Supporting Information

Diastereoselective construction of 4-indole substituted chromans bearing a ketal motif through a three-component Friedel-Crafts alkylation/ketalization sequence

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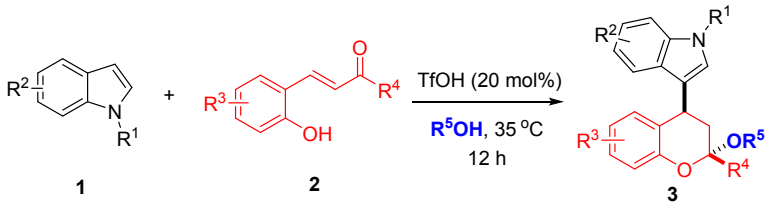
1. General methods

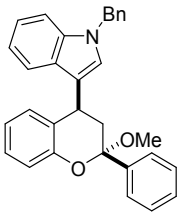
NMR spectra were recorded with tetramethylsilane as the internal standard. ^{1}H NMR spectra were recorded at 400 MHz, and ^{13}C NMR spectra were recorded at 100 MHz (Bruker Avance). ^{1}H NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane (TMS) with the solvent signal as the internal standard ($CDCl_3$ at 7.26 ppm, $(CD_3)_2SO$ at 2.50 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, $(CD_3)_2SO$ at 39.52 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 Thermo Fisher Nicolet Avatar 360 FTIR spectrometer on a KBr beam splitter. All the solvents were used directly without any purification.

2. Experimental data for 4-indole substituted chromans 3



1 2 3

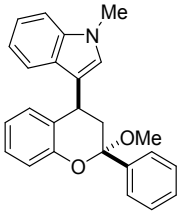
General procedure: To a 5.0 mL vial were successively added indole **1** (0.24 mmol), *ortho*-hydroxychalcone **2** (0.20 mmol), TfOH (6.0 mg, 0.04 mmol) and 1.0 mL alcohol. The resulting mixture was stirred at 35 °C for 12 h. For all cases, the precipitate was generated from the homogenous reaction system, and only a simple filtration was needed to purify them.



1-benzyl-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3a**)

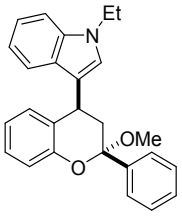
White solid; 86.2 mg, 97% yield; Reaction time = 12 h; mp 148.5-149.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (d, J = 8.0 Hz, 2H), 7.42-7.32 (m, 4H), 7.26-6.96 (m, 12H), 6.82 (t, J = 8.0 Hz, 1H), 5.25 (s, 2H), 4.82 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 3.17 (s, 3H), 2.52 (dd, J_1 = J_2 = 5.6 Hz,

1H), 2.31 (t, J = 13.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 141.2, 137.6, 137.1, 129.1, 128.8, 128.4, 128.2, 127.6, 127.5, 127.4, 126.8, 126.7, 126.5, 126.3, 121.8, 121.3, 120.0, 119.1, 117.1, 117.0, 109.9, 100.7, 50.4, 50.0, 42.8, 30.2. IR (KBr) v 3441, 3060, 3029, 2958, 2935, 2826, 1608, 1580, 1487, 1456, 1365, 1335, 1154, 1045, 1019, 908, 737, 699 cm^{-1}. HRMS (ESI) calcd for $C_{28}H_{29}NNaO_2$ $[M+Na]^+$ 468.1934, found 468.1936.



3-(2-methoxy-2-phenylchroman-4-yl)-1-methyl-1*H*-indole (**3b**)

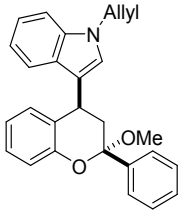
White solid; 68.3 mg, 92% yield; Reaction time = 12 h; mp 71.9-73.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.57-7.55 (m, 2H), 7.31-7.28 (m, 2H), 7.25-7.22 (m, 2H), 7.16 (d, J = 8.0 Hz, 1H), 7.07-7.00 (m, 3H), 6.95-6.86 (m, 2H), 6.81 (s, 1H), 6.72-6.70 (s, 1H), 4.74-4.70 (m, 1H), 3.59 (s, 3H), 3.08 (s, 3H), 2.44-2.39 (m, 1H), 2.24-2.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 141.2, 137.4, 129.2, 128.5, 128.2, 127.6, 127.4, 127.2, 126.7, 126.3, 121.6, 121.3, 119.9, 118.9, 117.2, 116.4, 109.4, 100.7, 50.4, 42.9, 32.7, 30.2. IR (KBr) v 3425, 3058, 2935, 2831, 1721, 1612, 1582, 1483, 1452, 1236, 1155, 1045, 1019, 907, 743, 701 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{23}NNaO_2$ $[M+Na]^+$ 392.1621, found 392.1607.



1-ethyl-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3c**)

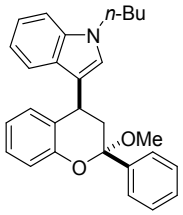
White solid; 72.2 mg, 94% yield; Reaction time = 12 h; mp 113.7-115.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (d, J = 8.0 Hz, 2H), 7.39-7.27 (m, 5H), 7.18-7.09 (m, 3H), 7.04 (d, J = 8.0 Hz, 1H), 6.97-6.95 (m, 2H), 6.80 (t, J = 8.0 Hz, 1H), 4.83 (dd, J_1 = J_2 = 5.6 Hz, 1H), 4.05 (q, J = 6.4 Hz, 2H), 3.17 (s, 3H), 2.52 (dd, J_1 = J_2 = 5.6 Hz, 1H), 2.31 (t, J = 12.0 Hz, 1H), 1.38 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 141.3, 136.5, 129.3, 128.5, 128.3, 127.6, 127.5, 126.8, 126.4, 125.6, 121.6, 121.4, 120.1, 118.9, 117.2, 116.5, 109.5, 100.8, 50.5, 43.0, 40.9, 30.3, 15.6. IR (KBr) v 3426, 3056, 2965, 2935, 2832, 1732, 1612, 1582, 1483, 1452, 1233, 1155, 1047, 1019,

908, 743, 703 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{25}NNaO_2$ $[M+Na]^+$ 406.1778, found 406.1777.



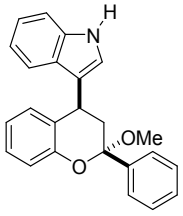
1-allyl-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3d**)

White solid; 76.6 mg, 97% yield; Reaction time = 12 h; mp 136.1-138.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.57 (d, J = 8.0 Hz, 2H), 7.33-7.17 (m, 5H), 7.11-7.06 (m, 2H), 7.02 (t, J = 8.0 Hz, 1H), 6.94 (t, J = 8.0 Hz, 1H), 6.89 (t, J = 8.0 Hz, 2H), 6.72 (t, J = 8.0 Hz, 1H), 5.91-5.81 (m, 1H), 5.07 (d, J = 10.4 Hz, 1H), 4.95 (d, J = 16.0 Hz, 1H), 4.73 (dd, $J_1 = J_2$ = 5.6 Hz, 1H), 4.55 (d, J = 5.2 Hz, 2H), 3.09 (s, 3H), 2.43 (dd, $J_1 = J_2$ = 5.6 Hz, 1H), 2.22 (t, J = 13.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 141.2, 136.9, 133.6, 129.2, 128.5, 128.2, 127.6, 127.4, 126.6, 126.4, 126.3, 121.7, 121.3, 120.0, 119.0, 117.3, 117.1, 116.8, 109.8, 100.7, 50.4, 48.8, 42.8, 30.1. IR (KBr) v 3431, 3059, 2962, 2935, 2832, 1582, 1485, 1455, 1337, 1155, 1048, 1020, 912, 760, 738 cm^{-1}. HRMS (ESI) calcd for $C_{27}H_{25}NNaO_2$ $[M+Na]^+$ 418.1778, found 418.1776.



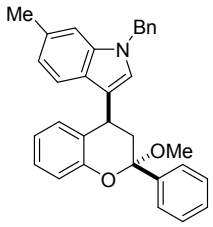
1-butyl-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3e**)

White solid; 80.2 mg, 97% yield; Reaction time = 12 h; mp 145.1-146.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.57 (d, J = 8.0 Hz, 2H), 7.31 (t, J = 8.0 Hz, 2H), 7.27-7.20 (m, 3H), 7.11-7.00 (m, 3H), 6.95 (d, J = 8.0 Hz, 1H), 6.89-6.86 (m, 2H), 6.72 (t, J = 8.0 Hz, 1H), 4.73 (dd, $J_1 = J_2$ = 8.0 Hz, 1H), 3.95 (t, J = 8.0 Hz, 2H), 3.09 (s, 3H), 2.42 (dd, $J_1 = J_2$ = 5.6 Hz, 1H), 2.21 (t, J = 13.2 Hz, 1H), 1.72-1.64 (m, 2H), 1.26-1.14 (m, 2H), 0.82 (t, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 141.2, 136.7, 129.2, 128.4, 128.2, 127.5, 127.3, 126.7, 126.3, 121.4, 121.3, 119.9, 118.7, 117.1, 116.2, 109.6, 100.7, (one carbon missing in the aromatic region), 50.4, 46.1, 42.9, 32.4, 30.1, 20.3, 13.8. IR (KBr) v 3431, 3058, 2964, 2933, 2830, 1580, 1482, 1451, 1342, 1154, 1050, 1015, 906, 758, 736 cm^{-1}. HRMS (ESI) calcd for $C_{28}H_{29}NNaO_2$ $[M+Na]^+$ 434.2091, found 434.2098.



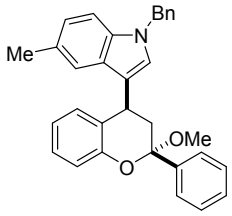
3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3f**)

White solid; 55.0 mg, 77% yield; Reaction time = 12 h; mp 188.3-189.4 ^{o}C; ^{1}H NMR (400 MHz, DMSO-d_6), δ 11.0 (s, 1H), 7.64 (d, J = 8.0 Hz, 2H), 7.47 (t, J = 8.0 Hz, 2H), 7.41-7.35 (m, 3H), 7.17-7.08 (m, 3H), 7.03 (t, J = 8.0 Hz, 1H), 6.87-6.77 (m, 3H), 4.70 (dd, J_1 = J_2 = 8.0 Hz, 1H), 3.05 (s, 3H), 2.42 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.28 (t, J = 13.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 151.8, 140.9, 137.2, 129.0, 128.9, 128.8, 128.0, 127.1, 126.5, 126.4, 124.3, 121.6, 121.4, 119.2, 118.9, 117.4, 115.8, 112.2, 100.6, 50.2, 42.0, 30.1. IR (KBr) v 3455, 3061, 3030, 2961, 2936, 2833, 1581, 1487, 1451, 1234, 1155, 1046, 1018, 907, 745, 702 cm^{-1}. HRMS (ESI) calcd for $C_{24}H_{21}NNaO_2$ $[M+Na]^+$ 378.1465, found 378.1456.



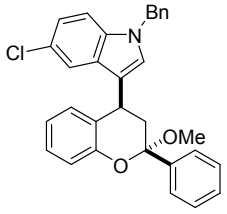
1-benzyl-3-(2-methoxy-2-phenylchroman-4-yl)-6-methyl-1*H*-indole (**3g**)

White solid; 85.5 mg, 93% yield; Reaction time = 12 h; mp 142.9-144.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (d, J = 8.0 Hz, 2H), 7.40 (t, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 1H), 7.30-7.16 (m, 5H), 7.10-7.04 (m, 5H), 6.95 (s, 1H), 6.82 (t, J = 4.0 Hz, 2H), 5.23 (s, 2H), 4.78 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.17 (s, 3H), 2.50 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.39 (s, 3H), 2.30 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 141.1, 137.8, 137.5, 131.6, 129.1, 128.8, 128.4, 128.2, 127.5, 127.4, 126.7, 126.6, 126.3, 126.1, 125.2, 121.2, 120.8, 119.7, 117.1, 116.9, 109.8, 100.7, 50.4, 49.8, 42.8, 30.2, 21.9. IR (KBr) v 3433, 3064, 3028, 2937, 2828, 1607, 1580, 1488, 1448, 1233, 1184, 1155, 1045, 1023, 762, 702 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2091, found 482.2067.



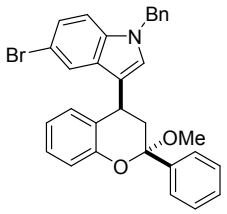
1-benzyl-3-(2-methoxy-2-phenylchroman-4-yl)-5-methyl-1*H*-indole (**3h**)

White solid; 87.2 mg, 95% yield; Reaction time = 12 h; mp 181.4-182.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.68-7.65 (m, 2H), 7.42-7.34 (m, 3H), 7.27-7.20 (m, 6H), 7.15-7.07 (m, 5H), 6.97 (d, *J* = 4.0 Hz, 1H), 6.84 (t, *J* = 8.0 Hz, 1H), 5.24 (s, 2H), 4.82-4.79 (m, 1H), 3.18 (d, *J* = 4.0 Hz, 3H), 2.55-2.49 (m, 1H), 2.36 (d, *J* = 4.0 Hz, 3H), 2.28 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 141.1, 137.7, 135.4, 129.0, 128.7, 128.4, 128.3, 128.2, 127.8, 127.5, 127.4, 126.7, 126.6, 126.3, 123.4, 121.2, 119.4, 117.0, 116.5, 116.4, 109.6, 100.6, 50.3, 50.0, 42.7, 29.9, 21.5. IR (KBr) *v* 3425, 3063, 3031, 2933, 1616, 1582, 1487, 1450, 1230, 1162, 1045, 1024, 760, 702 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2091, found 482.2100.



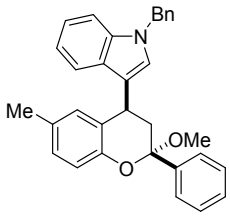
1-benzyl-5-chloro-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3i**)

White solid; 87.1 mg, 91% yield; Reaction time = 12 h; mp 163.9-165.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 2H), 7.27 (t, J = 8.0 Hz, 3H), 7.20 (t, *J* = 8.0 Hz, 1H), 7.15-7.04 (m, 6H), 7.00 (d, *J* = 8.0 Hz, 1H), 6.84 (t, *J* = 8.0 Hz, 1H), 5.24 (s, 2H), 4.77 (dd, $J_1 = J_2$ = 8.0 Hz, 1H), 3.17 (s, 3H), 2.49 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.24 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 138.8, 137.6, 137.1, 135.2, 129.8, 129.0, 128.8, 127.6, 127.5, 127.3, 126.8, 126.5, 121.8, 121.3, 120.7, 120.1, 119.1, 117.0, 116.8, 109.8, 100.8, one carbon missing in the aromatic region, 50.4, 50.0, 38.9, 29.7. IR (KBr) *v* 3429, 3065, 3031, 2960, 2938, 2831, 1580, 1458, 1347, 1236, 1156, 1024, 908, 758, 701 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}ClNNaO_2$ $[M+Na]^+$ 502.1544, found 502.1553.



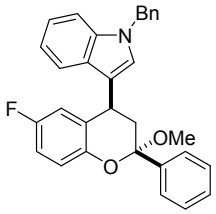
1-benzyl-5-bromo-3-(2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3j**)

White solid; 101.8 mg, 97% yield; Reaction time = 12 h; mp 163.8-165.4 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.58 (d, *J* = 4.0 Hz, 2H), 7.43 (s, 1H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 4.0 Hz, 1H), 7.20-7.11 (m, 5H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.96 (d, *J* = 4.0 Hz, 2H), 6.92 (d, *J* = 8.0 Hz, 2H), 6.77 (t, *J* = 8.0 Hz, 1H), 5.15 (s, 2H), 4.70 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.09 (s, 3H), 2.42 (dd, $J_1 = J_2$ = 5.6 Hz, 1H), 2.15 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 140.9, 137.1, 135.6, 129.3, 128.9, 128.8, 128.4, 128.2, 127.9, 127.8, 127.7, 126.7, 126.3, 126.0, 124.7, 122.3, 121.3, 117.3, 116.8, 112.6, 111.4, 100.5, 50.3, 50.2, 42.7, 29.9. IR (KBr) *v* 3430, 3067, 3031, 2936, 2835, 1608, 1581, 1477, 1450, 1355, 1308, 1157, 1046, 1022, 907, 759, 701 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}BrNNaO_2$ $[M+Na]^+$ 546.1039, found 546.1036.



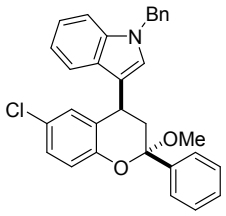
1-benzyl-3-(2-methoxy-6-methyl-2-phenylchroman-4-yl)-1*H*-indole (**3k**)

White solid; 87.6 mg, 95% yield; Reaction time = 12 h; mp 175.0-176.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.66 (t, *J* = 8.0 Hz, 2H), 7.43-7.38 (m, 3H), 7.35-7.23 (m, 5H), 7.17-7.08 (m, 3H), 7.02 (q, *J* = 8.0 Hz, 4H), 6.87 (d, *J* = 8.0 Hz, 1H), 5.27 (d, *J* = 4.0 Hz, 2H), 4.83-4.76 (m, 1H), 3.17 (d, *J* = 4.0 Hz, 3H), 2.54-2.47 (m, 1H), 2.33-2.24 (m, 1H), 2.14 (d, *J* = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.9, 141.2, 137.6, 137.0, 130.4, 129.3, 128.8, 128.4, 128.2, 128.1, 127.6, 127.5, 126.8, 126.7, 126.3, 126.2, 121.7, 120.0, 119.1, 117.3, 116.9, 109.8, 100.5, 50.3, 50.0, 43.1, 30.1, 20.8. IR (KBr) *v* 3402, 3029, 2930, 2835, 1608, 1490, 1456, 1341, 1237, 1157, 1045, 927, 736, 708 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2091, found 482.2100.



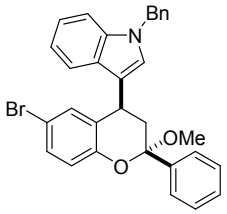
1-benzyl-3-(6-fluoro-2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3l**)

White solid; 90.7 mg, 98% yield; Reaction time = 12 h; mp 148.1-149.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.32-7.10 (m, 8H), 7.05-6.89 (m, 6H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 5.16 (s, 2H), 4.67 (s, 1H), 3.06 (s, 3H), 2.42-2.39 (m, 1H), 2,24-2.17 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.5 (d, *J* = 237.0 Hz, 1C), 148.0 (d, *J* = 2.0 Hz, 1C), 140.8, 137.5, 132.2, 128.9, 128.5, 128.3, 128.1 (d, *J* = 7.0 Hz, 1C), 127.7, 127.1, 126.8, 126.7, 126.3, 122.0, 119.9, 119.3, 118.4 (d, *J* = 8.0 Hz, 1C), 116.4, 115.2 (d, *J* = 23.0 Hz, 1C), 114.35 (d, *J* = 24.0 Hz, 1C), 110.0, 100.7, 50.4, 50.2, 42.4, 30.5. IR (KBr) *v* 3429, 3038, 2936, 2832, 1615, 1488, 1249, 1187, 1153, 1020, 933, 739, 700 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}FNNaO_2$ $[M+Na]^+$ 486.1840, found 486.1850.



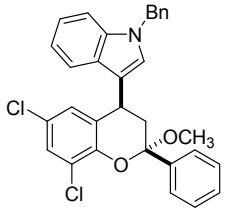
1-benzyl-3-(6-chloro-2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3m**)

White solid; 93.6 mg, 98% yield; Reaction time = 12 h; mp 145.3-147.2 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.43-7.34 (m, 4H), 7.31-7.25 (m, 4H), 7.17-7.09 (m, 4H), 7.04-7.02 (m, 4H), 5.29 (s, 2H), 4.78 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.16 (s, 3H), 2.53-2.47 (m, 1H), 2.29 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 140.6, 137.5, 137.1, 128.8, 128.7, 128.4, 128.3, 127.7, 127.6, 127.1, 126.8, 126.7, 126.2, 126.1, 121.9, 119.7, 119.2, 118.5, 116.2, 109.9, 100.9, 50.4, 50.0, 42.4, 30.2. IR (KBr) *v* 3429, 3058, 3029, 2938, 2836, 1475, 1342, 1247, 1155, 1039, 1019, 909, 742, 705 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}ClNNaO_2$ $[M+Na]^+$ 502.1544, found 502.1546.



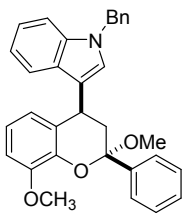
1-benzyl-3-(6-bromo-2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3n**)

White solid; 100.9 mg, 96% yield; Reaction time = 12 h; mp 171.1-172.4 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.62 (d, J = 8.0 Hz, 2H), 7.42-7.25 (m, 10H), 7.14 (d, J = 8.0 Hz, 2H), 7.09 (d, J = 8.0 Hz, 2H), 7.03-6.97 (m, 2H), 5.28 (s, 2H), 4.78 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.15 (s, 3H), 2.50 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.28 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.3, 140.6, 137.5, 137.1, 131.6, 130.5, 129.0, 128.8, 128.4, 128.3, 127.7, 127.1, 126.8, 126.8, 126.2, 121.9, 119.7, 119.3, 119.0, 116.2, 113.6, 109.9, 100.9, 50.4, 50.0, 42.5, 30.2. IR (KBr) v 3427, 3057, 3029, 2938, 2836, 1473, 1342, 1247, 1156, 1039, 1019, 908, 741, 703 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}BrNNaO_2$ $[M+Na]^+$ 546.1039, found 546.1045.



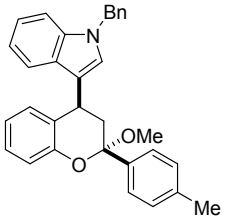
1-benzyl-3-(6,8-dichloro-2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**3o**)

White solid; 100.0 mg, 97% yield; Reaction time = 12 h; mp 186.2-187.7 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.70-7.67 (m, 2H), 7.43 (t, J = 8.0 Hz, 2H), 7.38-7.25 (m, 7H), 7.16 (t, J = 8.0 Hz, 1H), 7.10 (d, J = 8.0 Hz, 2H), 7.03 (t, J = 8.0 Hz, 2H), 6.93-6.90 (m, 1H), 5.29 (s, 2H), 4.79 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.15 (s, 3H), 2.60-2.54 (m, 1H), 2.37-2.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 139.9, 137.4, 137.1, 129.7, 128.8, 128.5, 128.4, 127.9, 127.7, 127.3, 126.9, 126.8, 126.3, 126.2, 125.7, 123.1, 122.0, 119.7, 119.4, 115.7, 110.0, 101.4, 50.5, 50.0, 42.0, 30.5. IR (KBr) v 3427, 3032, 2938, 2832, 1452, 1341, 1255, 1154, 1021, 974, 922, 741, 699 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{25}Cl_2NNaO_2$ $[M+Na]^+$ 536.1155, found 536.1156.



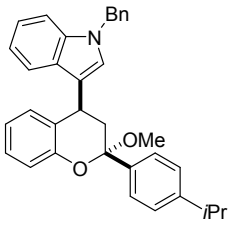
1-benzyl-3-(2,8-dimethoxy-2-phenylchroman-4-yl)-1*H*-indole (**3p**)

White solid; 89.7 mg, 94% yield; Reaction time = 12 h; mp 155.1-156.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.61 (d, J = 8.0 Hz, 2H), 7.33-7.12 (m, 8H), 7.01 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 3H), 6.90 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 2H), 6.72 (d, J = 8.0 Hz, 1H), 6.67 (t, J = 8.0 Hz, 1H), 6.58 (d, J = 8.0 Hz, 1H), 5.15 (s, 2H), 4.74 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 3.84 (s, 3H), 3.10 (s, 3H), 2.45 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.24 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 140.5, 140.0, 136.5, 135.9, 127.7, 127.3, 127.1, 126.5, 126.3, 125.7, 125.6, 125.3, 120.7, 119.9, 119.3, 118.9, 117.9, 116.1, 109.2, 108.7, 99.5, one carbon missing in the aromatic region, 55.3, 49.3, 48.9, 41.6, 29.2. IR (KBr) v 3431, 3036, 2936, 2833, 1586, 1467, 1339, 1264, 1212, 1158, 1045, 1023, 945, 738, 704 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_3$ $[M+Na]^+$ 498.2040, found 498.2054.



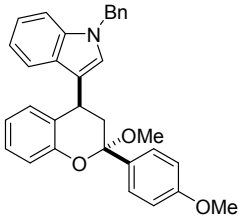
1-benzyl-3-(2-methoxy-2-(p-tolyl)chroman-4-yl)-1*H*-indole (**3q**)

White solid; 88.8 mg, 97% yield; Reaction time = 12 h; mp 168.2-169.3 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.46 (d, J = 8.0 Hz, 2H), 7.29 (d, J = 8.0 Hz, 1H), 7.22-7.07 (m, 8H), 7.05-7.00 (m, 3H), 6.98-6.89 (m, 3H), 6.74 (t, J = 8.0 Hz, 1H), 5.19 (s, 2H), 4.73 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 3.09 (s, 3H), 2.43 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.29 (s, 3H), 2.22 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 137.1, 136.8, 136.5, 135.9, 128.0, 127.9, 127.7, 127.4, 126.8, 126.5, 126.4, 125.7, 125.6, 125.5, 125.1, 120.7, 120.1, 118.9, 118.0, 116.0, 108.7, 99.6, 49.2, 48.9, 41.7, 29.0, 20.1. IR (KBr) v 3431, 3030, 2927, 1615, 1453, 1343, 1264, 1222, 1154, 1103, 1023, 977, 908, 812, 732 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2091, found 482.2086.



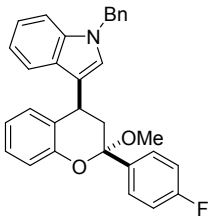
1-benzyl-3-(2-(4-isopropylphenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3r**)

White solid; 85.4 mg, 88% yield; Reaction time = 12 h; mp 173.5-174.4 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 8.0 Hz, 6H), 7.12-6.90 (m, 8H), 6.74 (t, *J* = 8.0 Hz, 1H), 5.18 (s, 2H), 4.73 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 3.11 (s, 3H), 2.88-2.81 (m, 1H), 2.43 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.23 (t, *J* = 12.0 Hz, 1H), 1.18 (d, *J* = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 148.8, 138.5, 137.6, 137.0, 129.1, 128.8, 128.7, 127.6, 127.5, 127.4, 126.8, 126.7, 126.6, 126.4, 126.2, 121.8, 121.2, 120.0, 119.0, 117.1, 109.8, 100.7, 50.3, 50.0, 42.8, 33.9, 30.1, 24.1. IR (KBr) *v* 3435, 3033, 2963, 1582, 1480, 1456, 1340, 1264, 1220, 1156, 1107, 1025, 968, 908, 834, 736 cm^{-1}. HRMS (ESI) calcd for $C_{34}H_{33}NNaO_2$ $[M+Na]^+$ 510.2404, found 510.2407.



1-benzyl-3-(2-methoxy-2-(4-methoxyphenyl)chroman-4-yl)-1*H*-indole (**3s**)

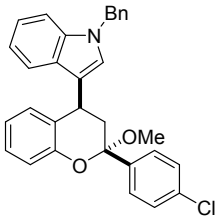
White solid; 85.8 mg, 90% yield; Reaction time = 12 h; mp 81.1-82.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.50 (t, *J* = 8.0 Hz, 2H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.19-6.84 (m, 14H), 6.74 (t, *J* = 8.0 Hz, 1H), 5.19 (s, 2H), 4.74 (s, 1H), 3.74 (d, *J* = 4.0 Hz, 3H), 3.09 (d, *J* = 8.0 Hz, 3H), 2.47-2.41 (m, 1H), 2.27-2.18 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 152.1, 137.6, 137.0, 133.3, 129.1, 128.8, 127.6, 127.5, 127.5, 127.5, 127.4, 126.8, 126.7, 126.6, 121.8, 121.2, 120.0, 119.1, 117.1, 113.7, 109.9, 100.6, 55.3, 50.2, 50.0, 42.9, 30.2. IR (KBr) *v* 3424, 3032, 2933, 2834, 1609, 1582, 1485, 1458, 1337, 1306, 1252, 1171, 1024, 970, 905, 835, 741 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_3$ $[M+Na]^+$ 498.2040, found 498.2030.



1-benzyl-3-(2-(4-fluorophenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3t**)

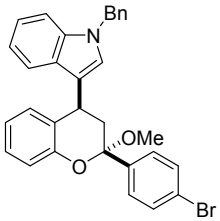
White solid; 91.7 mg, 99% yield; Reaction time = 12 h; mp 137.9-139.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.53 (t, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 1H), 7.17 (t, *J* = 8.0 Hz, 4H), 7.12-6.88 (m, 10H), 6.74 (t, *J* = 8.0 Hz, 1H), 5.16 (s, 2H), 4.72 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.07 (s, 3H), 2.41 (dd,

J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.20 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.7 (d, J = 245.0 Hz, 1C), 151.9, 137.6, 137.1, 129.1, 128.8, 128.3, 128.2, 127.7, 127.6, 127.4, 126.8, 126.7, 126.4, 121.9, 121.4, 120.0, 119.1, 117.1, 116.9, 115.3 (d, J = 21.0 Hz, 1C), 109.9, 100.4, 50.3, 50.0, 42.9, 30.2. IR (KBr) v 3427, 3061, 3032, 2935, 2834, 1607, 1507, 1485, 1457, 1337, 1264, 1225, 1155, 1106, 1044, 1021, 908, 838, 809, 738, 698 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}FNNaO_2$ $[M+Na]^+$ 486.1840, found 486.1839.



1-benzyl-3-(2-(4-chlorophenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3u**)

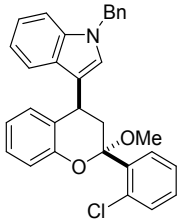
White solid; 89.1 mg, 93% yield; Reaction time = 12 h; mp 157.4-158.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.50 (d, J = 8.0 Hz, 2H), 7.27 (dd, J_1 = J_2 = 8.0 Hz, 4H), 7.20-7.14 (m, 4H), 7.12-6.88 (m, 9H), 6.74 (t, J = 8.0 Hz, 1H), 5.16 (s, 2H), 4.72 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.06 (s, 3H), 2.39 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.19 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 138.6, 136.5, 136.0, 133.0, 128.0, 127.7, 127.5, 127.4, 126.8, 126.5, 126.2, 125.7, 125.6, 125.3, 120.8, 120.3, 118.8, 118.0, 116.0, 115.7, 108.8, 99.2, 49.2, 48.9, 41.6, 29.0. IR (KBr) v 3431, 3059, 3032, 2931, 2834, 1607, 1585, 1484, 1455, 1341, 1263, 1219, 1156, 1099, 1050, 1019, 969, 910, 815, 731 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}ClNNaO_2$ $[M+Na]^+$ 502.1544, found 502.1555.



1-benzyl-3-(2-(4-bromophenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3v**)

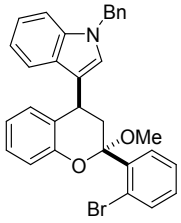
White solid; 95.7 mg, 91% yield; Reaction time = 12 h; mp 163.4-164.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.44 (s, 4H), 7.25 (d, J = 8.0 Hz, 1H), 7.21-7.14 (m, 4H), 7.10-6.88 (m, 8H), 6.75 (t, J = 8.0 Hz, 1H), 5.18 (s, 2H), 4.72 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.07 (s, 3H), 2.39 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.19 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 139.2, 136.5, 136.0, 130.5, 128.0, 127.7, 127.1, 126.6, 126.5, 126.2, 125.7, 125.6, 125.3, 121.3, 120.8, 120.3, 118.8, 118.0, 116.0, 115.7, 108.8, 99.2, 49.2, 48.9, 41.5, 29.0. IR (KBr) v 3433, 3033, 2963, 1585, 1481,

1457, 1339, 1262, 1206, 1158, 1101, 1040, 805, 745 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}BrNNaO_2$ $[M+Na]^+$ 546.1039, found 546.1052.



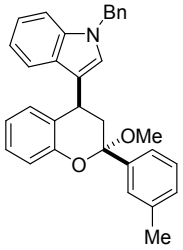
1-benzyl-3-(2-(2-chlorophenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3w**)

White solid; 82.8 mg, 86% yield; Reaction time = 12 h; mp 179.3-180.8 ^oC; ^1H NMR (400 MHz, $CDCl_3$), δ 7.89 (d, J = 8.0 Hz, 1H), 7.31 (t, J = 4.0 Hz, 1H), 7.27-7.13 (m, 7H), 7.11-6.97 (m, 7H), 6.91 (d, J = 8.0 Hz, 1H), 6.76 (d, J = 4.0 Hz, 1H), 5.19 (s, 2H), 4.74 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.14 (s, 3H), 2.87 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.31-2.23 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 137.6, 137.3, 137.1, 132.1, 131.6, 129.7, 129.6, 129.0, 128.8, 127.6, 127.5, 126.9, 126.8, 126.6, 121.8, 121.3, 120.1, 119.1, 117.0, 116.9, 109.9, 100.5, 50.4, 50.0, 38.8, 29.7. IR (KBr) *v* 3420, 3060, 2934, 1583, 1486, 1458, 1338, 1264, 1235, 1158, 1043, 1015, 906, 758, 744 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}ClNNaO_2$ $[M+Na]^+$ 502.1544, found 502.1558.



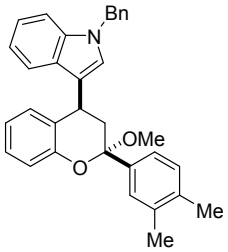
1-benzyl-3-(2-(2-bromophenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3x**)

White solid; 101.6 mg, 97% yield; Reaction time = 12 h; mp 125.5-127.1 ^oC; ^1H NMR (400 MHz, $CDCl_3$), δ 7.96 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.41-7.36 (m, 2H), 7.31-7.24 (m, 4H), 7.20-7.18 (m, 2H), 7.12 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 4H), 7.06 (t, J = 8.0 Hz, 2H), 6.99 (t, J = 8.0 Hz, 1H), 6.83 (t, J = 8.0 Hz, 1H), 5.28 (s, 2H), 4.81 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 3.22 (s, 3H), 2.92 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.38 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 140.9, 137.1, 135.4, 128.9, 128.8, 128.5, 128.4, 128.2, 128.0, 127.8, 127.7, 126.7, 126.3, 126.0, 124.9, 122.1, 121.3, 119.2, 117.2, 116.8, 110.9, 100.5, 50.3, 50.2, 42.7, 30.0. IR (KBr) *v* 3440, 3061, 3030, 2961, 2933, 2829, 1584, 1487, 1458, 1337, 1265, 1235, 1207, 1157, 1117, 1038, 1012, 966, 906, 813, 744 cm^{-1}. HRMS (ESI) calcd for $C_{31}H_{26}BrNNaO_2$ $[M+Na]^+$ 546.1039, found 546.1020.



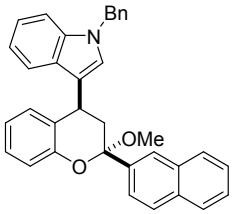
1-benzyl-3-(2-methoxy-2-(m-tolyl)chroman-4-yl)-1*H*-indole (**3y**)

White solid; 85.5 mg, 93% yield; Reaction time = 12 h; mp 149.0-150.9 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.45 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 4.0 Hz, 2H), 7.17-7.10 (m, 6H), 7.03-6.95 (m, 5H), 6.91 (d, J = 12.0 Hz, 2H), 6.72 (t, J = 8.0 Hz, 1H), 5.15 (s, 2H), 4.73 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 3.08 (s, 3H), 2.42 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.27 (s, 3H), 2.21 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 137.1, 136.8, 136.5, 135.9, 128.0, 127.9, 127.7, 127.4, 126.7, 126.6, 126.5, 126.4, 125.7, 125.6, 125.5, 125.1, 123.6, 120.7, 120.1, 118.9, 118.0, 116.0, 108.7, 99.6, 49.2, 48.9, 41.7, 29.0, 20.1. IR (KBr) *v* 3431, 3032, 2932, 1730, 1611, 1481, 1457, 1340, 1264, 1235, 1157, 1107, 1042, 1023, 971, 906, 816, 742 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2091, found 482.2072.



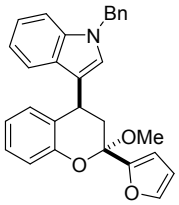
1-benzyl-3-(2-(3,4-dimethylphenyl)-2-methoxychroman-4-yl)-1*H*-indole (**3z**)

White solid; 92.9 mg, 98% yield; Reaction time = 12 h; mp 123.7-125.6 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.34 (s, 1H), 7.30 (d, J = 8.0 Hz, 2H), 7.22-7.14 (m, 4H), 7.10-6.89 (m, 9H), 6.72 (t, J = 8.0 Hz, 1H), 5.19 (s, 2H), 4.73 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.10 (s, 3H), 2.43 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.25-2.18 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 137.5, 136.5, 135.9, 135.5, 135.4, 128.6, 128.0, 127.7, 126.5, 126.4, 126.3, 125.7, 125.6, 125.5, 122.6, 120.7, 120.1, 118.9, 117.9, 116.1, 116.0, 115.9, 108.7, 99.6, 49.2, 48.9, 41.8, 29.0, 18.9, 18.5. IR (KBr) *v* 3431, 3057, 3029, 2957, 2930, 2832, 1610, 1580, 1483, 1454, 1337, 1264, 1232, 1156, 1048, 1029, 909, 806, 737 cm^{-1}. HRMS (ESI) calcd for $C_{33}H_{31}NNaO_2$ $[M+Na]^+$ 496.2247, found 496.2248.



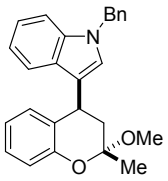
1-benzyl-3-(2-methoxy-2-(naphthalen-2-yl)chroman-4-yl)-1*H*-indole (**3aa**)

White solid; 94.0 mg, 95% yield; Reaction time = 12 h; mp 169.4-170.9 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.21 (s, 1H), 7.91-7.82 (m, 3H), 7.69 (d, J = 8.0 Hz, 1H), 7.51-7.46 (m, 2H), 7.38 (d, J = 8.0 Hz, 1H), 7.25-7.17 (m, 6H), 7.13-6.96 (m, 6H), 6.84 (t, J = 8.0 Hz, 1H), 5.23 (s, 2H), 4.88 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.21 (s, 3H), 2.63 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.37 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 138.6, 137.6, 137.1, 133.2 (2C), 129.2, 128.8, 128.5, 128.3, 127.7, 127.6, 127.5, 126.8, 126.7, 126.6, 126.4, 126.3, 125.8, 124.0, 121.8, 121.4, 120.0, 119.1, 117.2, 117.0, 109.9, 100.8, one carbon missing in the aromatic region, 50.5, 50.0, 42.7, 30.2. IR (KBr) v 3435, 3056, 3029, 2932, 2835, 1609, 1581, 1452, 1342, 1271, 1226, 1157, 1044, 907, 862, 823, 741, 699 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{30}NO_2$ $[M+H]^+$ 496.2271, found 496.2281.



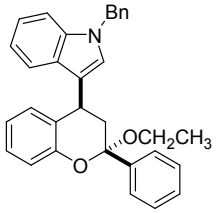
1-benzyl-3-(2-(furan-2-yl)-2-methoxychroman-4-yl)-1*H*-indole (**3ab**)

White solid; 86.4 mg, 99% yield; Reaction time = 12 h; mp 192.7-194.1 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.41 (s, 1H), 7.32-7.21 (m, 5H), 7.16-7.03 (m, 7H), 6.97 (t, J = 8.0 Hz, 1H), 6.81 (t, J = 8.0 Hz, 1H), 6.63 (d, J = 4.0 Hz, 1H), 6.39 (s, 1H), 5.27 (s, 2H), 4.76 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.23 (s, 3H), 2.73 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.40 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 151.4, 142.5, 137.6, 137.1, 129.2, 128.8, 127.6 (2C), 127.3, 126.9, 126.8, 126.4, 121.8, 121.5, 120.1, 119.1, 117.1, 116.8, 110.2, 109.9, 108.5, 97.5, 50.8, 50.0, 39.5, 29.5. IR (KBr) v 3434, 3038, 2940, 1609, 1584, 1456, 1343, 1265, 1233, 1157, 1039, 1007, 905, 815, 747, 698 cm^{-1}. HRMS (ESI) calcd for $C_{29}H_{26}NO_3$ $[M+H]^+$ 436.1907, found 436.1901.



1-benzyl-3-(2-methoxy-2-methylchroman-4-yl)-1*H*-indole (**3ac**)

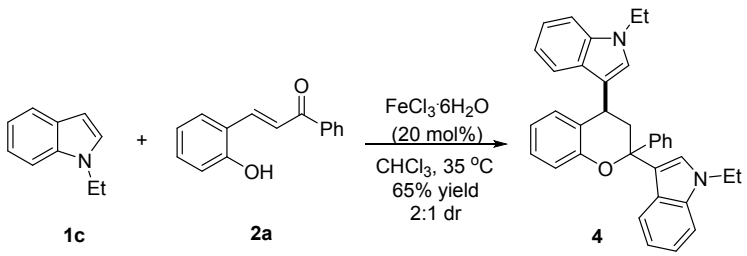
White solid; 68.3 mg, 89% yield; Reaction time = 36 h; mp 158.7-160.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.31-7.19 (m, 5H), 7.17-7.09 (m, 4H), 6.99 (q, J = 8.0 Hz, 3H), 6.91 (d, J = 8.0 Hz, 1H), 6.75 (t, J = 8.0 Hz, 1H), 5.26 (s, 2H), 4.63 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.34 (s, 3H), 2.32-2.23 (m, 2H), 1.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 137.7, 137.2, 129.1, 128.8, 127.7, 127.4, 127.3, 126.9, 126.8, 126.3, 121.8, 120.9, 120.1, 119.1, 117.5, 116.8, 109.9, 98.7, 50.0, 49.2, 40.7, 29.6, 23.2. IR (KBr) *v* 3433, 3055, 3032, 2985, 2935, 1609, 1582, 1480, 1456, 1345, 1225, 1191, 1065, 885, 806, 742 cm^{-1}. HRMS (ESI) calcd for $C_{26}H_{26}NO_2$ $[M+H]^+$ 384.1958, found 384.1957.



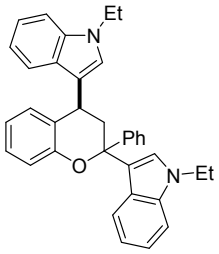
1-benzyl-3-(2-ethoxy-2-phenylchroman-4-yl)-1*H*-indole (**3ad**)

White solid; 89.1 mg, 97% yield; Reaction time = 12 h; mp 154.5-155.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.67 (t, J = 8.0 Hz, 2H), 7.41-6.98 (m, 16H), 6.82 (d, J = 8.0 Hz, 1H), 5.27 (s, 2H), 4.86 (s, 1H), 3.54 (d, J = 8.0 Hz, 1H), 3.39 (d, J = 8.0 Hz, 1H), 2.51-2.25 (m, 2H), 1.09 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 142.1, 137.6, 137.1, 129.0, 128.8, 128.4, 128.1, 127.6, 127.5, 127.4, 126.8, 126.7, 126.5, 126.2, 121.8, 121.1, 120.1, 119.0, 117.1, 117.0, 109.8, 100.6, 58.5, 50.0, 42.9, 30.2, 15.4. IR (KBr) *v* 3428, 3062, 3031, 2975, 2929, 2886, 1611, 1581, 1487, 1456, 1337, 1264, 1233, 1161, 1058, 1018, 931, 896, 748, 702 cm^{-1}. HRMS (ESI) calcd for $C_{32}H_{29}NNaO_2$ $[M+Na]^+$ 482.2089, found 482.2091.

3. Experimental data for bis-indole substituted chromans 4-7

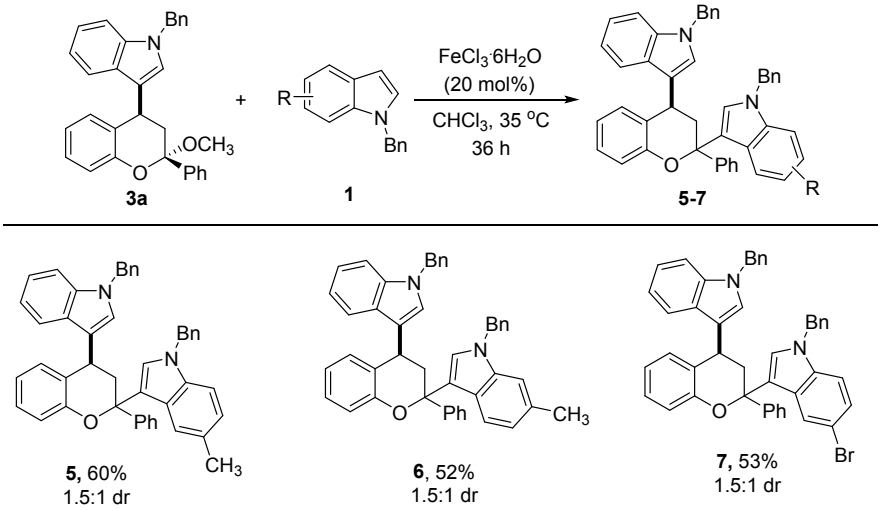


General procedure for the synthesis of 4 bearing two same indole substituents： To a 5.0 mL vial were successively added indole **1c** (0.44 mmol), *ortho*-hydroxychalcone **2a** (0.20 mmol), $FeCl_3 \cdot 6H_2O$ (10.8 mg, 0.04 mmol) and 1.0 mL $CHCl_3$. The resulting mixture was stirred at 35 °C till almost full consumption of **2a** monitored by thin layer chromatography, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate = 100:1 to 80:1) to afford the corresponding products **4** in 65% yield with 2:1 dr.



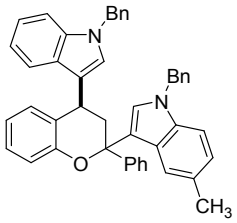
3,3'-(2-phenylchromane-2,4-diyl)bis(1-ethyl-1*H*-indole) (**4**)

White solid; 64.5 mg, 65% yield; Reaction time = 12 h; dr = 2:1; mp 87.8-88.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.75-7.61 (m, 1H), 7.50-7.45 (m, 2H), 7.25-6.81 (m, 14H), 6.73-6.60 (m, 2H), 4.32-3.90 (m, 5H), 3.24-3.09 (m, 1H), 2.93-2.77 (m, 1H), 1.33-1.24 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 144.9, 135.7, 135.2, 128.1, 127.3, 126.9, 126.6, 126.3, 125.8, 125.2, 125.1, 124.9, 124.6, 124.2, 124.0, 120.5, 120.0, 119.5, 119.0, 118.8, 118.3, 117.7, 116.1, 115.9, 108.3, 79.5, 39.8, 39.7, 30.6, 29.7, 14.4, 14.3. IR (KBr) *v* 3428, 3055, 2975, 2932, 2878, 1610, 1581, 1546, 1477, 1456, 1346, 1232, 906, 742, 706 cm^{-1}. HRMS (ESI) calcd for $C_{35}H_{32}N_2NaO$ $[M+Na]^+$ 519.2407, found 519.2402.



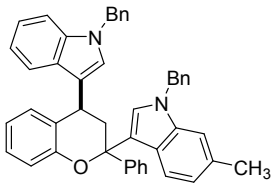
General procedure for the synthesis of 5-7 bearing two different indole substituents：

To a 5.0 mL vial were successively added mono-indole substituted chroman **3a** (0.10 mmol), substituted indole (0.11 mmol), $FeCl_3 \cdot 6H_2O$ (5.4 mg, 0.02 mmol) and 1.0 mL $CHCl_3$. The resulting mixture was stirred at 35 °C for 36 h, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate = 100:1 to 80:1) to afford the corresponding products **5-7**. Among them, the two isomers of **7** could be separated by gel column chromatography, while for **5-6**, they could not be separated. The dr value was determined by ^{1}H NMR.



1-benzyl-3-(4-(1-benzyl-1*H*-indol-3-yl)-2-phenylchroman-2-yl)-5-methyl-1*H*-indole (**5**)

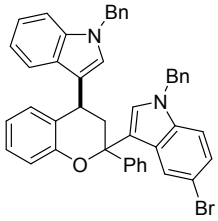
White solid; 38.3 mg, 60% yield; Reaction time = 36 h; dr = 1.5:1; mp 107.3-108.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.52 (d, J = 8.0 Hz, 2H), 7.24-6.80 (m, 25H), 6.63 (t, J = 8.0 Hz, 1H), 5.12 (dd, J_1 = 12.0 Hz, J_2 = 16.0 Hz, 4H), 4.34-3.98 (m, 1H), 3.28-3.07 (m, 1H), 2.94-2.74 (m, 1H), 2.28 (dd, $J_1 = J_2$ = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 142.9, 136.9, 136.7, 136.6, 136.4, 128.3, 127.8, 127.7, 127.5, 127.2, 126.8, 126.6, 126.5, 126.3, 126.0, 125.8, 125.7, 125.6, 125.5, 125.4, 125.2, 124.8, 124.6, 122.7, 122.5, 120.3, 119.9, 116.2, 116.0, 108.9, 108.7, 119.3, 118.2, 80.2, 57.6, 49.1, 39.3, 30.8, 20.7. IR (KBr) *v* 3432, 3058, 3030, 2923, 2860, 1610, 1582, 1485, 1451, 1302, 1234, 1176, 1102, 1030, 907, 799, 739, 701 cm^{-1}. HRMS (ESI) calcd for $C_{46}H_{38}N_2NaO$ $[M+Na]^+$ 657.2876, found 657.2871.



1-benzyl-3-(4-(1-benzyl-1*H*-indol-3-yl)-2-phenylchroman-2-yl)-6-methyl-1*H*-indole (**6**)

White solid; 32.9 mg, 52% yield; Reaction time = 36 h; dr = 1.5:1; mp 106.6-108.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.63-7.49 (m, 3H), 7.24-6.73 (m, 24H), 6.63 (dd, J_1 J_2 = 4.0 Hz, 1H), 5.17-5.07 (m, 4H), 4.34-3.94 (m, 1H), 3.22-3.03 (m, 1H), 2.92-2.74 (m, 1H), 2.30 (dd, $J_1 = J_2$ = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 146.0, 143.9, 137.8, 137.7, 137.4, 136.9, 131.9, 131.7,

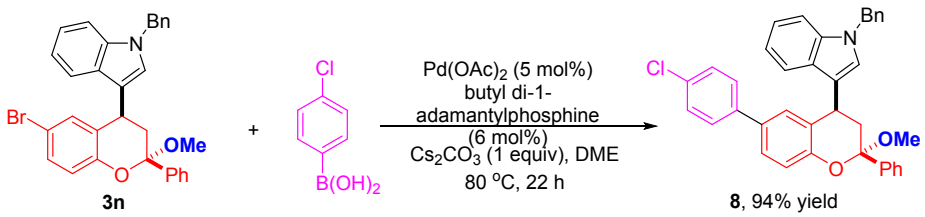
129.2, 128.8, 128.4, 128.1, 127.7, 127.6, 127.3, 127.1, 126.9, 126.8, 126.7, 126.6, 126.3, 126.1, 125.6, 123.9, 121.9, 121.8, 121.5, 120.9, 120.2, 119.8, 117.7, 117.0, 109.8, 80.6, 58.5, 49.8, 40.4, 30.8, 21.9. IR (KBr) *v* 3433, 3059, 3030, 2923, 2861, 1612, 1583, 1478, 1454, 1300, 1235, 1174, 1106, 1029, 906, 802, 736, 702 cm^{-1}. HRMS (ESI) calcd for $C_{46}H_{38}N_2NaO$ $[M+Na]^+$ 657.2876, found 657.2866.



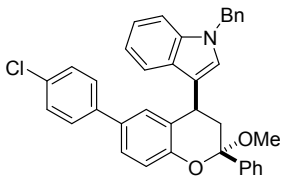
1-benzyl-3-(4-(1-benzyl-1*H*-indol-3-yl)-2-phenylchroman-2-yl)-5-bromo-1*H*-indole (**7**)

White solid; 37.5 mg, 53% yield; Reaction time = 36 h; dr = 1.5:1; mp 215.7-212.3 °C (major isomer), 219.8-221.1 °C (minor isomer); ^{1}H NMR (400 MHz, $CDCl_3$) for major isomer δ 7.88 (s, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.28-7.01 (m, 17H), 6.92 (t, *J* = 8.0 Hz, 5H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.73 (s, 1H), 6.65 (d, *J* = 4.0 Hz, 1H), 5.17 (s, 2H), 5.06 (s, 2H), 4.01 (t, *J* = 4.0 Hz, 1H), 3.13 (t, *J* = 12.0 Hz, 1H), 2.92 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) for major isomer δ 154.0, 143.4, 137.6, 137.0, 136.8, 136.0, 129.2, 128.9, 128.8, 128.6, 127.9, 127.8, 127.7, 127.6, 127.2, 127.1, 126.8, 126.7, 126.6, 126.5, 126.2, 125.4, 125.0, 124.1, 121.9, 121.1,120.5, 119.9, 119.2, 117.4, 117.1, 113.2, 111.5, 109.9, 80.3, 58.6, 50.3, 40.4, 30.7. ^{1}H NMR (400 MHz, $CDCl_3$) for minor isomer δ 7.81 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.18-7.11 (m, 12 H), 7.08-6.98 (m, 6H), 6.96-6.92 (m, 2H), 6.89-6.86 (m, 3H), 6.81 (s, 1H), 6.63 (t, *J* = 8.0 Hz, 1H), 5.15 (d, *J* = 4.0 Hz, 4H), 4.35 (dd, J_1 = J_2 = 8.0 Hz, 1H), 3.01 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.73 (t, *J* = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) for minor isomer δ 153.1, 144.5, 136.5, 135.8, 134.7, 128.1, 127.9, 127.8, 127.7, 127.5, 127.2, 126.9, 126.7, 126.6, 126.5, 126.3, 125.7, 125.5, 125.4, 125.3, 124.8, 124.2, 123.9, 122.6, 120.8, 119.4, 118.5, 118.2, 116.6, 116.4, 116.1, 112.2, 110.3, 108.8, 79.6, 57.4, 48.9, 41.0, 30.6. IR (KBr) for major isomer *v* 3429, 3059, 3031, 2924, 2860, 1610, 1548, 1457, 1346, 1232, 1178, 1103, 1035, 906, 797, 735, 698 cm^{-1}; IR (KBr) for minor isomer *v* 3434, 3060, 3031, 2958, 2926, 2861, 1723, 1608, 1582, 1546, 1456, 1389, 1340, 1298, 1260, 1234, 1179, 1075, 1025, 800, 736, 698 cm^{-1}. HRMS (ESI) calcd for $C_{45}H_{36}BrN_2O$ $[M+H]^+$ 699.2006, found 699.1997.

4. Experimental data for derivations of 3n and 3v

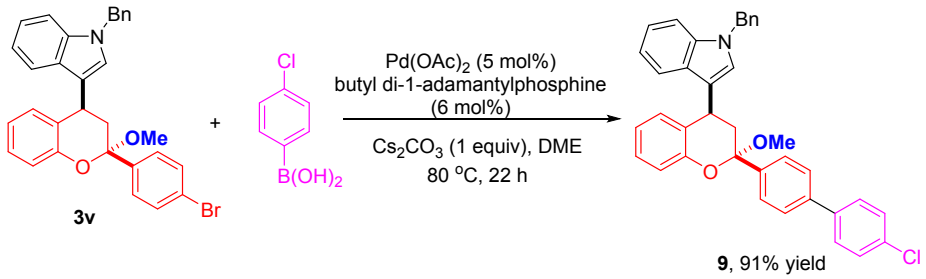


General procedure for the synthesis of 8: Under nitrogen atmosphere, compound **3n** (104.9 mg, 0.20 mmol), 4-chlorophenyl boronic acid (1.5 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 22 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 product **8**.

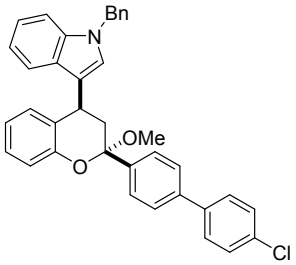


1-benzyl-3-(6-(4-chlorophenyl)-2-methoxy-2-phenylchroman-4-yl)-1*H*-indole (**8**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 100:1); 104.7mg, 94% yield; Reaction time = 22 h; mp 194.8-196.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.66 (d, J = 8.0 Hz, 2H), 7.44-7.31 (m, 5H), 7.27-7.15 (m, 10H), 7.12 (t, J = 8.0 Hz, 1H), 7.04-6.97 (m, 4H), 5.22 (s, 2H), 4.89 (dd, $J_1 = J_2$ = 8.0 Hz, 1H), 3.19 (s, 3H), 2.57 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.30 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 140.9, 139.6, 137.7, 137.1, 133.0, 132.5, 128.8, 128.7, 128.5, 128.3, 128.0, 127.7, 127.4, 127.0, 126.8, 126.7, 126.3 (2C), 122.0, 119.8, 119.2, 117.8, 117.0, 109.9, 100.9, one carbon missing in the aromatic region, 50.5, 49.9, 43.1, 30.3. IR (KBr) v 3432, 3031, 2961, 2931, 1610, 1476, 1337, 1251, 1209, 1156, 1042, 1015, 969, 909, 815, 735, 699 cm^{-1}. HRMS (ESI) calcd for $C_{37}H_{31}ClNO_2$ $[M+H]^+$ 556.2038, found 556.2041.

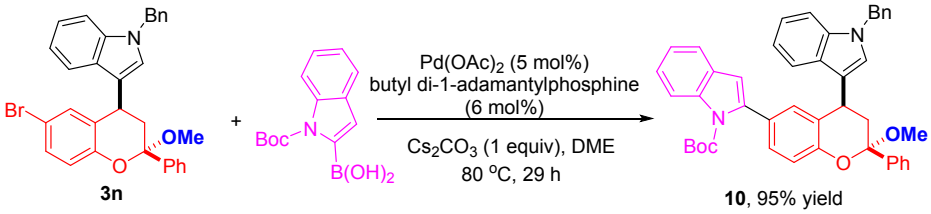


General procedure for the synthesis of 9: Under nitrogen atmosphere, compound **3v** (104.9 mg, 0.20 mmol), 4-chlorophenyl boronic acid (1.5 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 22 h till almost full consumption of **3v** 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 product **9**.

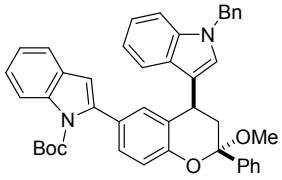


1-benzyl-3-(2-(4'-chloro-[1,1'-biphenyl]-4-yl)-2-methoxychroman-4-yl)-1*H*-indole (**9**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 100:1); 100.8 mg, 91% yield; Reaction time = 22 h; mp 222.8-223.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.64 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.0 Hz, 2H), 7.30 (t, J = 8.0 Hz, 3H), 7.18-7.09 (m, 5H), 7.04-6.89 (m, 7H), 6.75 (t, J = 8.0 Hz, 1H), 5.17 (s, 2H), 4.76 (dd, J_1 = J_2 = 4.0 Hz, 1H), 3.13 (s, 3H), 2.46 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.25 (t, J = 12.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 140.6, 139.8, 139.2, 137.6, 137.1, 133.6, 129.1, 129.0, 128.8, 128.4, 127.6 (2C), 127.4, 127.0, 126.9, 126.8, 126.7, 126.5, 121.8, 121.3, 120.0, 119.1, 117.1, 117.0, 109.9, 100.6, 50.4, 50.0, 42.8, 30.2. IR (KBr) v 3434, 3032, 2962, 2931, 1610, 1581, 1480, 1457, 1388, 1345, 1297, 1263, 1225, 1154, 1100, 1040, 1017, 967, 906, 852, 816 cm^{-1}. HRMS (ESI) calcd for $C_{37}H_{31}ClNO_2$ $[M+H]^+$ 556.2038, found 556.2042.

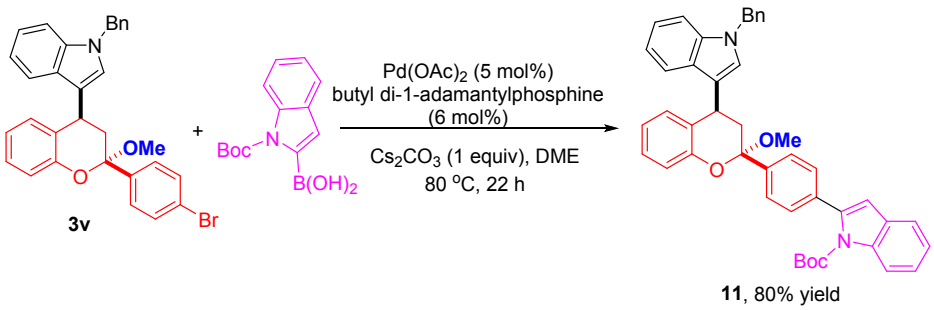


General procedure for the synthesis of 10: Under nitrogen atmosphere, compound **3n** (104.9 mg, 0.20 mmol), 2-indolyl boronic acid (1.7 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 29 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 product **10**.



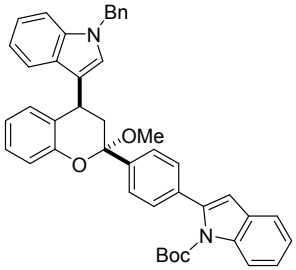
tert-butyl 2-(4-(1-benzyl-1*H*-indol-3-yl)-2-methoxy-2-phenylchroman-6-yl)-1*H*-indole-1-carboxylate (**10**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 100:1 to 80:1); 124.9 mg, 95% yield; Reaction time = 29 h; mp 205.4-206.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.14 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.0 Hz, 2H), 7.45-7.33 (m, 5H), 7.27-7.14 (m, 7H), 7.11-7.04 (m, 5H), 7.01 (s, 1H), 6.96 (t, J = 8.0 Hz, 1H), 6.32 (s, 1H), 5.23 (s, 2H), 4.84 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.17 (s, 3H), 2.55 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 2.36 (t, J = 12.0 Hz, 1H), 1.32 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 150.3, 140.9, 140.7, 137.5, 137.3, 137.2, 129.4, 129.2, 128.8, 128.4, 128.3, 128.2, 127.9, 127.6, 127.2, 126.8, 126.7, 126.3, 126.0, 124.0, 122.8, 121.9, 120.2, 119.8, 119.1, 116.7, 116.6, 115.2, 109.9, 109.3, 100.9, 83.1, 50.3, 49.9, 42.9, 30.4, 27.7. IR (KBr) v 3425, 3058, 2974, 2933, 1726, 1610, 1486, 1455, 1365, 1330, 1257, 1217, 1161, 1126, 1042, 1022, 907, 813, 739, 703 cm^{-1}. HRMS (ESI) calcd for $C_{44}H_{41}N_2O_4$ $[M+H]^+$ 661.3061, found 661.3060.



11, 80% yield

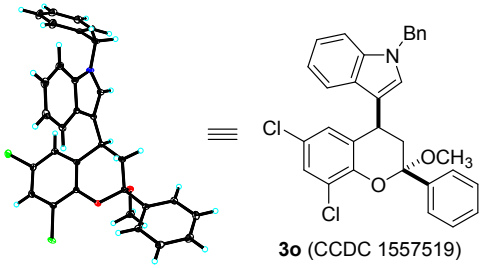
General procedure for the synthesis of 11: Under nitrogen atmosphere, compound **3v** (104.9 mg, 0.20 mmol), 2-indolyl boronic acid (1.8 equiv), Cs_2CO_3 (2.0 equiv), $Pd(OAc)_2$ (0.05 equiv) and butyl di-1-adamantylphosphine (0.06 equiv) were successively added to a 15 mL dried tube, followed by adding 2.0 mL DME. The resulting mixture was stirred at 80 °C for 22 h till almost full consumption of **3v** 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 product **11**.



tert-butyl 2-(4-(1-benzyl-1*H*-indol-3-yl)-2-methoxychroman-2-yl)phenyl)-1*H*-indole-1-carboxylate (**11**)

White solid obtained by column chromatography (petroleum ether/ethyl acetate = 100:1 to 80:1); 105.8 mg, 80% yield; Reaction time = 22 h; mp 229.8-230.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.23 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.38 (d, J = 8.0 Hz, 1H), 7.35-6.98 (m, 14H), 6.83 (t, J = 8.0 Hz, 1H), 6.56 (s, 1H), 5.26 (s, 2H), 4.85 (dd, $J_1 = J_2$ = 4.0 Hz, 1H), 3.22 (s, 3H), 2.55 (dd, J_1 = 4.0 Hz, J_2 = 8.0 Hz, 1H), 2.32 (t, J = 12.0 Hz, 1H), 1.28 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 150.2, 140.6, 140.1, 137.6 (2C), 137.1, 134.9, 129.3, 129.1, 128.8, 127.7, 127.6, 127.5, 126.9, 126.7, 126.6, 125.8, 124.5, 123.0, 121.9, 121.3, 120.5, 120.0, 119.1, 117.1, 117.0, 115.3, 110.3, 109.9, 100.6, one carbon missing in the aromatic region, 83.5, 50.4, 50.0, 42.8, 30.2, 27.7. IR (KBr) ν 3427, 3071, 3033,2979, 2935, 1721, 1583, 1456, 1363, 1330, 1264, 1227, 1161, 1037, 967, 905, 849, 816, 745 cm^{-1}. HRMS (ESI) calcd for $C_{44}H_{41}N_2O_4$ $[M+H]^+$ 661.3061, found 661.3074.

5. Crystal data for 3o



3o (CCDC 1557519)

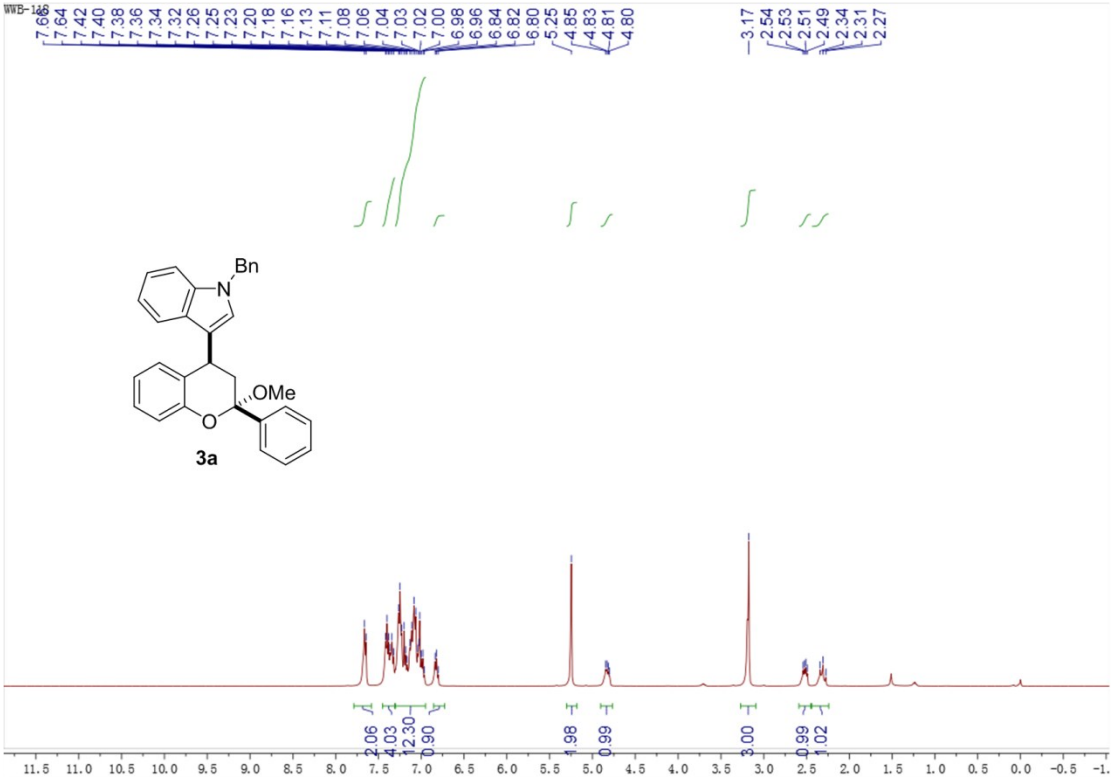
Displacement ellipsoids are drawn at the 30% probability level.

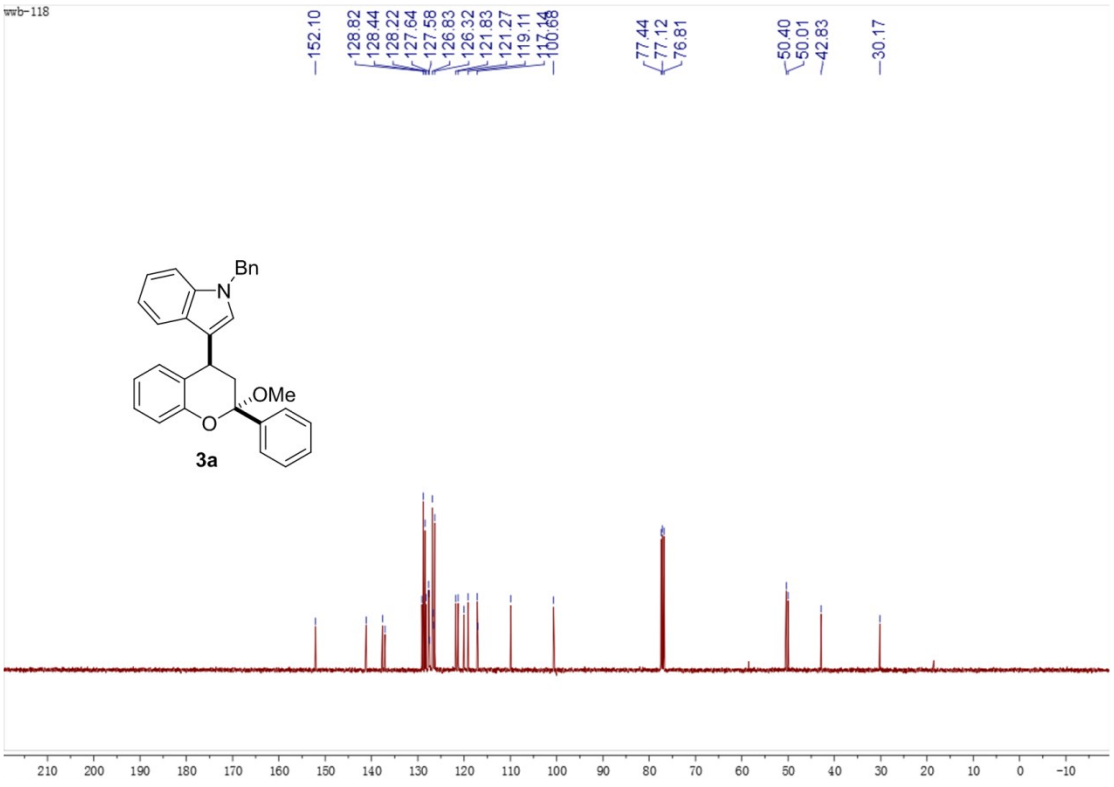
Table S1. Crystal data and structure refinement for **3o**.

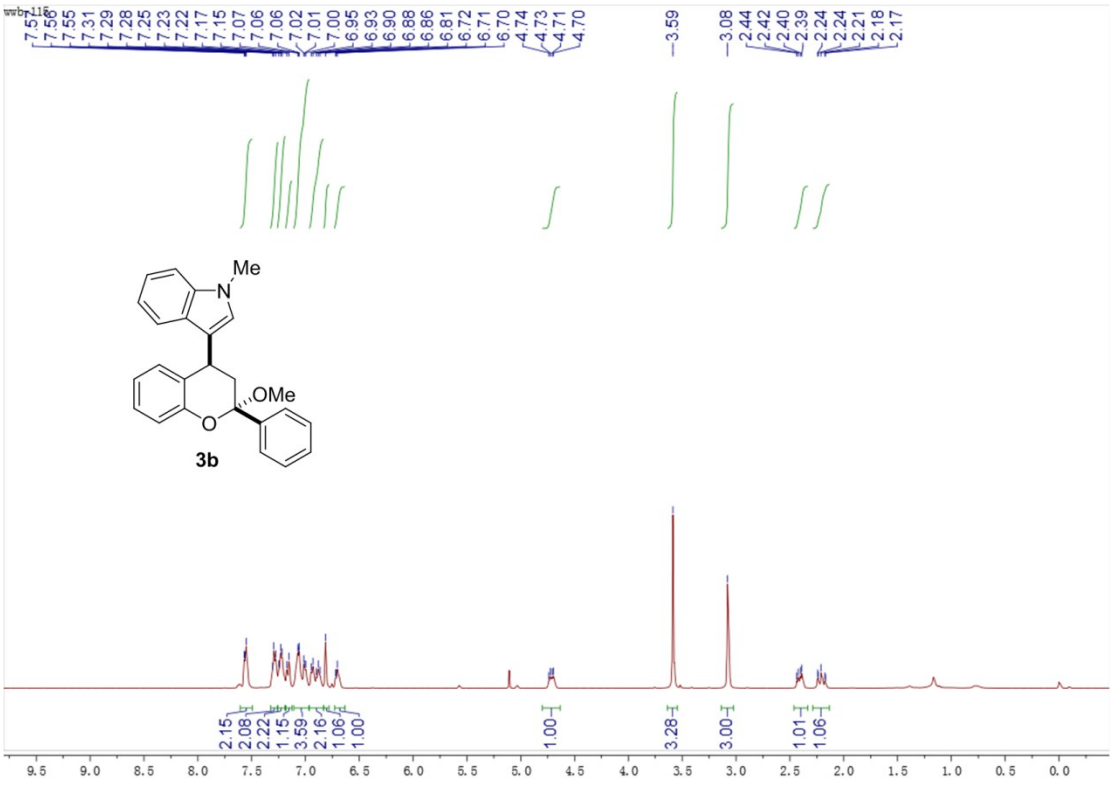
Identification code	**3o**	
Empirical formula	$C_{31}H_{25}Cl_2NO_2$	
Formula weight	514.42	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3851(6) Å	α = 95.0880(10)°.
	b = 11.5543(8) Å	β = 91.1550(10)°.
	c = 12.0921(8) Å	γ=104.0260(10)°.
Volume	1265.96(15) $Å^3$	
Z	2	
Density (calculated)	1.350 Mg/m^3	
Absorption coefficient	0.286 mm^{-1}	
F(000)	536	
Crystal size	0.280 x 0.240 x 0.210 mm^3	
Theta range for data collection	1.692 to 31.044°.	
Index ranges	-13<=h<=13, -15<=k<=16, -16<=l<=16	
Reflections collected	19072	
Independent reflections	7379 [R(int) = 0.0291]	
Completeness to theta = 25.242°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7379 / 0 / 326	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0992	
R indices (all data)	R1 = 0.0513, wR2 = 0.1070	
Extinction coefficient	n/a	

Largest diff. peak and hole	0.384 and -0.258 e.Å^{-3}

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



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7.06
7.06
7.02
7.01
7.00
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6.90
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6.86
6.81
6.72
6.71
6.70
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4.73
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4.70
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2.17
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OMe
O
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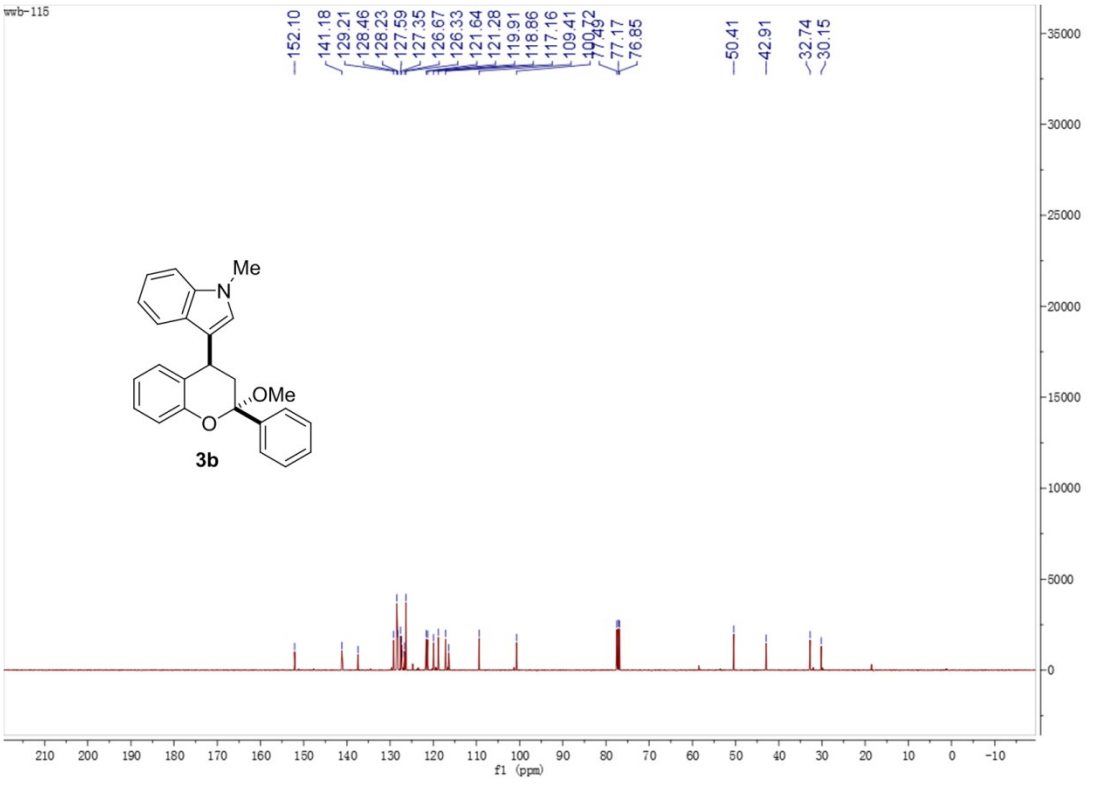
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200
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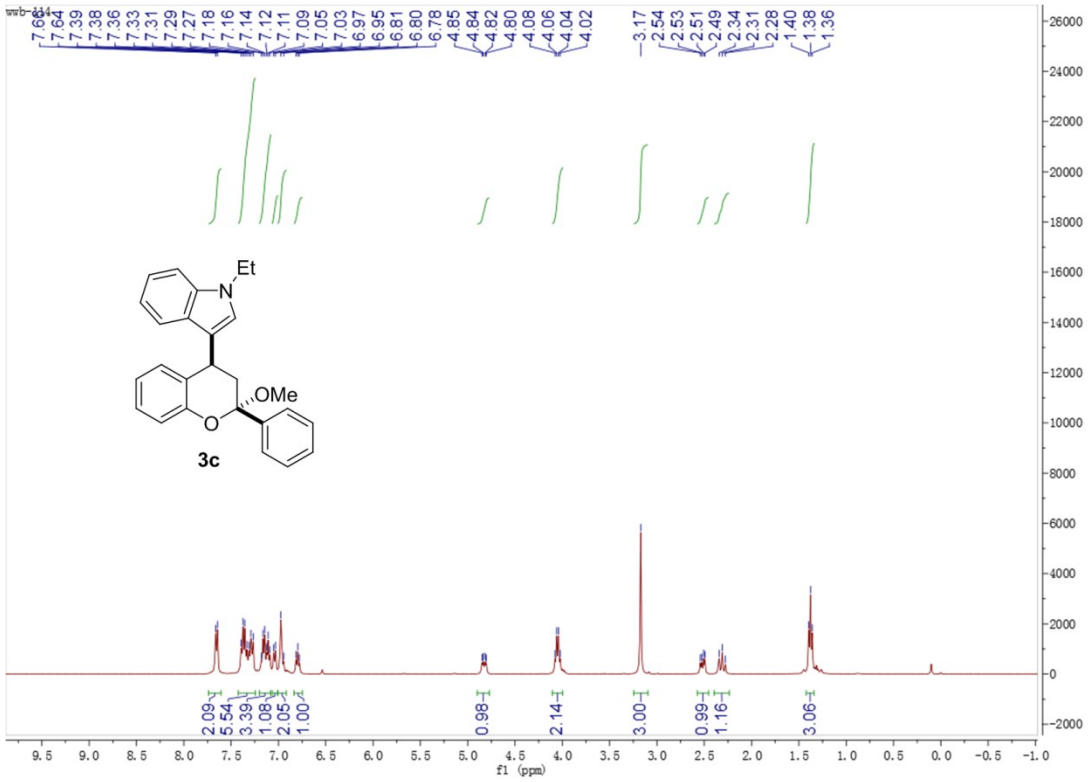
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6.80
6.78
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4.84
4.82
4.80
4.08
4.06
4.04
4.02
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O
3c
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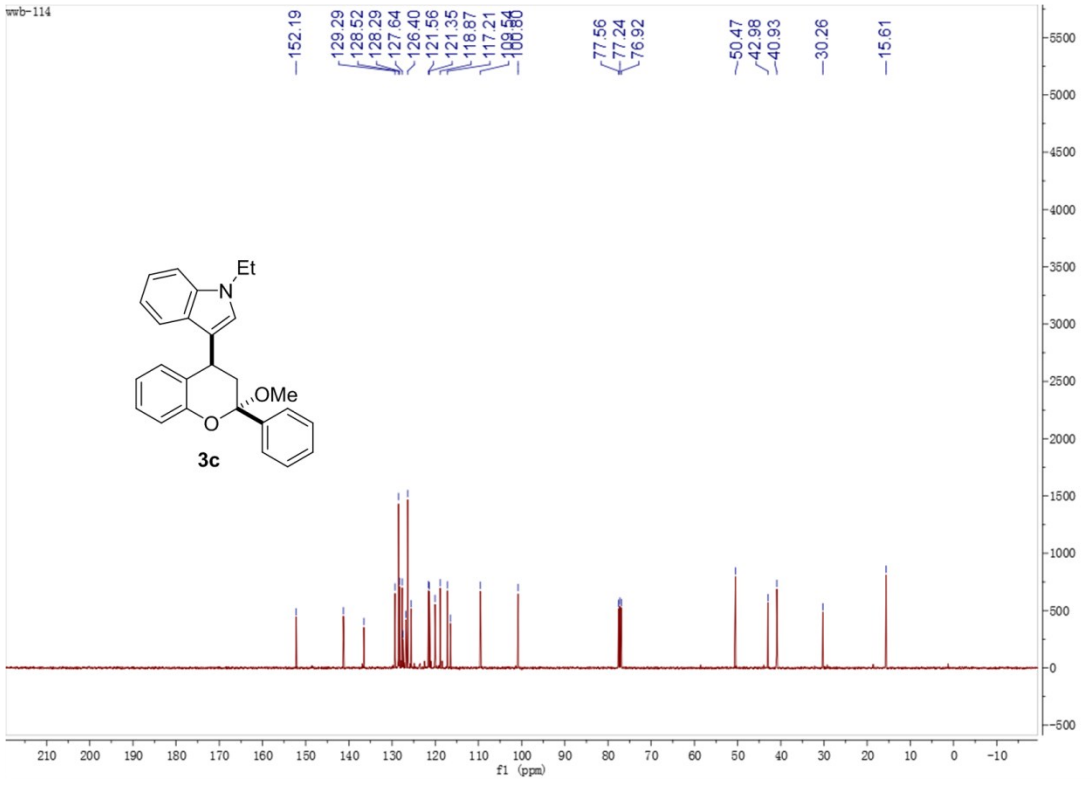
f1 (ppm)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O
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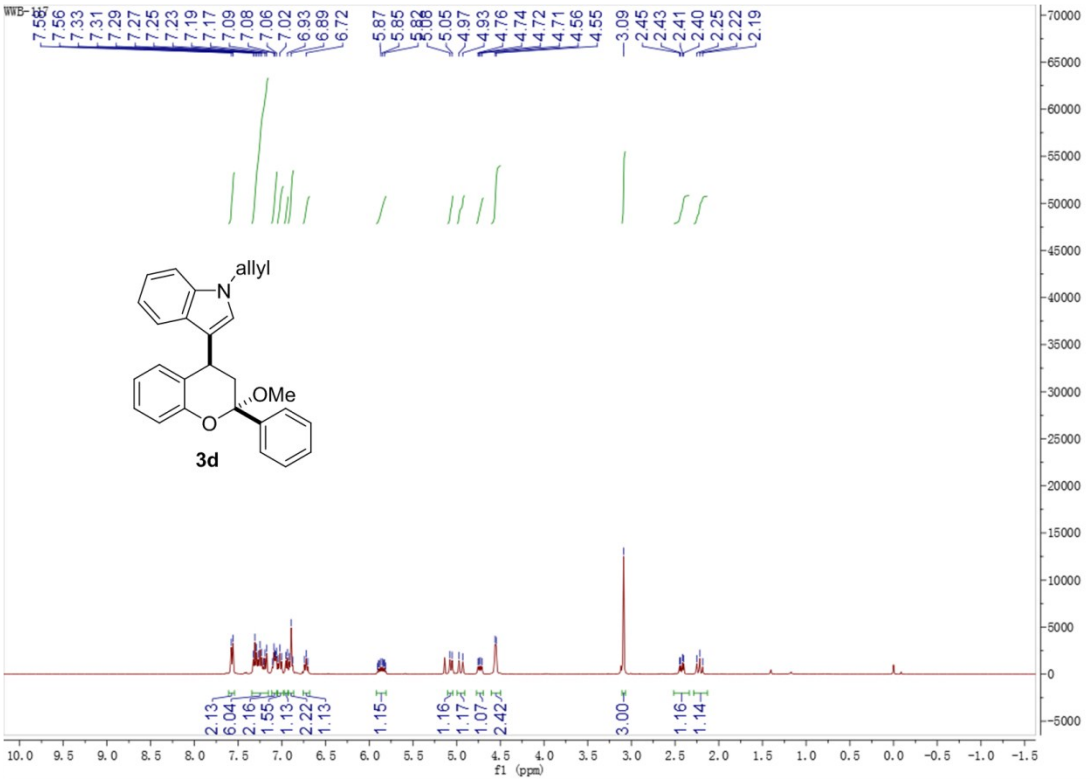
f1 (ppm)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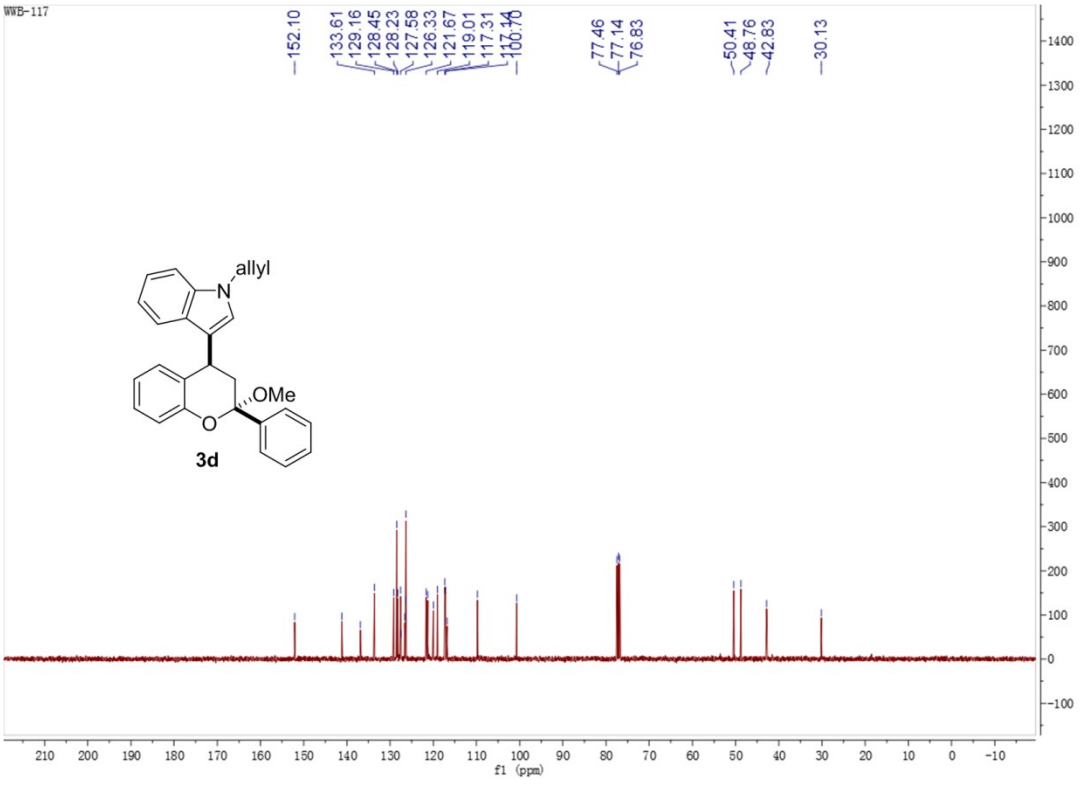
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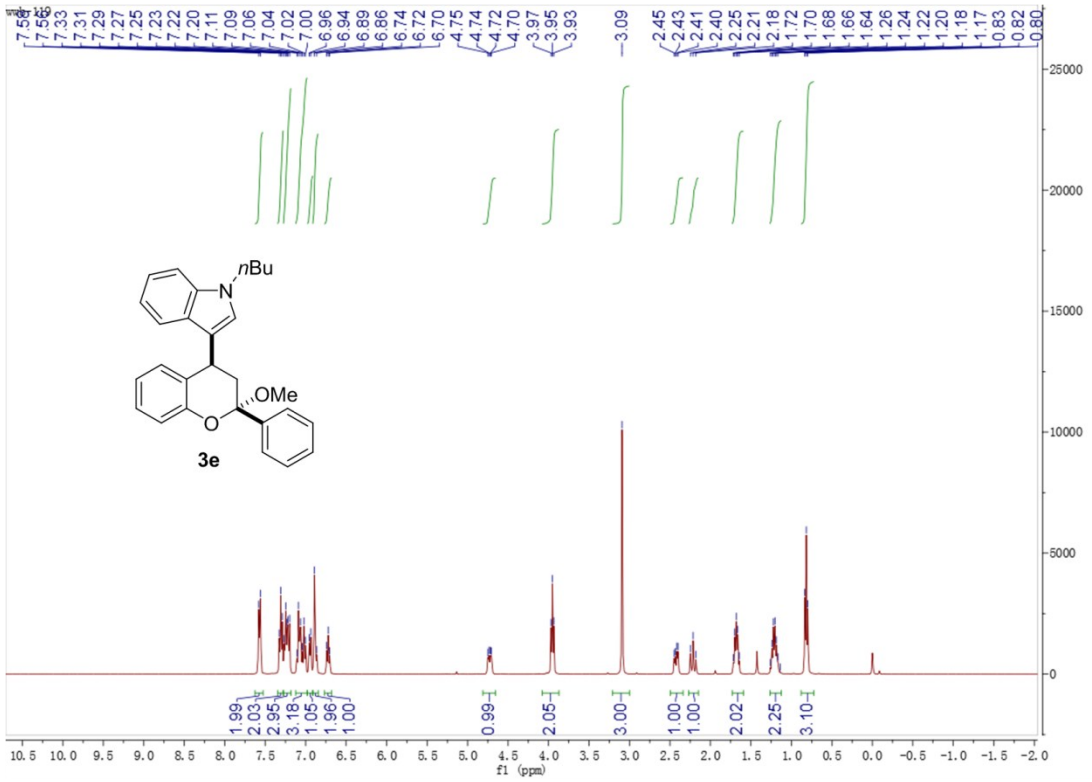
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O
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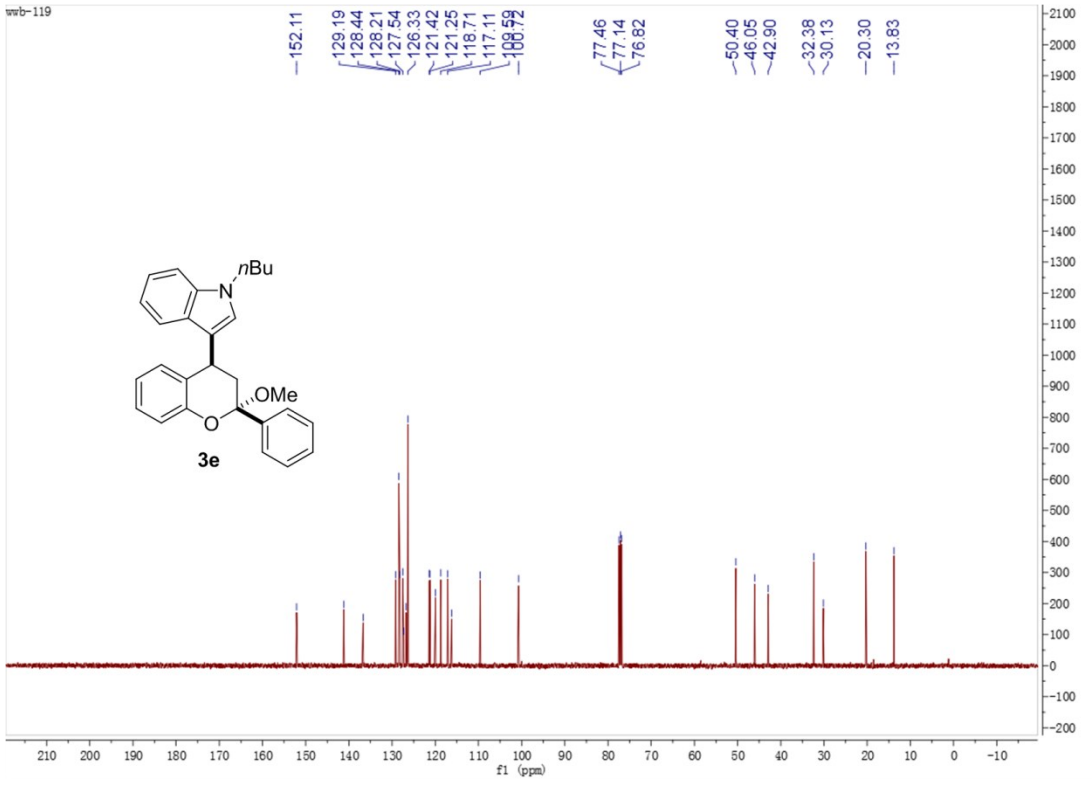
f1 (ppm)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O
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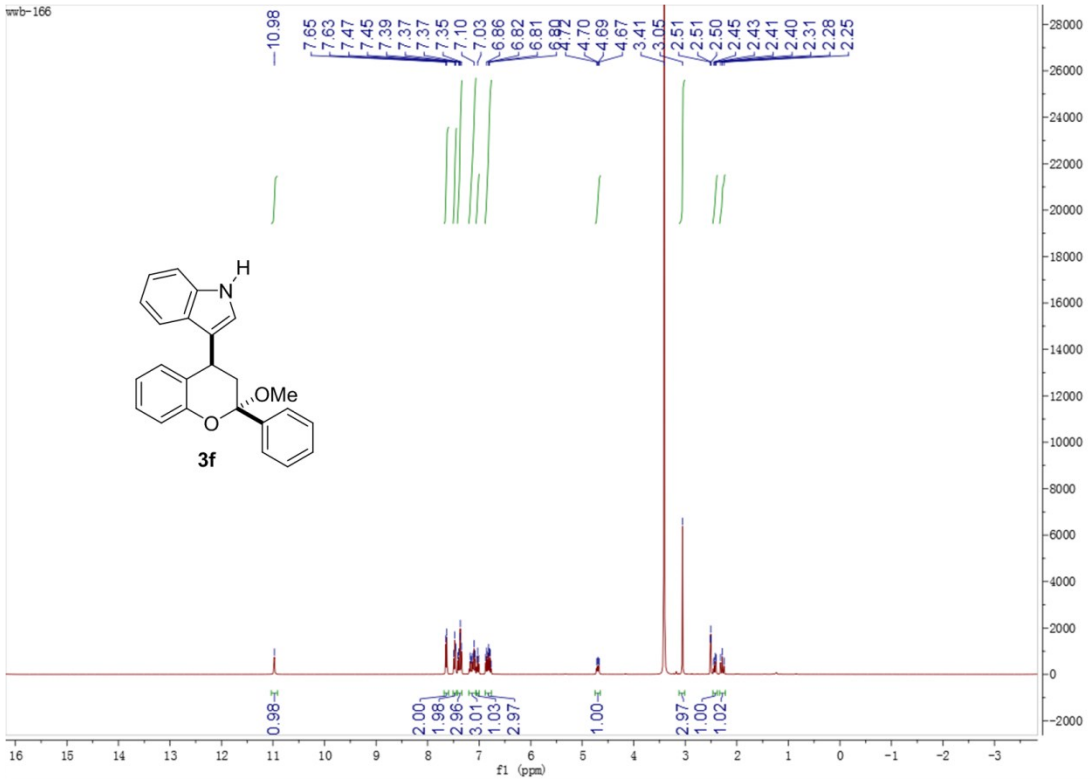
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H
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OMe
O
3f
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2.97
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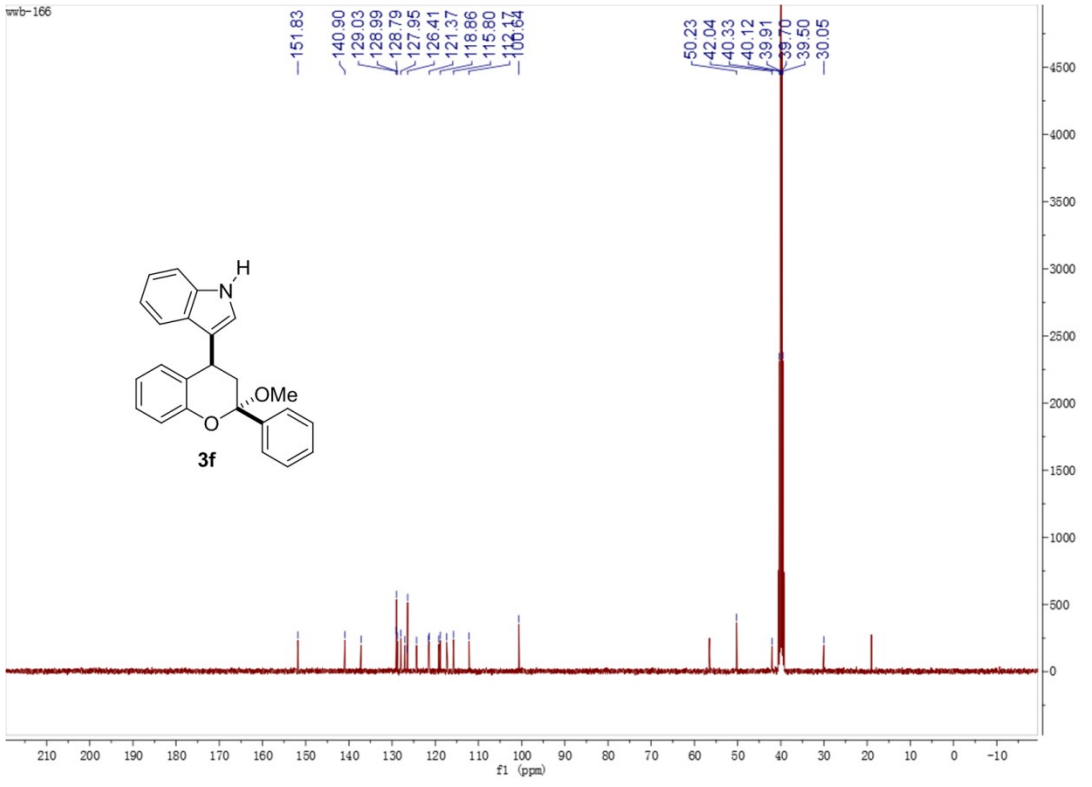
f1 (ppm)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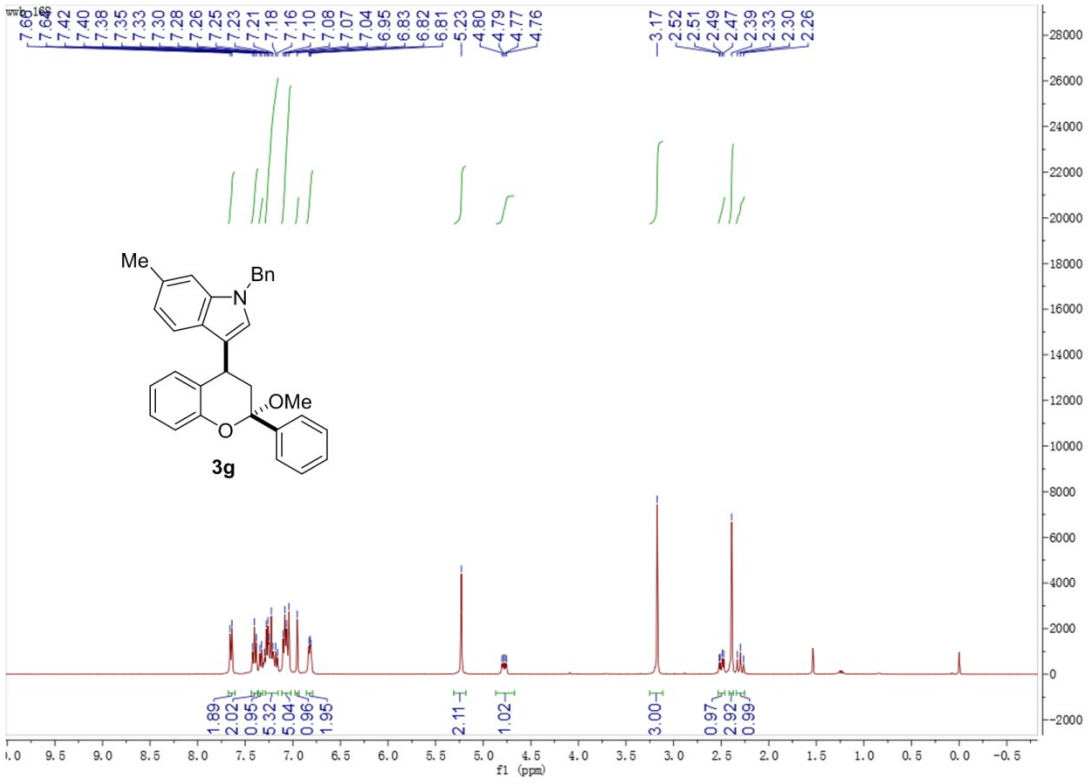
H
N
OMe
O
3f
f1 (ppm)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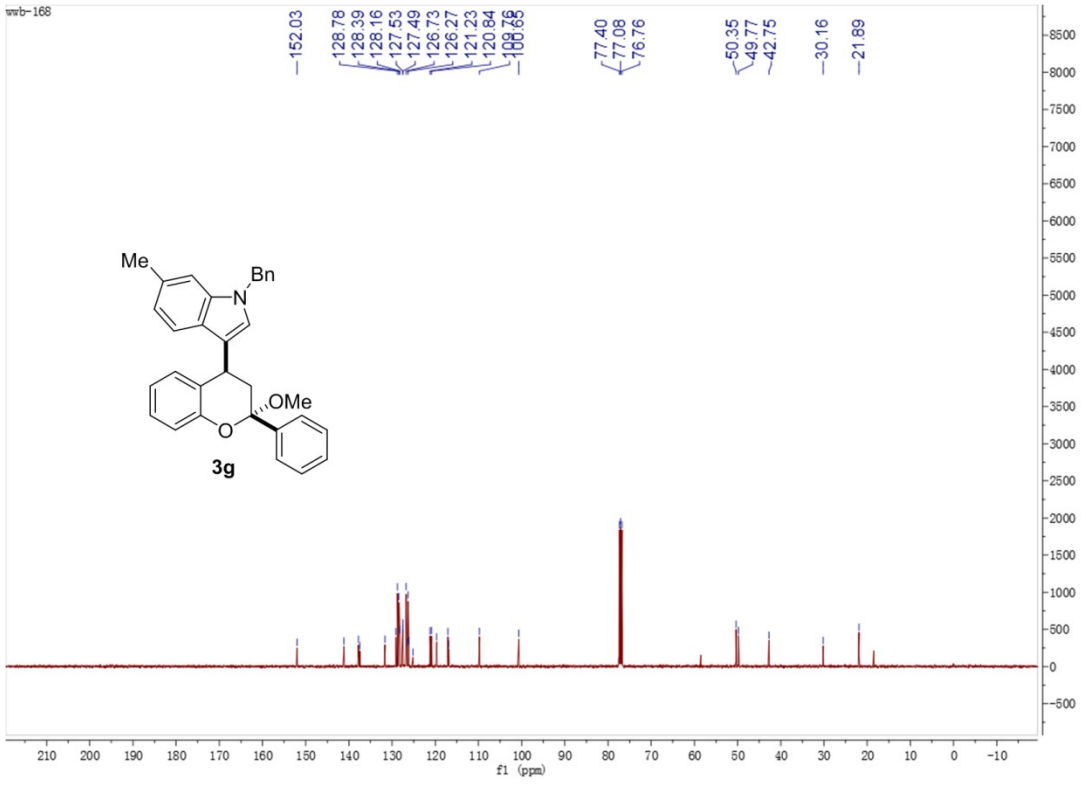
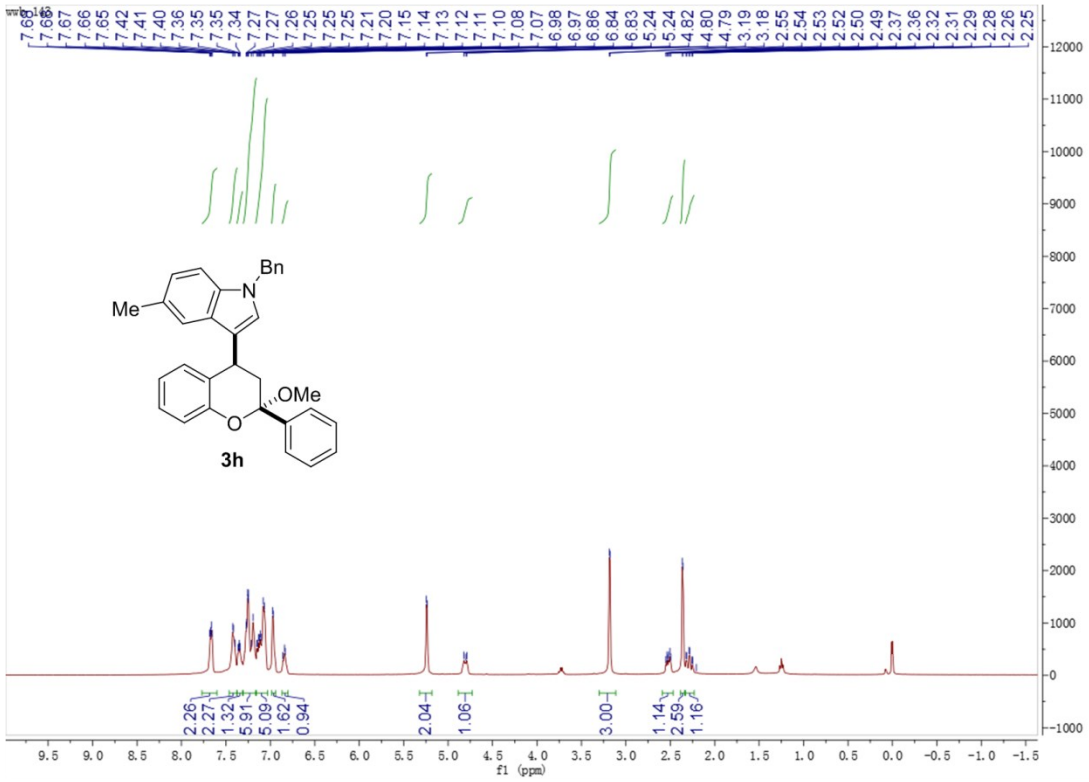
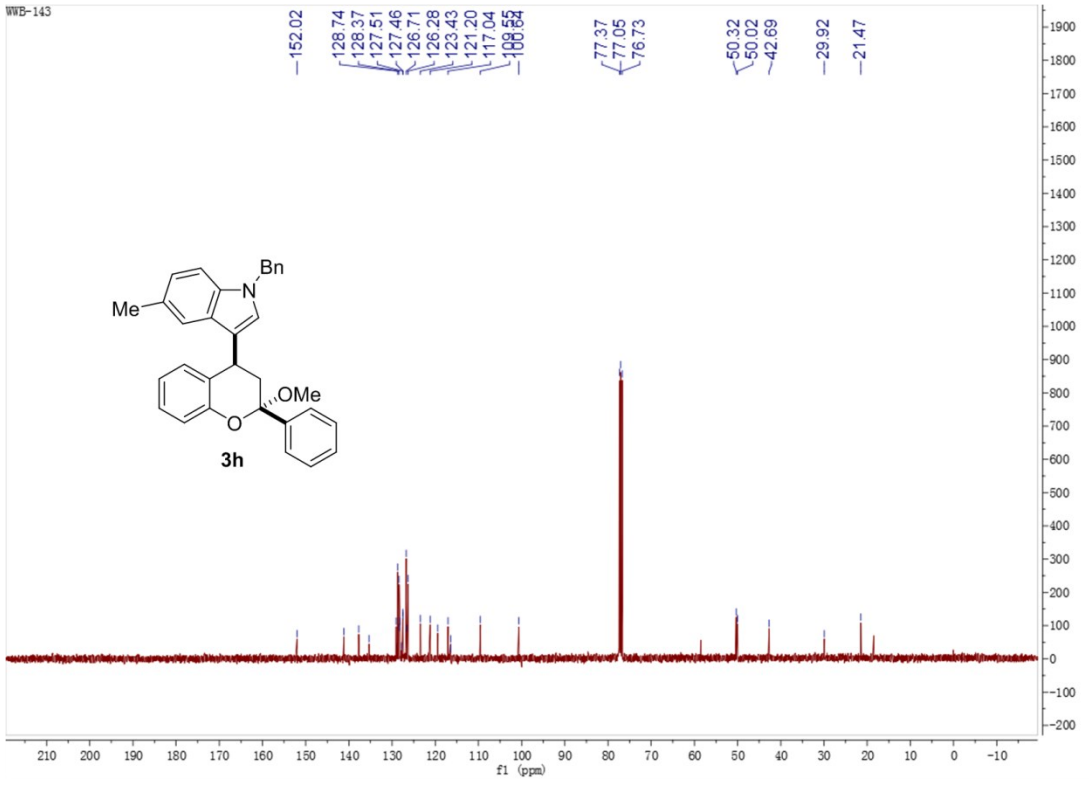
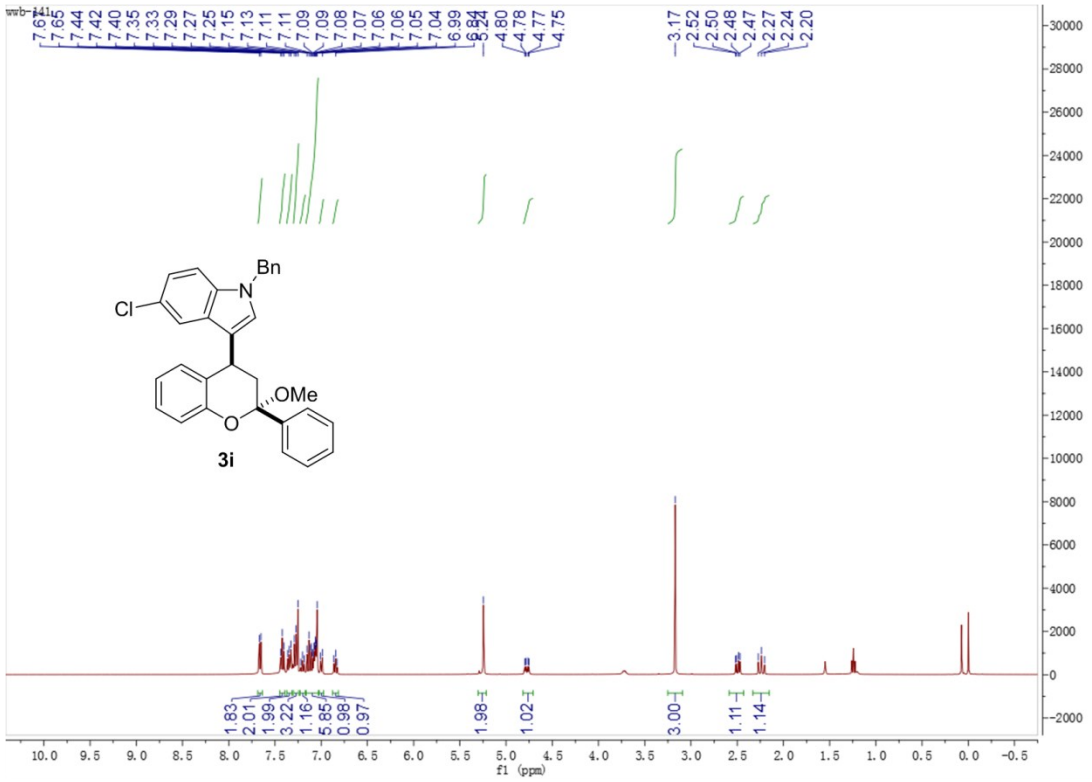
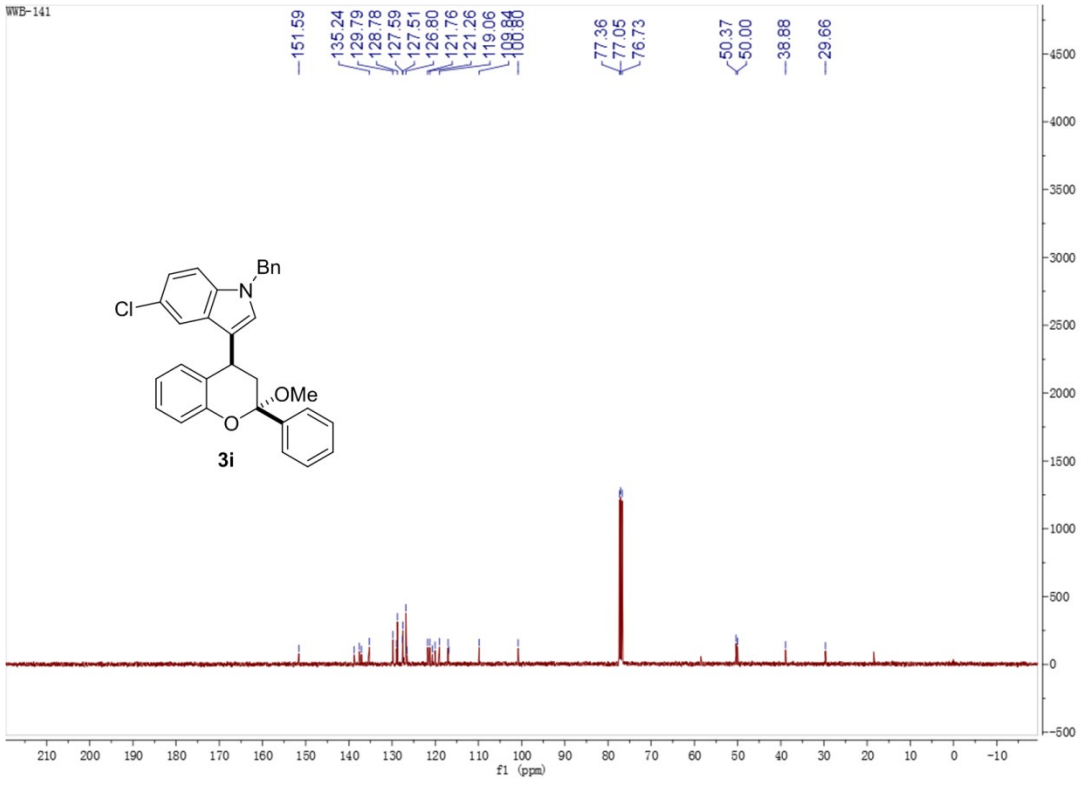
1.02
3.00
0.97
2.92
0.99
f1 (ppm)

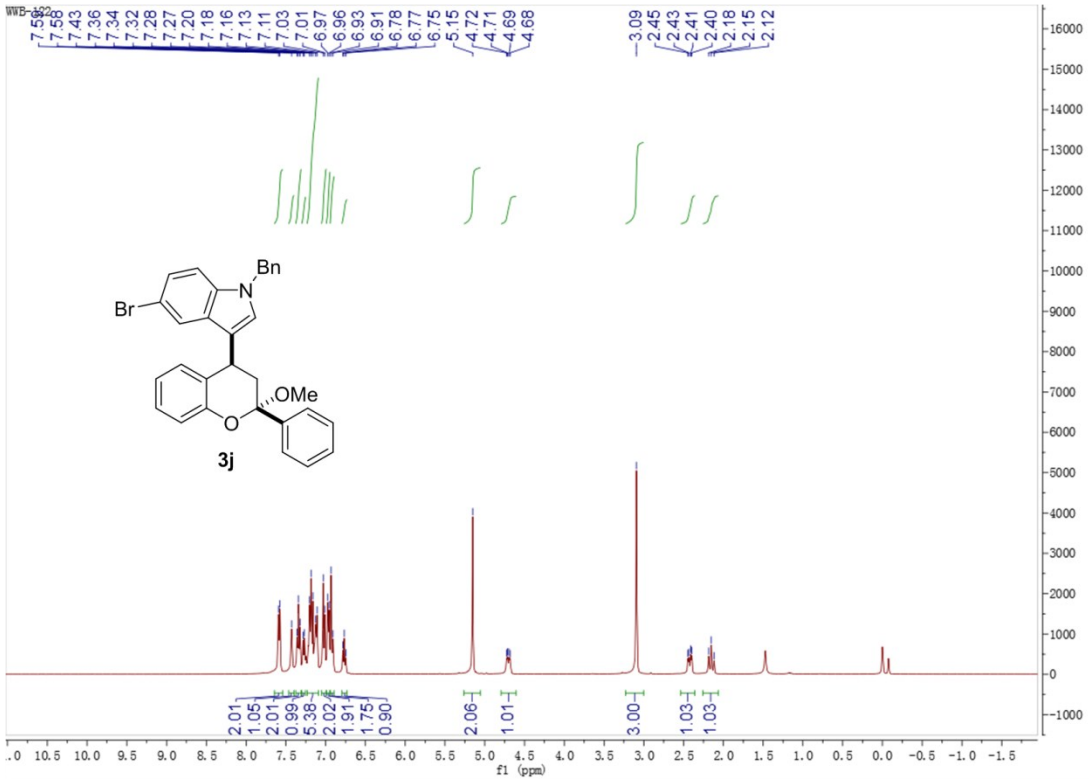

wwb-168
152.03
128.78
128.39
128.16
127.53
127.49
126.73
126.27
121.23
120.84
77.40
77.08
76.76
50.35
49.77
42.75
30.16
21.89
Me
N
Bn
OMe
O
3g
f1 (ppm)

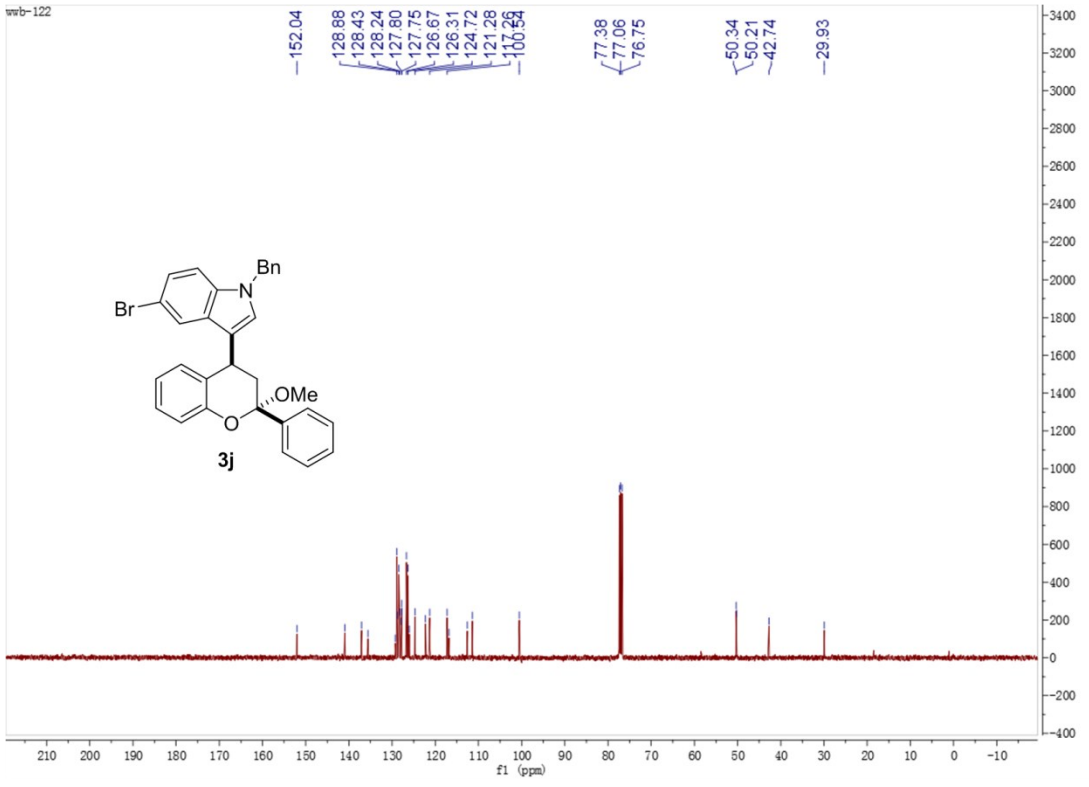

Bn
N
Me
OMe
O
3h
f1 (ppm)

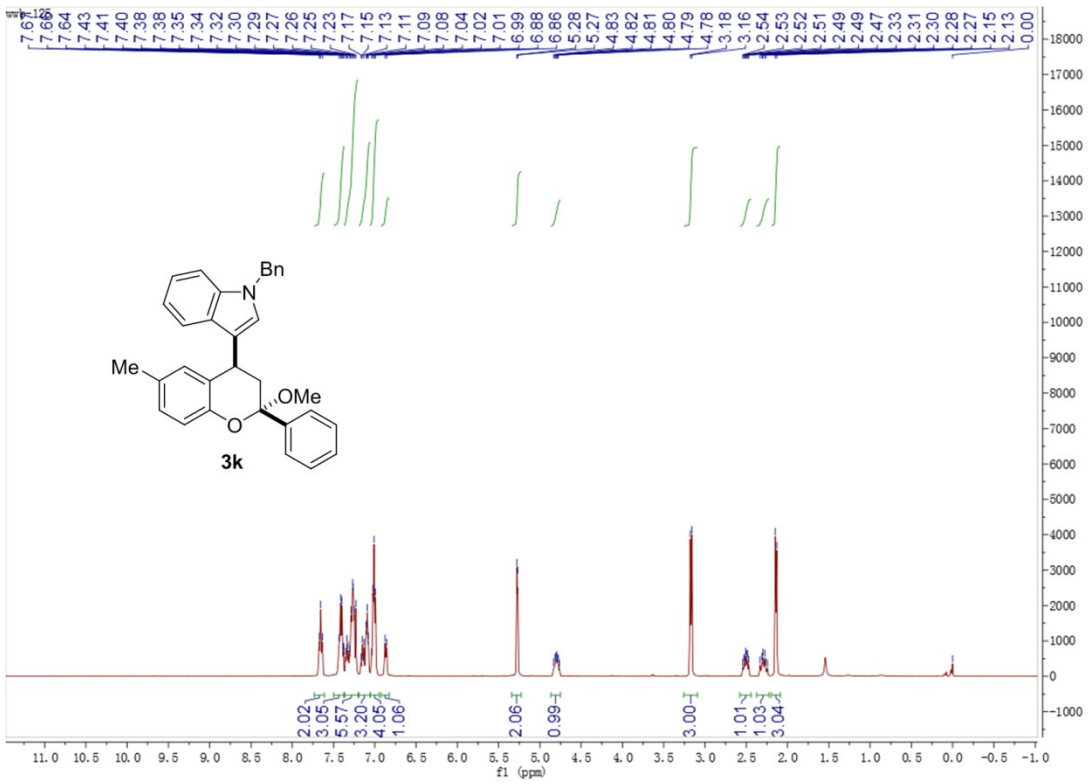

WWB-143
Bn
N
Me
OMe
O
3h
f1 (ppm)

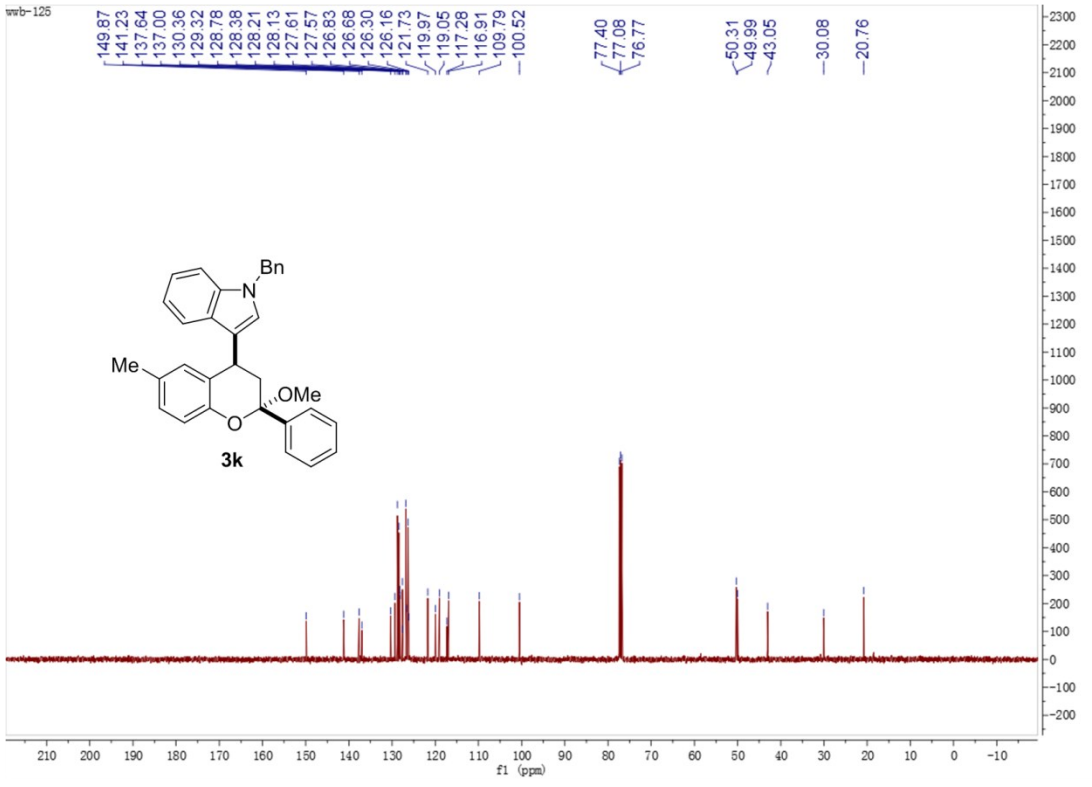

7.65
7.44
7.42
7.40
7.35
7.33
7.29
7.27
7.25
7.15
7.13
7.11
7.11
7.09
7.09
7.08
7.07
7.06
7.06
7.05
7.04
6.99
6.84
5.24
4.80
4.78
4.77
4.75
3.17
2.52
2.50
2.48
2.47
2.27
2.24
2.20
Bn
N
Cl
OMe
O
3i
1.83
2.01
1.99
3.22
1.16
5.85
0.98
0.97
1.98
1.02
3.00
1.11
1.14
f1 (ppm)

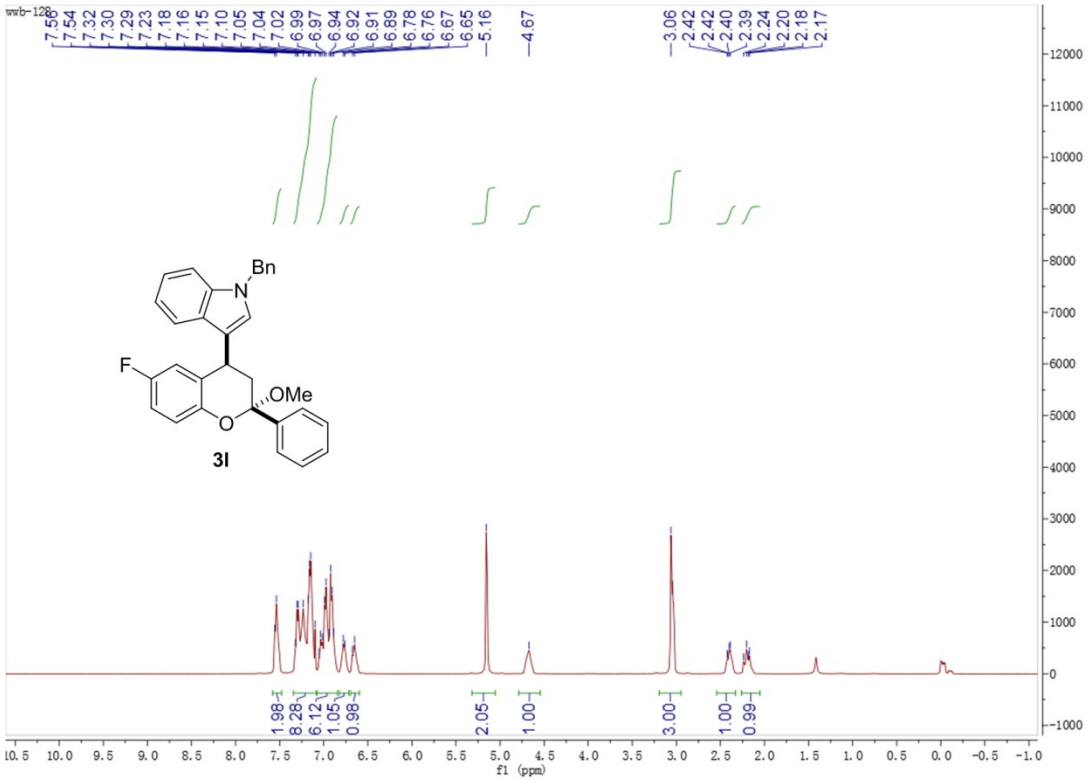

WWB-141
151.59
135.24
129.79
128.78
127.59
127.51
126.80
121.76
121.26
119.06
77.36
77.05
76.73
50.37
50.00
38.88
29.66
Bn
N
Cl
OMe
O
3i
f1 (ppm)

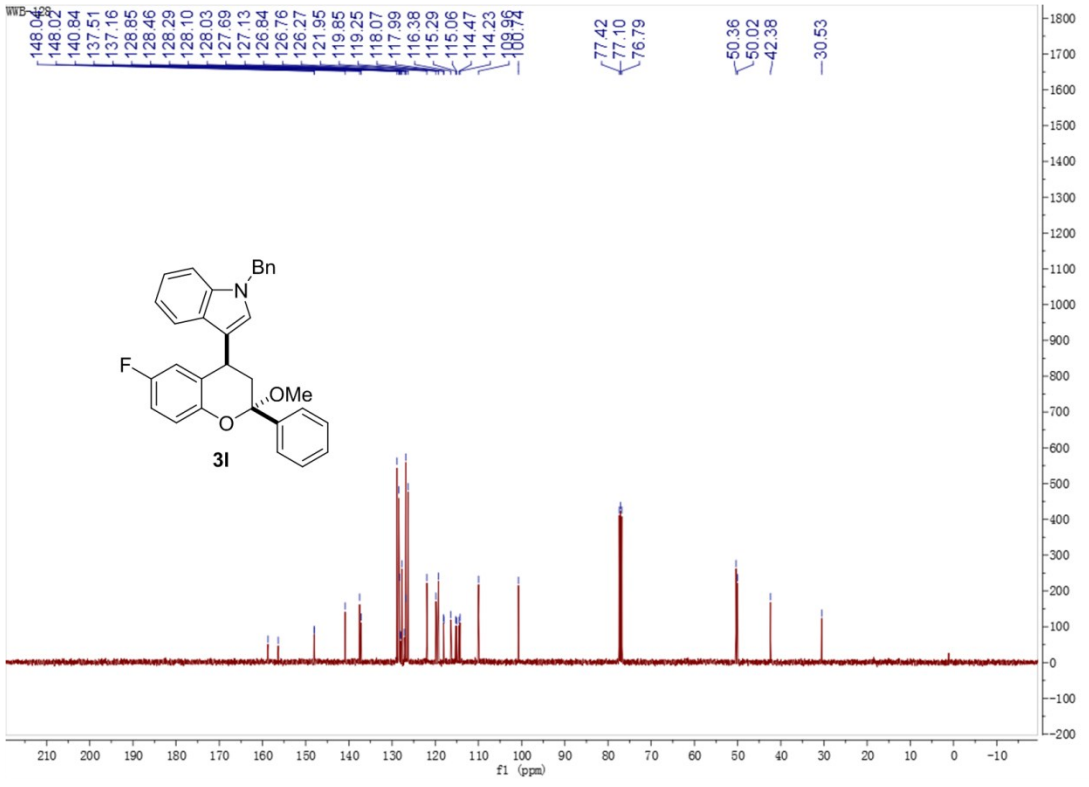

7.59
7.58
7.43
7.36
7.34
7.32
7.28
7.27
7.20
7.18
7.16
7.13
7.11
7.03
7.01
6.97
6.96
6.93
6.91
6.78
6.77
6.75
5.15
4.72
4.71
4.69
4.68
3.09
2.45
2.43
2.41
2.40
2.18
2.15
2.12
Bn
N
Br
OMe
O
3j
2.01
1.05
2.01
0.99
5.38
2.02
1.91
1.75
0.90
2.06
1.01
3.00
1.03
1.03
f1 (ppm)

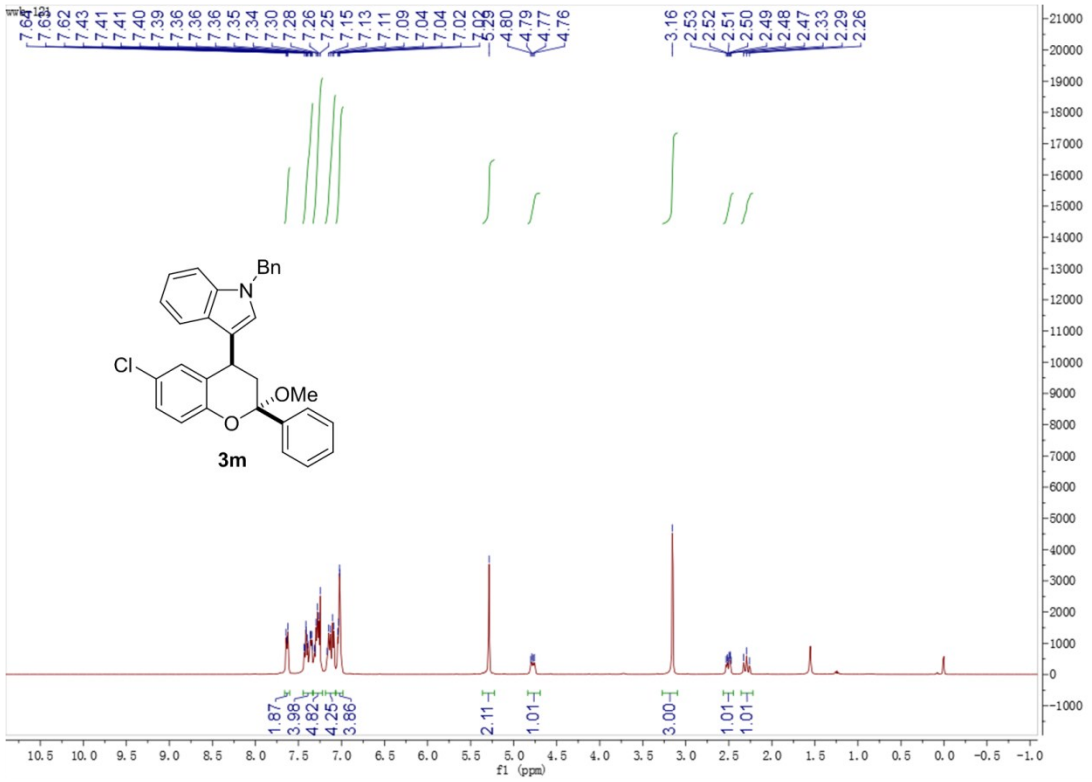

wwb-122
152.04
128.88
128.43
128.24
127.80
127.75
126.67
126.31
124.72
121.28
77.38
77.06
76.75
50.34
50.21
42.74
29.93
Bn
N
Br
OMe
O
3j
f1 (ppm)

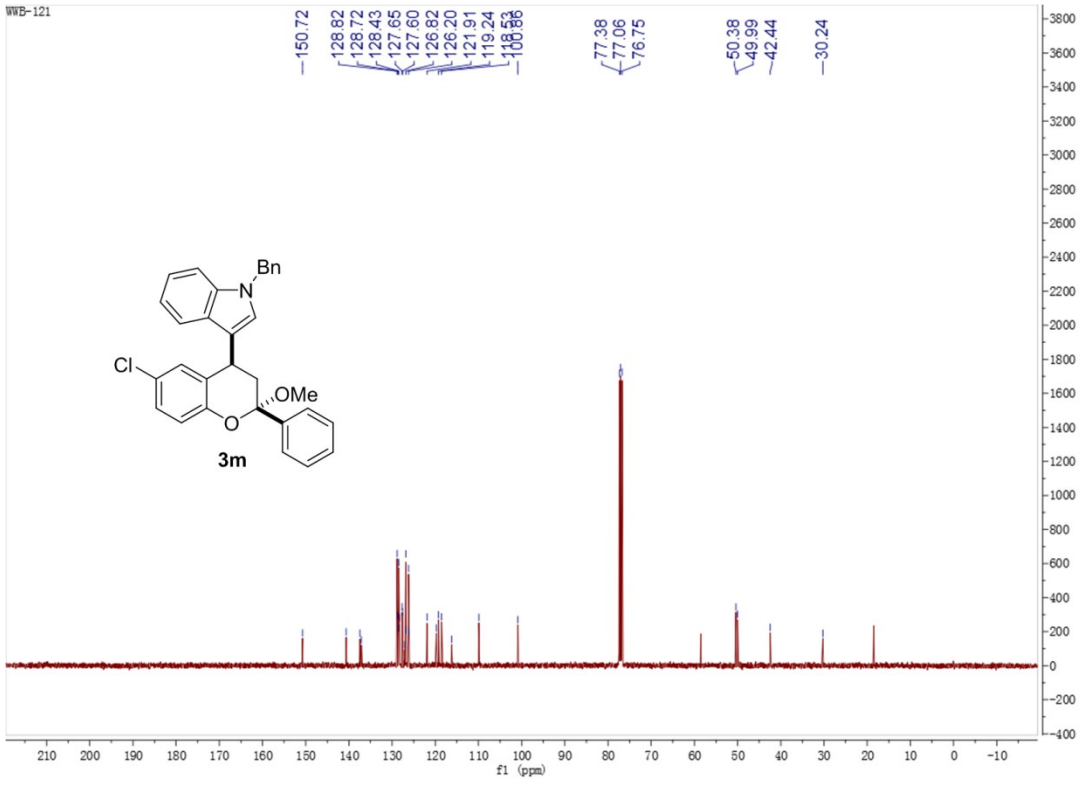

wwb-126
7.66
7.64
7.43
7.41
7.40
7.38
7.35
7.34
7.32
7.30
7.29
7.27
7.26
7.25
7.23
7.17
7.15
7.13
7.11
7.09
7.08
7.04
7.02
7.01
6.99
6.88
6.86
5.28
5.27
4.83
4.82
4.81
4.80
4.79
4.78
3.18
3.16
2.54
2.53
2.52
2.51
2.49
2.47
2.33
2.31
2.30
2.28
2.27
2.15
2.13
0.00
Bn
N
Me
OMe
O
3k
2.02
3.05
5.57
3.20
4.05
1.06
2.06
0.99
3.00
1.01
1.03
3.04
f1 (ppm)

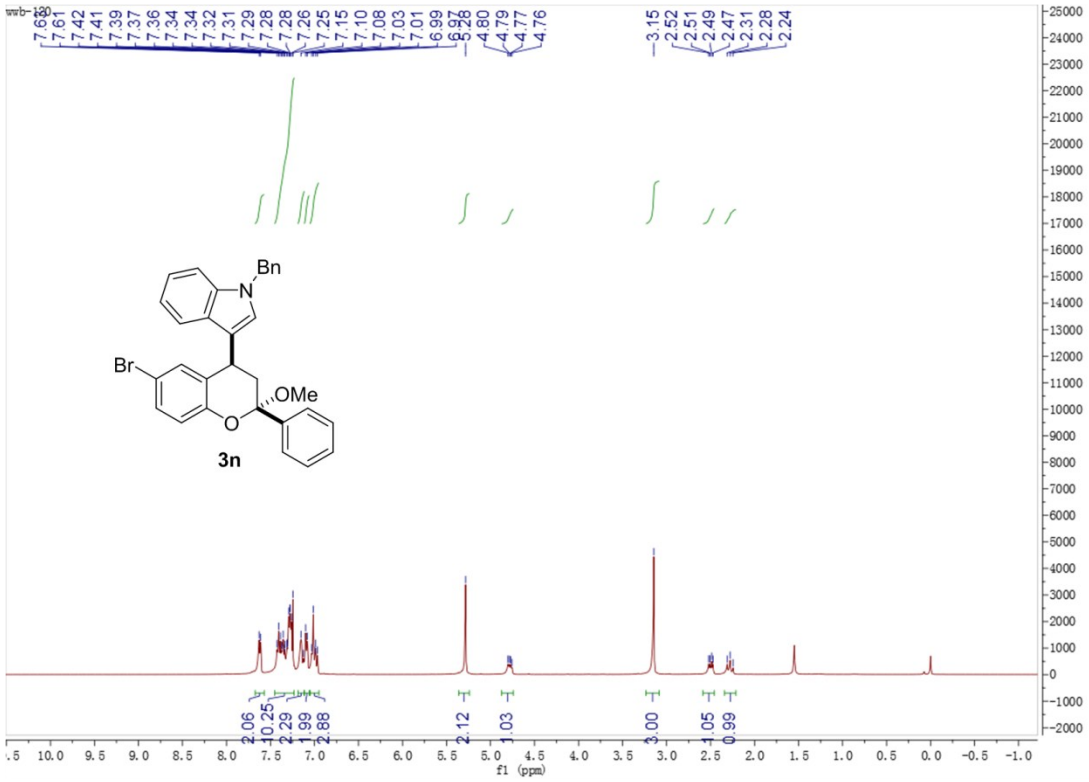

wwb-125
149.87
141.23
137.64
137.00
130.36
129.32
128.78
128.38
128.21
128.13
127.61
127.57
126.83
126.68
126.30
126.16
121.73
119.97
119.05
117.28
116.91
109.79
100.52
77.40
77.08
76.77
50.31
49.99
43.05
30.08
20.76
Bn
N
Me
OMe
O
3k
f1 (ppm)

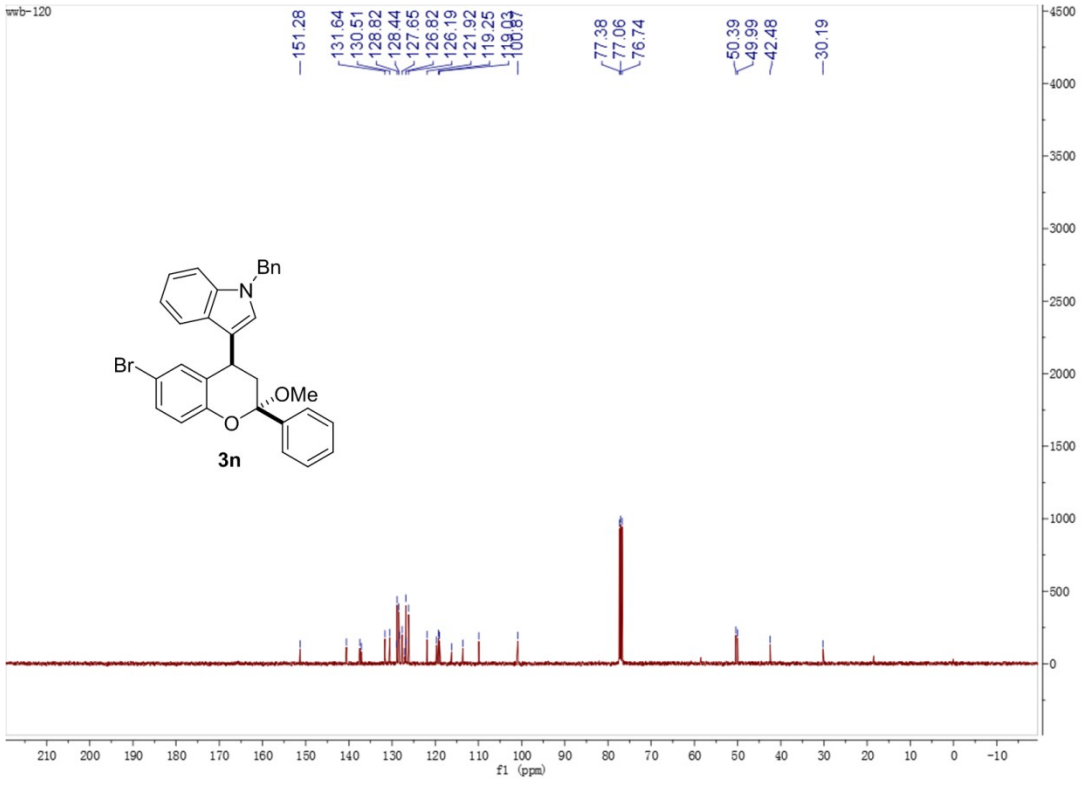

wwb-128
7.58
7.54
7.32
7.30
7.29
7.23
7.18
7.16
7.15
7.10
7.05
7.04
7.02
6.99
6.97
6.94
6.92
6.91
6.89
6.78
6.76
6.67
6.65
5.16
4.67
3.06
2.42
2.42
2.40
2.39
2.24
2.20
2.18
2.17
Bn
N
F
OMe
O
3l
1.98
8.28
6.12
1.05
0.98
2.05
1.00
3.00
1.00
0.99
f1 (ppm)

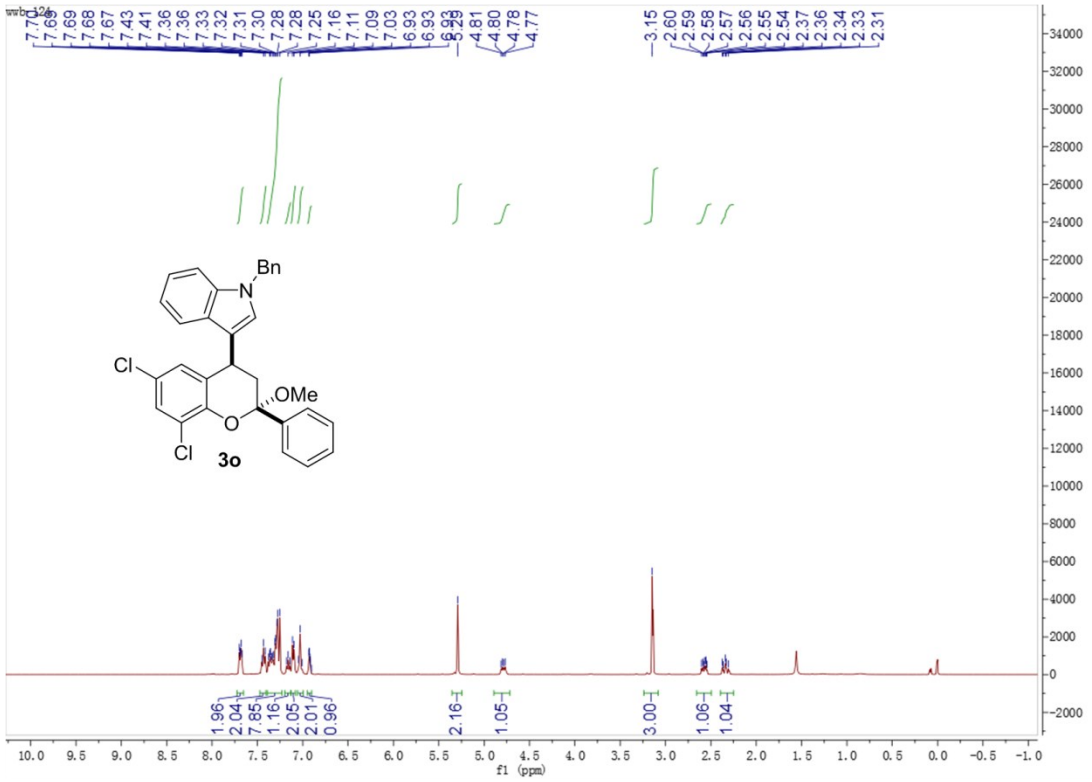

WWB-128
148.04
148.02
140.84
137.51
137.16
128.85
128.46
128.29
128.10
128.03
127.69
127.13
126.84
126.76
126.27
121.95
119.85
119.25
118.07
117.99
116.38
115.29
115.06
114.47
114.23
100.74
77.42
77.10
76.79
50.36
50.02
42.38
30.53
Bn
N
F
OMe
O
3l
f1 (ppm)

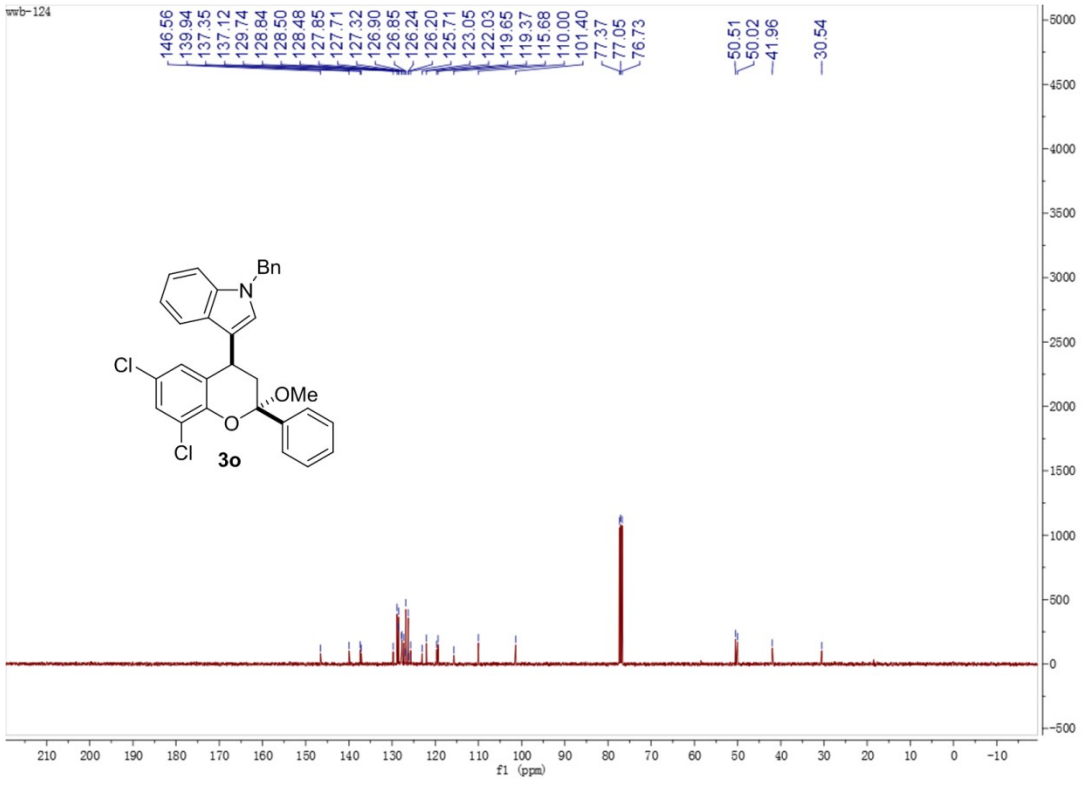

Bn
N
Cl
OMe
O
3m
f1 (ppm)

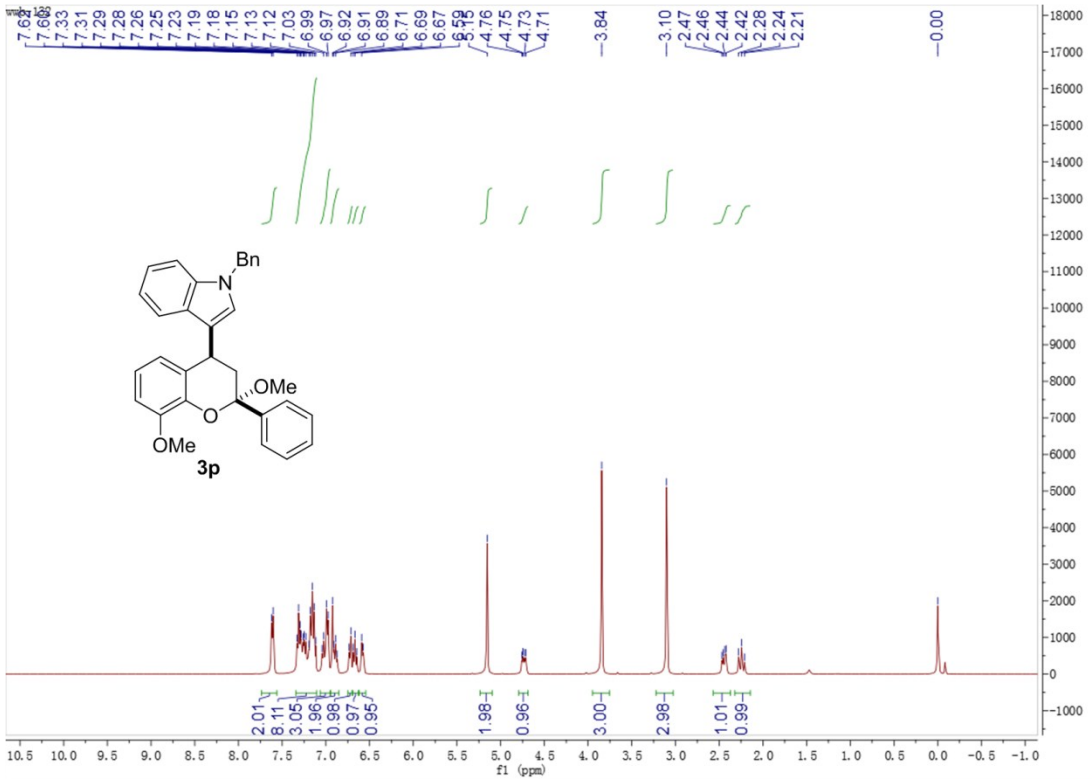

WWB-121
Bn
N
Cl
OMe
O
3m
f1 (ppm)

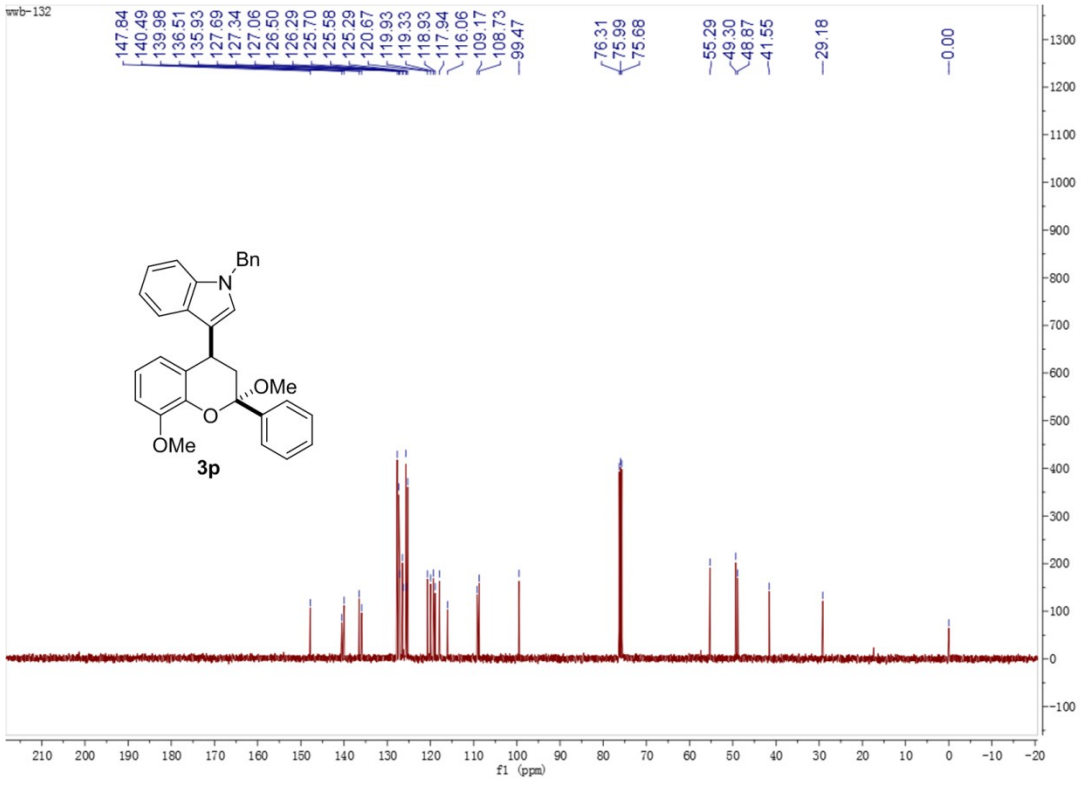

wrb-120
7.65
7.61
7.42
7.41
7.39
7.37
7.36
7.34
7.34
7.32
7.31
7.29
7.28
7.28
7.26
7.25
7.15
7.10
7.08
7.03
7.01
6.99
6.97
5.28
4.80
4.79
4.77
4.76
3.15
2.52
2.51
2.49
2.47
2.31
2.28
2.24
Bn
N
Br
OMe
O
3n
2.06
10.25
2.29
1.99
2.88
2.12
1.03
3.00
1.05
0.99
f1 (ppm)

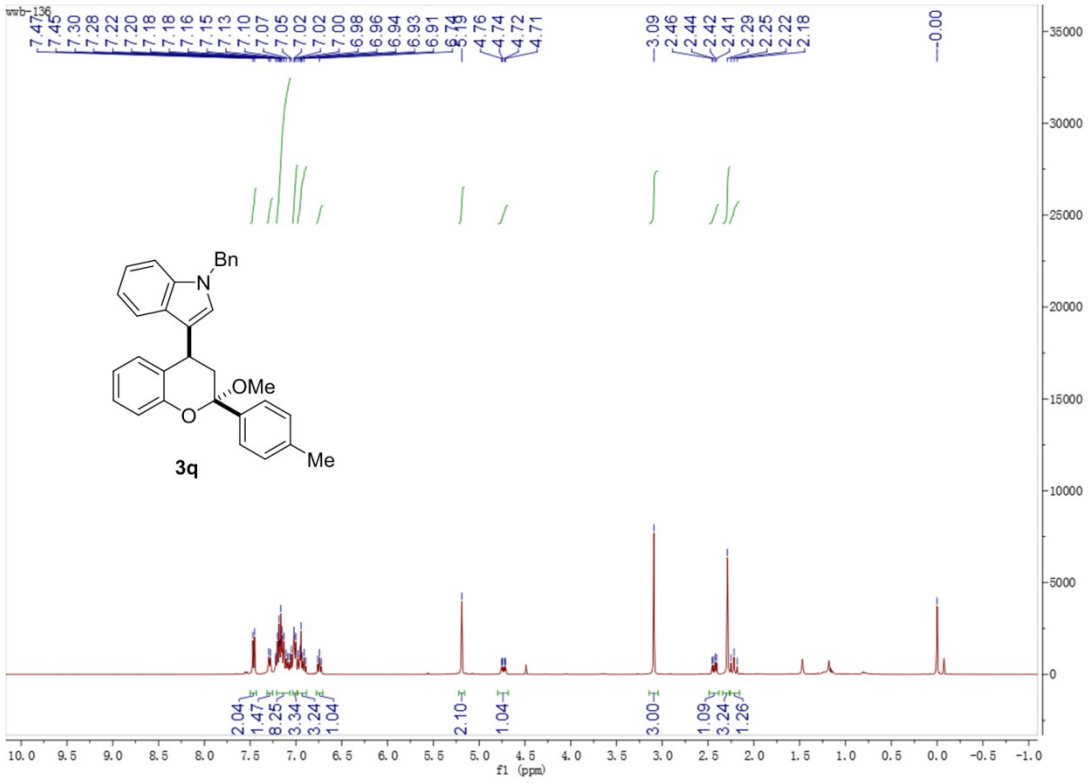

wrb-120
151.28
131.64
130.51
128.82
128.44
127.65
126.82
126.19
121.92
119.25
109.03
100.87
77.38
77.06
76.74
50.39
49.99
42.48
30.19
Bn
N
Br
OMe
O
3n
f1 (ppm)

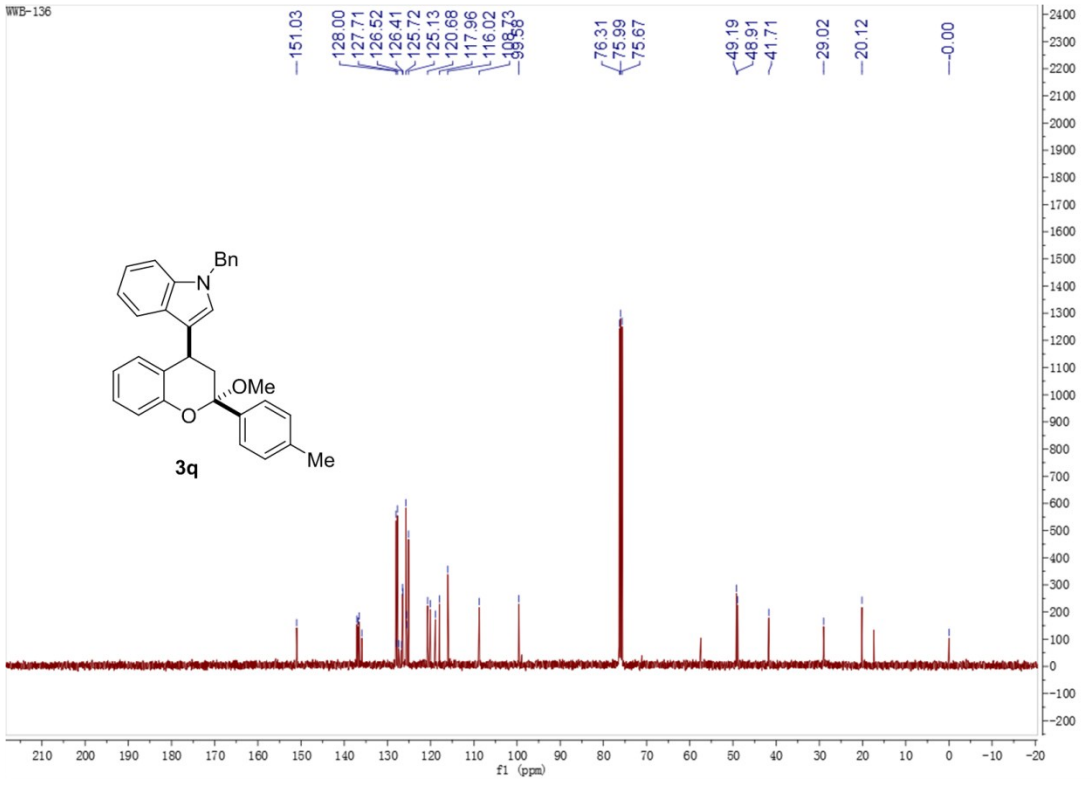

wrb-124
7.70
7.69
7.69
7.68
7.67
7.43
7.41
7.36
7.36
7.33
7.32
7.31
7.30
7.28
7.28
7.25
7.16
7.11
7.09
7.03
6.93
6.93
6.93
6.93
4.81
4.80
4.78
4.77
3.15
2.60
2.59
2.58
2.57
2.56
2.55
2.54
2.37
2.36
2.34
2.33
2.31
Bn
N
Cl
OMe
O
Cl
3o
1.96
2.04
7.85
1.16
2.05
2.01
0.96
2.16
1.05
3.00
1.06
1.04
f1 (ppm)

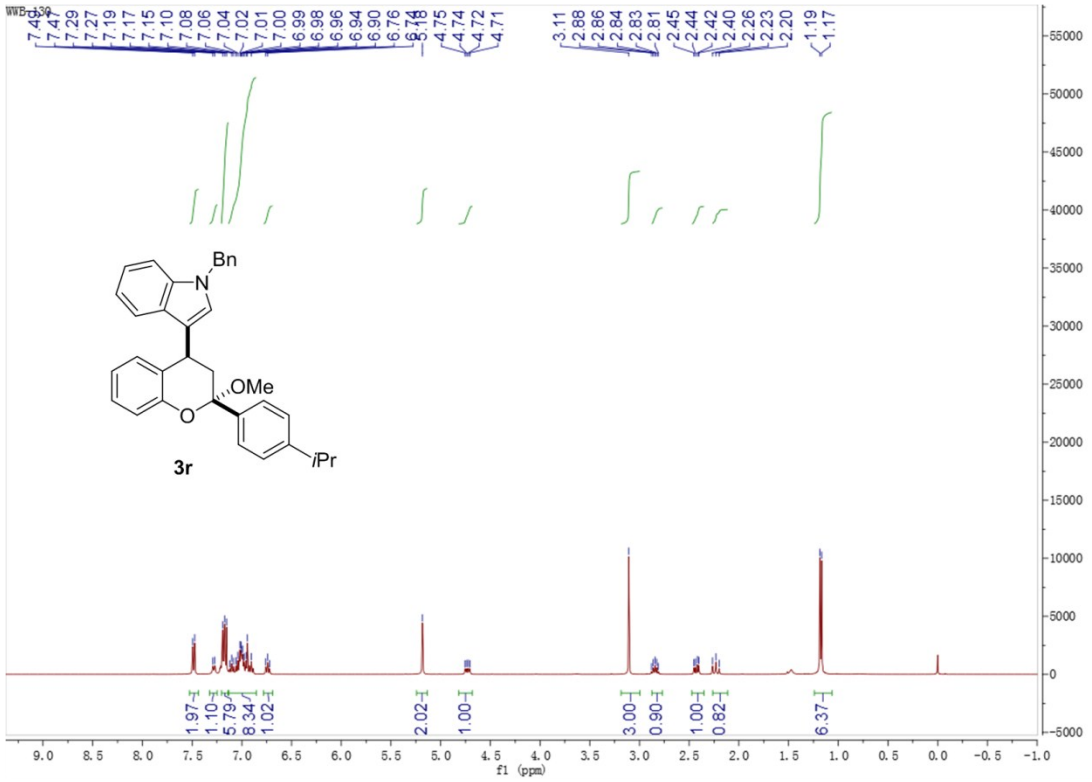

wrb-124
146.56
139.94
137.35
137.12
129.74
128.84
128.50
128.48
127.85
127.71
127.32
126.90
126.85
126.24
126.20
125.71
123.05
122.03
119.65
119.37
115.68
110.00
101.40
77.37
77.05
76.73
50.51
50.02
41.96
30.54
Bn
N
Cl
OMe
O
Cl
3o
f1 (ppm)

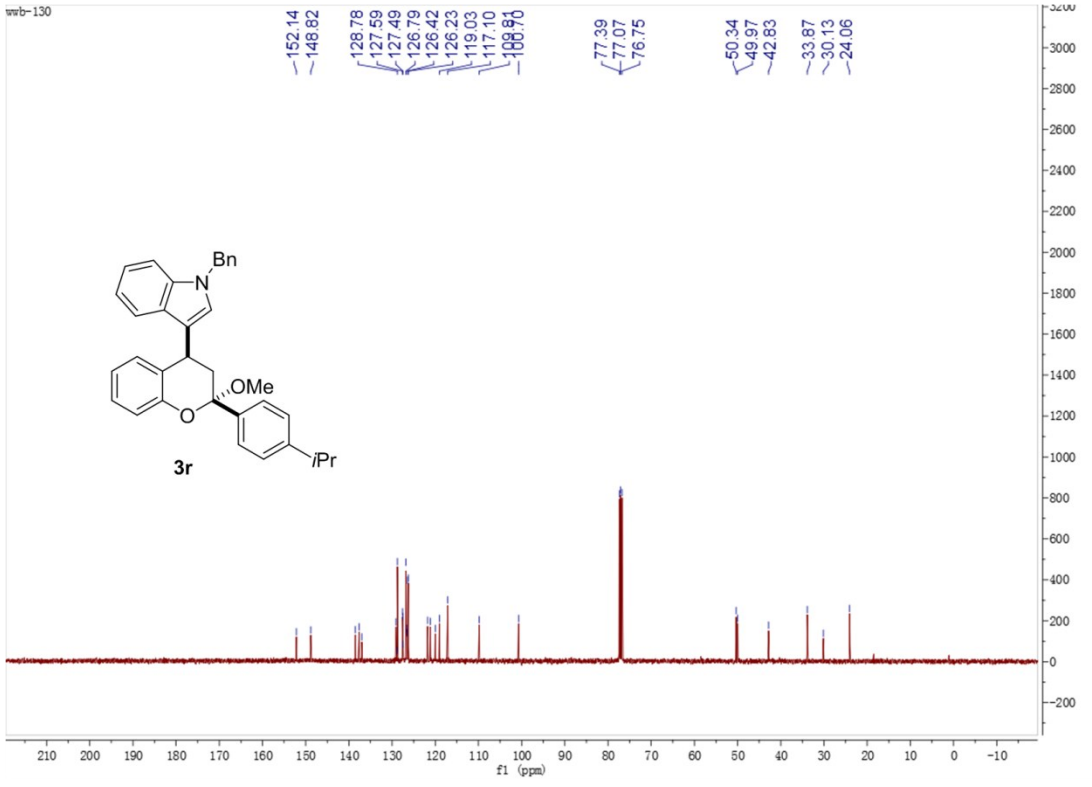

7.67
7.66
7.33
7.31
7.29
7.28
7.26
7.25
7.23
7.19
7.18
7.15
7.13
7.12
7.03
6.99
6.97
6.92
6.91
6.89
6.71
6.69
6.67
6.59
4.76
4.75
4.73
4.71
3.84
3.10
2.47
2.46
2.44
2.42
2.28
2.24
2.21
0.00
Bn
N
OMe
O
OMe
3p
2.01
8.11
3.05
1.96
0.98
0.97
0.95
1.98
0.96
3.00
2.98
1.01
0.99
f1 (ppm)

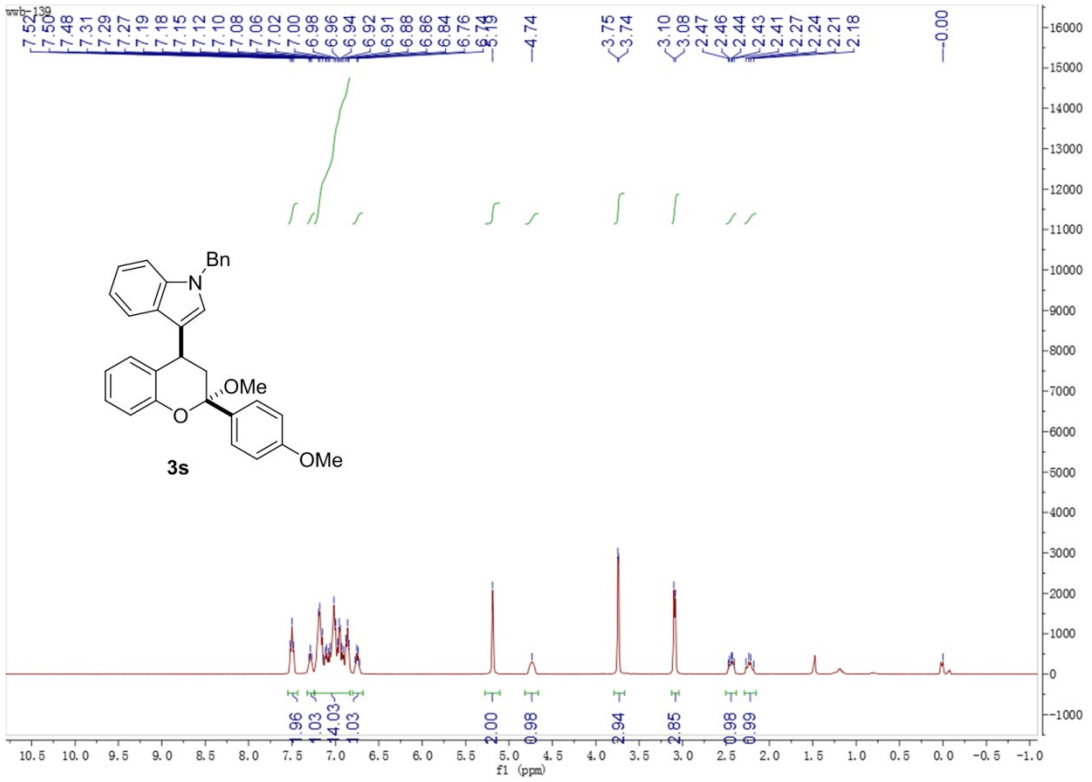

wwb-132
147.84
140.49
139.98
136.51
135.93
127.69
127.34
127.06
126.50
126.29
125.70
125.58
125.29
120.67
119.93
119.33
118.93
117.94
116.06
109.17
108.73
99.47
76.31
75.99
75.68
55.29
49.30
48.87
41.55
29.18
0.00
Bn
N
OMe
O
OMe
3p
f1 (ppm)

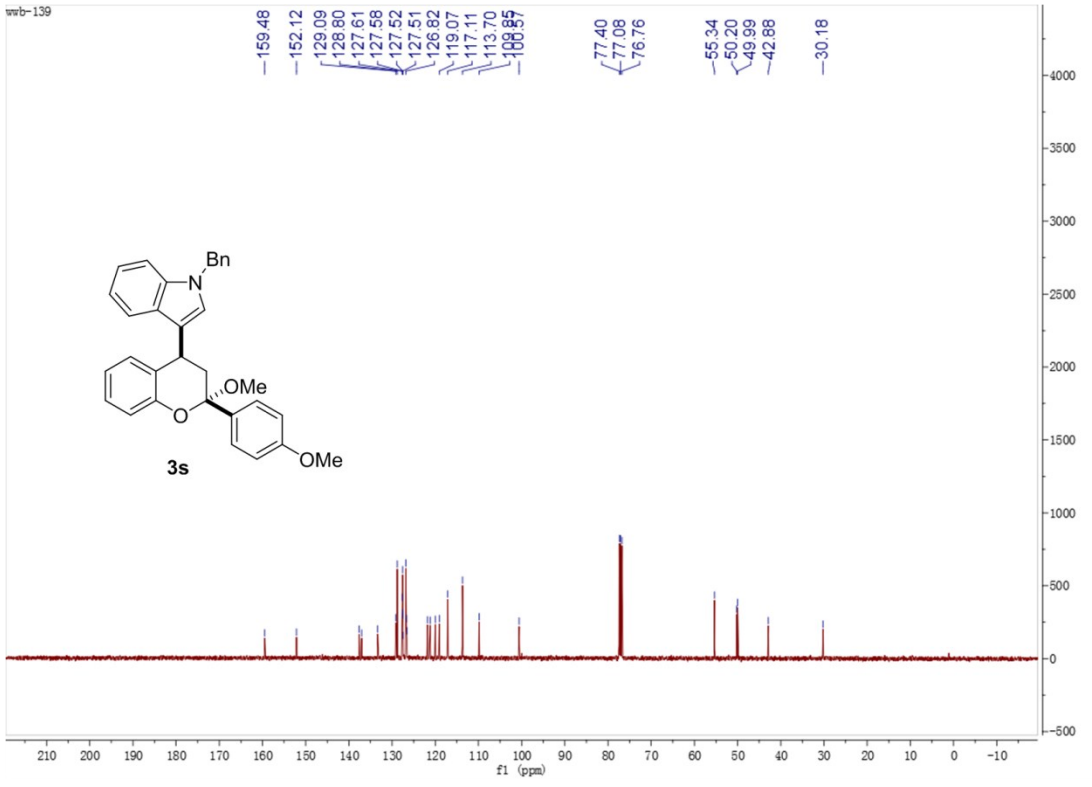

wwb-136
7.47
7.45
7.30
7.28
7.22
7.20
7.18
7.18
7.16
7.15
7.13
7.10
7.07
7.05
7.02
7.02
7.00
6.98
6.96
6.94
6.93
6.91
6.74
5.19
4.76
4.74
4.72
4.71
3.09
2.46
2.44
2.42
2.41
2.29
2.25
2.22
2.18
0.00
Bn
N
OMe
O
Me
3q
2.04
1.47
8.25
3.34
3.24
1.04
2.10
1.04
3.00
1.09
3.24
1.26
f1 (ppm)

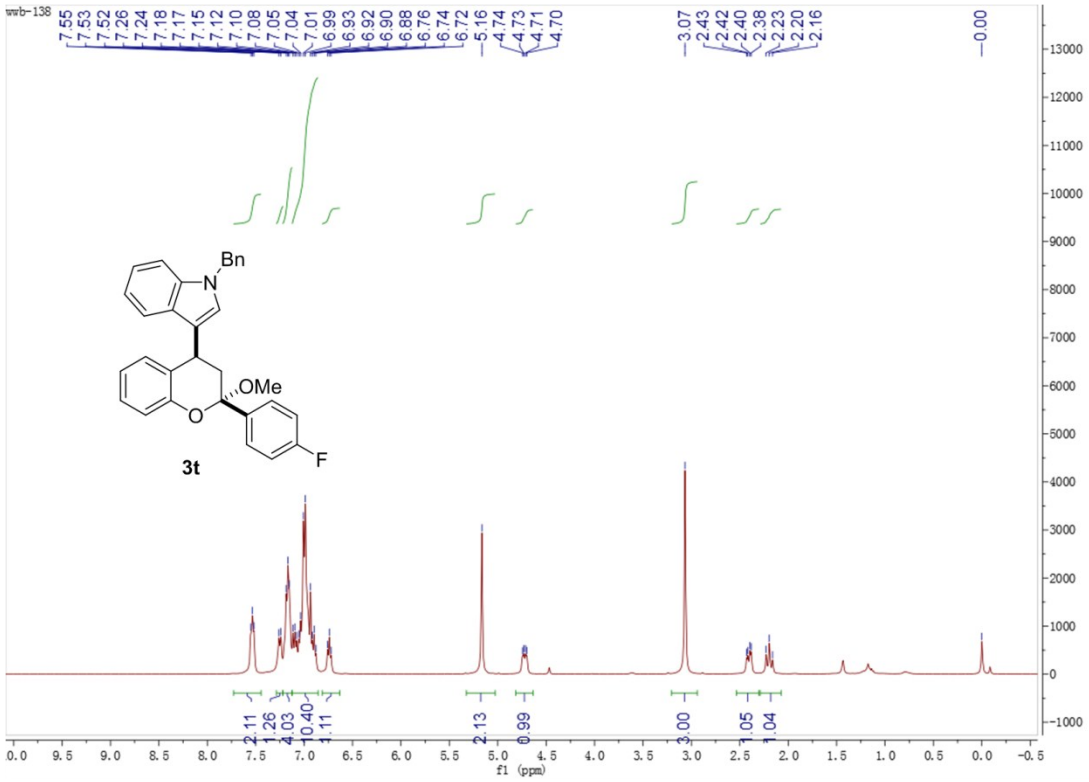

WWB-136
151.03
128.00
127.71
126.52
126.41
125.72
125.13
120.68
117.96
116.02
108.73
99.58
76.31
75.99
75.67
49.19
48.91
41.71
29.02
20.12
0.00
Bn
N
OMe
O
Me
3q
f1 (ppm)

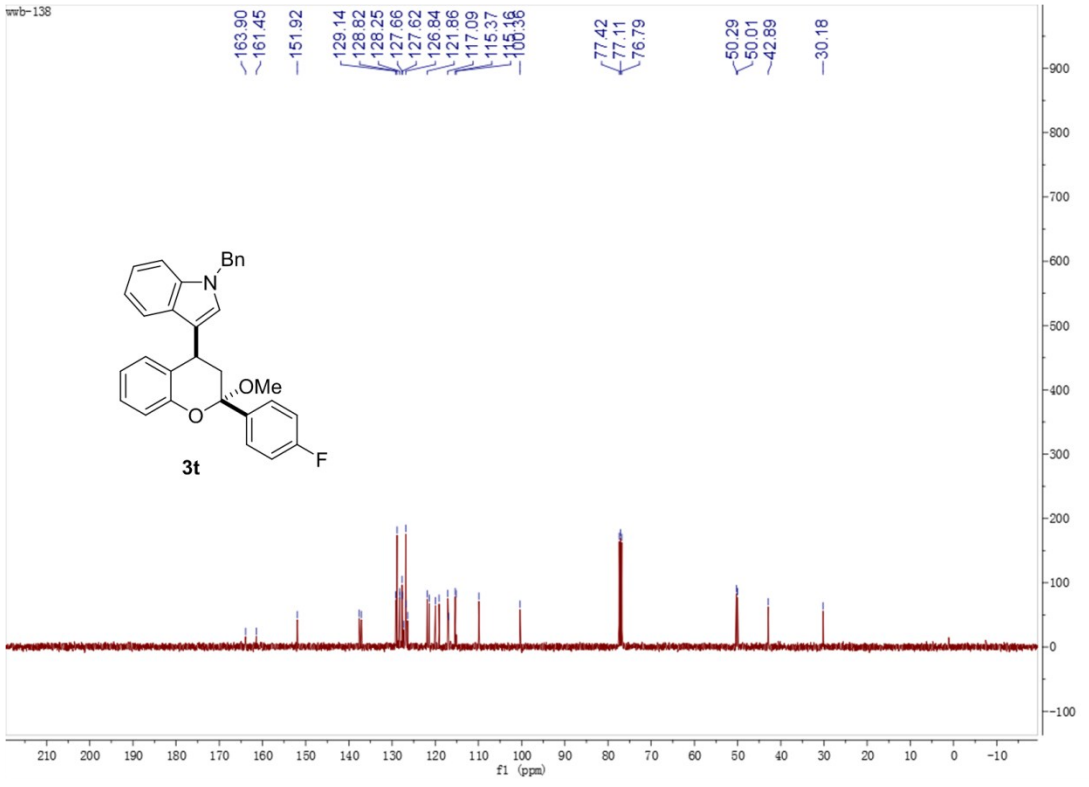

Bn
OMe
iPr
3r
f1 (ppm)

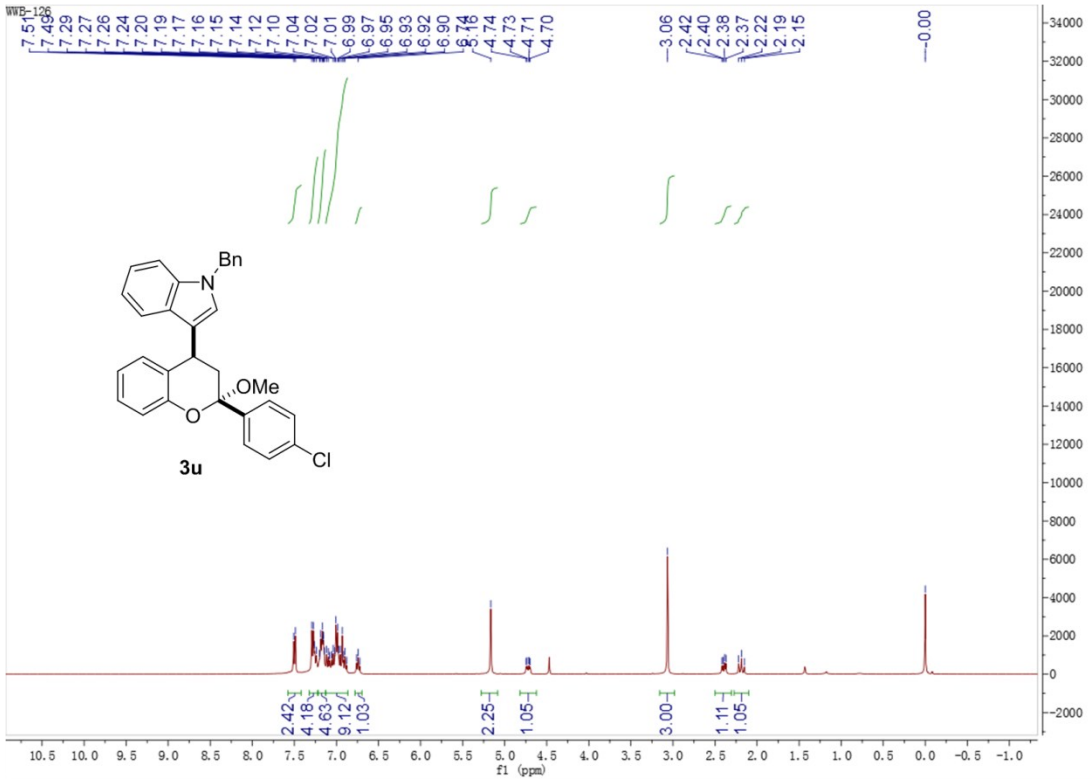

Bn
OMe
iPr
3r
f1 (ppm)

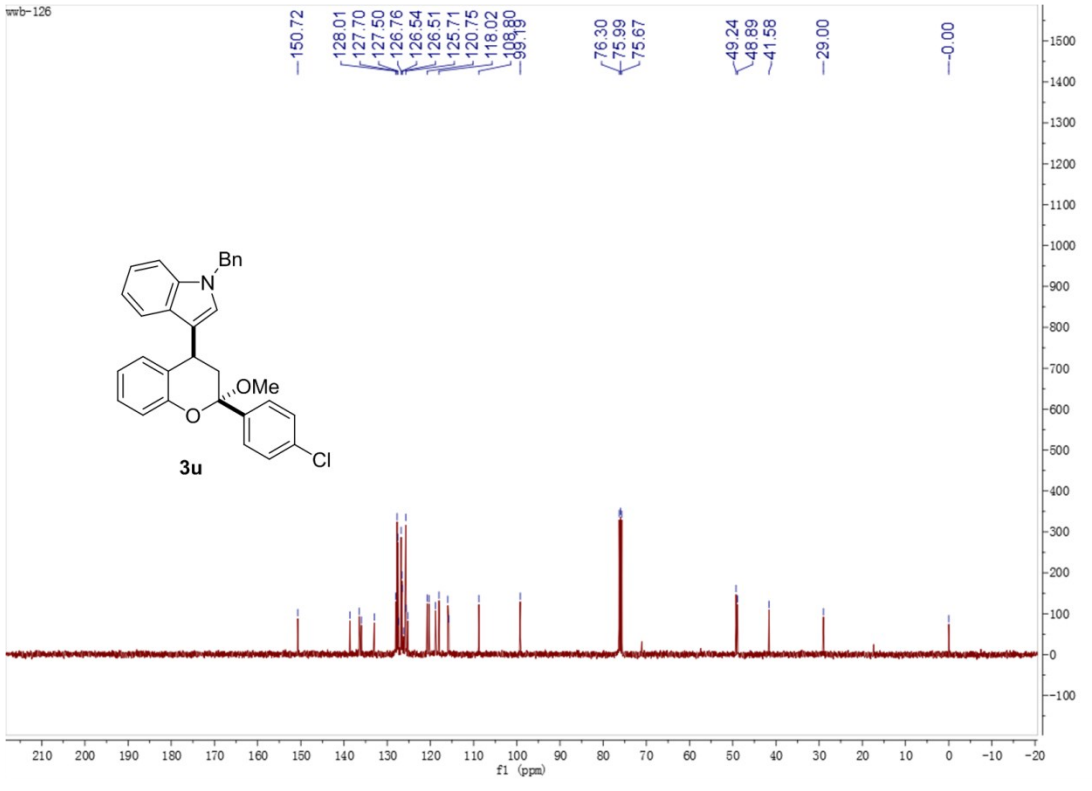

wwb-139
7.52
7.50
7.48
7.31
7.29
7.27
7.19
7.18
7.15
7.12
7.10
7.08
7.06
7.02
7.00
6.98
6.96
6.94
6.92
6.91
6.88
6.86
6.84
6.76
6.74
5.19
4.74
3.75
3.74
3.10
3.08
2.47
2.46
2.44
2.43
2.41
2.27
2.24
2.21
2.18
0.00
Bn
N
OMe
O
OMe
3s
1.96
1.03
14.03
1.03
2.00
0.98
2.94
2.85
0.98
0.99
f1 (ppm)

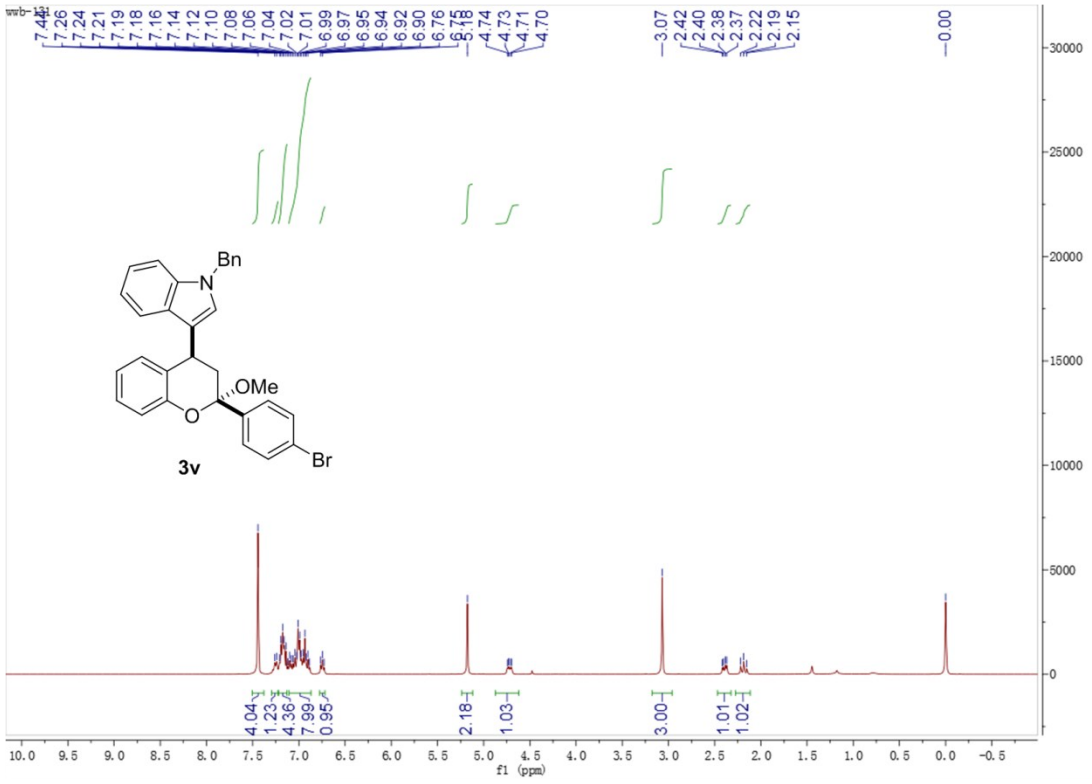

wwb-139
159.48
152.12
129.09
128.80
127.61
127.58
127.52
127.51
126.82
119.07
117.11
113.70
77.40
77.08
76.76
55.34
50.20
49.99
42.88
30.18
Bn
N
OMe
O
OMe
3s
f1 (ppm)

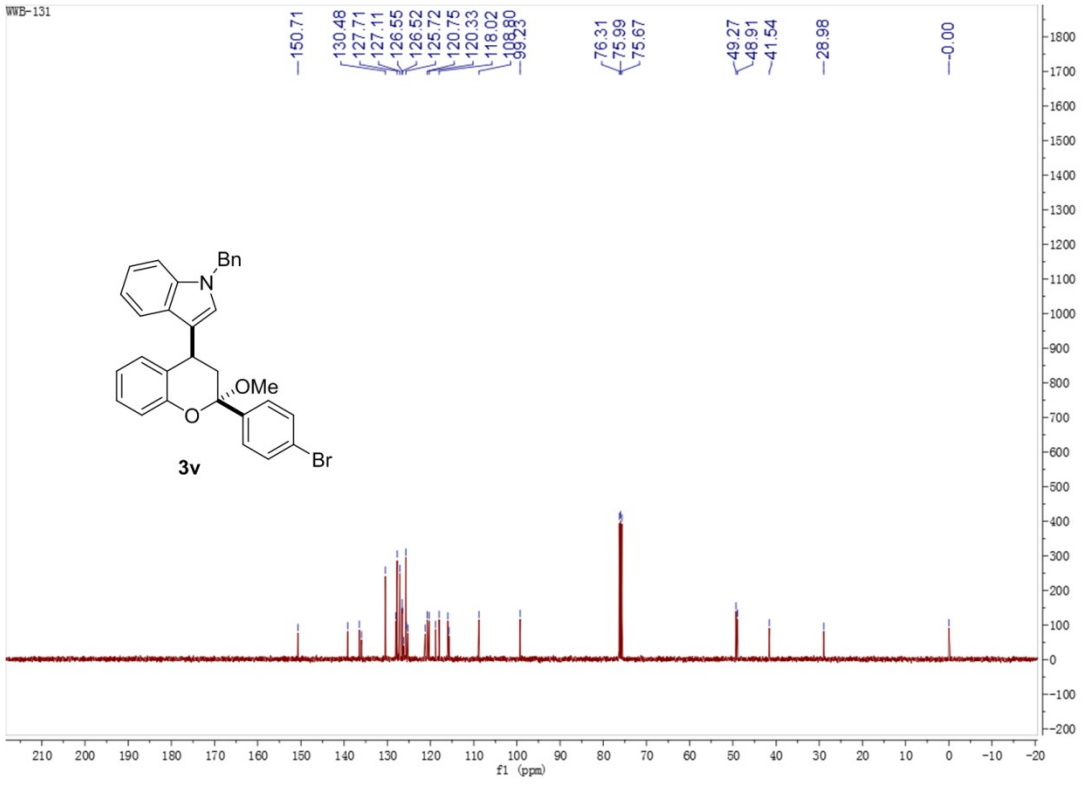

wwb-138
7.55
7.53
7.52
7.26
7.24
7.18
7.17
7.15
7.12
7.10
7.08
7.05
7.04
7.01
6.99
6.93
6.92
6.90
6.88
6.76
6.74
6.72
5.16
4.74
4.73
4.71
4.70
3.07
2.43
2.42
2.40
2.38
2.23
2.20
2.16
0.00
Bn
N
OMe
O
F
3t
2.11
1.26
4.03
10.40
1.11
2.13
0.99
3.00
1.05
1.04
f1 (ppm)

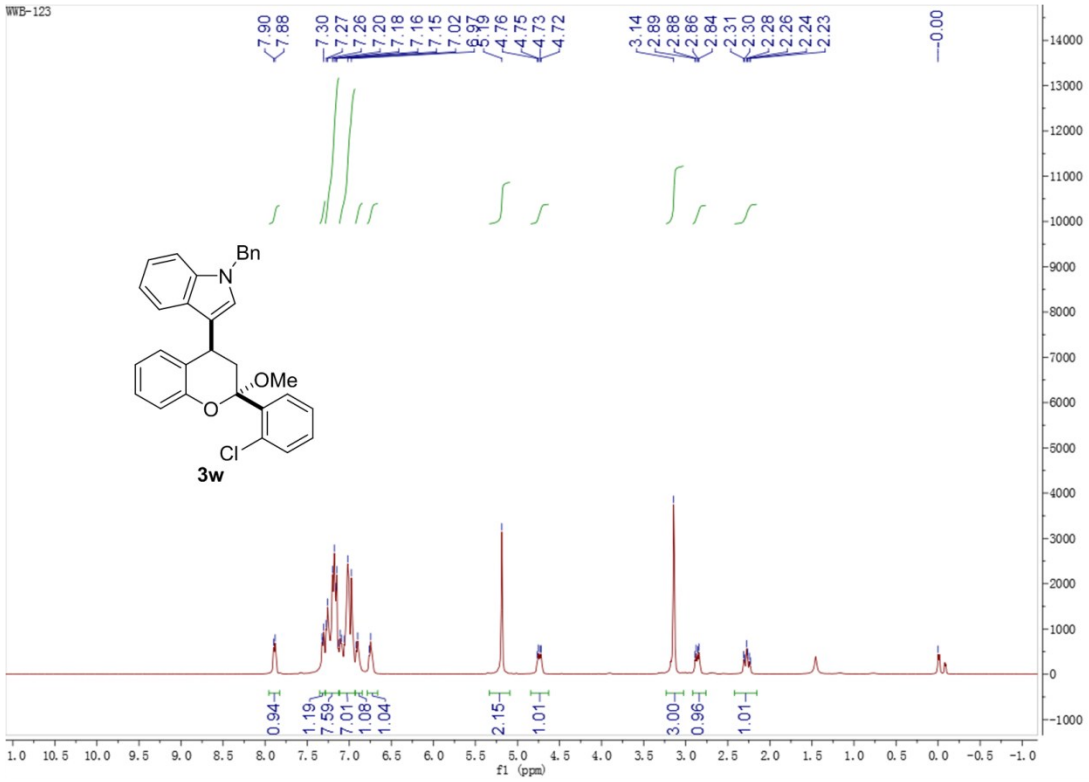

wwb-138
163.90
161.45
151.92
129.14
128.82
128.25
127.66
127.62
126.84
121.86
117.09
115.37
115.16
100.36
77.42
77.11
76.79
50.29
50.01
42.89
30.18
Bn
N
OMe
O
F
3t
f1 (ppm)

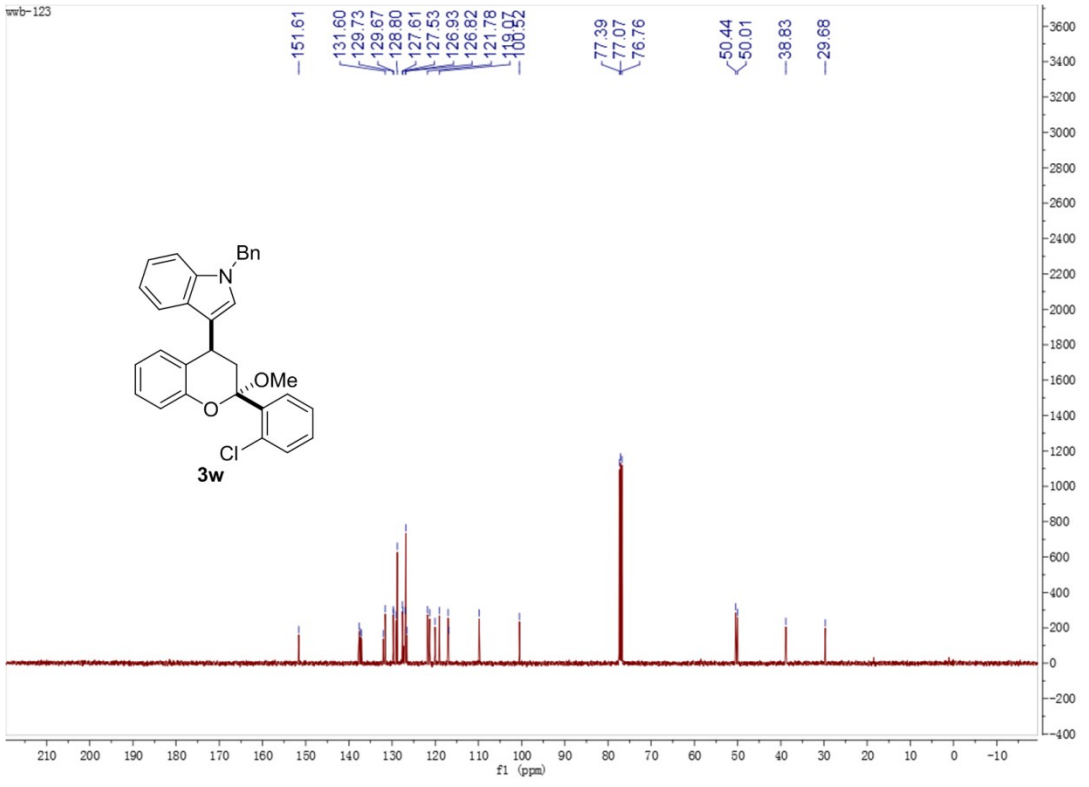

WWB-126
7.51
7.49
7.29
7.27
7.26
7.24
7.20
7.19
7.17
7.16
7.15
7.14
7.12
7.10
7.04
7.02
7.01
6.99
6.97
6.95
6.93
6.92
6.90
4.74
4.73
4.71
4.70
3.06
2.42
2.40
2.38
2.37
2.22
2.19
2.15
0.00
Bn
N
OMe
O
Cl
3u
2.42
4.18
4.63
9.12
1.03
2.25
1.05
3.00
1.11
1.05
f1 (ppm)

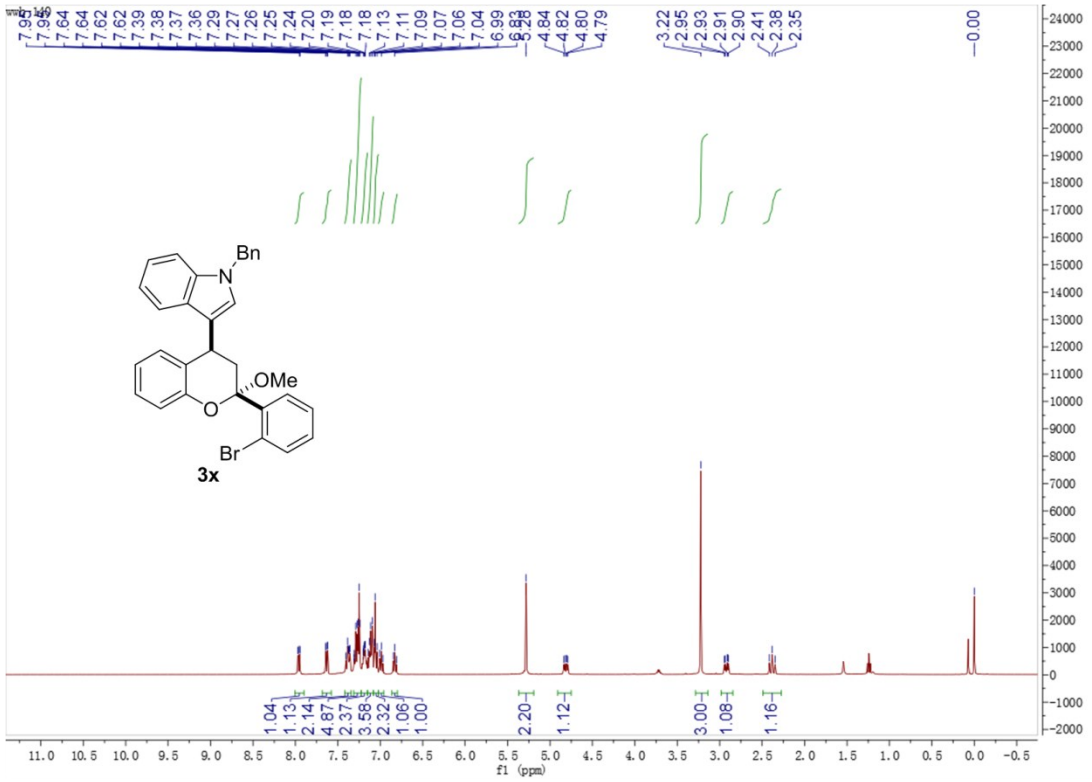

wwb-126
150.72
128.01
127.70
127.50
126.76
126.54
126.51
125.71
120.75
118.02
108.80
99.19
76.30
75.99
75.67
49.24
48.89
41.58
29.00
0.00
Bn
N
OMe
O
Cl
3u
f1 (ppm)

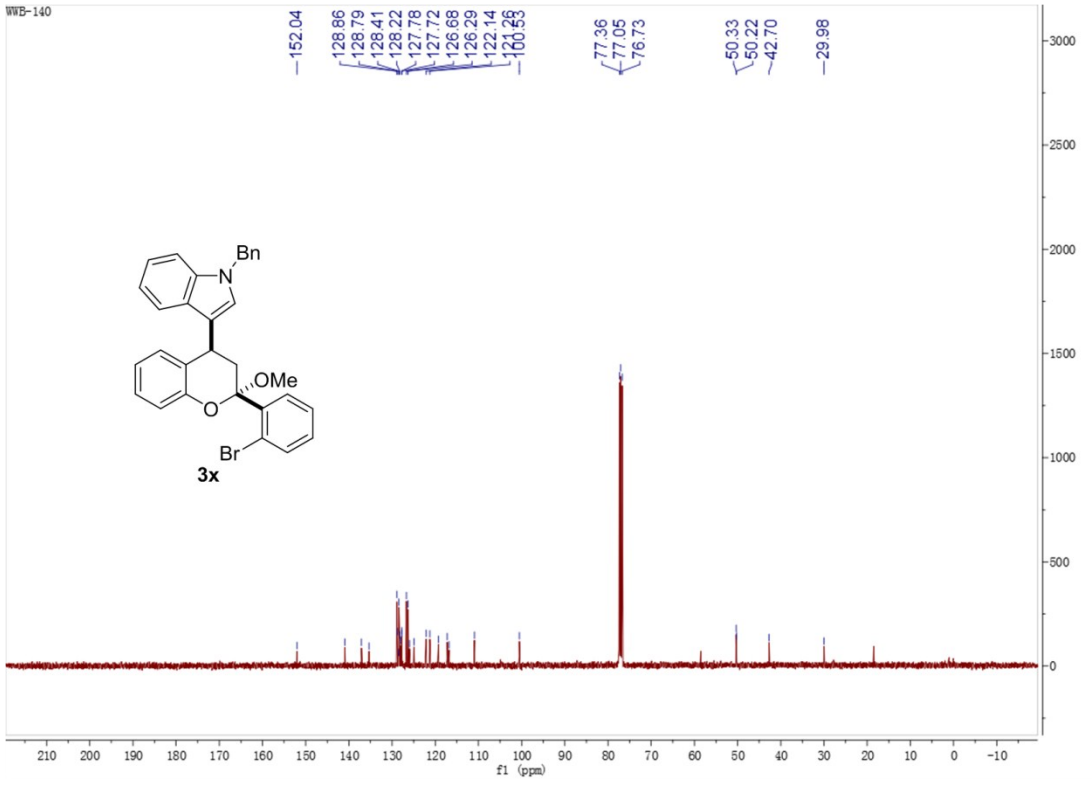

7.44
7.26
7.24
7.21
7.19
7.18
7.16
7.14
7.12
7.10
7.08
7.06
7.04
7.02
7.01
6.99
6.97
6.95
6.94
6.92
6.90
6.76
6.75
5.18
4.74
4.73
4.71
4.70
3.07
2.42
2.40
2.38
2.37
2.22
2.19
2.15
0.00
Bn
N
OMe
O
Br
3v
4.04
1.23
4.36
7.99
0.95
2.18
1.03
3.00
1.01
1.02
f1 (ppm)

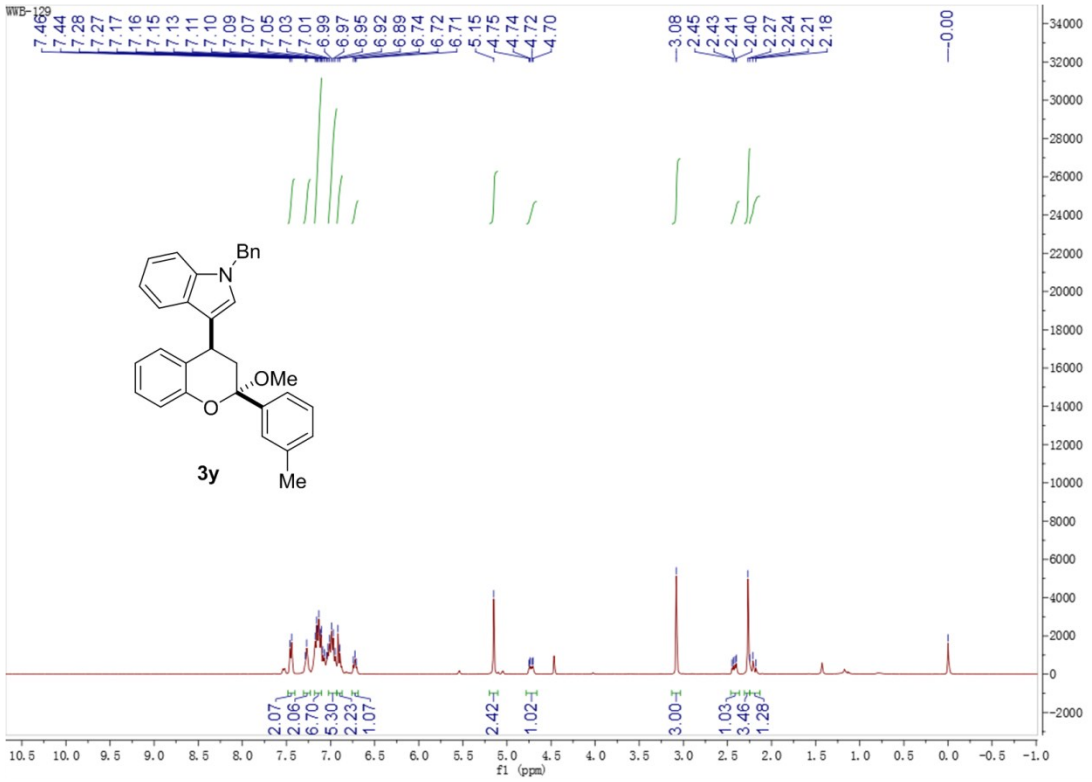

WWB-131
150.71
130.48
127.71
127.11
126.55
126.52
125.72
120.75
120.33
118.02
108.80
99.23
76.31
75.99
75.67
49.27
48.91
41.54
28.98
0.00
Bn
N
OMe
O
Br
3v
f1 (ppm)

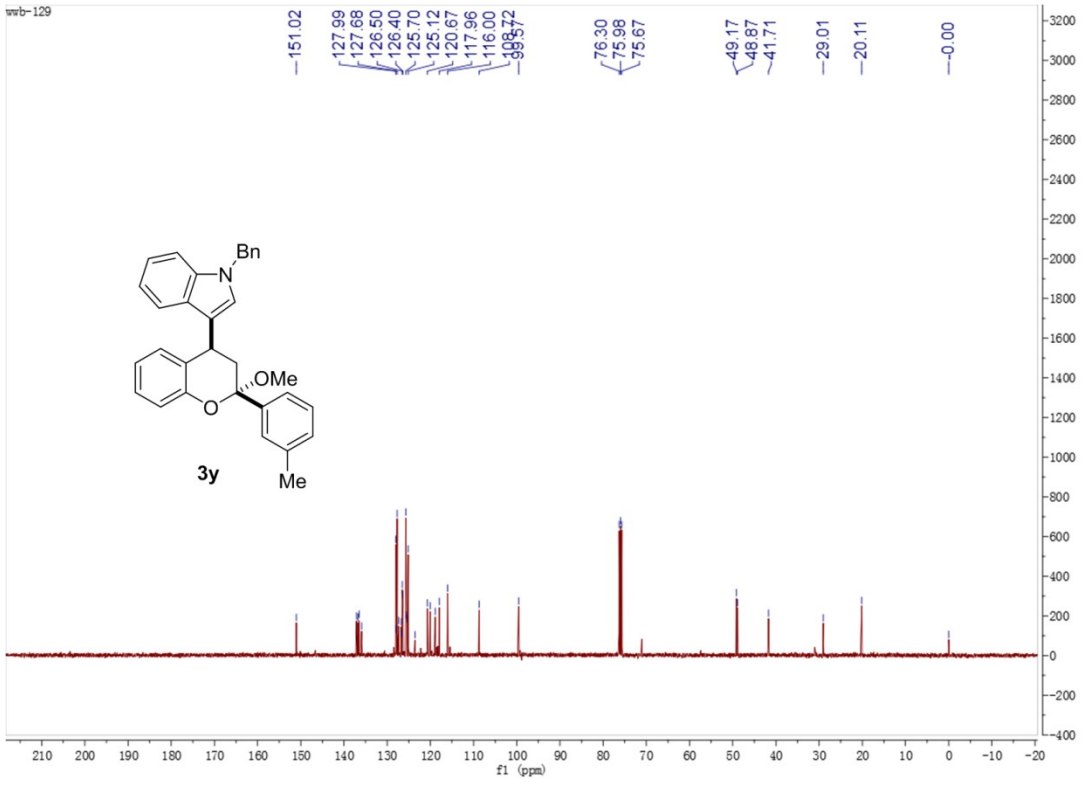

WWB-123
7.90
7.88
7.30
7.27
7.26
7.20
7.18
7.16
7.15
7.02
6.97
6.95
4.76
4.75
4.73
4.72
3.14
2.89
2.88
2.86
2.84
2.31
2.30
2.28
2.26
2.24
2.23
0.00
Bn
N
OMe
O
Cl
3w
0.94
1.19
7.59
7.01
1.08
1.04
2.15
1.01
3.00
0.96
1.01
f1 (ppm)

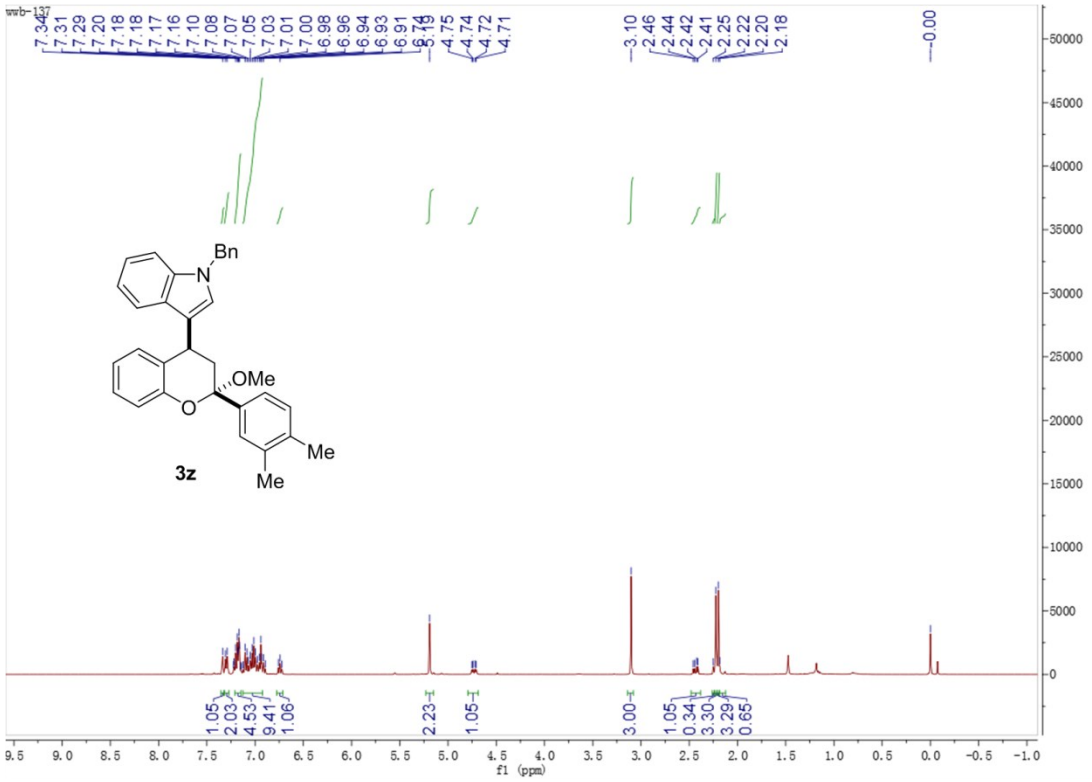

wwb-123
151.61
131.60
129.73
129.67
128.80
127.61
127.53
126.93
126.82
121.78
119.07
100.52
77.39
77.07
76.76
50.44
50.01
38.83
29.68
Bn
N
OMe
O
Cl
3w
f1 (ppm)

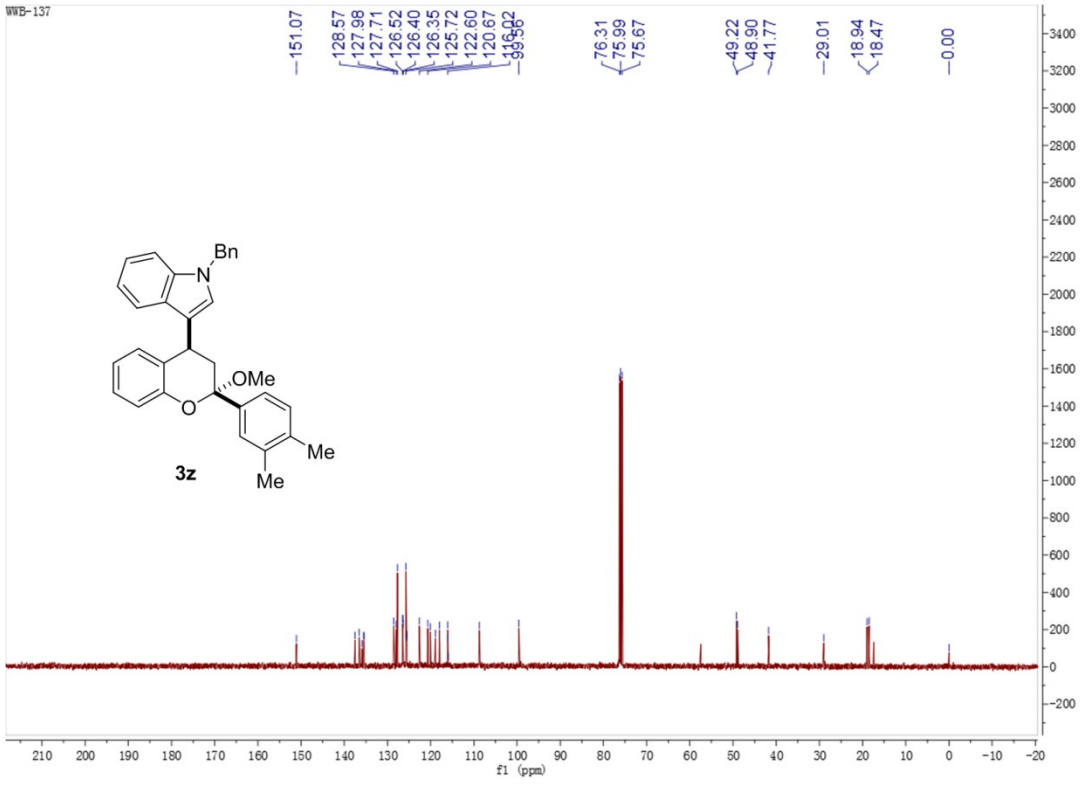

Bn
N
OMe
O
Br
3x
f1 (ppm)

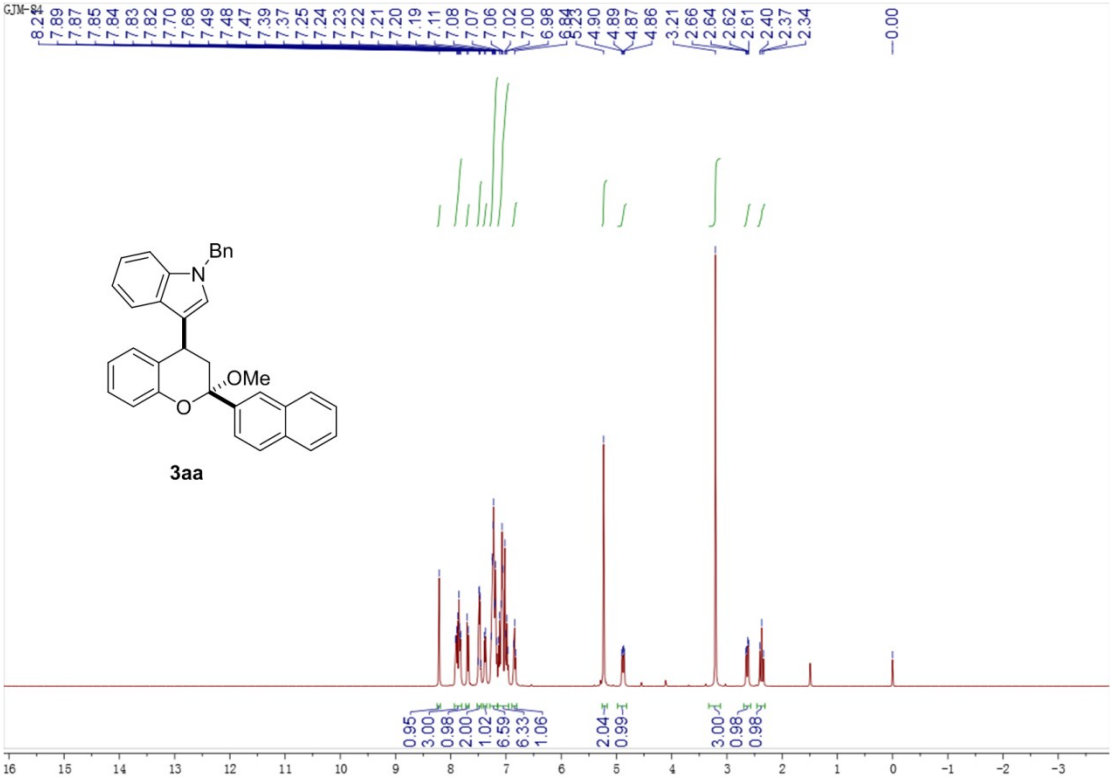

WWB-140
Bn
N
OMe
O
Br
3x
f1 (ppm)

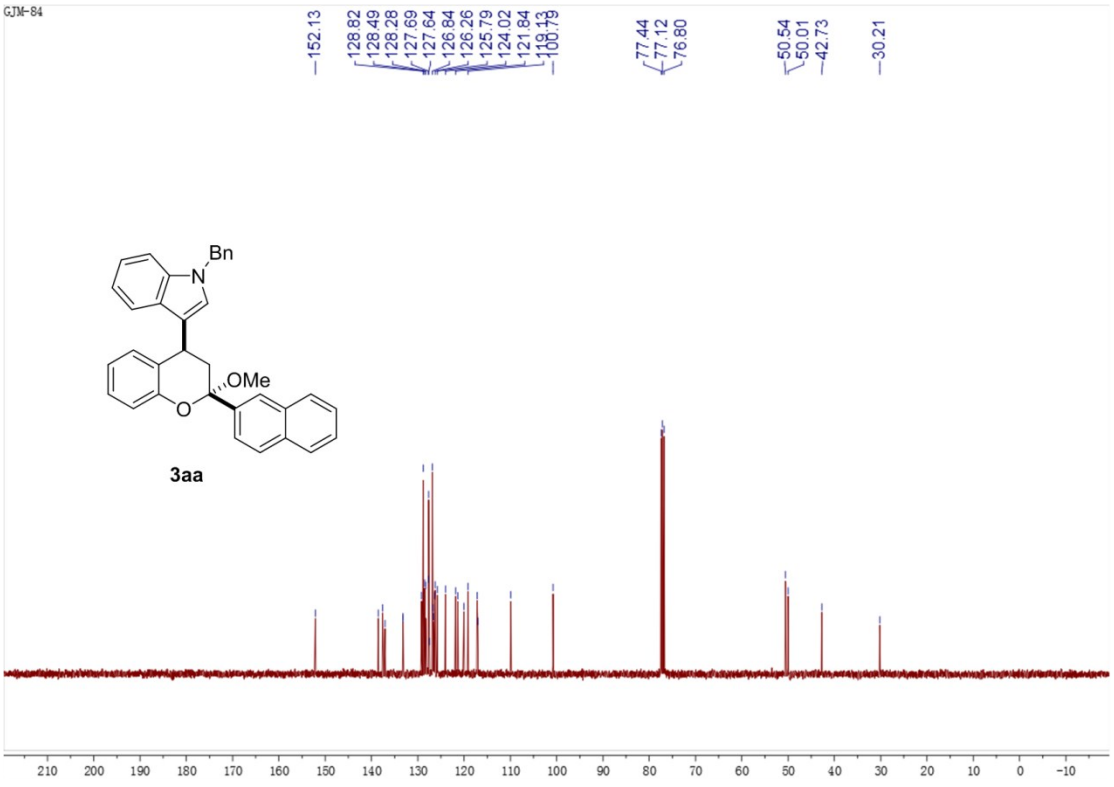

WWB-129
7.46
7.44
7.28
7.27
7.17
7.16
7.15
7.13
7.11
7.10
7.09
7.07
7.05
7.03
7.01
6.99
6.97
6.95
6.92
6.89
6.74
6.72
6.71
5.15
4.75
4.74
4.72
4.70
3.08
2.45
2.43
2.41
2.40
2.27
2.24
2.21
2.18
0.00
Bn
N
OMe
O
3y
Me
2.07
2.06
6.70
5.30
2.23
1.07
2.42
1.02
3.00
1.03
3.46
1.28
f1 (ppm)

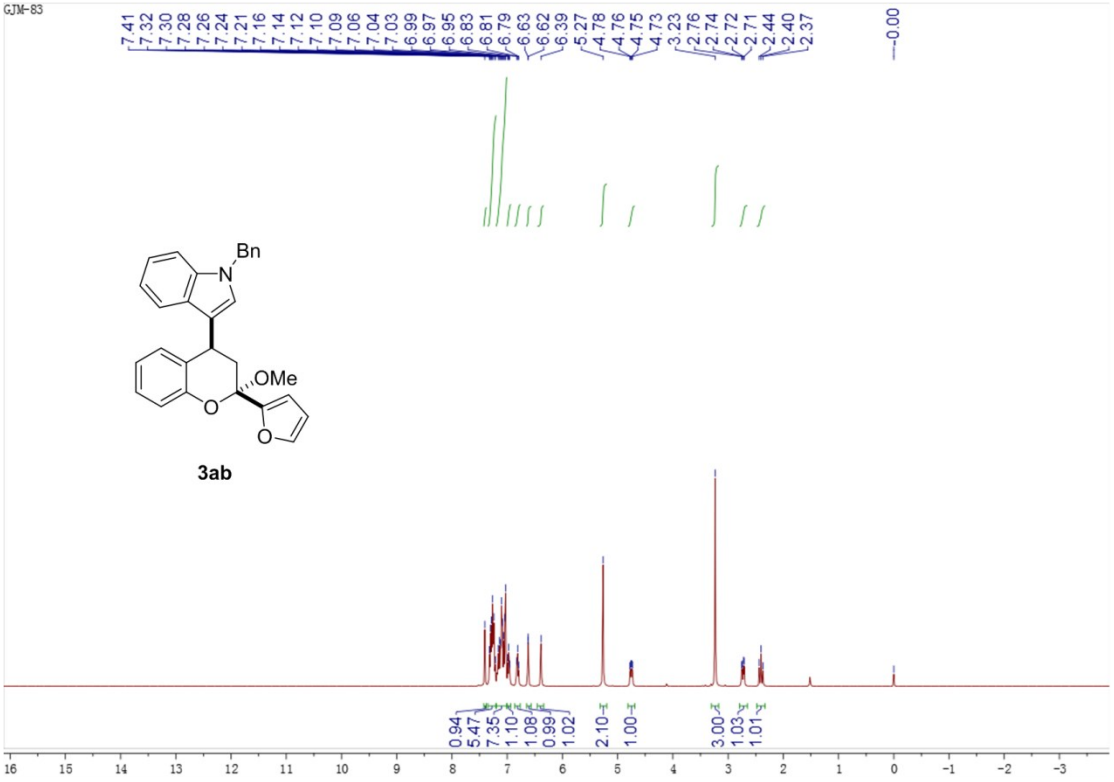

wwb-129
151.02
127.99
127.68
126.50
126.40
125.70
125.12
120.67
117.96
116.00
108.72
99.57
76.30
75.98
75.67
49.17
48.87
41.71
29.01
20.11
0.00
Bn
N
OMe
O
3y
Me
f1 (ppm)

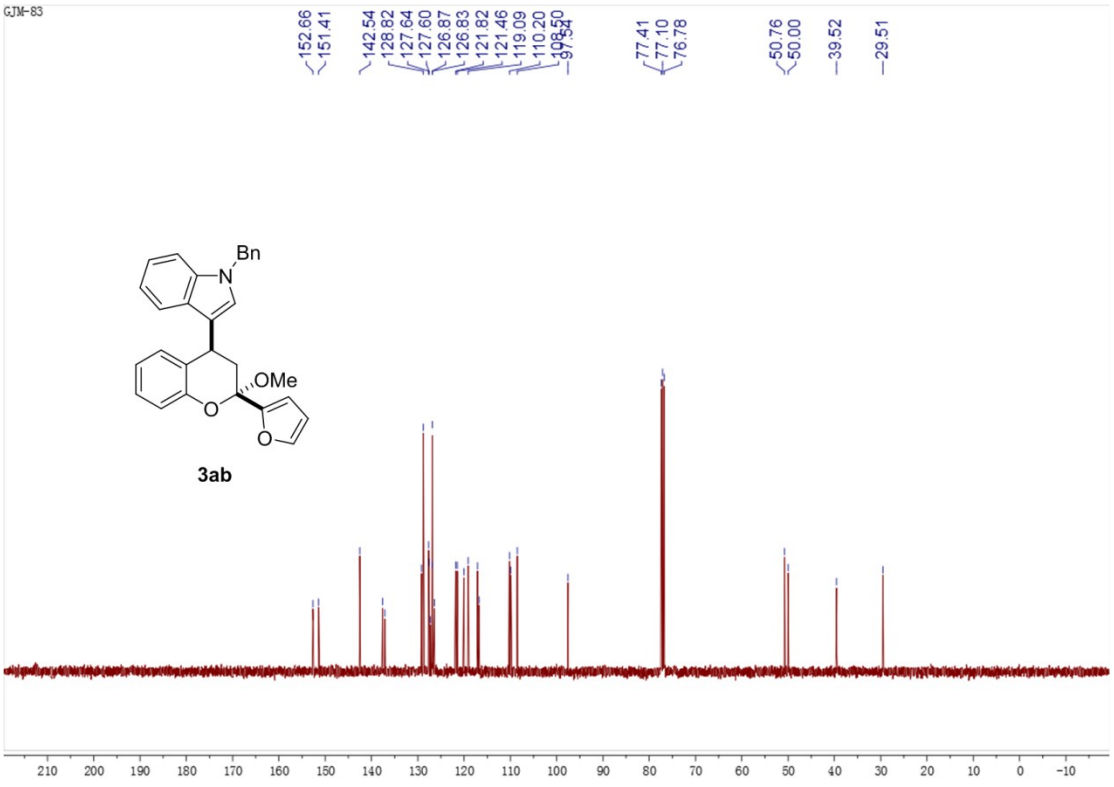

wwb-137
7.34
7.31
7.29
7.20
7.18
7.18
7.17
7.16
7.10
7.08
7.07
7.05
7.03
7.01
7.00
6.98
6.96
6.94
6.93
6.91
6.74
4.75
4.74
4.72
4.71
3.10
2.46
2.44
2.42
2.41
2.25
2.22
2.20
2.18
0.00
Bn
N
OMe
O
Me
Me
3z
1.05
2.03
4.53
9.41
1.06
2.23
1.05
3.00
1.05
0.34
3.30
3.29
0.65
f1 (ppm)

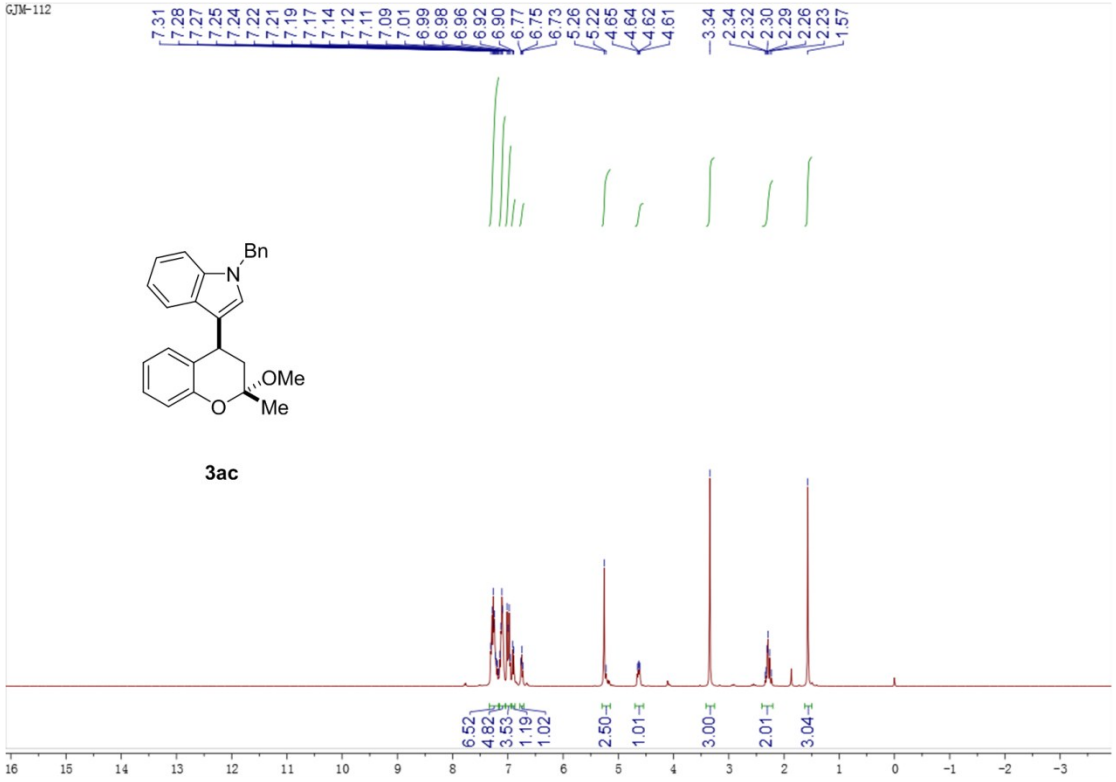

WWB-137
151.07
128.57
127.98
127.71
126.52
126.40
126.35
125.72
122.60
120.67
116.02
99.56
76.31
75.99
75.67
49.22
48.90
41.77
29.01
18.94
18.47
0.00
Bn
N
OMe
O
Me
Me
3z
f1 (ppm)

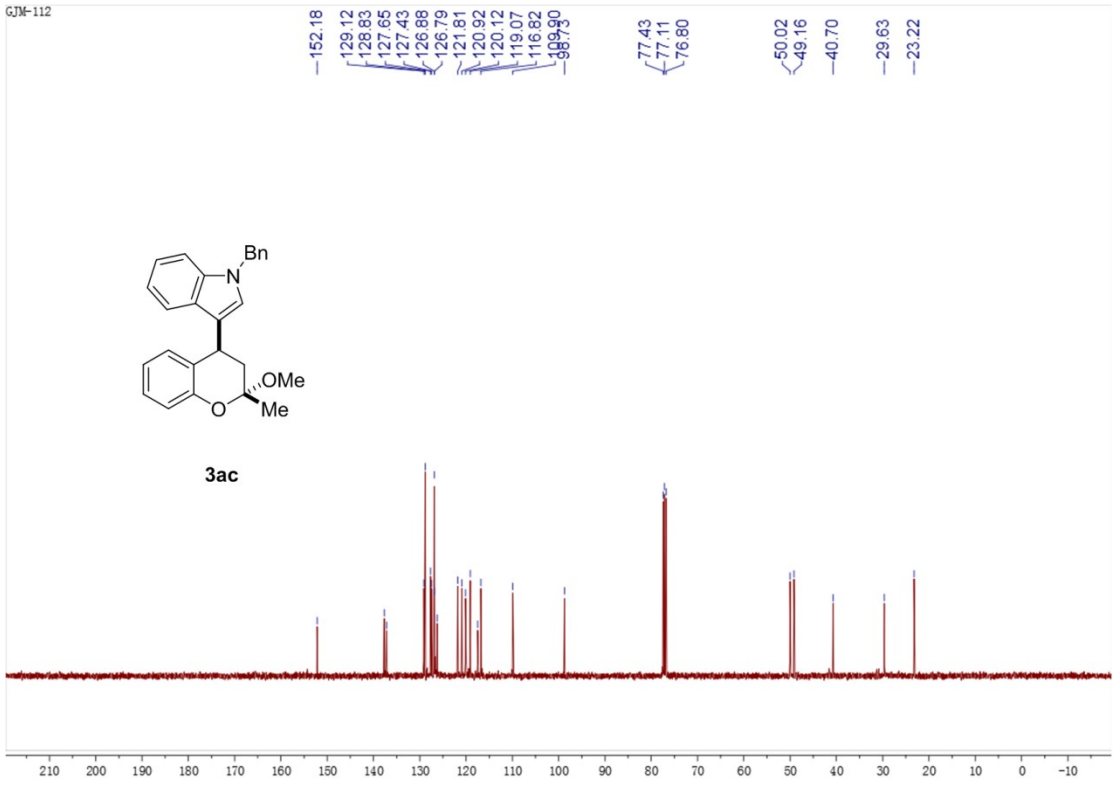

GJM-84
Bn
N
OMe
O
3aa

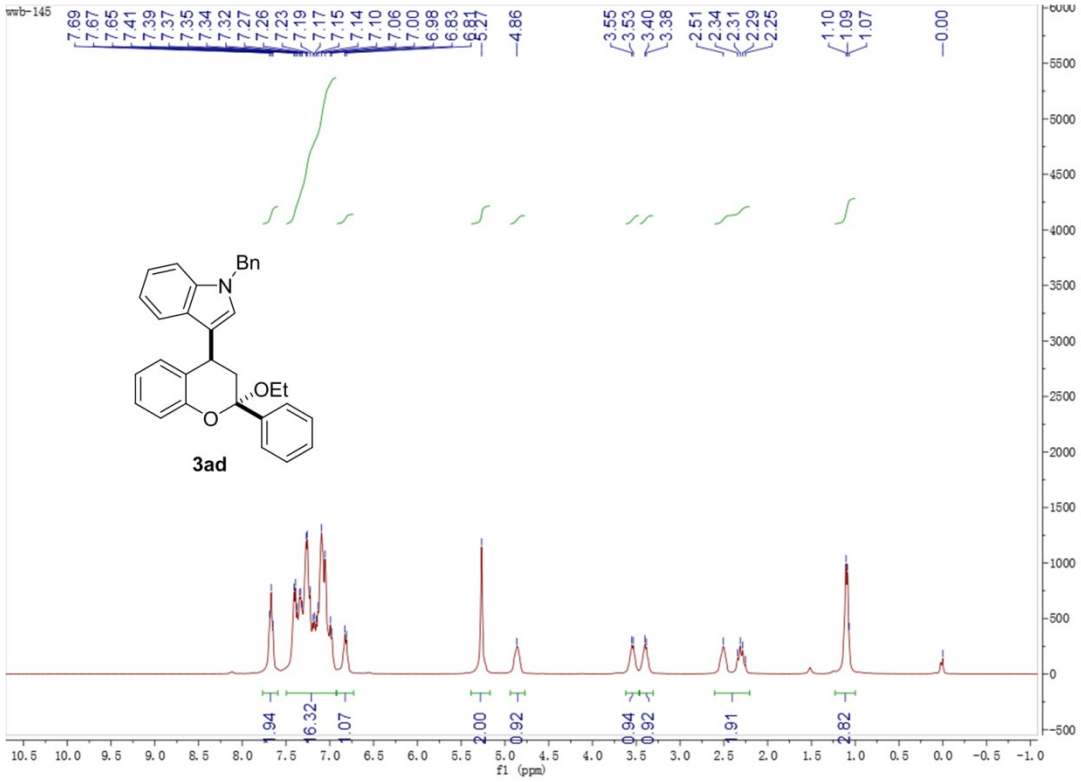

GJM-84
Bn
N
OMe
O
3aa

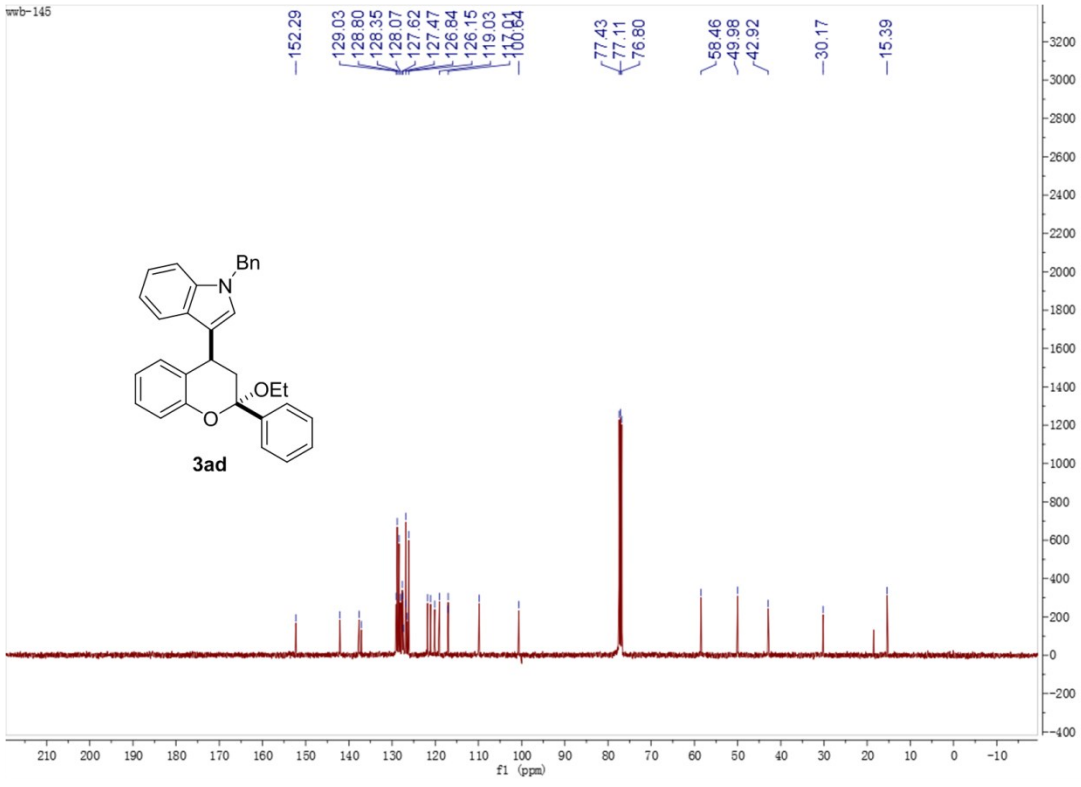

GJM-83
7.41
7.32
7.30
7.28
7.26
7.24
7.21
7.16
7.14
7.12
7.10
7.09
7.06
7.04
7.03
6.99
6.97
6.95
6.83
6.81
6.79
6.63
6.62
6.39
5.27
4.78
4.76
4.75
4.73
3.23
2.76
2.74
2.72
2.71
2.44
2.40
2.37
0.00
Bn
N
OMe
O
O
3ab
0.94
5.47
7.35
1.10
1.08
0.99
1.02
2.10
1.00
3.00
1.03
1.01

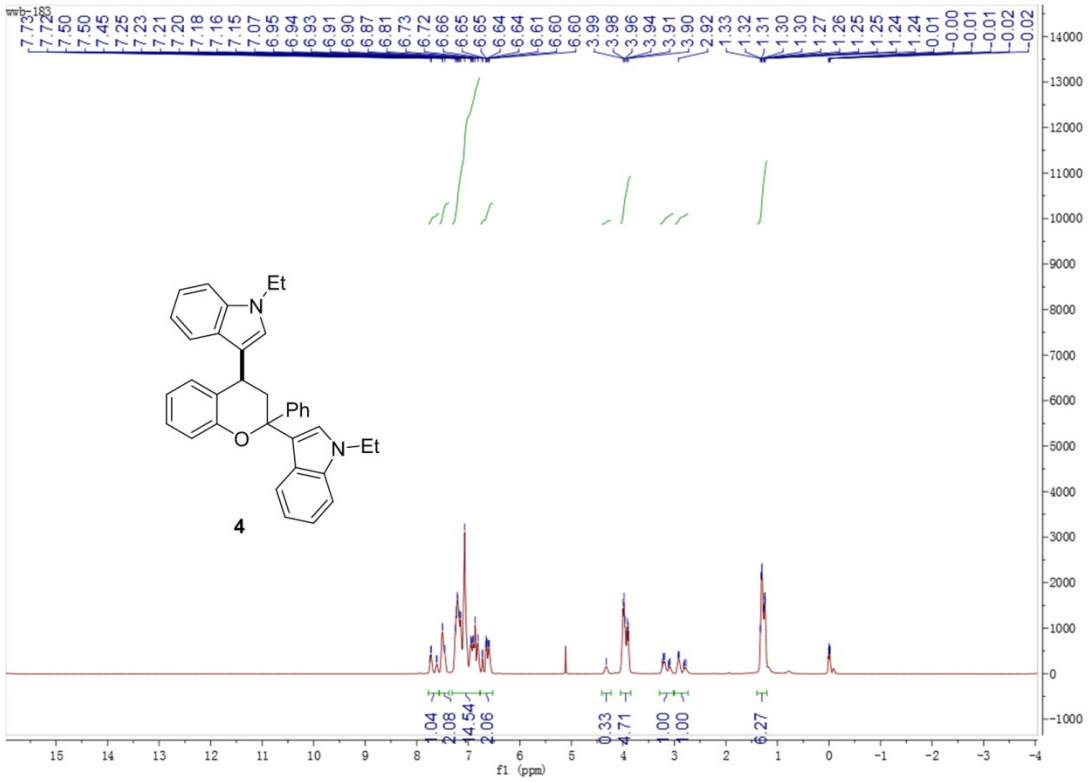

GJM-83
152.66
151.41
142.54
128.82
127.64
127.60
126.87
126.83
121.82
121.46
119.09
110.20
108.50
97.54
77.41
77.10
76.78
50.76
50.00
39.52
29.51
Bn
N
OMe
O
O
3ab

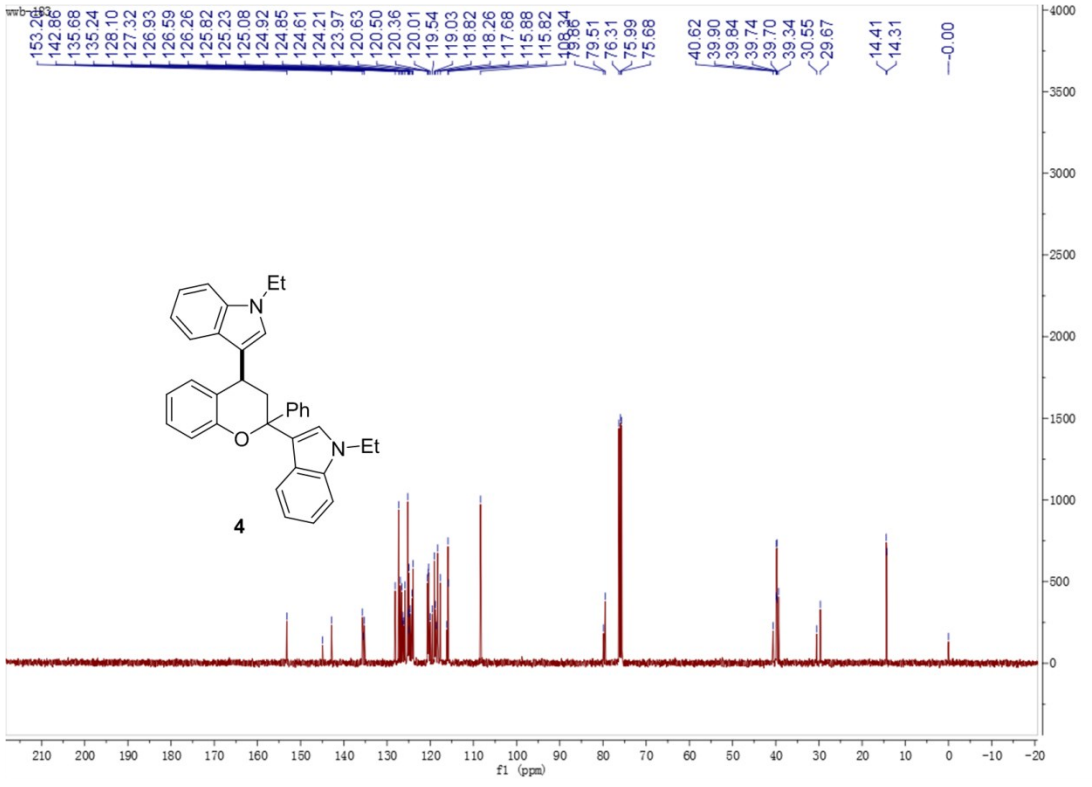

GJM-112
7.31
7.28
7.27
7.25
7.24
7.22
7.21
7.19
7.17
7.14
7.12
7.11
7.09
7.01
6.99
6.98
6.96
6.92
6.90
6.77
6.75
6.73
5.26
5.22
4.65
4.64
4.62
4.61
3.34
2.34
2.32
2.30
2.29
2.26
2.23
1.57
Bn
N
OMe
Me
O
3ac
6.52
4.82
3.53
1.19
1.02
2.50
1.01
3.00
2.01
3.04
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
−2
−3

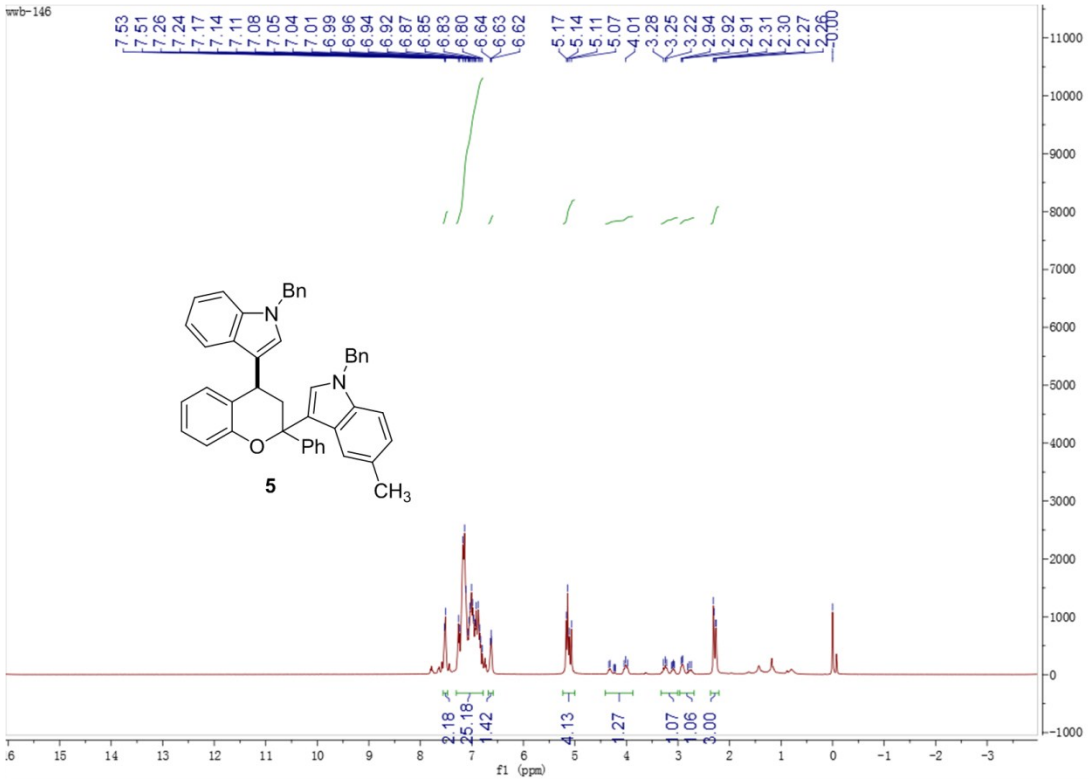

GJM-112
152.18
129.12
128.83
127.65
127.43
126.88
126.79
121.81
120.92
120.12
119.07
116.82
109.90
98.73
77.43
77.11
76.80
50.02
49.16
40.70
29.63
23.22
Bn
N
OMe
Me
O
3ac
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10

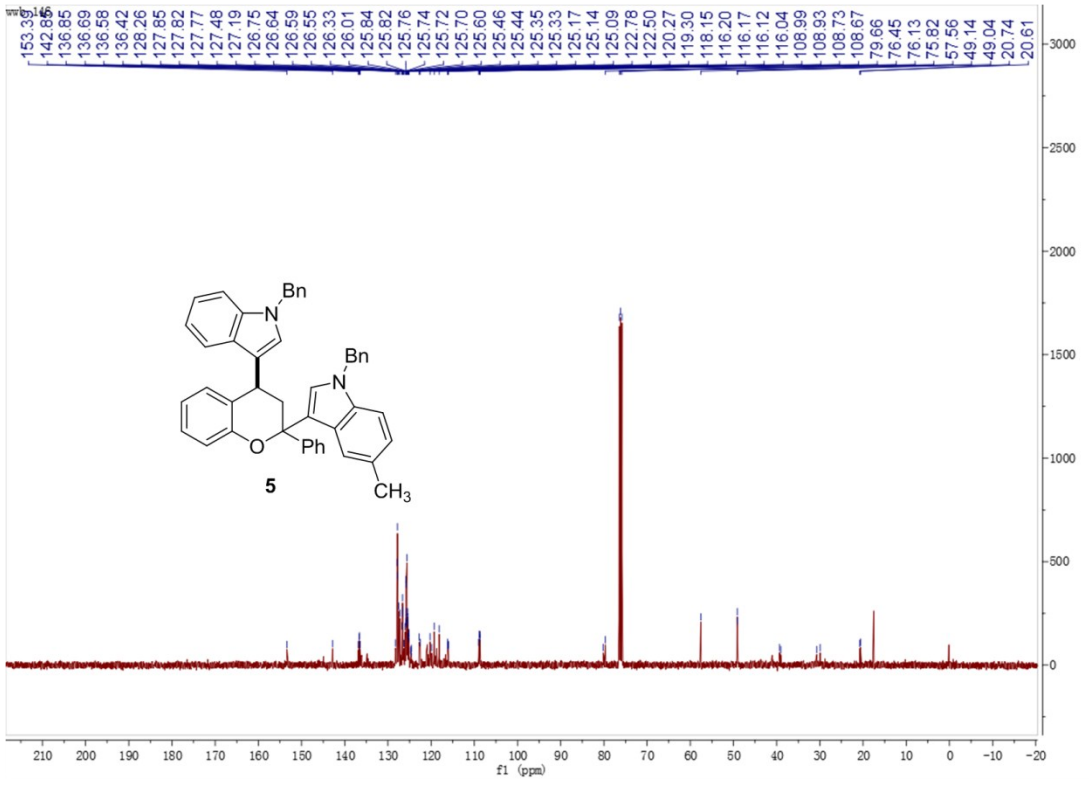

wwb-145
7.69
7.67
7.65
7.41
7.39
7.37
7.35
7.34
7.32
7.27
7.26
7.23
7.19
7.17
7.15
7.14
7.10
7.06
7.00
6.98
6.83
6.81
5.27
4.86
3.55
3.53
3.40
3.38
2.51
2.34
2.31
2.29
2.25
1.10
1.09
1.07
0.00
Bn
N
OEt
O
3ad
1.94
16.32
1.07
2.00
0.92
0.94
0.92
1.91
2.82
f1 (ppm)

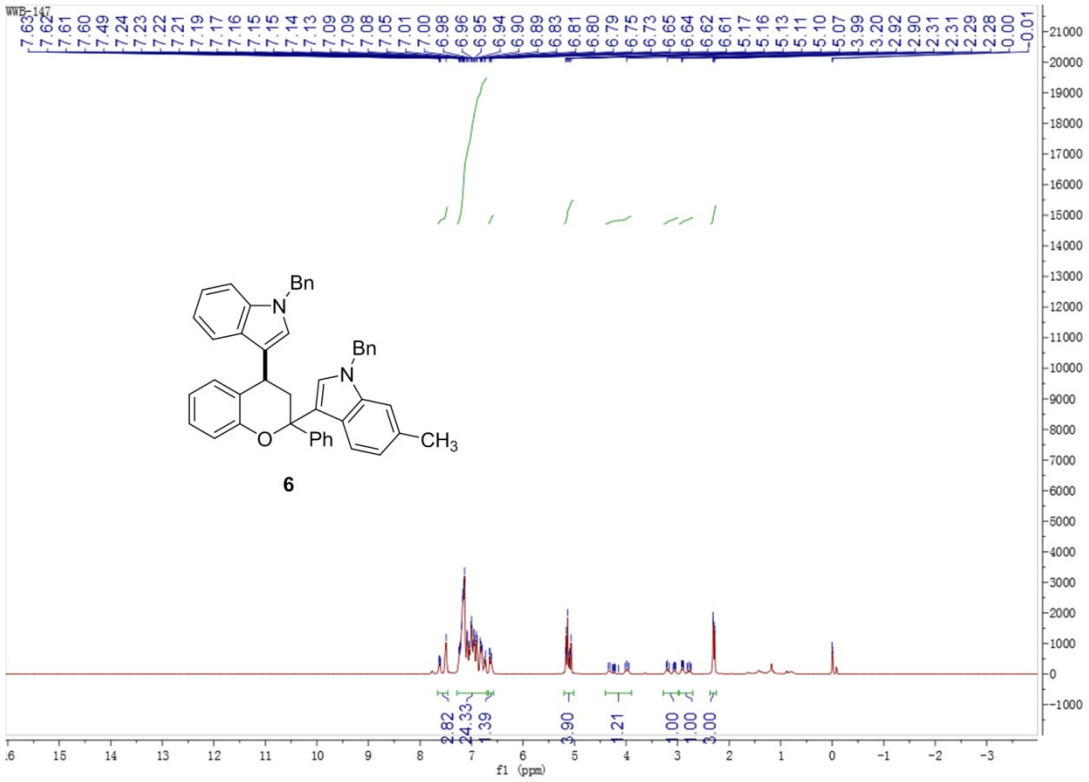

wwb-145
152.29
129.03
128.80
128.35
128.07
127.62
127.47
126.84
126.15
119.03
77.43
77.11
76.80
58.46
49.98
42.92
30.17
15.39
Bn
N
OEt
O
3ad
f1 (ppm)

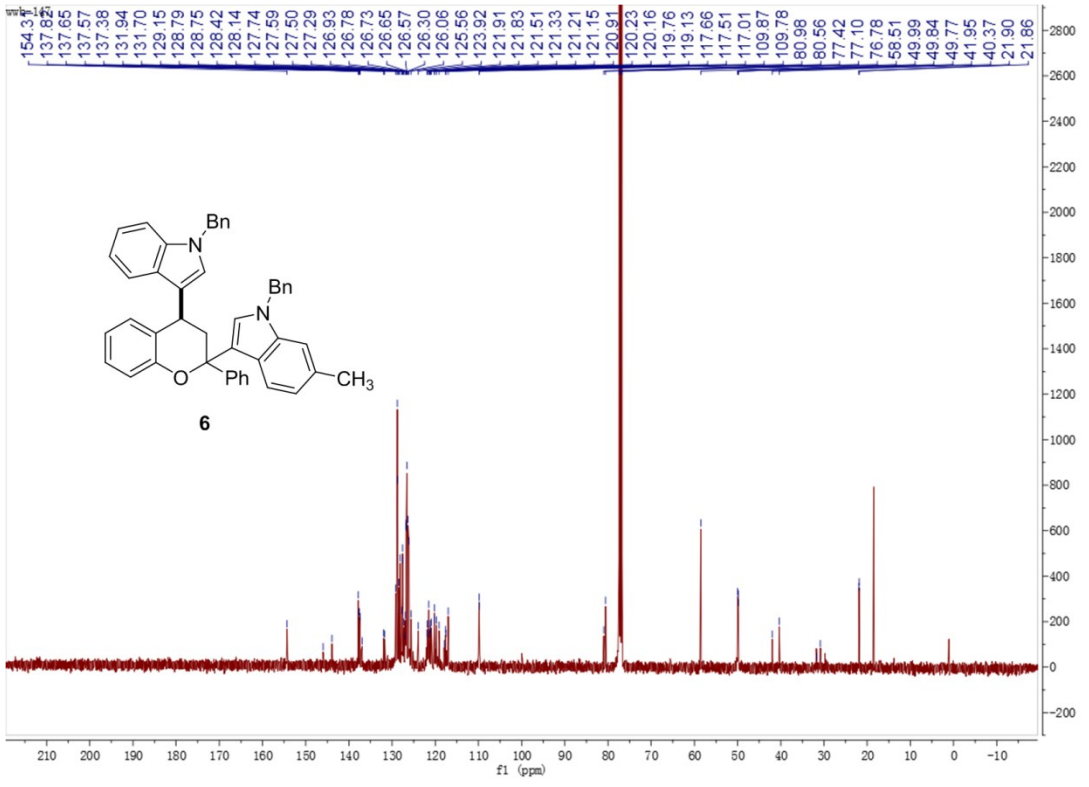

wrb-183
Et
N
Ph
O
N–Et
4
f1 (ppm)

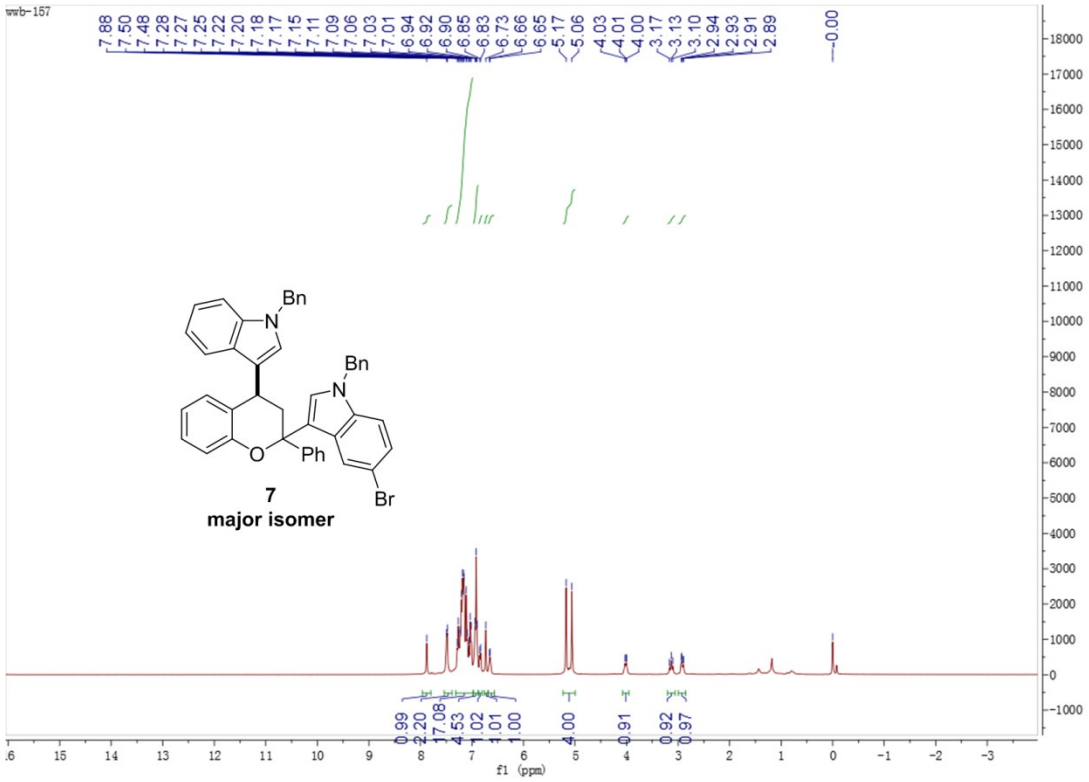

wrb-183
Et
N
Ph
O
N–Et
4
f1 (ppm)

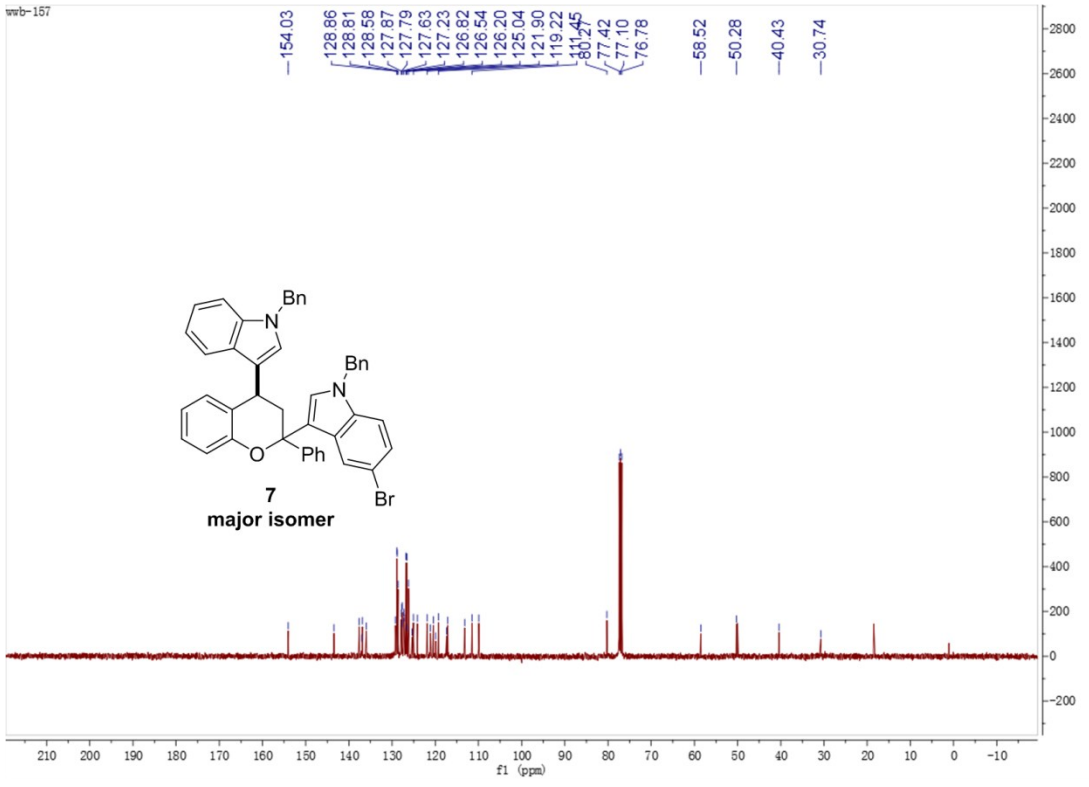

wwb-146
7.53
7.51
7.26
7.24
7.17
7.14
7.11
7.08
7.05
7.04
7.01
6.99
6.96
6.94
6.92
6.87
6.85
6.83
6.80
6.64
6.63
6.62
5.17
5.14
5.11
5.07
4.01
3.28
3.25
3.22
2.94
2.92
2.91
2.31
2.30
2.27
2.26
0.00
Bn
N
Bn
N
O
Ph
CH3
5
2.18
5.18
1.42
4.13
1.27
1.07
1.06
3.00
f1 (ppm)

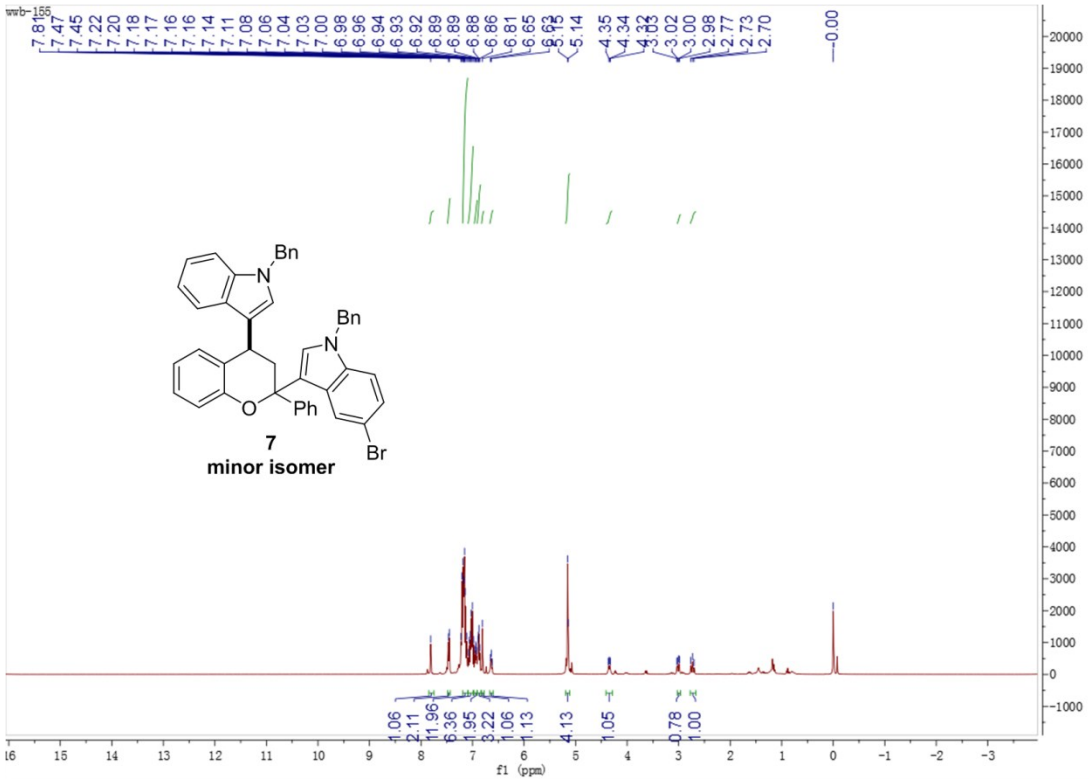

153.39
142.85
136.85
136.69
136.58
136.42
128.26
127.85
127.82
127.77
127.48
127.19
126.75
126.64
126.59
126.55
126.33
126.01
125.84
125.82
125.76
125.74
125.72
125.70
125.60
125.46
125.44
125.35
125.33
125.17
125.14
125.09
122.78
122.50
120.27
119.30
118.15
116.20
116.17
116.12
116.04
108.99
108.93
108.73
108.67
79.66
76.45
76.13
75.82
57.56
49.14
49.04
20.74
20.61
Bn
N
Bn
N
O
Ph
CH3
5
f1 (ppm)

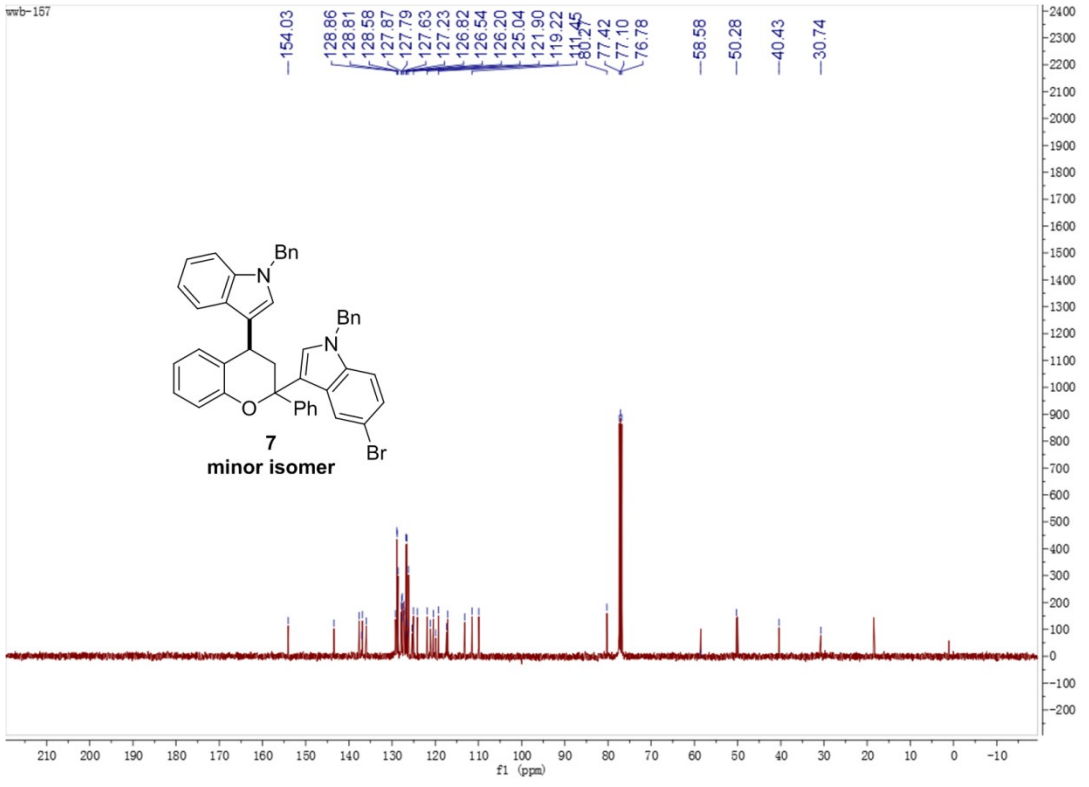

Bn
N
Bn
N
O
Ph
CH3
6
f1 (ppm)

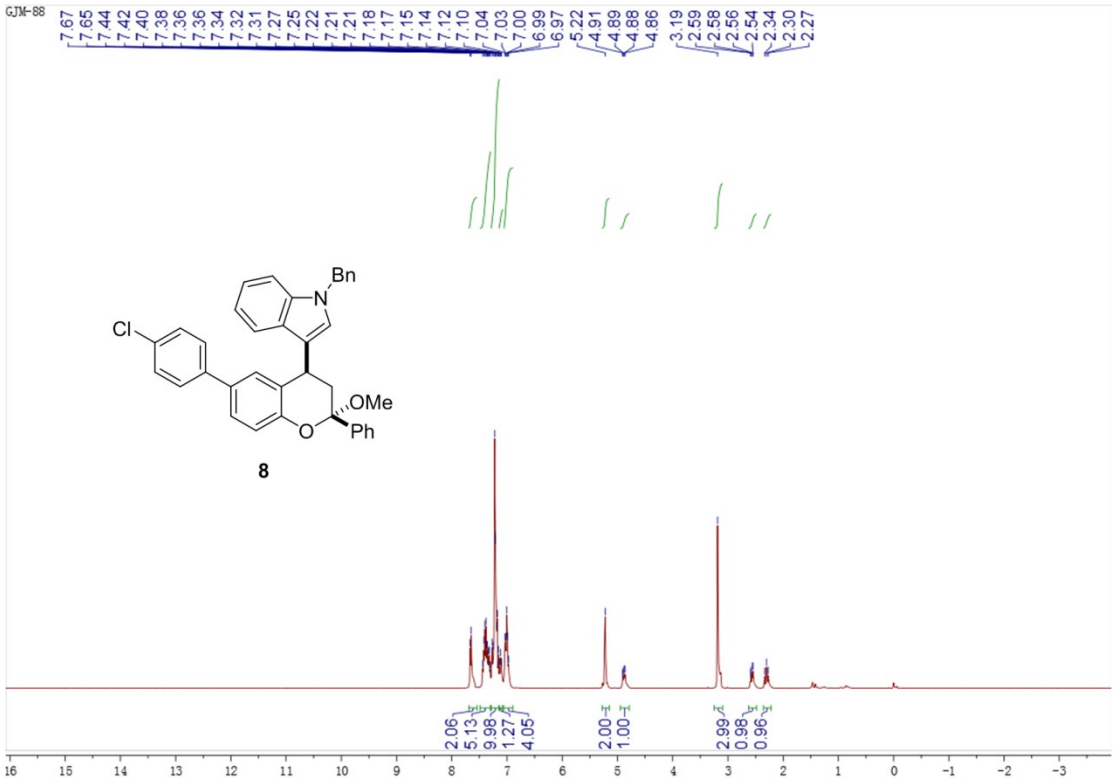

Bn
N
Bn
N
O
Ph
CH3
6
f1 (ppm)

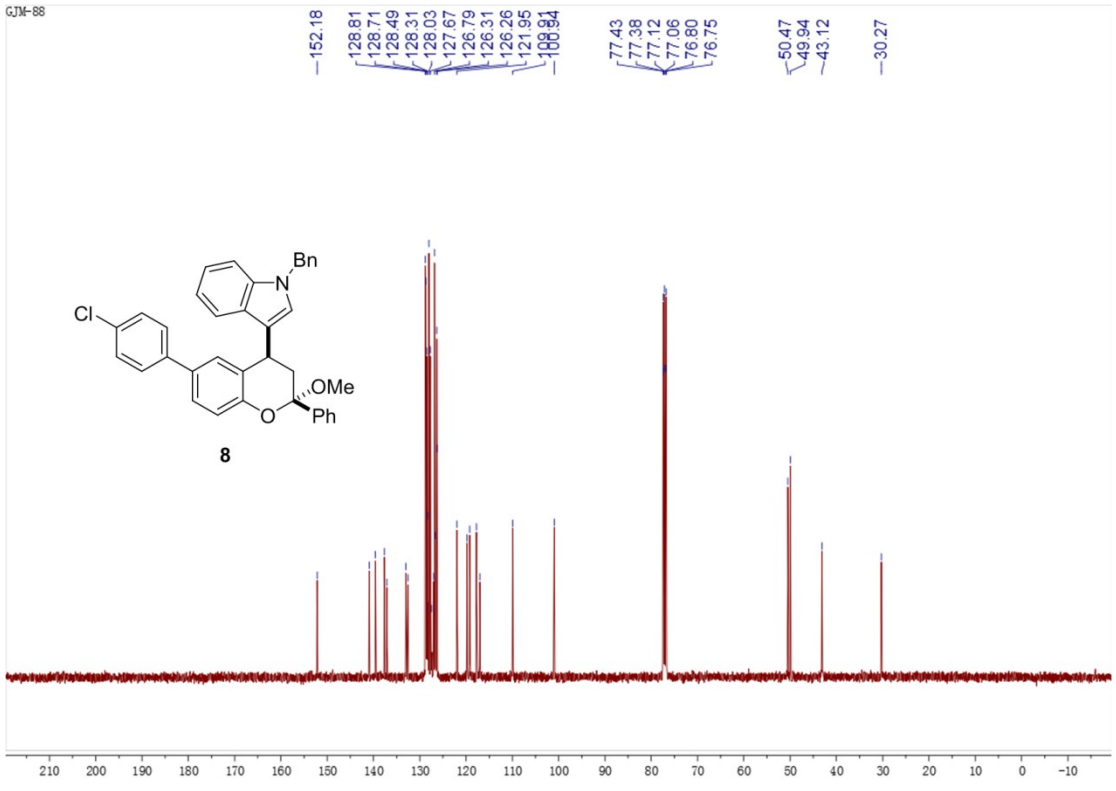

wwb-157
7.88
7.50
7.48
7.28
7.27
7.25
7.22
7.20
7.18
7.17
7.15
7.11
7.09
7.06
7.03
7.01
6.94
6.92
6.90
6.85
6.83
6.73
6.66
6.65
5.17
5.06
4.03
4.01
4.00
3.17
3.13
3.10
2.94
2.93
2.91
2.89
0.00
Bn
N
Bn
N
O
Ph
Br
7
major isomer
0.99
2.20
17.08
4.53
1.02
1.01
1.00
4.00
0.91
0.92
0.97
f1 (ppm)

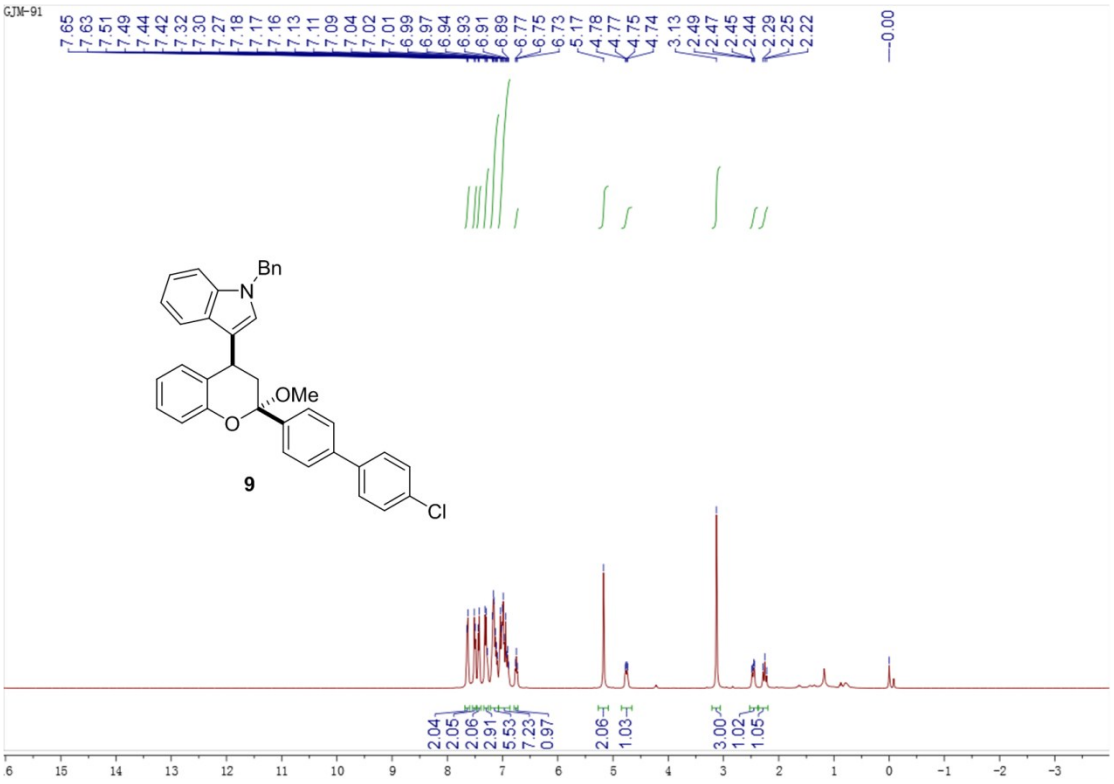

wwb-157
154.03
128.86
128.81
128.58
127.87
127.79
127.63
127.23
126.82
126.54
126.20
125.04
121.90
119.22
111.45
80.27
77.42
77.10
76.78
58.52
50.28
40.43
30.74
Bn
N
Bn
N
O
Ph
Br
7
major isomer
f1 (ppm)

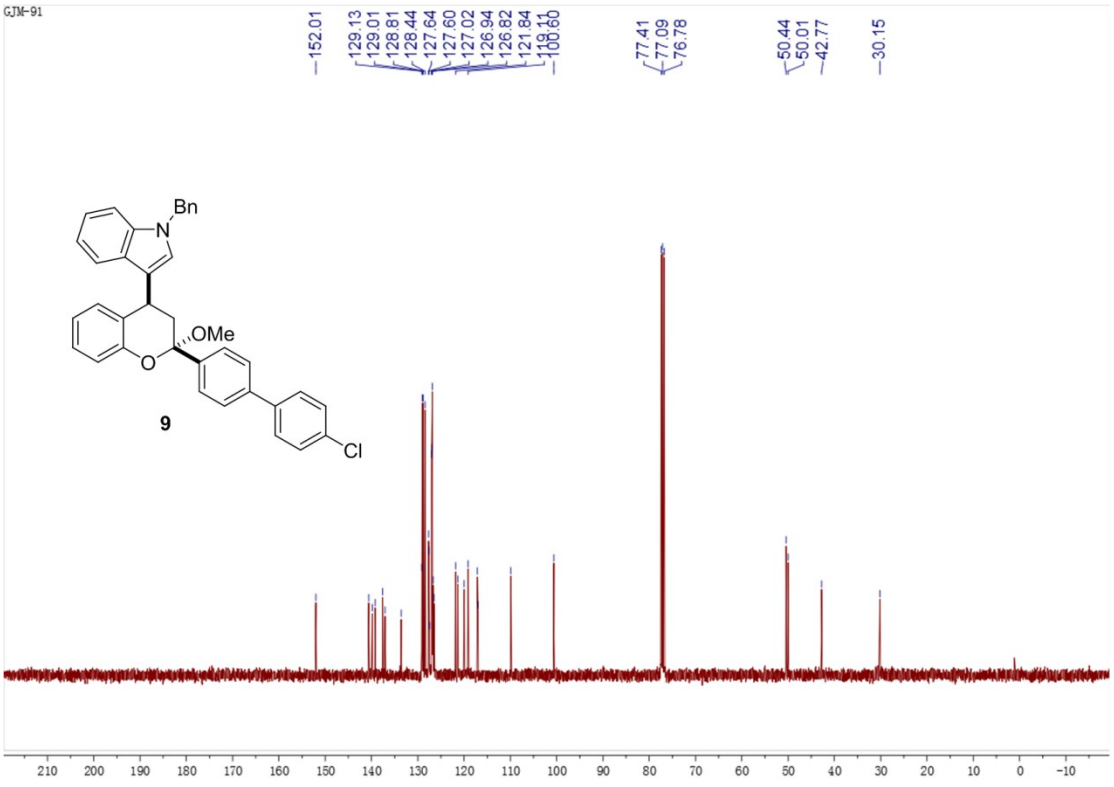

wwb-156
Bn
N
Bn
N
O
Ph
Br
7
minor isomer
f1 (ppm)

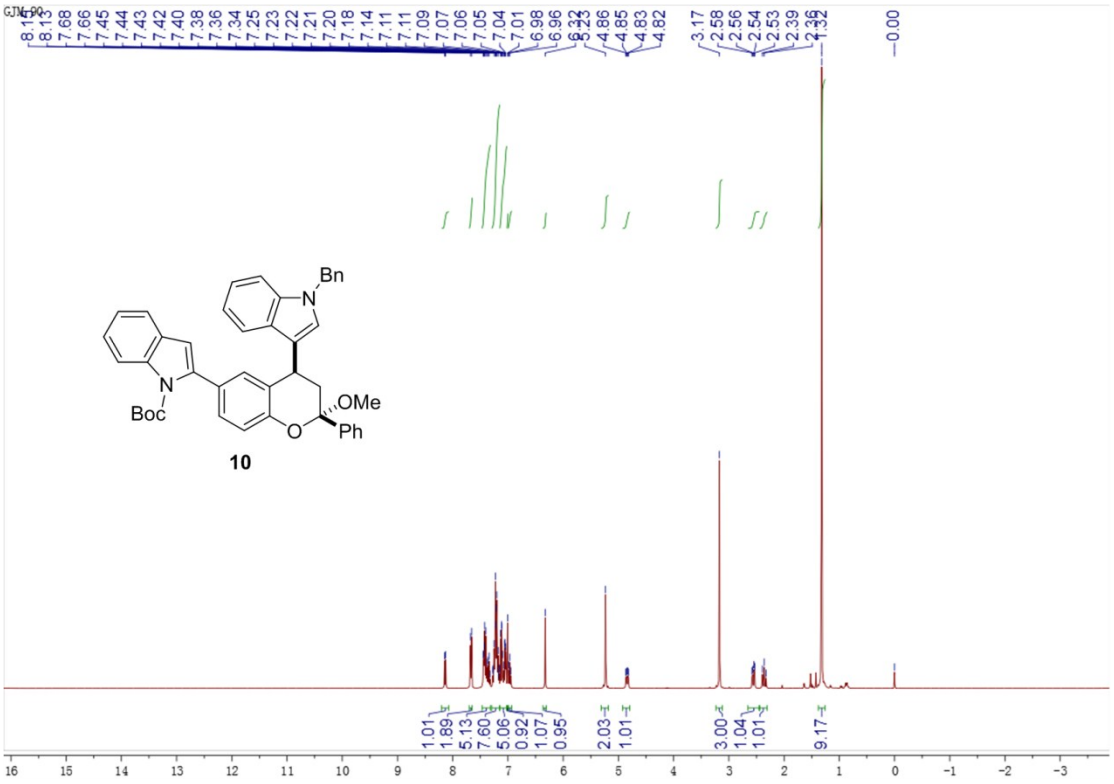

wwb-157
Bn
N
Bn
N
O
Ph
Br
7
minor isomer
f1 (ppm)

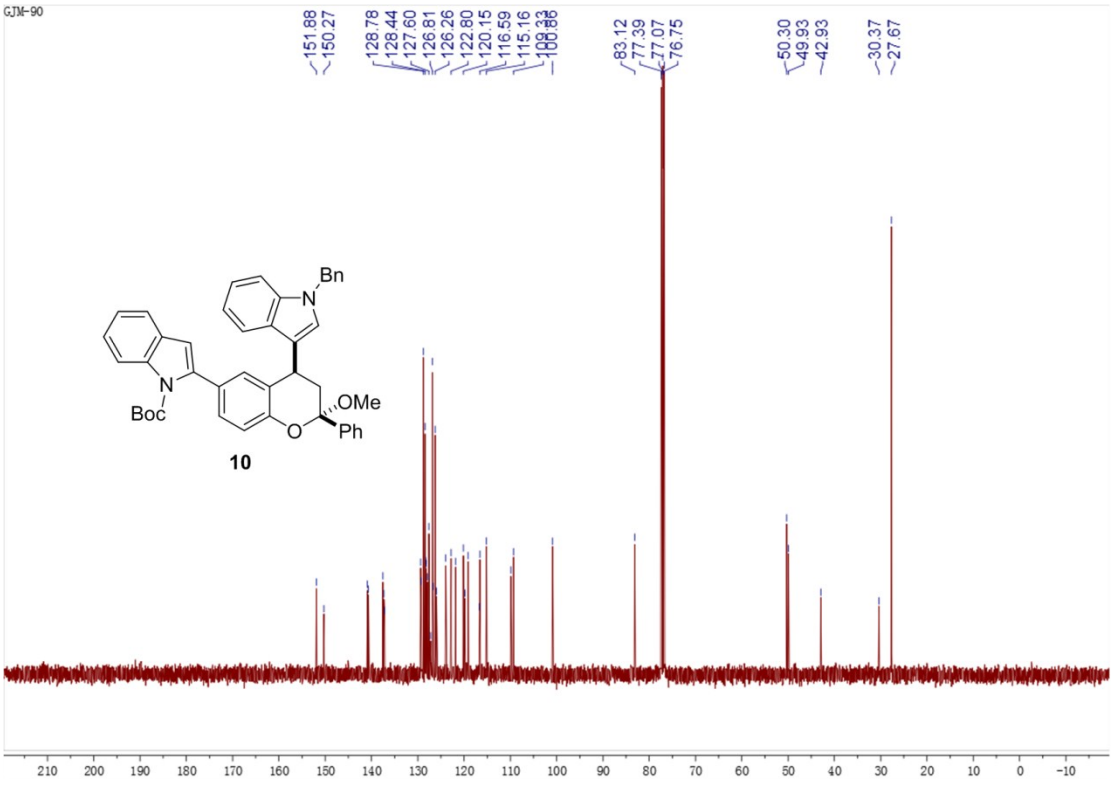

GJM-88
7.67
7.65
7.44
7.42
7.40
7.38
7.36
7.36
7.34
7.32
7.31
7.27
7.25
7.22
7.21
7.21
7.18
7.17
7.15
7.14
7.12
7.10
7.04
7.03
7.00
6.99
6.97
5.22
4.91
4.89
4.88
4.86
3.19
2.59
2.58
2.56
2.54
2.34
2.30
2.27
Bn
N
Cl
OMe
Ph
O
8
2.06
5.13
9.98
1.27
4.05
2.00
1.00
2.99
0.98
0.96

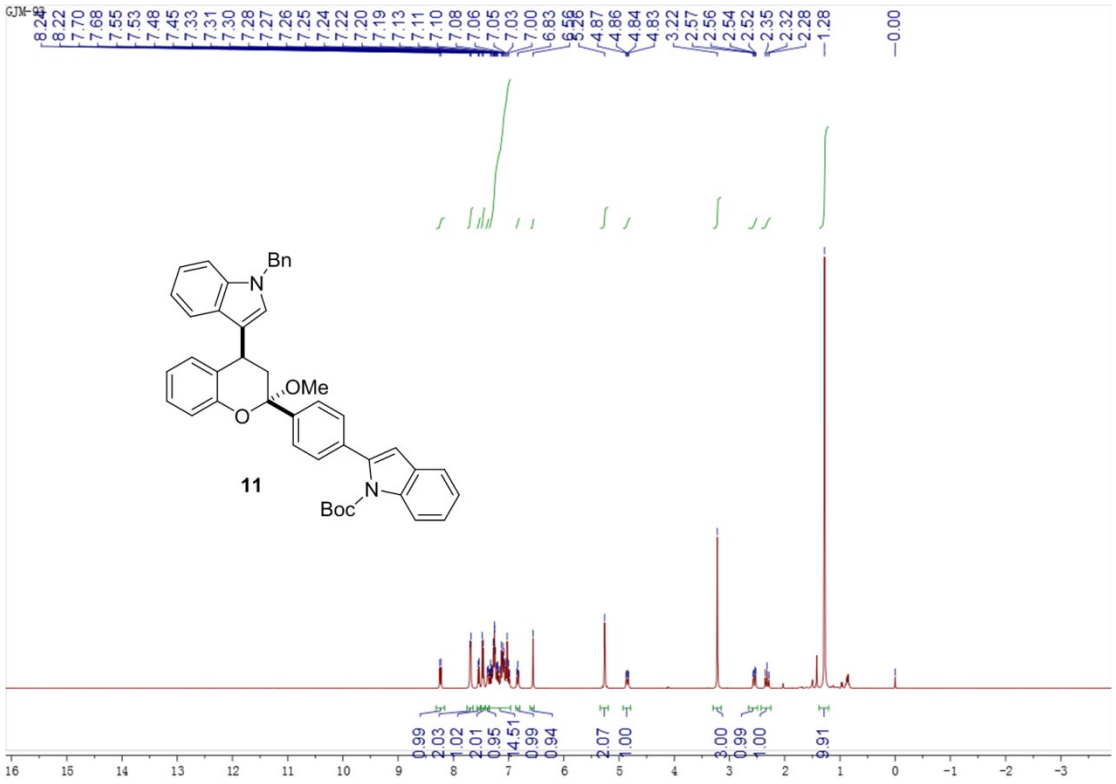

GJM-88
152.18
128.81
128.71
128.49
128.31
128.03
127.67
126.79
126.31
126.26
121.95
77.43
77.38
77.12
77.06
76.80
76.75
50.47
49.94
43.12
30.27
Bn
N
Cl
OMe
Ph
O
8

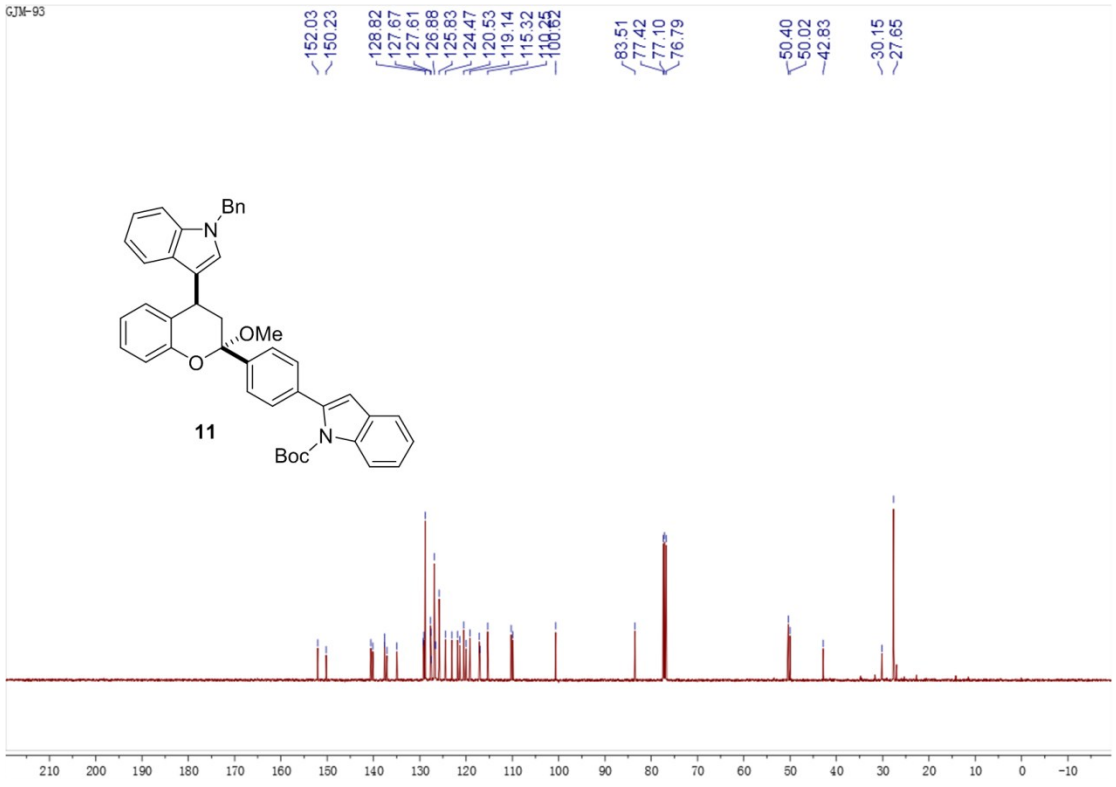

GJM-91
7.65
7.63
7.51
7.49
7.44
7.42
7.32
7.30
7.27
7.18
7.17
7.16
7.13
7.11
7.09
7.04
7.02
7.01
6.99
6.97
6.94
6.93
6.91
6.89
6.77
6.75
6.73
5.17
4.78
4.77
4.75
4.74
3.13
2.49
2.47
2.45
2.44
2.29
2.25
2.22
0.00
Bn
N
OMe
O
Cl
9
2.04
2.05
2.06
2.91
5.53
7.23
0.97
2.06
1.03
3.00
1.02
1.05


GJM-91
152.01
129.13
129.01
128.81
128.44
127.64
127.60
127.02
126.94
126.82
121.84
119.11
100.60
77.41
77.09
76.78
50.44
50.01
42.77
30.15
Bn
N
OMe
O
Cl
9


GJM-90
Bn
N
N
Boc
OMe
O
Ph
10


GJM-90
Bn
N
N
Boc
OMe
O
Ph
10


GJM-93
Bn
OMe
O
N
Boc
11


GJM-93
Bn
OMe
O
N
Boc
11