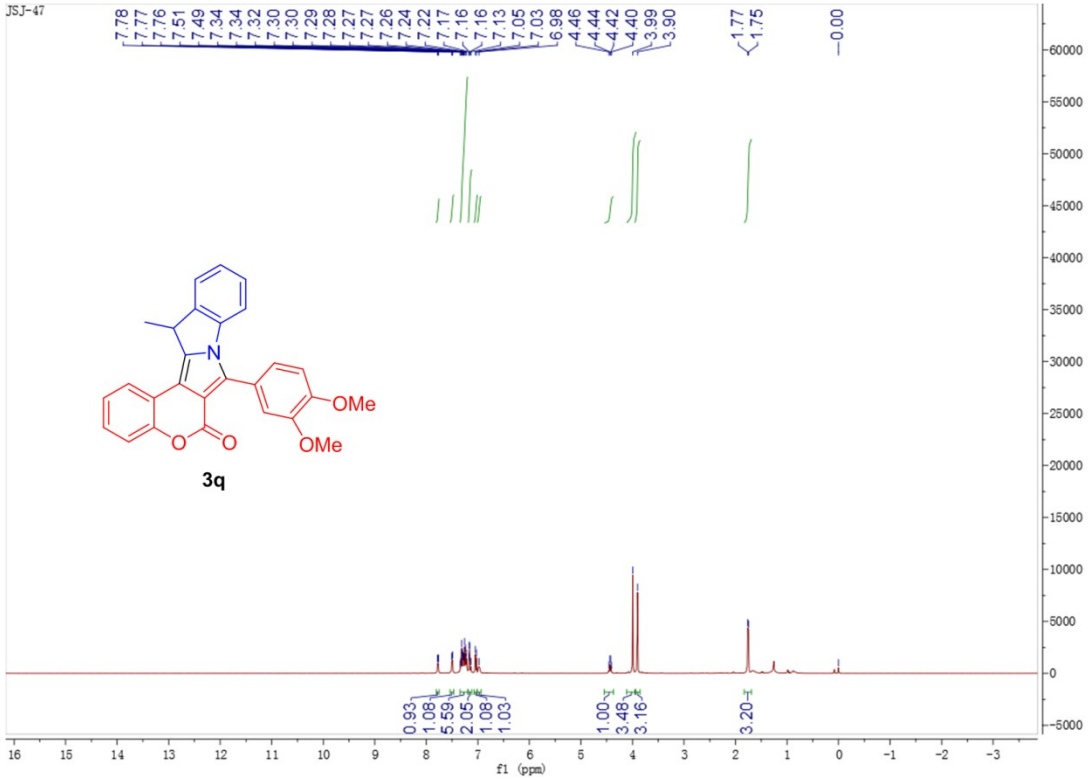

JSJ-42
158.03
151.64
141.66
138.74
134.36
129.63
129.20
128.43
127.87
127.06
126.05
125.23
124.77
120.67
119.91
116.25
113.62
77.38
77.07
76.75
35.60
17.94
Ph
Br
O
O
N
3n
f1 (ppm)

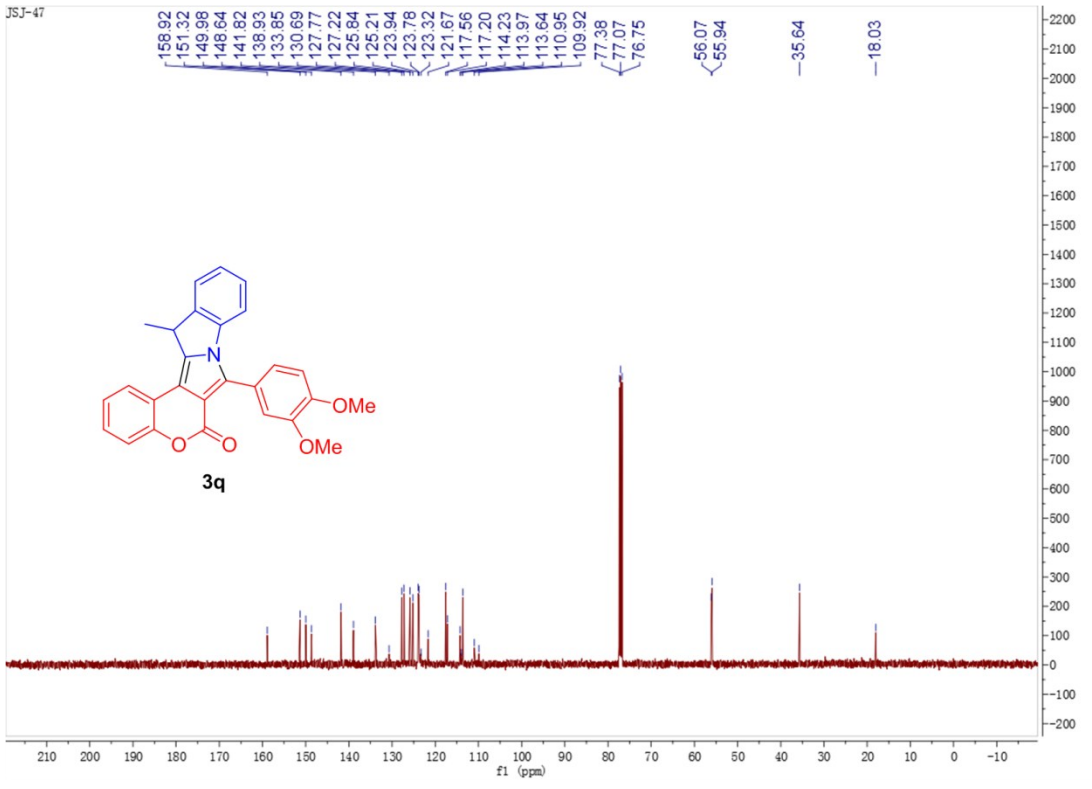

JSJ-53
7.76
7.75
7.74
7.73
7.53
7.52
7.47
7.45
7.34
7.32
7.31
7.29
7.29
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.20
7.18
7.13
7.11
7.10
6.93
6.91
4.41
4.39
4.37
4.35
2.47
1.73
1.71
Me
O
O
N
3o
0.93
1.93
0.98
5.05
1.08
1.04
0.96
1.00
2.95
3.23
f1 (ppm)

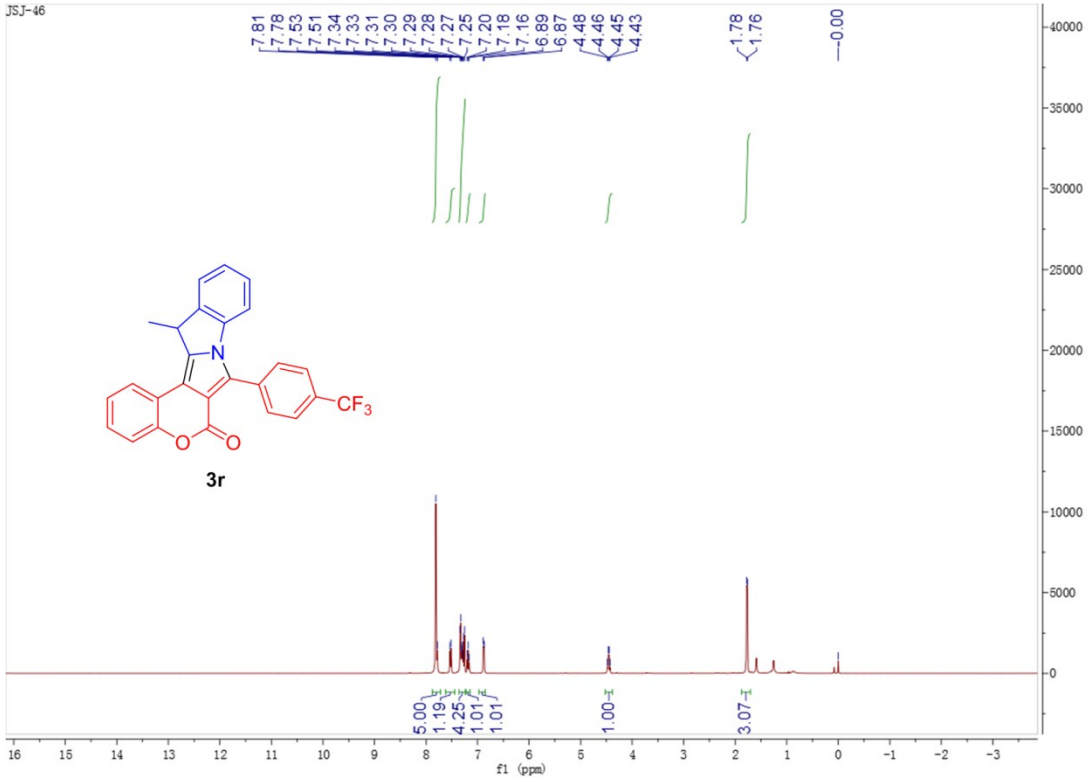

JSJ-53
158.85
151.34
141.82
139.45
138.92
134.01
129.15
127.73
127.16
126.45
125.80
125.17
123.91
123.79
117.52
117.23
113.60
77.43
77.11
76.80
35.60
21.62
18.05
Me
O
O
N
3o
f1 (ppm)

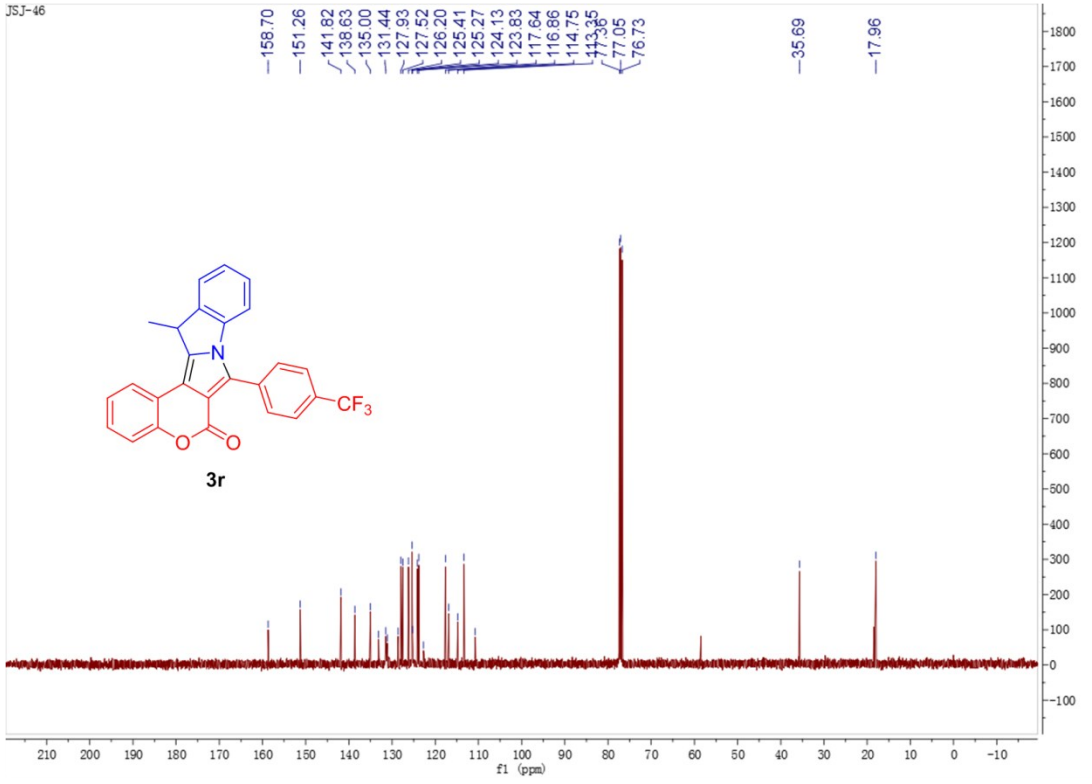

JSJ-44
7.75
7.74
7.73
7.57
7.55
7.47
7.45
7.31
7.31
7.29
7.27
7.27
7.26
7.26
7.24
7.22
7.21
7.19
7.14
7.12
7.11
7.06
7.04
6.94
6.92
4.41
4.39
4.37
4.36
3.90
1.73
1.71
OMe
O
O
N
3p
1.05
2.08
1.08
3.07
1.18
1.08
2.01
1.02
1.00
3.16
3.32
f1 (ppm)

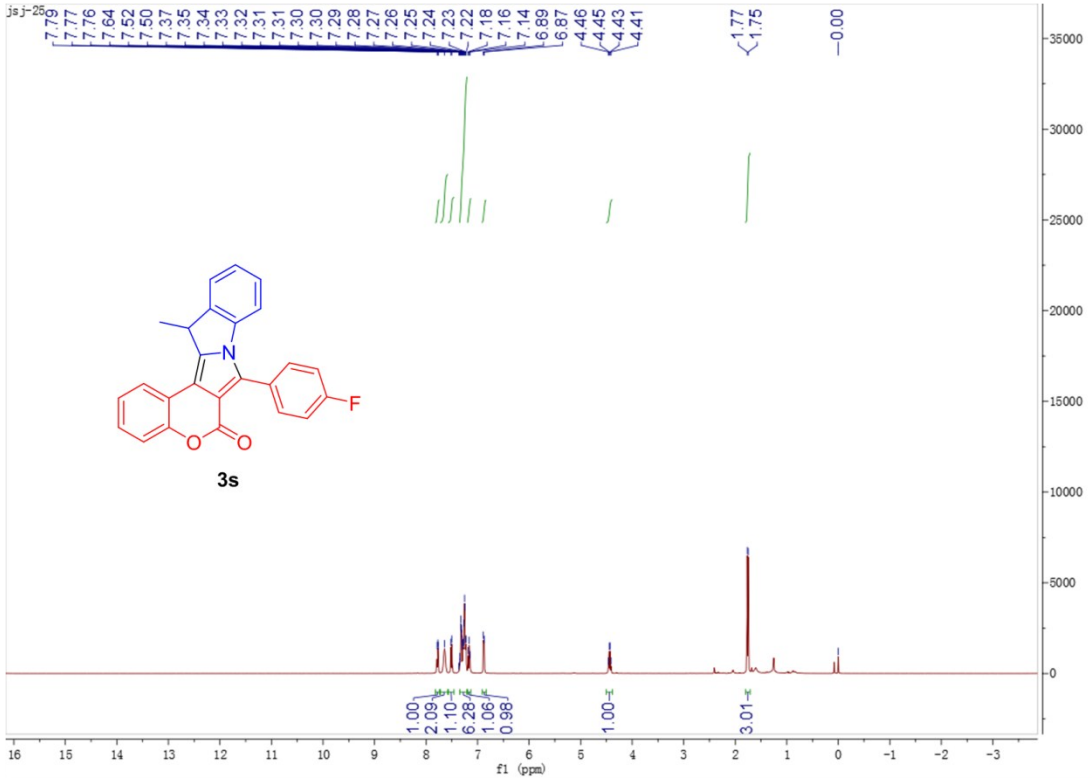

JSJ-44
160.45
158.94
151.31
141.82
138.92
133.88
127.75
127.16
125.80
125.20
123.92
123.79
121.51
117.52
117.24
113.88
113.55
77.44
77.32
77.12
76.80
55.37
35.60
18.05
OMe
O
O
N
3p
f1 (ppm)

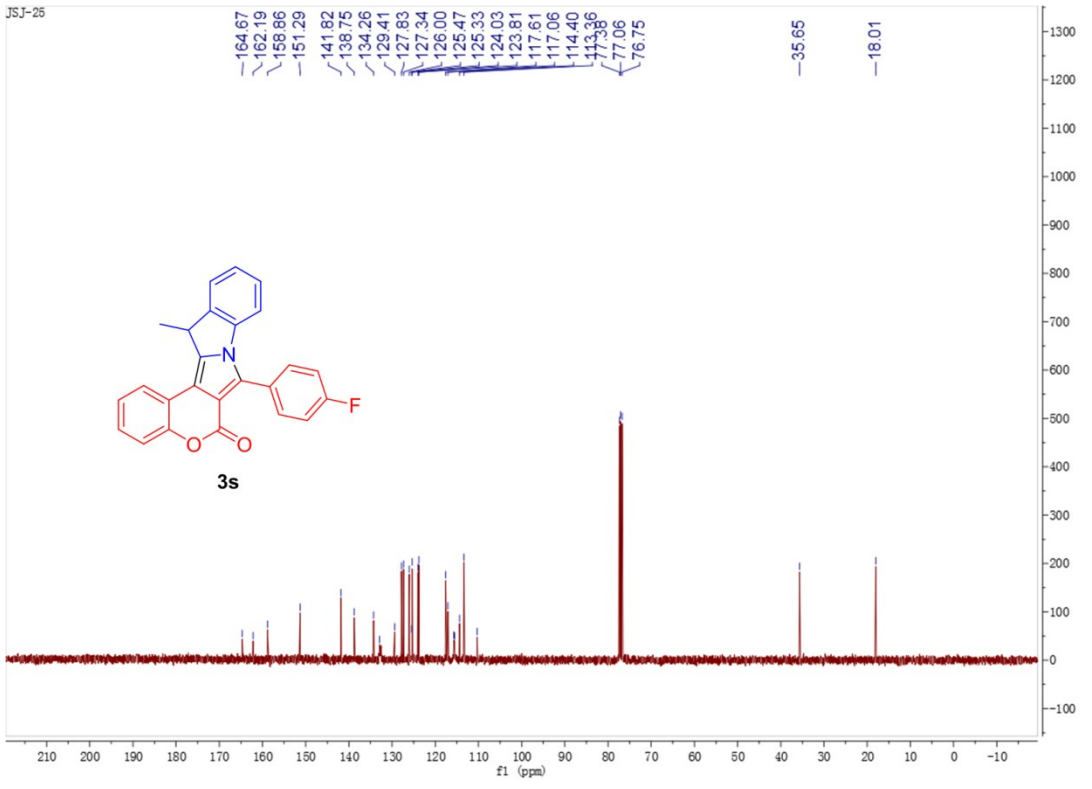

JSJ-47
7.78
7.77
7.76
7.51
7.49
7.34
7.34
7.32
7.30
7.30
7.29
7.28
7.27
7.27
7.26
7.24
7.22
7.17
7.16
7.16
7.13
7.05
7.03
6.98
4.46
4.44
4.42
4.40
3.99
3.90
1.77
1.75
0.00
OMe
OMe
O
O
N
3q
0.93
1.08
5.59
2.05
1.08
1.03
1.00
3.48
3.16
3.20
f1 (ppm)

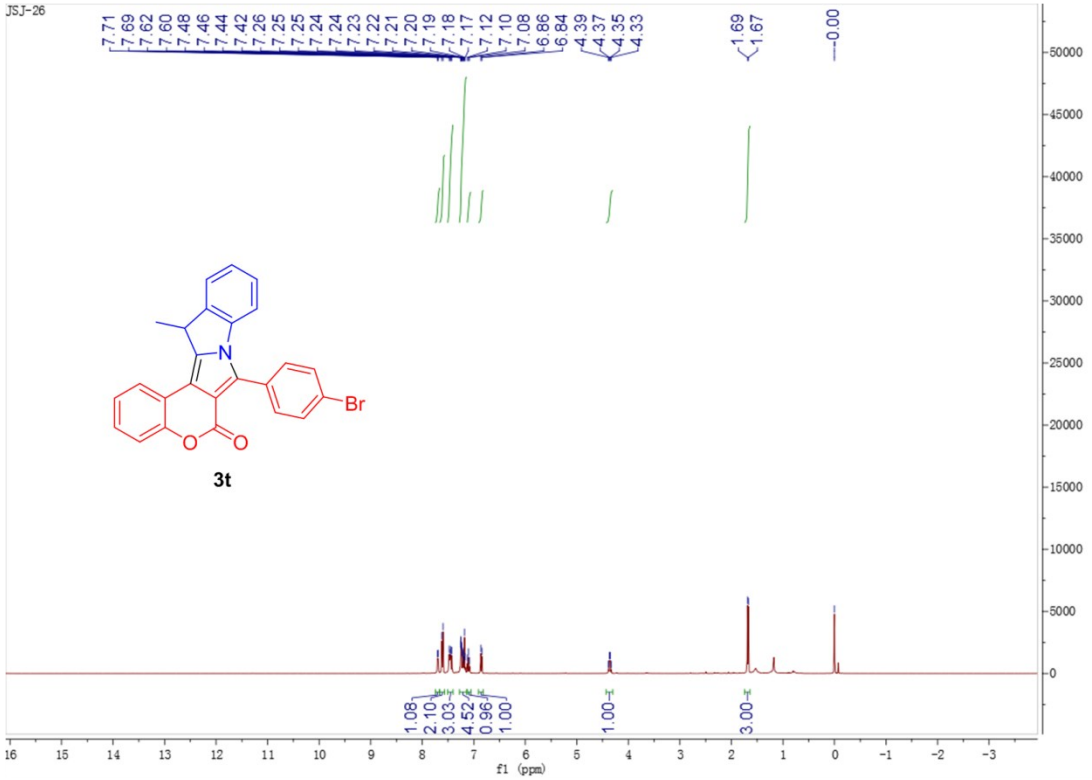

JSJ-47
158.92
151.32
149.98
148.64
141.82
138.93
133.85
130.69
127.77
127.22
125.84
125.21
123.94
123.78
123.32
121.67
117.56
117.20
114.23
113.97
113.64
110.95
109.92
77.38
77.07
76.75
56.07
55.94
35.64
18.03
OMe
OMe
O
O
N
3q
f1 (ppm)

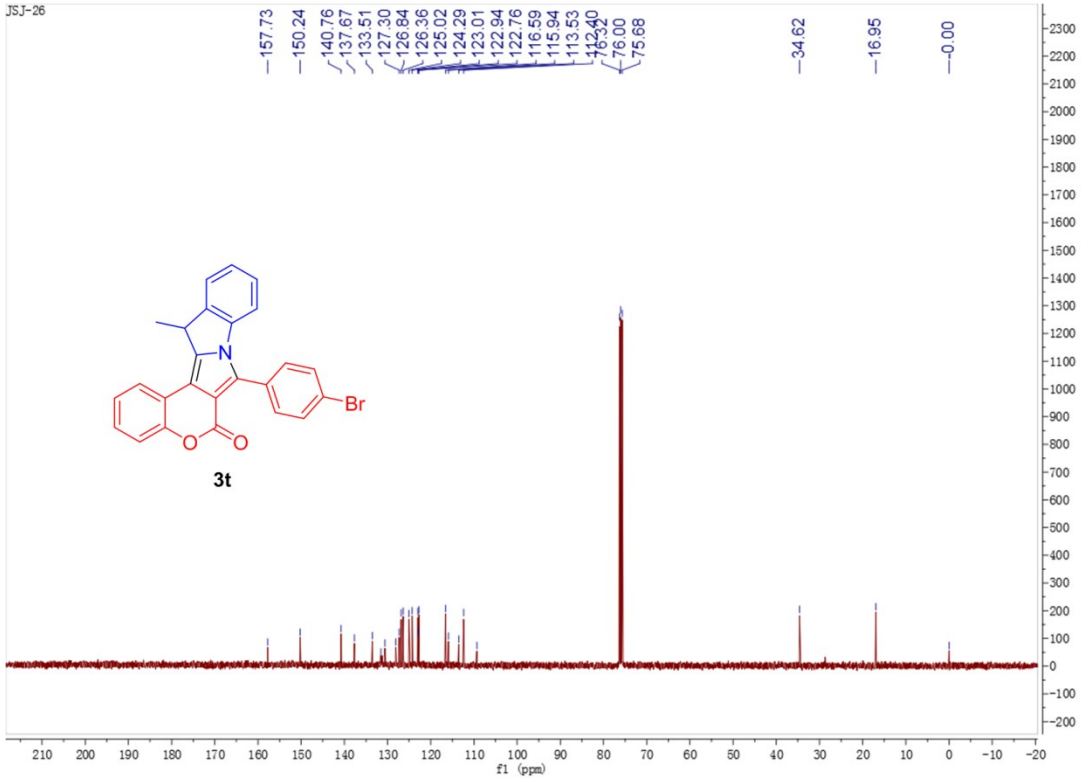

JSJ-46
7.81
7.78
7.53
7.51
7.34
7.33
7.31
7.30
7.29
7.28
7.27
7.25
7.20
7.18
7.16
6.89
6.87
4.48
4.46
4.45
4.43
1.78
1.76
0.00
CF3
O
O
N
3r
5.00
1.19
4.25
1.01
1.01
1.00
3.07
f1 (ppm)

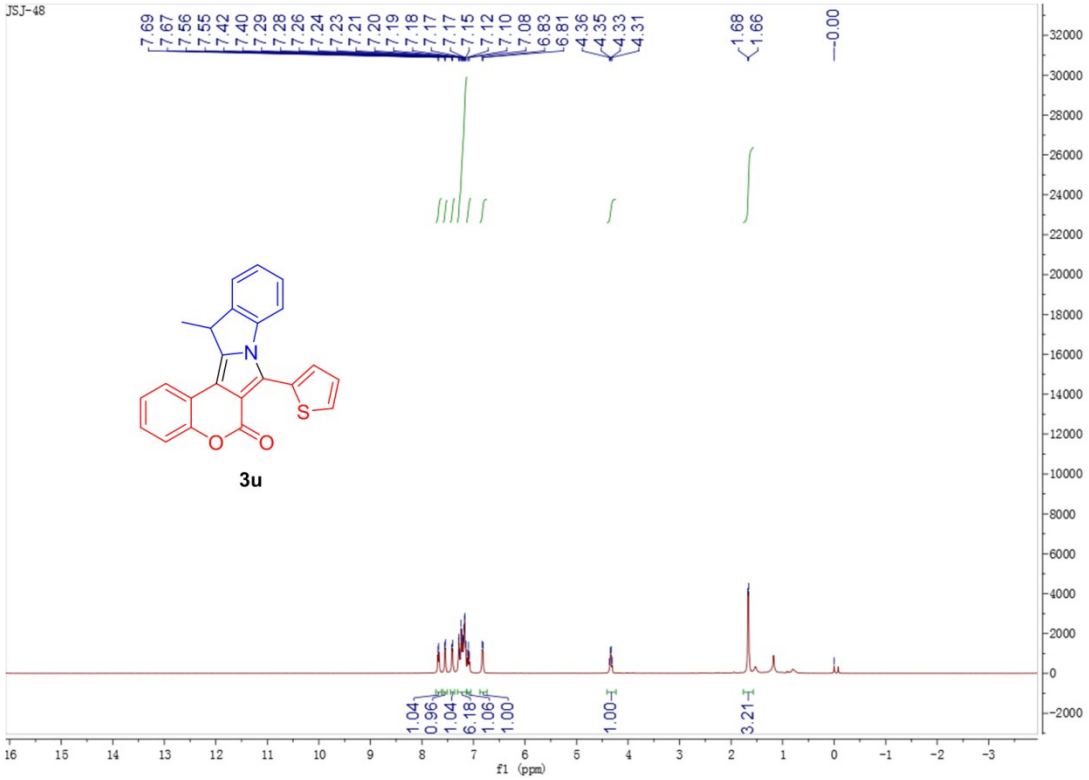

JSJ-46
158.70
151.26
141.82
138.63
135.00
131.44
127.93
127.52
126.20
125.41
125.27
124.13
123.83
117.64
116.86
114.75
77.36
77.05
76.73
35.69
17.96
CF3
O
O
N
3r
f1 (ppm)

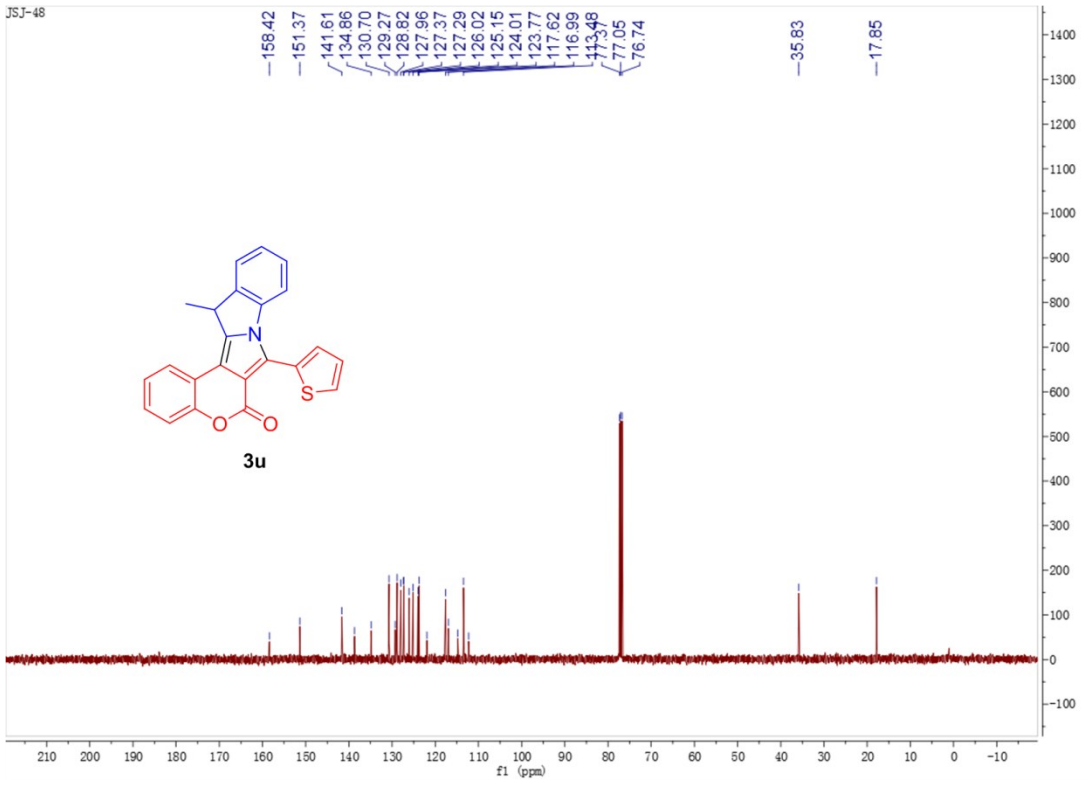

jsj-25
7.79
7.77
7.76
7.64
7.52
7.50
7.37
7.35
7.34
7.33
7.32
7.31
7.31
7.30
7.30
7.29
7.28
7.27
7.26
7.25
7.24
7.23
7.22
7.18
7.16
7.14
6.89
6.87
4.46
4.45
4.43
4.41
1.77
1.75
0.00
N
F
O
O
3s
1.00
2.09
1.10
6.28
1.06
0.98
1.00
3.01
f1 (ppm)

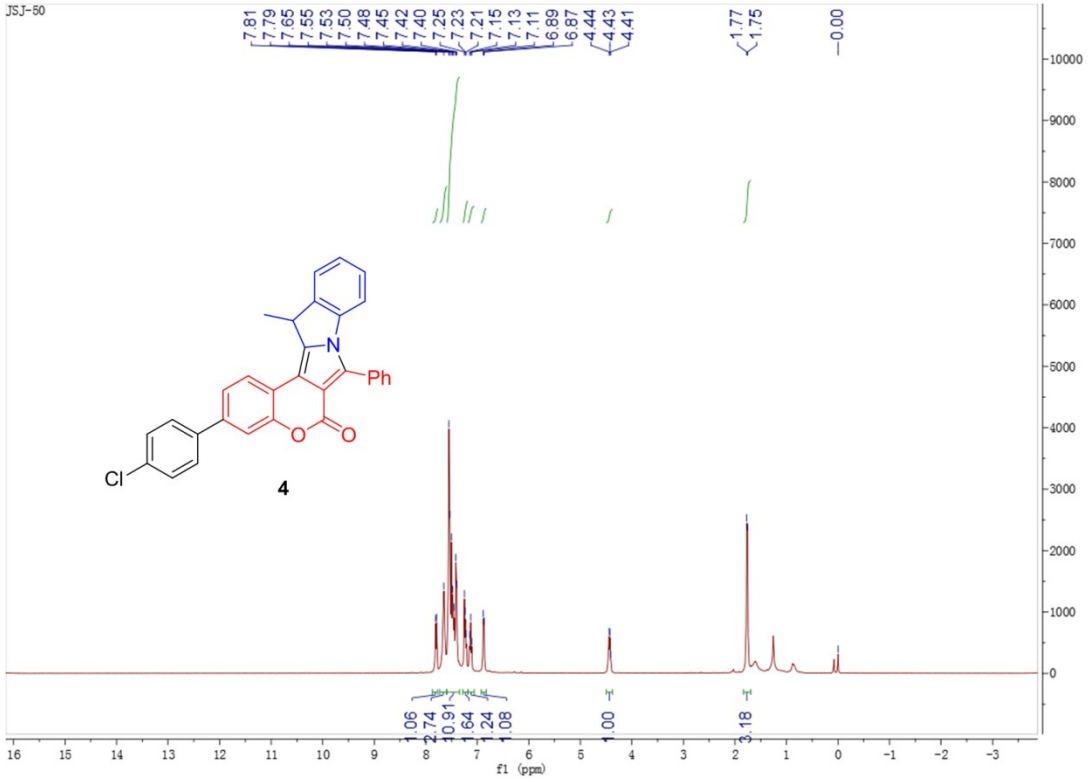

JSJ-25
164.67
162.19
158.86
151.29
141.82
138.75
134.26
129.41
127.83
127.34
126.00
125.47
125.33
124.03
123.81
117.61
117.06
114.40
114.16
77.38
77.06
76.75
35.65
18.01
N
F
O
O
3s
f1 (ppm)

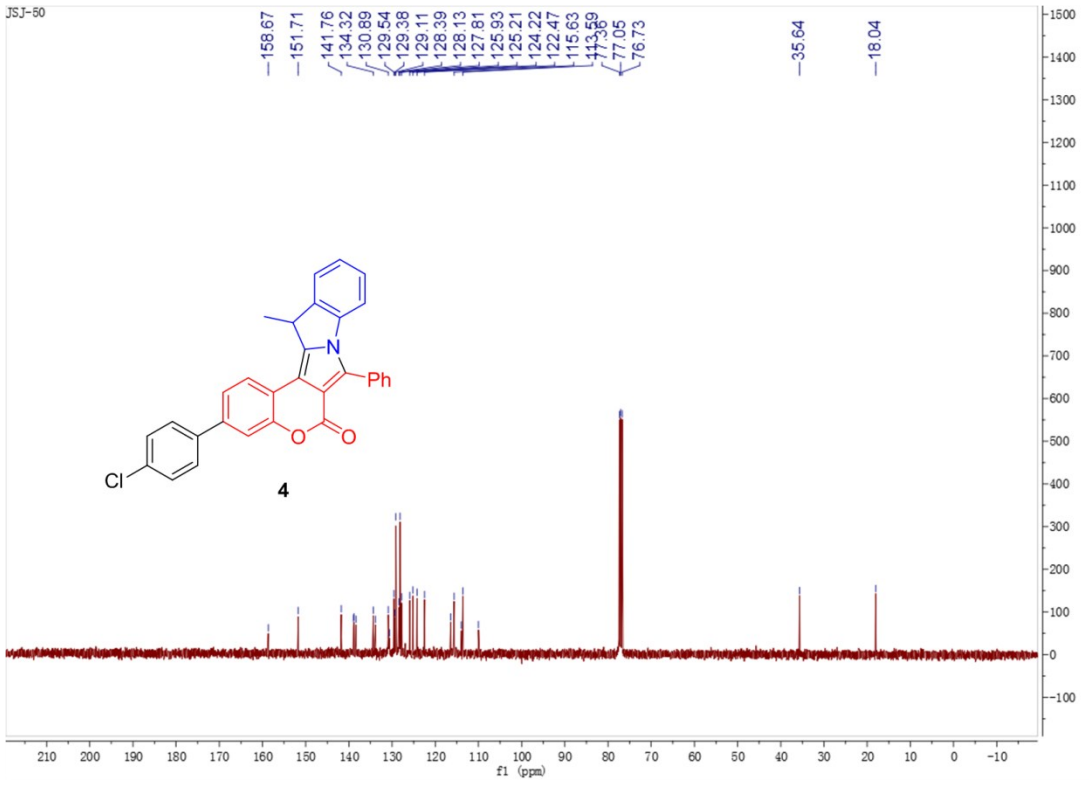

JSJ-26
7.71
7.69
7.62
7.60
7.48
7.46
7.44
7.42
7.26
7.25
7.25
7.24
7.24
7.23
7.22
7.21
7.20
7.19
7.18
7.17
7.12
7.10
7.08
6.86
6.84
4.39
4.37
4.35
4.33
1.69
1.67
0.00
N
Br
O
O
3t
1.08
2.10
3.03
4.52
0.96
1.00
1.00
3.00
f1 (ppm)

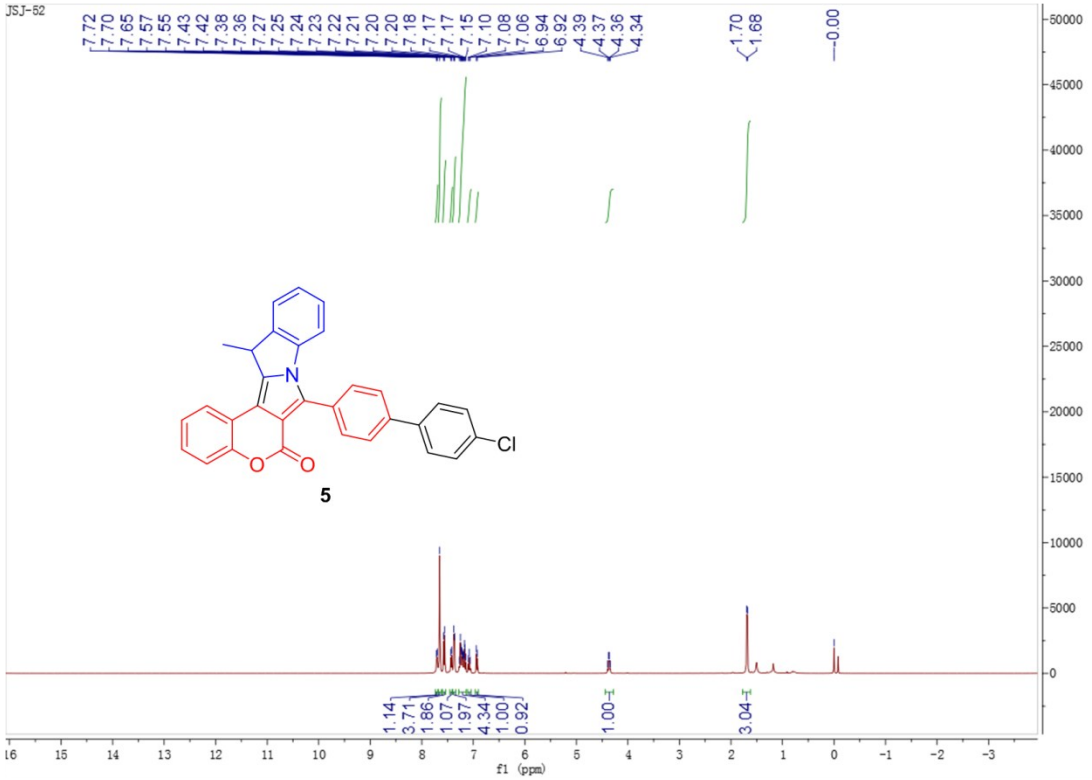

JSJ-26
157.73
150.24
140.76
137.67
133.51
127.30
126.84
126.36
125.02
124.29
123.01
122.94
122.76
116.59
115.94
113.53
112.40
76.32
76.00
75.68
34.62
16.95
0.00
N
Br
O
O
3t
f1 (ppm)

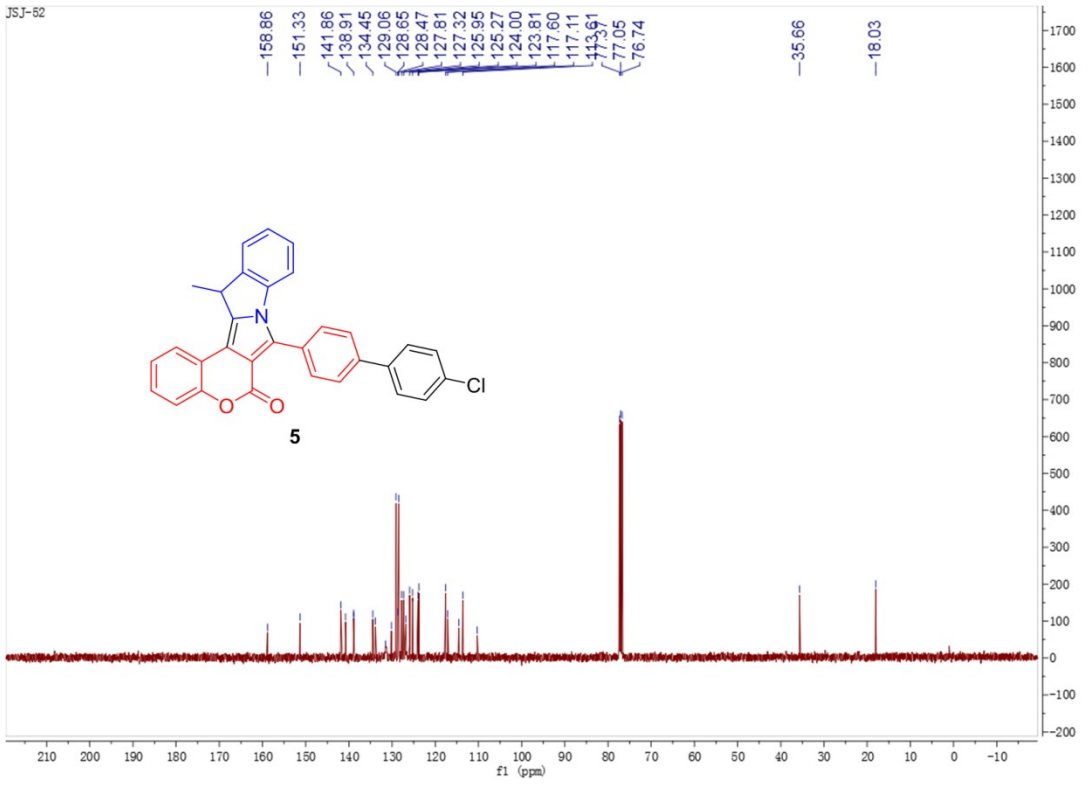

JSJ-48
7.69
7.67
7.56
7.55
7.42
7.40
7.29
7.28
7.26
7.24
7.23
7.21
7.20
7.19
7.18
7.17
7.17
7.15
7.12
7.10
7.08
6.83
6.81
4.36
4.35
4.33
4.31
1.68
1.66
0.00
3u
1.04
0.96
1.04
6.18
1.06
1.00
1.00
3.21
f1 (ppm)


JSJ-48
158.42
151.37
141.61
134.86
130.70
129.27
128.82
127.96
127.37
127.29
126.02
125.15
124.01
123.77
117.62
116.99
113.48
77.37
77.05
76.74
35.83
17.85
3u
f1 (ppm)


JSJ-50
7.81
7.79
7.65
7.55
7.53
7.50
7.48
7.45
7.42
7.40
7.25
7.23
7.21
7.15
7.13
7.11
6.89
6.87
4.44
4.43
4.41
1.77
1.75
0.00
Ph
O
O
N
Cl
4
1.06
2.74
10.91
1.64
1.24
1.08
1.00
3.18
f1 (ppm)


JSJ-50
158.67
151.71
141.76
134.32
130.89
129.54
129.38
129.11
128.39
128.13
127.81
125.93
125.21
124.22
122.47
115.63
113.59
77.36
77.05
76.73
35.64
18.04
Ph
O
O
N
Cl
4
f1 (ppm)


JSJ-52
7.72
7.70
7.65
7.57
7.55
7.43
7.42
7.38
7.36
7.27
7.25
7.24
7.23
7.22
7.21
7.20
7.20
7.18
7.17
7.17
7.15
7.10
7.08
7.06
6.94
6.92
4.39
4.37
4.36
4.34
1.70
1.68
0.00
N
O
O
Cl
5
1.14
3.71
1.86
1.07
1.97
4.34
1.00
0.92
1.00
3.04
f1 (ppm)


JSJ-52
158.86
151.33
141.86
138.91
134.45
129.06
128.65
128.47
127.81
127.32
125.95
125.27
124.00
123.81
117.60
117.11
113.61
77.37
77.05
76.74
35.66
18.03
N
O
O
Cl
5
f1 (ppm)