Supporting Information for

A $FeCl_3$-catalyzed Highly Regioselective 1,2-Addition/Substitution Sequence for the Construction of Coumarin-substituted Bis(indolyl)methanes

Wen-Bo Wang, Yan-Shuo Zhu, Sheng-Qiang Guo, Qi-Lin Wang *, Zhan-Wei Bu *

Institute of Environmental and Analytical Sciences, College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475004, China

E-mail: wangqilin@henu.edu.cn ; buzhanwei@henu.edu.cn.

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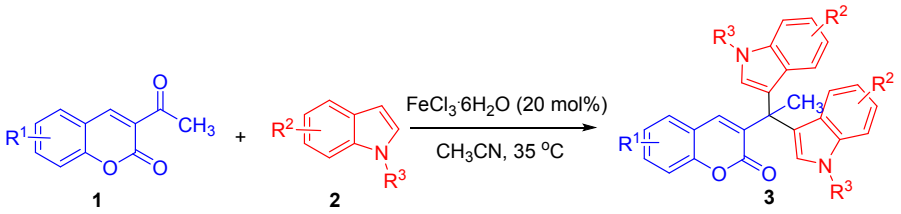
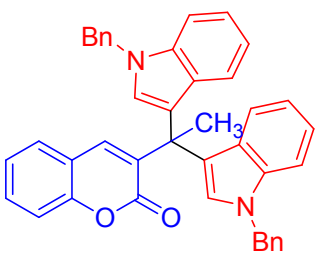
1. General methods

NMR spectra were recorded with tetramethylsilane as the internal standard. ^{1}H NMR spectra were recorded at 300 MHz, and ^{13}C NMR spectra were recorded at 75 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 ThermoFisherNicolet Avatar 360 FTIR spectrometer on a KBr beamsplitter.

2. Experimental data for bis(indolyl)methanes 3

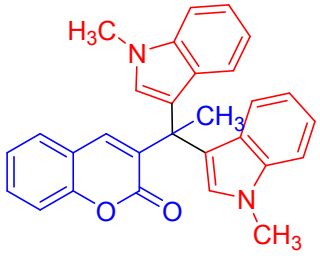


General procedure: To a 5.0 mL vial were successively added 3-acylcoumarin **1** (0.12 mmol), indole **2** (0.30 mmol), $FeCl_3{\cdot}6H_2O$ (6.5 mg, 0.024 mmol) and 1.0 mL CH_3CN. The resulting mixture was stirred for 10-72 h at 35 °C till almost full consumption of **1** by TLC analysis, and then the reaction mixture was directly subjected to flash column chromatography on silica gel (petroleum ether/ ethyl acetate) to afford the corresponding products **3**.



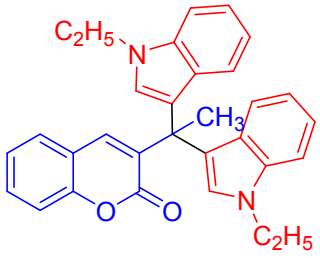
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3a)

Product **3a** was obtained in 98% yield as a white solid. Reaction time = 12 h; m. p. 234.1-235.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.64 (s, 1H), 7.31 (d, *J* = 8.0 Hz, 3H), 7.19-7.13 (m, 11H), 7.02-6.97 (m, 6H), 6.88 (s, 2H), 6.84 (t, *J* = 4.0 Hz, 2H), 5.18 (s, 4H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 152.6, 152.5, 139.5, 136.6, 136.3, 127.7, 127.2, 127.1, 126.4, 125.7, 125.4, 122.8, 120.7, 120.2, 118.9, 117.9, 114.9, 109.1, 48.9, 42.4, 24.9. IR (KBr) *v* 3437, 3121, 3054, 2916, 1727, 1610, 1457, 1178, 1094, 740, 705 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{32}N_2NaO_2$ $[M+Na]^+$: 607.2356, Found: 607.2338.



3-(1,1-bis(1-methyl-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3b)

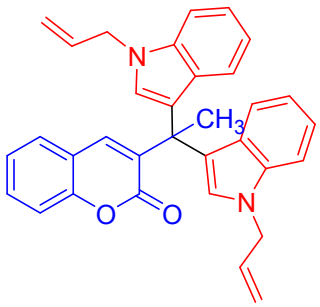
Product **3b** was obtained in 98% yield as a yellow solid. Reaction time = 10 h; m. p. 230.2-231.5 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.31 (t, *J* = 8.0 Hz, 3H), 7.24 (d, *J* = 8.0 Hz, 2H),7.17 (d, *J* = 8.0 Hz, 2H), 7.12-7.04 (m, 3H), 6.87 (t, *J* = 8.0 Hz, 2H), 6.70 (s, 2H), 3.64 (s, 6H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 152.7, 139.6, 136.8, 132.0, 129.7, 127.7, 127.1, 125.5, 122.9, 120.7, 120.1, 118.5, 118.3, 117.8, 115.0, 108.6, 42.5, 31.9, 25.1. IR (KBr) *v* 3428, 3116, 3053, 2926, 1728, 1609, 1460, 1170, 1097, 737 cm^{-1}. HRMS (ESI) Calcd. for $C_{29}H_{24}N_2NaO_2$ $[M+Na]^+$: 455.1730, Found: 455.1728



3-(1,1-bis(1-ethyl-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3c)

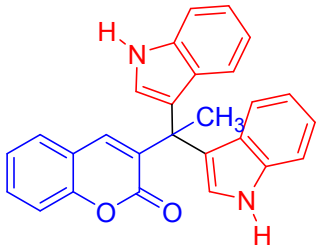
Product **3c** was obtained in 98% yield as a yellow solid. Reaction time = 10 h; m. p. 243.8-244.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.31-7.26 (m, 5H), 7.17-7.14 (m, 2H), 7.09-7.04

(m, 3H), 6.86-6.82 (m, 2H), 6.78 (s, 2H), 4.02 (q, J = 8.0 Hz, 4H), 2.35 (s, 3H), 1.32 (t, J = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 152.5, 139.4, 135.7, 131.8, 129.5, 127.0, 126.1, 125.6, 122.7, 120.7, 119.8, 118.3, 117.5, 114.9, 108.5, 108.4, 42.4, 39.9, 25.0, 14.5. IR (KBr) v 3435, 3052, 2979, 2937, 1730, 1612, 1459, 1202, 978, 746 cm^{-1}. HRMS (ESI) Calcd. for $C_{31}H_{28}N_2NaO_2$ $[M+Na]^+$: 483.2043, Found: 483.2050.



3-(1,1-bis(1-allyl-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3d)

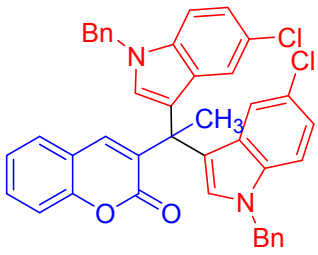
Product **3d** was obtained in 61% yield as a white solid. Reaction time = 31 h; m. p. 176.3-178.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.35-7.29 (m, 3H), 7.24 (d, J = 8.0 Hz, 2H), 7.19-7.17 (m, 2H), 7.09-7.04 (m, 3H), 6.87-6.84 (m, 2H), 6.77 (s, 2H), 5.93-5.83 (m, 2H), 5.07 (d, J = 12.0 Hz, 2H), 4.95 (d, J = 16.0 Hz, 2H), 4.60-4.59 (m, 4H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 152.6, 139.5, 136.1, 132.5, 131.8, 129.6, 127.0, 126.8, 125.6, 122.7, 120.7, 120.0, 118.6, 118.2, 117.8, 115.9, 114.9, 108.9, 47.7, 42.4, 24.9. IR (KBr) v 34336, 3049, 2982, 1732, 1610, 1463, 1188, 984, 742 cm^{-1}. HRMS (ESI) Calcd. for $C_{33}H_{28}N_2NaO_2$ $[M+Na]^+$: 507.2043, Found: 507.2020.



3-(1,1-di(1H-indol-3-yl)ethyl)-2H-chromen-2-one (3e)

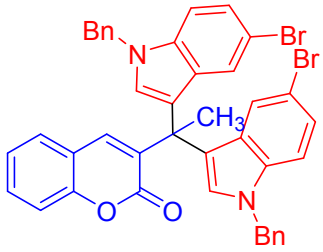
Product **3e** was obtained in 94% yield as a white solid. Reaction time = 72 h; m. p. 277.3-278.1 °C; ^{1}H NMR (400 MHz, DMSO-d_6), δ 10.91 (s, 2H), 7.63 (s, 1H), 7.53-7.49 (s, 1H), 7.38 (t, J = 4 Hz, 3H), 7.34 (d, J = 8 Hz, 1H), 7.28 (d, J = 8 Hz, 2H), 7.20 (t, J = 8 Hz, 1H), 7.02 (t, J = 8 Hz, 2H), 6.88 (d, J = 1 Hz, 2H), 6.81 (t, J = 8 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) 159.3, 153.5, 140.6, 137.5, 133.4, 131.5, 128.9, 126.1, 124.7, 124.6, 121.1, 121.0, 120.1, 119.2, 118.8,

115.9, 112.3, 43.4, 26.2. IR (KBr) *v* 3408, 2923, 1709, 1611, 1455, 1421, 1110, 986, 742 cm^{-1}. HRMS (ESI) Calcd. for $C_{27}H_{20}N_2NaO_2$ $[M+Na]^+$: 427.1417, Found: 427.1419.



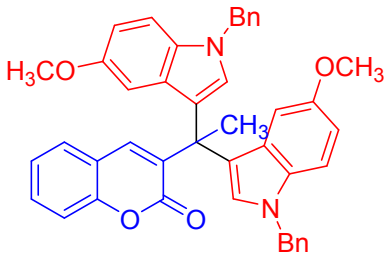
3-(1,1-bis(1-benzyl-5-chloro-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3f)

Product **3f** was obtained in 99% yield as a white solid. Reaction time = 67 h; m.p. 146.6-148.6 °C; ^1H NMR (400 MHz, $CDCl_3$), δ 7.57 (s, 1H), 7.28 (t, *J* = 8 Hz, 1H), 7.30-7.23 (m, 10H), 7.16-7.12 (m, 3H), 7.07-7.00 (m, 8H), 5.26 (s, 4H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 153.6, 140.7, 137.1, 135.7, 132.6, 131.1, 129.3, 129.0, 128.3, 127.7, 126.4, 124.9, 124.1, 121.9, 120.7, 119.2, 119.1, 116.1, 111.3, 50.4, 43.3, 26.0 (one carbon missing). IR (KBr) ν 3431, 3030, 2926, 1727, 1610, 1470, 1178, 980, 793, 755 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{30}Cl_2N_2NaO_2$ $[M+Na]^+$: 675.2140, Found: 675.2136.



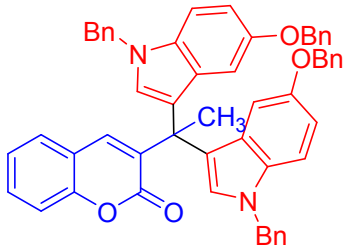
3-(1,1-bis(1-benzyl-5-bromo-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3g)

Product **3g** was obtained in 99% yield as a yellow solid. Reaction time = 72 h; m. p. 152.2-153.9 °C; ^1H NMR (400 MHz, $CDCl_3$), δ 7.49 (s, 1H), 7.39-7.33 (m, 3H), 7.24-7.13 (m, 8H), 7.09-7.06 (m, 3H), 7.02-6.96 (m, 6H), 6.89 (s, 2H), 5.16 (s, 4H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 152.5, 139.6, 135.9, 134.8, 131.4, 130.0, 128.1, 127.9, 127.3, 127.2, 126.6, 125.4, 123.3, 123.1, 122.7, 118.0, 117.9, 115.0, 111.5, 110.7, 49.3, 42.1, 24.9. IR (KBr) *v* 3432, 3029, 2928, 1725, 1610, 1461, 1358, 1179, 982, 795, 729 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{30}Br_2N_2NaO_2$ $[M+Na]^+$: 763.0566, Found: 763.0574.



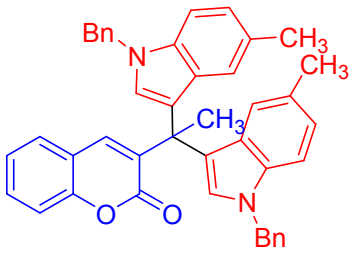
3-(1,1-bis(1-benzyl-5-methoxy-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3h)

Product **3h** was obtained in 56% yield as a white solid. Reaction time = 50 h; m. p. 89.2-91.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.36-7.31 (m, 1H), 7.21-7.13 (m, 8H), 7.08-7.03 (m, 3H), 6.98 (d, J = 8 Hz, 4H), 6.88 (s, 2H), 6.74 (d, J = 4 Hz, 2H), 6.67 (dd, $J_1 = J_2$= 4 Hz, 2H), 5.15 (s, 4H), 3.46 (s, 6H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 152.6, 152.3, 139.4, 136.7, 131.6, 131.5, 129.7, 127.9, 127.7, 126.8, 126.4, 126.1, 125.4, 122.9, 118.2, 118.1, 114.9, 110.1, 109.8, 102.8, 54.6, 49.2, 42.3, 24.6. IR (KBr) ν 3441, 2937, 2832, 1727, 1613, 1486, 1447, 1222, 1176, 1110, 1032, 797, 733 cm^{-1}. HRMS (ESI) Calcd. for $C_{43}H_{36}N_2NaO_4$ $[M+Na]^+$: 667.2567, Found: 667.2546.



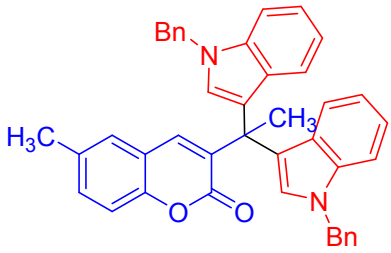
3-(1,1-bis(1-benzyl-5-(benzyloxy)-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3i)

Product **3i** was obtained in 77% yield as a white solid. Reaction time = 10 h; m.p. 88.2-90.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.64 (s, 1H), 7.43 (t, J = 8 Hz, 1H), 7.22 (t, J = 8 Hz, 14H), 7.17 (t, J = 8 Hz, 5H), 7.12 (d, J = 8 Hz, 2H), 7.05 (d, J = 8 Hz, 4H), 6.93 (s, 2H), 6.90 (d, J = 4 Hz, 2H), 6.83 (dd, $J_1 = J_2$ = 4 Hz, 2H), 5.21 (s, 4H), 4.75 (s, 4H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 153.7, 152.6, 140.5, 137.8, 137.5, 132.8, 132.6, 130.8, 129.0, 128.8, 128.4, 128.1, 127.1, 127.5, 127.4, 127.1, 126.5, 124.0, 119.3, 119.2, 116.0, 112.0, 110.9, 105.5, 70.1, 50.3, 43.4, 25.7. IR (KBr) ν 3433, 3031, 2922, 1728, 1613, 1484, 1451, 1206, 1116, 1024, 734, 701 cm^{-1}. HRMS (ESI) Calcd. for $C_{55}H_{44}N_2NaO_4$ $[M+Na]^+$: 819.3880, Found: 819.3871.



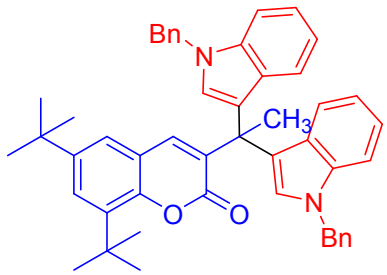
3-(1,1-bis(1-benzyl-5-methyl-1H-indol-3-yl)ethyl)-2H-chromen-2-one (3j)

Product **3j** was obtained in 89% yield as a white solid. Reaction time = 4 h; m.p. 126.8-128.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.62 (d, J = 4 Hz, 1H), 7.33 (t, J = 8 Hz, 1H), 7.20-7.12 (m, 10H), 7.08-7.03 (m, 3H), 6.98 (d, J = 8 Hz, 4H), 6.83 (d, J = 8 Hz, 4H), 5.15 (s, 4H), 2.39 (s, 3H), 2.19 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 152.6, 139.5, 136.8, 134.7, 132.0, 129.5, 127.7, 127.4, 127.0, 126.9, 126.3, 126.0, 125.4, 122.7, 121.8, 120.5, 118.3, 118.2, 114.9, 108.7, 49.0, 42.5, 25.0, 20.6. IR (KBr) ν 3432, 3029, 2919, 1728, 1610, 1487, 1450, 1260, 1097, 1026, 798, 702 cm^{-1}. HRMS (ESI) Calcd. for $C_{43}H_{36}N_2NaO_2$ $[M+Na]^+$: 635.3194, Found: 635.3188.



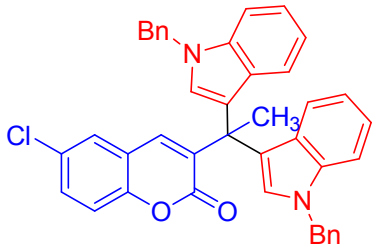
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6-methyl-2H-chromen-2-one (3k)

Product **3k** was obtained in 93% yield as a white solid. Reaction time = 72 h; m. p. 234.2-234.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.60 (s, 1H), 7.31 (d, J = 8 Hz, 2H), 7.20-7.13 (m, 9H), 7.08 (d, J = 8 Hz, 1H), 7.00 (dd, $J_1 = J_2$ = 8 Hz, 7H), 6.86 (dd, $J_1 = J_2$ = 8 Hz, 4H), 5.20 (q, J = 12 Hz, 4H), 2.39 (s, 3H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 150.7, 139.6, 136.7, 136.3, 132.4, 131.7, 130.6, 127.7, 127.2, 126.9, 126.4, 125.8, 125.5, 120.7, 120.2, 119.0, 117.9, 117.8, 114.6, 109.1, 49.0, 42.4, 24.9, 19.6. IR (KBr) ν 3433, 2964, 1727, 1261, 1096, 1023, 803, 739 cm^{-1}. HRMS (ESI) Calcd. for $C_{42}H_{34}N_2NaO_2$ $[M+Na]^+$: 621.2512, Found: 621.2494.



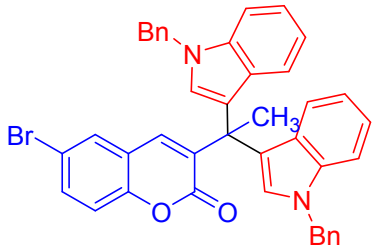
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6,8-di-tert-butyl-2H-chromen-2-one (3l)

Product **3l** was obtained in 90% yield as a white solid. Reaction time = 30 h; m. p. 145.7-147.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.60 (s, 1H), 7.40 (d, J = 4 Hz, 1H), 7.35 (d, J= 8 Hz, 2H), 7.18-7.09 (m, 8H), 6.99 (dd, $J_1 = J_2$ = 8 Hz, 7H), 6.85 (dd, J_1 = 4 Hz, J_2 = 8 Hz, 4H), 5.16 (s, 4H), 2.39 (s, 3H), 1.41 (s, 9H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 150.4, 146.1, 141.9, 137.8, 137.4, 136.5, 131.9, 128.8, 128.3, 127.5, 127.0, 126.7, 126.0, 122.8, 122.1, 121.3, 120.3, 119.2, 119.0, 110.1, 50.1, 43.4, 35.1, 34.7, 31.5, 30.1, 26.3. IR (KBr) v 3435, 2960, 1725, 1463, 1361, 1183, 735 cm^{-1}. HRMS (ESI) Calcd. for $C_{49}H_{48}N_2NaO_2$ $[M+Na]^+$: 719.3608, Found: 719.3592.



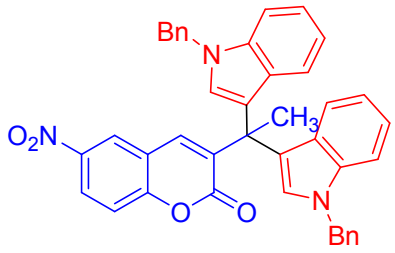
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6-chloro-2H-chromen-2-one (3m)

Product **3m** was obtained in 99% yield as a yellow solid. Reaction time = 72 h; m. p. 130.5-131.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.58 (s, 1H), 7.25 (dd, J_1 = 8 Hz, J_2 = 4 Hz, 3H), 7.19-7.08 (m, 10H), 6.99 (dd, $J_1 = J_2$ = 8 Hz, , 6H), 6.85 (t, J = 8 Hz, 4H), 5.17 (t, J = 16 Hz, 4H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 150.9, 138.2, 136.5, 136.3, 133.0, 129.5, 127.9, 127.7, 127.3, 126.4, 126.2, 125.6, 125.5, 120.5, 120.3, 119.3, 118.4, 118.0, 116.3, 109.2, 49.0, 42.5, 24.8. IR (KBr) v 3434, 2923, 1734, 1461, 1179, 983, 818, 738, 696 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{31}ClN_2NaO_2$ $[M+Na]^+$: 641.1966, Found: 641.1970.



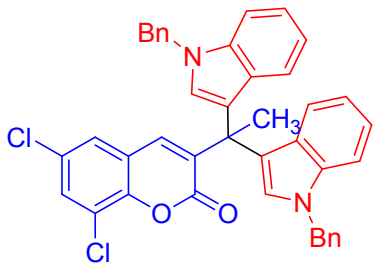
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6-bromo-2H-chromen-2-one (3n)

Product **3n** was obtained in 98% yield as a yellow solid. Reaction time = 72 h; m. p. 195.6-197.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.58 (s, 1H), 7.38 (dd, $J_1 = J_2 = 2$ Hz, 1H), 7.28 (t, $J = 8$ Hz, 3H), 7.19-7.11 (m, 8H), 7.00 (ddd, $J_1 = J_2 = J_3 = 8$ Hz, 7H), 6.85 (t, $J = 8$ Hz, 4H), 5.17 (t, $J = 16$ Hz, 4H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 151.4, 138.1, 136.5, 136.3, 133.0, 132.3, 129.2, 127.7, 127.3, 126.4, 125.6, 125.5, 120.5, 120.3, 119.8, 118.4, 118.0, 116.6, 115.3, 109.2, 49.0, 42.5, 24.8. IR (KBr) ν 3440, 3058, 2933, 1734, 1607, 1470, 1329, 1179, 1069, 985, 740 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{31}BrN_2NaO_2$ $[M+Na]^+$: 685.1461, Found: 685.1468.



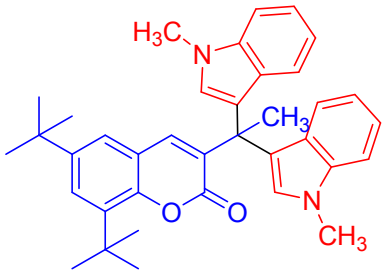
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6-nitro-2H-chromen-2-one (3o)

Product **3o** was obtained in 98% yield as a yellow solid. Reaction time = 72 h; m. p. 141.0-142.6 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 8.25 (dd, $J_1 = J_2 = 4$ Hz, 1H), 8.18 (d, $J = 4$ Hz, 1H), 7.83 (s, 1H), 7.36-7.22 (m, 11H), 7.14-7.06 (m, 6H), 6.96 (dd, $J_1 = 4$ Hz, $J_2 = 12$ Hz, 4H), 5.27 (t, J = 20 Hz, 4H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 157.1, 143.7, 139.1, 137.5, 137.3, 135.0, 128.7, 128.5, 127.5, 126.5, 126.4, 125.5, 123.9, 121.5, 121.4, 119.3, 119.2, 118.8, 117.0, 110.3, 50.0, 43.7, 25.6. IR (KBr) ν 3438, 3058, 1734, 1530, 1461, 1346, 1178, 966, 739 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{31}N_3NaO_4$ $[M+Na]^+$: 652.2207, Found: 652.2189.



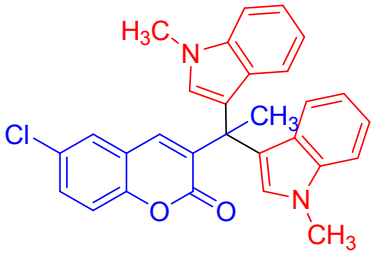
3-(1,1-bis(1-benzyl-1H-indol-3-yl)ethyl)-6,8-dichloro-2H-chromen-2-one (3p)

Product **3p** was obtained in 99% yield as a yellow solid. Reaction time = 41 h; m. p. 213.9-215.7 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.43 (d, J = 4 Hz, 1H), 7.33 (d, J = 8 Hz, 2H), 7.28-7.20 (m, 8H), 7.13-7.05 (m, 7H), 6.95 (dd, J_1 = 4 Hz, J_2 = 8 Hz, 4H), 5.26 (t, J = 16 Hz, 4H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 148.0, 139.0, 137.6, 137.4, 134.9, 130.6, 128.8, 128.7, 128.5, 127.6, 126.6, 125.9, 121.7, 121.5, 121.4, 121.1, 119.2, 119.1, 110.4, 50.1, 43.7, 25.6 (one carbon missing). IR (KBr) v 3436, 3062, 2933, 1734, 1458, 1181, 993, 738 cm^{-1}. HRMS (ESI) Calcd. for $C_{41}H_{30}Cl_2N_2NaO_2$ $[M+Na]^+$: 675.1577, Found: 675.1596.



3-(1,1-bis(1-methyl-1H-indol-3-yl)ethyl)-6,8-di-tert-butyl-2H-chromen-2-one (3q)

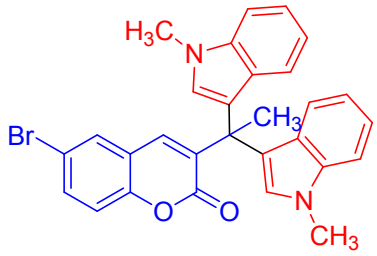
Product **3q** was obtained in 90% yield as a yellow solid. Reaction time = 55 h; m. p. 323.0-324.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.65 (s, 1H), 7.39 (s, 1H), 7.34 (d, J = 8 Hz, 2H), 7.23 (d, J = 8 Hz, 2H), 7.10 (dd, J_1 = J_2 = 8 Hz, 2H), 6.97 (s, 1H), 6.87 (t, J = 8 Hz, 2H), 6.70 (s, 2H), 3.62 (s, 6 H), 2.35 (s, 3H), 1.39 (s, 9H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 149.2, 144.9, 140.7, 136.7, 135.4, 130.6, 127.6, 125.5, 124.8, 121.6, 120.8, 119.9, 118.6, 118.1, 117.6, 108.4, 42.1, 33.9, 33.6, 31.8, 30.4, 28.9, 25.1. IR (KBr) v 3431, 2955, 1726, 1474, 1367, 1208, 1008, 742 cm^{-1}. HRMS (ESI) Calcd. for $C_{37}H_{40}N_2NaO_2$ $[M+Na]^+$: 567.2982, Found: 567.3000.



3-(1,1-bis(1-methyl-1H-indol-3-yl)ethyl)-6-chloro-2H-chromen-2-one (3r)

Product **3r** was obtained in 97% yield as a yellow solid. Reaction time = 48 h; m. p. 173.0-174.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.60 (s, 1H), 7.27-7.23 (m, 5H), 7.16-7.08 (m, 4H), 6.87 (t, J =

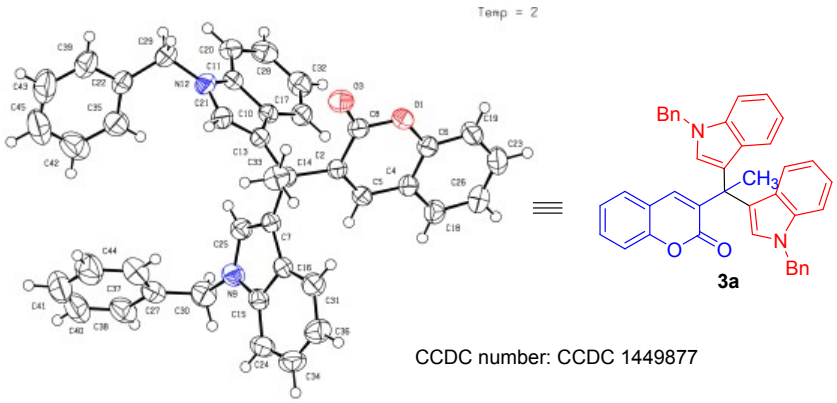
8 Hz, 2H), 6.70 (s, 2H), 3.63 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.1, 151.0, 138.3, 136.8, 133.1, 129.5, 128.0, 127.6, 126.2, 125.3, 120.4, 120.1, 119.3, 118.1, 117.8, 116.3, 108.6, 42.5, 31.8, 24.9. IR (KBr) *v* 3418, 3057, 2940, 1734, 1610, 1539, 1478, 1328, 1248, 1211, 986, 910, 732 cm^{-1}. HRMS (ESI) Calcd. for $C_{29}H_{23}ClN_2NaO_2$ $[M+Na]^+$: 489.1340, Found: 489.1332.



3-(1,1-bis(1-methyl-1H-indol-3-yl)ethyl)-6-bromo-2H-chromen-2-one (3s)

Product **3s** was obtained in 95% yield as a yellow solid. Reaction time = 48 h; m. p. 250.3-252.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$), δ 7.60 (s, 1H), 7.31-7.25 (m, 5H), 7.17 (s, 1H), 7.12 (t, *J* = 8 Hz, 2H), 7.05 (d, *J* = 8 Hz, 1H), 6.89 (t, *J* = 8 Hz, 2H), 6.71 (s, 2H), 3.65 (s, 6H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 151.4, 138.2, 136.7, 133.1, 132.3, 129.2, 127.6, 125.3, 120.4, 120.1, 119.8, 118.0, 117.8, 116.7, 115.3, 108.6, 42.4, 31.8, 24.8. IR (KBr) *v* 3437, 2923, 1733, 1475, 1250, 1098, 985, 906, 735 cm^{-1}. HRMS (ESI) Calcd. for $C_{29}H_{23}BrN_2NaO_2$ $[M+Na]^+$: 533.0835, Found: 533.0821.

3. Crystal data for 3a



CCDC number: CCDC 1449877

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

Identification code	**3a**
Empirical formula	C41 H32 N2 O2

Formula weight	584.69
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.9786(15) A alpha = 76.842(2) deg. b = 12.3683(16) A beta = 66.138(2) deg. c = 12.7772(17) A gamma = 62.478(2) deg.
Volume	1533.3(3) A^3
Z, Calculated density	2, 1.266 Mg/m^3
Absorption coefficient	0.078 mm^-1
F(000)	616
Crystal size	0.40 x 0.25 x 0.20 mm
Theta range for data collection	1.74 to 25.00 deg.
Limiting indices	-10<=h<=14, -13<=k<=14, -9<=l<=15
Reflections collected / unique	7881 / 5368 [R(int) = 0.0163]
Completeness to theta = 25.00	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9846 and 0.9696
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5368 / 0 / 406
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0416, wR2 = 0.1180
R indices (all data)	R1 = 0.0533, wR2 = 0.1292
Largest diff. peak and hole	0.217 and -0.188 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3a**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	X	Y	Z	U(eq)
O(1)	3507(1)	-3681(1)	658(1)	48(1)
C(2)	1792(1)	-1898(1)	1748(1)	36(1)
O(3)	4121(1)	-2826(1)	1524(1)	58(1)
C(4)	1233(2)	-2950(1)	763(1)	39(1)
C(5)	885(2)	-2012(1)	1469(1)	39(1)
C(6)	2567(2)	-3777 (1)	371(1)	41(1)
C(7)	-41(1)	-49(1)	2836(1)	36(1)
C(8)	3193(2)	-2790(1)	1336(1)	42(1)
N(9)	-2054(1)	1557(1)	3126(1)	46(1)
C(10)	2459(1)	220(1)	360(1)	36(1)
C(11)	3173(1)	966(1)	15(1)	38(1)
N(12)	3342(1)	1121(1)	961(1)	46(1)
C(13)	2204(1)	-65(1)	1574(1)	36(1)
C(14)	1470(1)	-826(1)	2395(1)	37(1)
C(15)	-2288(2)	640(1)	3906(1)	40(1)
C(16)	-1049(2)	-388(1)	3739(1)	37(1)
C(17)	2212(2)	-92 (2)	-490(1)	42(1)
C(18)	321(2)	-3067(2)	426(2)	48(1)
C(19)	3003(2)	-4721(2)	-305(1)	52(1)
C(20)	3621(2)	1396(2)	-1116(2)	48(1)
C(21)	2768(2)	494(2)	1876(1)	44(1)
C(22)	3163(2)	2866(2)	1758(1)	43(1)
C(23)	2077(2)	-4822(2)	-610(2)	57(1)
C(24)	-3487(2)	629(2)	4716(2)	51(1)
C(25)	-702(2)	1118(1)	2498(1)	43(1)
C(26)	745(2)	-3991(2)	-258(2)	54(1)
C(27)	-3106(2)	3789(2)	3471(1)	48(1)
C(28)	3361(2)	1060(2)	-1915(2)	53(1)

C(29)	4043(2)	1796(2)	1010(2)	53(1)
C(30)	-3054(2)	2766(2)	2971(2)	56(1)
C(31)	-1053(2)	-1461(2)	4400(2)	49(1)
C(32)	2674(2)	318(2)	-1609(2)	51(1)
C(33)	1931(2)	-1291(2)	3453(2)	52(1)
C(34)	-3437(2)	-438(2)	5348(2)	60(1)
C(35)	1794(2)	3438(2)	2020(2)	57(1)
C(36)	-2240(2)	-1474(2)	5188(2)	59(1)
C(37)	-2231(2)	3614(2)	3994(2)	62(1)
C(38)	-4054(2)	4968(2)	3372(2)	62(1)
C(39)	3754(2)	3320(2)	2175(2)	60(1)
C(40)	-4115(3)	5937(2)	3778(2)	77(1)
C(41)	-3238(3)	5757(2)	4288(2)	86(1)
C(42)	1034(2)	4454(2)	2673(2)	78(1)
C(43)	2994(3)	4327(2)	2830(2)	82(1)
C(44)	-2300(3)	4598(2)	4404(2)	82(1)
C(45)	1643(3)	4889(2)	3077(2)	88(1)

Table S3. Bond lengths [A] and angles [deg] for **3a**.

O(1)-C(8)	1.376(2)	O(1)-C(6)	1.3762(19)
C(2)-C(5)	1.343(2)	C(2)-C(8)	1.467(2)
C(2)-C(14)	1.536(2)	O(3)-C(8)	1.2084(19)
C(4)-C(6)	1.387(2)	C(4)-C(18)	1.399(2)
C(4)-C(5)	1.435(2)	C(5)-H(5A)	0.9300
C(6)-C(19)	1.382(2)	C(7)-C(25)	1.354(2)
C(7)-C(16)	1.444(2)	C(7)-C(14)	1.527(2)
N(9)-C(25)	1.377(2)	N(9)-C(15)	1.382(2)
N(9)-C(30)	1.453(2)	C(10)-C(17)	1.405(2)
C(10)-C(11)	1.421(2)	C(10)-C(13)	1.447(2)

C(11)-N(12)	1.371(2)	C(11)-C(20)	1.395(2)
N(12)-C(21)	1.368(2)	N(12)-C(29)	1.455(2)
C(13)-C(21)	1.359(2)	C(13)-C(14)	1.525(2)
C(14)-C(33)	1.555(2)	C(15)-C(24)	1.394(2)
C(15)-C(16)	1.410(2)	C(16)-C(31)	1.402(2)
C(17)-C(32)	1.377(2)	C(17)-H(17A)	0.9300
C(18)-C(26)	1.373(2)	C(18)-H(18A)	0.9300
C(19)-C(23)	1.377(3)	C(19)-H(19A)	0.9300
C(20)-C(28)	1.371(3)	C(20)-H(20A)	0.9300
C(21)-H(21A)	0.9300	C(22)-C(35)	1.376(2)
C(22)-C(39)	1.382(2)	C(22)-C(29)	1.499(2)
C(23)-C(26)	1.385(3)	C(23)-H(23A)	0.9300
C(24)-C(34)	1.370(3)	C(24)-H(24A)	0.9300
C(25)-H(25A)	0.9300	C(26)-H(26A)	0.9300
C(27)-C(37)	1.373(3)	C(27)-C(38)	1.391(2)
C(27)-C(30)	1.509(3)	C(28)-C(32)	1.396(3)
C(28)-H(28A)	0.9300	C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700	C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700	C(31)-C(36)	1.375(2)
C(31)-H(31A)	0.9300	C(32)-H(32A)	0.9300
C(33)-H(33A)	0.9600	C(33)-H(33B)	0.9600
C(33)-H(33C)	0.9600	C(34)-C(36)	1.387(3)
C(34)-H(34A)	0.9300	C(35)-C(42)	1.381(3)
C(35)-H(35A)	0.9300	C(36)-H(36A)	0.9300
C(37)-C(44)	1.387(3)	C(37)-H(37A)	0.9300
C(38)-C(40)	1.373(3)	C(38)-H(38A)	0.9300
C(39)-C(43)	1.374(3)	C(39)-H(39A)	0.9300
C(40)-C(41)	1.360(4)	C(40)-H(40A)	0.9300
C(41)-C(44)	1.374(4)	C(41)-H(41A)	0.9300

C(42)-C(45)	1.372(4)	C(42)-H(42A)	0.9300
C(43)-C(45)	1.360(4)	C(43)-H(43A)	0.9300
C(44)-H(44A)	0.9300	C(45)-H(45A)	0.9300
C(8)-O(1)-C(6)	123.06(12)	C(5)-C(2)-C(8)	118.50(14)
C(5)-C(2)-C(14)	123.75(13)	C(8)-C(2)-C(14)	117.56(13)
C(6)-C(4)-C(18)	118.05(15)	C(6)-C(4)-C(5)	117.72(14)
C(18)-C(4)-C(5)	124.22(14)	C(2)-C(5)-C(4)	122.90(14)
C(2)-C(5)-H(5A)	118.5	C(4)-C(5)-H(5A)	118.5
O(1)-C(6)-C(19)	117.66(14)	O(1)-C(6)-C(4)	120.13(14)
C(19)-C(6)-C(4)	122.20(16)	C(25)-C(7)-C(16)	105.94(13)
C(25)-C(7)-C(14)	127.01(14)	C(16)-C(7)-C(14)	126.98(13)
O(3)-C(8)-O(1)	115.64(14)	O(3)-C(8)-C(2)	126.69(15)
O(1)-C(8)-C(2)	117.66(13)	C(25)-N(9)-C(15)	107.99(13)
C(25)-N(9)-C(30)	125.53(15)	C(15)-N(9)-C(30)	126.47(14)
C(17)-C(10)-C(11)	117.54(14)	C(17)-C(10)-C(13)	135.83(14)
C(11)-C(10)-C(13)	106.59(13)	N(12)-C(11)-C(20)	129.38(14)
N(12)-C(11)-C(10)	107.85(14)	C(20)-C(11)-C(10)	122.75(15)
C(21)-N(12)-C(11)	108.31(12)	C(21)-N(12)-C(29)	124.46(14)
C(11)-N(12)-C(29)	127.20(14)	C(21)-C(13)-C(10)	105.64(13)
C(21)-C(13)-C(14)	124.81(14)	C(10)-C(13)-C(14)	129.54(13)
C(13)-C(14)-C(7)	110.49(12)	C(13)-C(14)-C(2)	108.20(12)
C(7)-C(14)-C(2)	110.30(12)	C(13)-C(14)-C(33)	109.55(12)
C(7)-C(14)-C(33)	107.30(12)	C(2)-C(14)-C(33)	111.02(13)
N(9)-C(15)-C(24)	129.91(15)	N(9)-C(15)-C(16)	107.63(13)
C(24)-C(15)-C(16)	122.43(15)	C(31)-C(16)-C(15)	117.73(14)
C(31)-C(16)-C(7)	135.09(15)	C(15)-C(16)-C(7)	107.13(13)
C(32)-C(17)-C(10)	119.52(15)	C(32)-C(17)-H(17A)	120.2
C(10)-C(17)-H(17A)	120.2	C(26)-C(18)-C(4)	120.27(16)
C(26)-C(18)-H(18A)	119.9	C(4)-C(18)-H(18A)	119.9

C(23)-C(19)-C(6)	118.37(17)	C(23)-C(19)-H(19A)	120.8
C(6)-C(19)-H(19A)	120.8	C(28)-C(20)-C(11)	117.51(16)
C(28)-C(20)-H(20A)	121.2	C(11)-C(20)-H(20A)	121.2
C(13)-C(21)-N(12)	111.60(14)	C(13)-C(21)-H(21A)	124.2
N(12)-C(21)-H(21A)	124.2	C(35)-C(22)-C(39)	118.50(17)
C(35)-C(22)-C(29)	122.77(16)	C(39)-C(22)-C(29)	118.71(16)
C(19)-C(23)-C(26)	120.80(16)	C(19)-C(23)-H(23A)	119.6
C(26)-C(23)-H(23A)	119.6	C(34)-C(24)-C(15)	117.61(17)
C(34)-C(24)-H(24A)	121.2	C(15)-C(24)-H(24A)	121.2
C(7)-C(25)-N(9)	111.29(14)	C(7)-C(25)-H(25A)	124.4
N(9)-C(25)-H(25A)	124.4	C(18)-C(26)-C(23)	120.27(17)
C(18)-C(26)-H(26A)	119.9	C(23)-C(26)-H(26A)	119.9
C(37)-C(27)-C(38)	118.25(18)	C(37)-C(27)-C(30)	122.84(16)
C(38)-C(27)-C(30)	118.88(17)	C(20)-C(28)-C(32)	121.32(17)
C(20)-C(28)-H(28A)	119.3	C(32)-C(28)-H(28A)	119.3
N(12)-C(29)-C(22)	113.93(14)	N(12)-C(29)-H(29A)	108.8
C(22)-C(29)-H(29A)	108.8	N(12)-C(29)-H(29B)	108.8
C(22)-C(29)-H(29B)	108.8	H(29A)-C(29)-H(29B)	107.7
N(9)-C(30)-C(27)	115.72(15)	N(9)-C(30)-H(30A)	108.4
C(27)-C(30)-H(30A)	108.4	N(9)-C(30)-H(30B)	108.4
C(27)-C(30)-H(30B)	108.4	H(30A)-C(30)-H(30B)	107.4
C(36)-C(31)-C(16)	119.72(17)	C(36)-C(31)-H(31A)	120.1
C(16)-C(31)-H(31A)	120.1	C(17)-C(32)-C(28)	121.35(16)
C(17)-C(32)-H(32A)	119.3	C(28)-C(32)-H(32A)	119.3
C(14)-C(33)-H(33A)	109.5	C(14)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5	C(14)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5	H(33B)-C(33)-H(33C)	109.5
C(24)-C(34)-C(36)	121.47(17)	C(24)-C(34)-H(34A)	119.3
C(36)-C(34)-H(34A)	119.3	C(22)-C(35)-C(42)	120.6(2)

C(22)-C(35)-H(35A)	119.7	C(42)-C(35)-H(35A)	119.7
C(31)-C(36)-C(34)	121.02(17)	C(31)-C(36)-H(36A)	119.5
C(34)-C(36)-H(36A)	119.5	C(27)-C(37)-C(44)	120.2(2)
C(27)-C(37)-H(37A)	119.9	C(44)-C(37)-H(37A)	119.9
C(40)-C(38)-C(27)	121.2(2)	C(40)-C(38)-H(38A)	119.4
C(27)-C(38)-H(38A)	119.4	C(43)-C(39)-C(22)	120.8(2)
C(43)-C(39)-H(39A)	119.6	C(22)-C(39)-H(39A)	119.6
C(41)-C(40)-C(38)	120.1(2)	C(41)-C(40)-H(40A)	119.9
C(38)-C(40)-H(40A)	119.9	C(40)-C(41)-C(44)	119.6(2)
C(40)-C(41)-H(41A)	120.2	C(44)-C(41)-H(41A)	120.2
C(45)-C(42)-C(35)	119.9(2)	C(45)-C(42)-H(42A)	120.1
C(35)-C(42)-H(42A)	120.1	C(45)-C(43)-C(39)	120.1(2)
C(45)-C(43)-H(43A)	119.9	C(39)-C(43)-H(43A)	119.9
C(41)-C(44)-C(37)	120.6(2)	C(41)-C(44)-H(44A)	119.7
C(37)-C(44)-H(44A)	119.7	C(43)-C(45)-C(42)	120.1(2)
C(43)-C(45)-H(45A)	119.9	C(42)-C(45)-H(45A)	119.9

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for **3a**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

Atom	U11	U22	U33	U23	U13	U12
O(1)	33(1)	41(1)	62(1)	-12(1)	-10(1)	-10(1)
C(2)	33(1)	32(1)	39(1)	0(1)	-11(1)	-13(1)
O(3)	33(1)	56(1)	83(1)	-13(1)	21(1)	-12(1)
C(4)	39(1)	33(1)	44(1)	-1 (1)	-13(1)	-15(1)
C(5)	31(1)	33(1)	46(1)	-5(1)	-11(1)	-9(1)
C(6)	39(1)	36(1)	45(1)	-1(1)	-10(1)	-16(1)
C(7)	36(1)	37(1)	33(1)	-5(1)	-10(1)	-15(1)
C(8)	35(1)	37(1)	48(1)	-1(1)	-11(1)	-15(1)

N(9)	39(1)	38(1)	53(1)	-2(1)	-15(1)	-10(1)
C(10)	29(1)	34(1)	40(1)	-7(1)	-11(1)	-10(1)
C(11)	32(1)	38(1)	42(1)	-10(1)	-8(1)	-13(1)
N(12)	46(1)	55(1)	46(1)	-11(1)	-9(1)	-30(1)
C(13)	33(1)	38(1)	38(1)	-6(1)	-11(1)	-14(1)
C(14)	35(1)	38(1)	38(1)	-2(1)	-14(1)	-14(1)
C(15)	41(1)	44(1)	36(1)	-9(1)	-11(1)	-17(1)
C(16)	39(1)	39(1)	33(1)	-7(1)	-10(1)	-15(1)
C(17)	40(1)	45(1)	45(1)	-6(1)	-17(1)	-17(1)
C(18)	47(1)	38(1)	60(1)	-3(1)	-22(1)	-16(1)
C(19)	51(1)	39(1)	52(1)	-101(1)	-7(1)	-14(1)
C(20)	41(1)	48(1)	49(2)	-4 (1)	-6(1)	-21(1)
C(21)	46(1)	54(1)	40(1)	-9(1)	13(1)	-25(1)
C(22)	50(1)	43(1)	42(1)	2(1)	-17(1)	-26(1)
C(23)	74(1)	44(1)	54(1)	-9(1)	-18(1)	-27(1)
C(24)	38(1)	64(1)	48(1)	-16(1)	-7(1)	-17(1)
C(25)	42(1)	41(1)	43(1)	0(1)	-12(1)	-19(1)
C(26)	66(1)	47(1)	61(1)	-2(1)	-29(1)	-28(1)
C(27)	42(1)	45(1)	42(1)	-2(1)	-9(1)	-12(1)
C(28)	49(1)	60(1)	39(1)	-11(1)	-8(1)	-20(1)
C(29)	46(1)	60(1)	65(1)	-14 (1)	-13(1)	-31(1)
C(30)	48(1)	47(1)	68(1)	1(1)	-28(1)	-11(1)
C(31)	51(1)	45(1)	46(1)	0(1)	-13(1)	-20(1)
C(32)	52(1)	57(1)	44(1)	-9(1)	-20(1)	-17(1)
C(33)	52(1)	61(1)	48(1)	4(1)	-25 (1)	-25(1)
C(34)	53(1)	81(1)	45(1)	-7(1)	-3(1)	-38(1)
C(35)	54(1)	54(1)	62(1)	-2(1)	-21(1)	-22(1)
C(36)	66(1)	63(1)	48(1)	6(1)	-11(1)	-37(1)
C(37)	61(1)	59(1)	56(1)	-10(1)	-20(1)	-13(1)

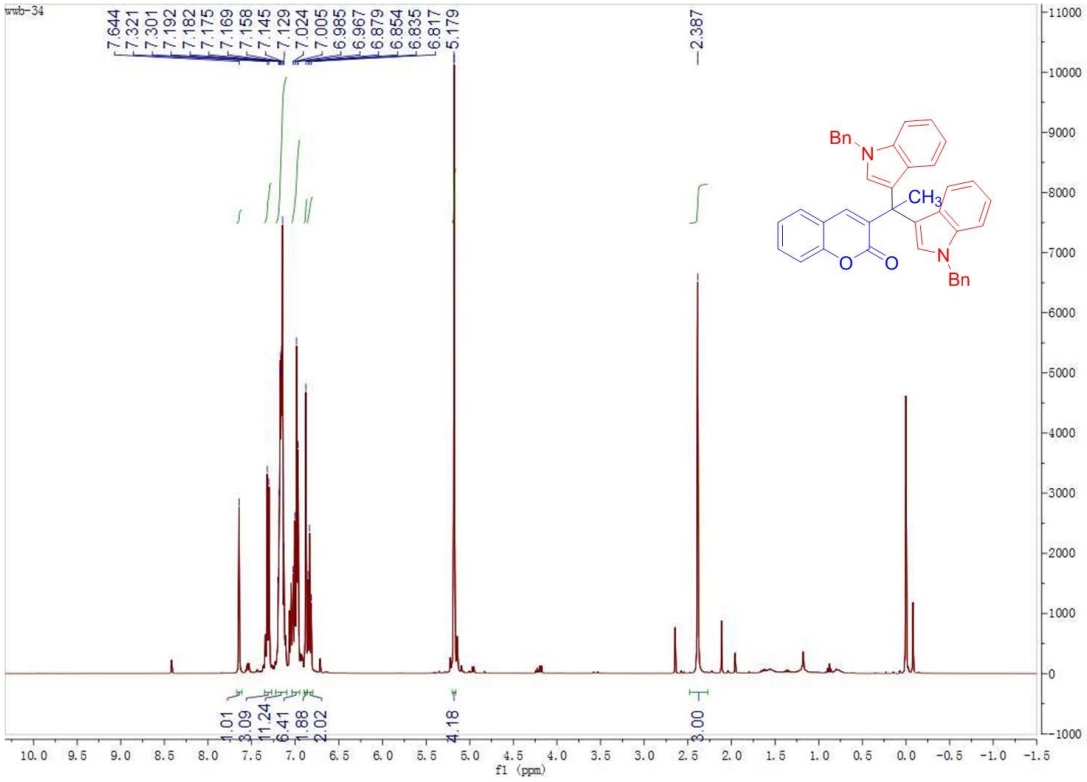
C(38)	54(1)	50(1)	60(1)	-3 (1)	-14(1)	-9(1)
C(39)	75(1)	65(1)	60(1)	-1(1)	-27(1)	-43(1)
C(40)	84(2)	47(1)	70(2)	-13 (1)	-10(1)	-13(1)
C(41)	100(2)	67(2)	82(2)	-28(1)	-12(2)	-33(1)
C(42)	69(1)	57(1)	75(2)	-4(1)	-11(1)	-12(1)
C(43)	121(2)	76(2)	72(2)	-14(1)	-29(2)	-58(2)
C(44)	85(2)	91(2)	75(2)	-27(1)	-26(1)	-32(1)
C(45)	124(2)	52(1)	70(2)	-14(1)	-18(2)	-32(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3a.**

Atom	X	Y	Z	U(eq)
H(5A)	-8	-1459	1746	47
H(17A)	1740	-573	-299	51
H(18A)	-577	-2517	666	57
H(19A)	3899	-5274	-548	62
H(20A)	4078	1891	-1321	57
H(21A)	2764	456	2613	53
H(23A)	2350	-5456	-1057	68
H(24A)	-4292	1321	4823	62
H(25A)	-296	1566	1917	52
H(26A)	136	-4059	-486	65
H(28A)	3649	1333	-2676	64
H(29A)	4440	2085	240	64
H(29B)	4767	1244	1292	64
H(30A)	-3930	2745	3313	67
H(30B)	-2884	2952	2156	67
H(31A)	-256	-2160	4306	59
H(32A)	2525	96	-2173	61

H(33A)	1725	-606	3839	78
H(33B)	2881	-1782	3205	78
H(33C)	1471	-1772	3967	78
H(34A)	-4222	-467	5896	71
H(35A)	1377	3139	1756	69
H(36A)	-2240	-2190	5619	71
H(37A)	-1590	2833	4074	75
H(38A)	-4659	5102	3024	74
H(39A)	4678	2940	2010	72
H(40A)	-4757	6719	3704	92
H(41A)	-3272	6414	4557	104
H(42A)	111	4842	2838	94
H(43A)	3405	4624	3104	99
H(44A)	-1706	4472	4760	99
H(45A)	1131	5569	3521	105

4. Copies of ^{1}H NMR and ^{13}C NMR spectra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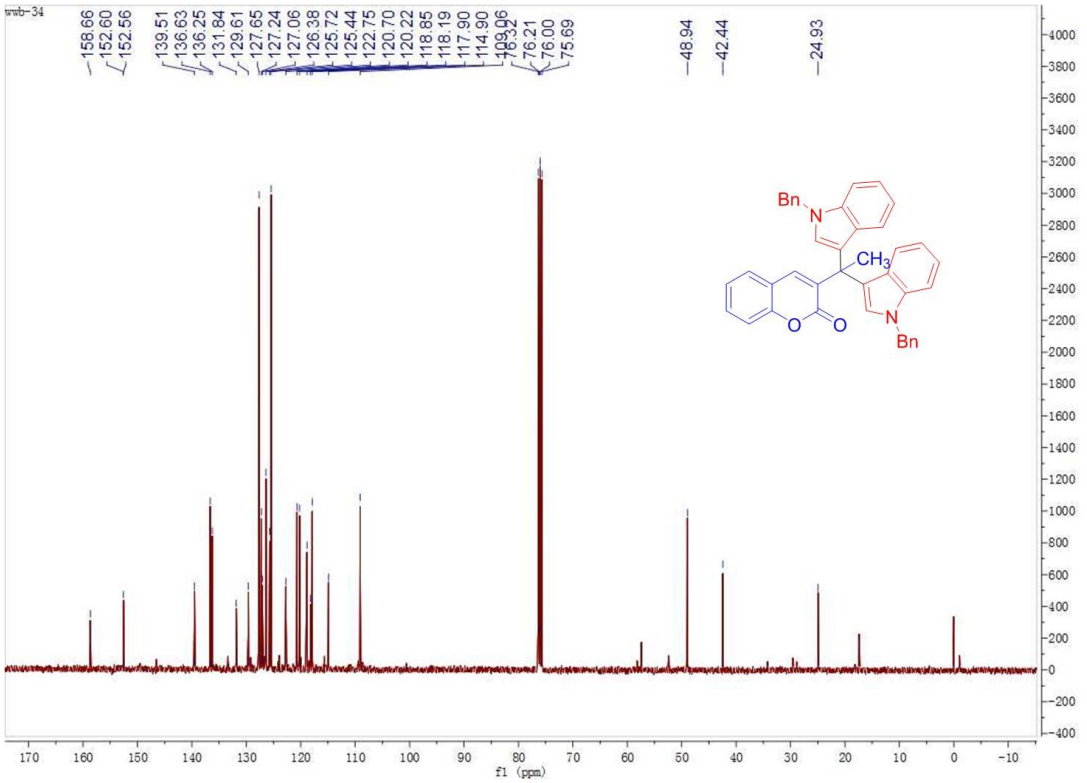
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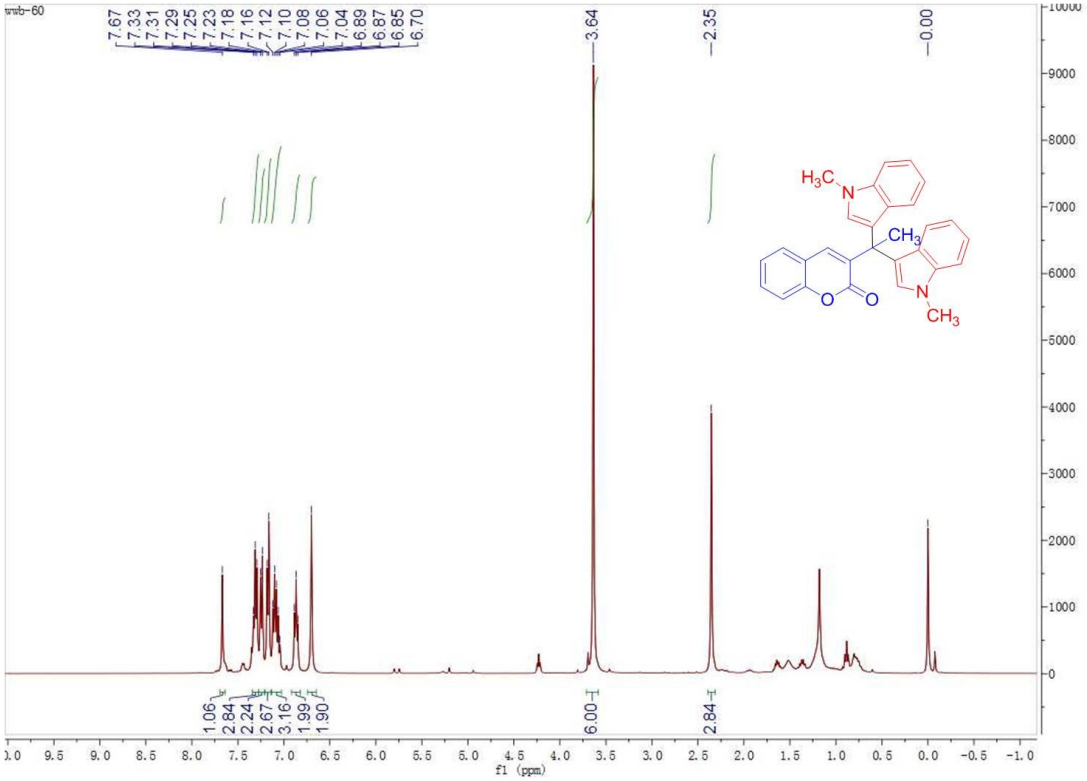
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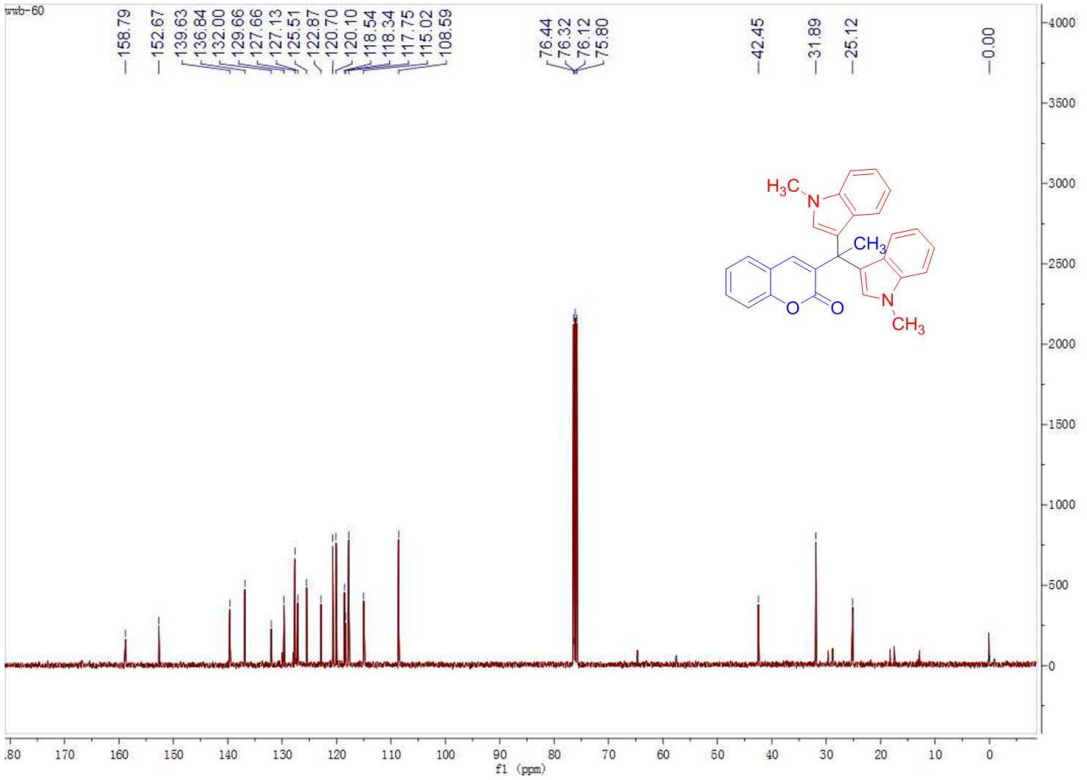
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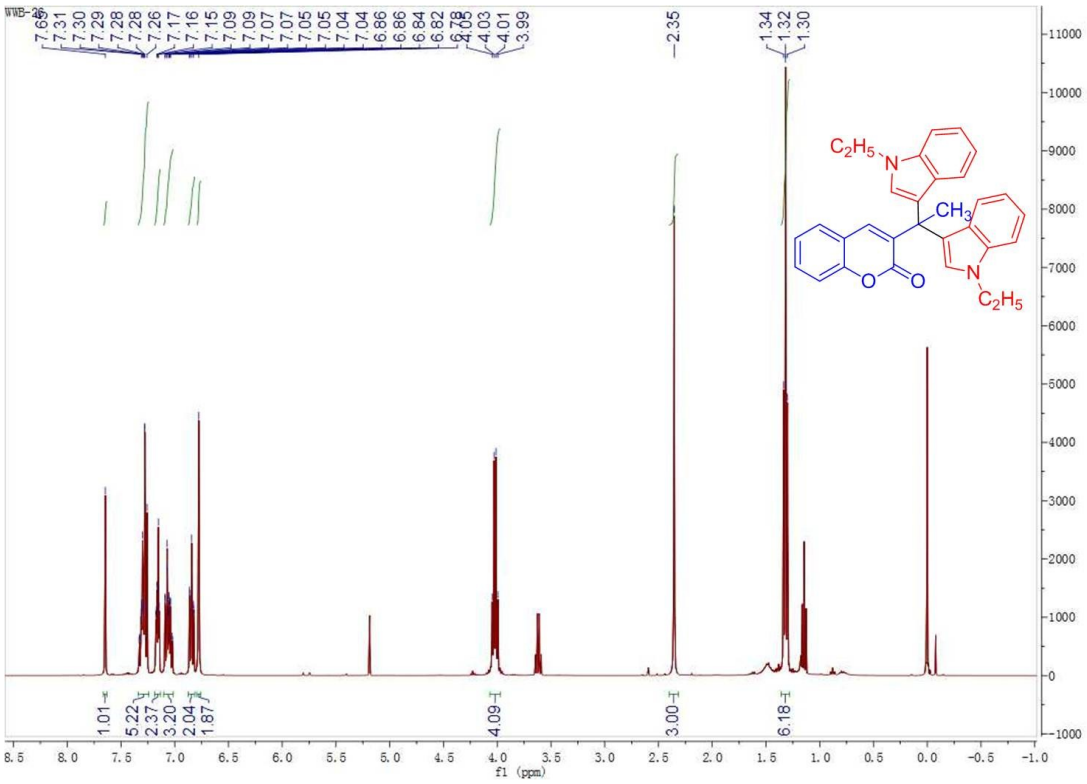
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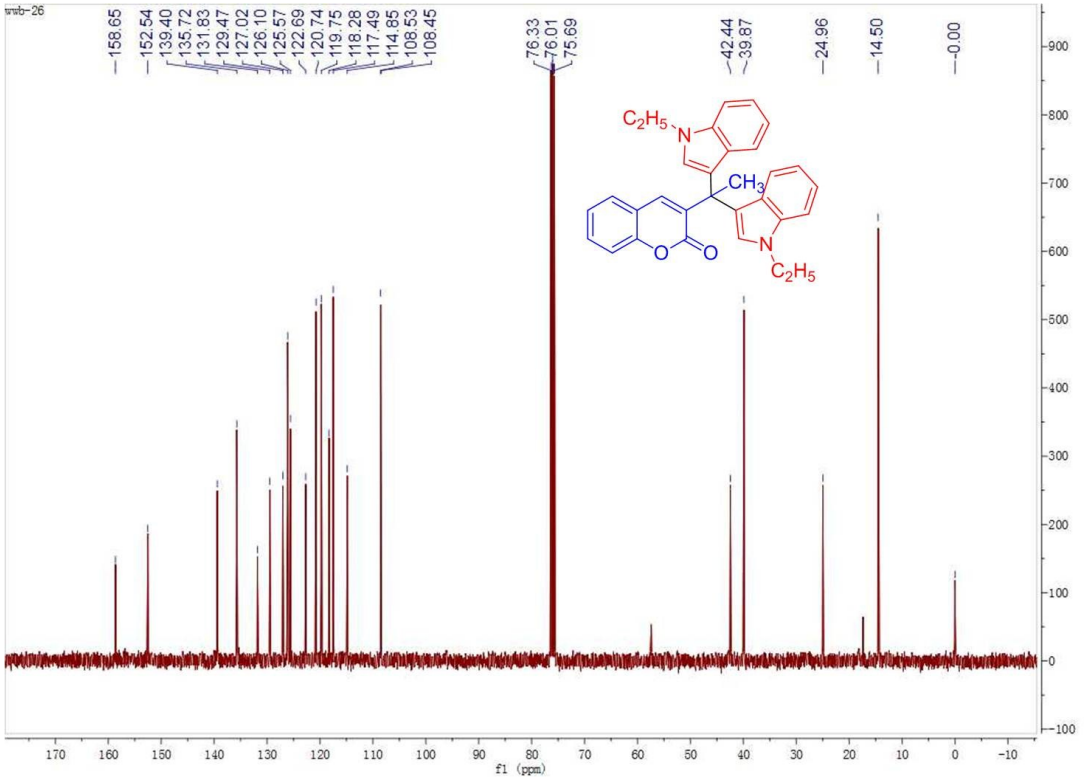
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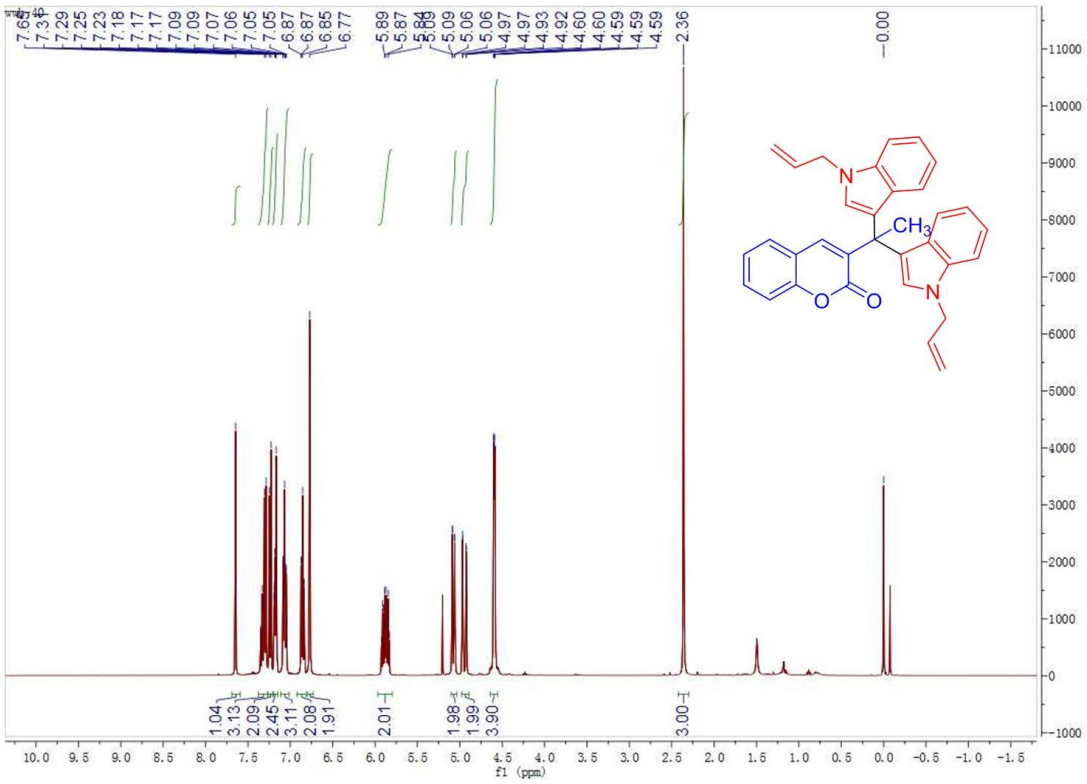
f1 (ppm)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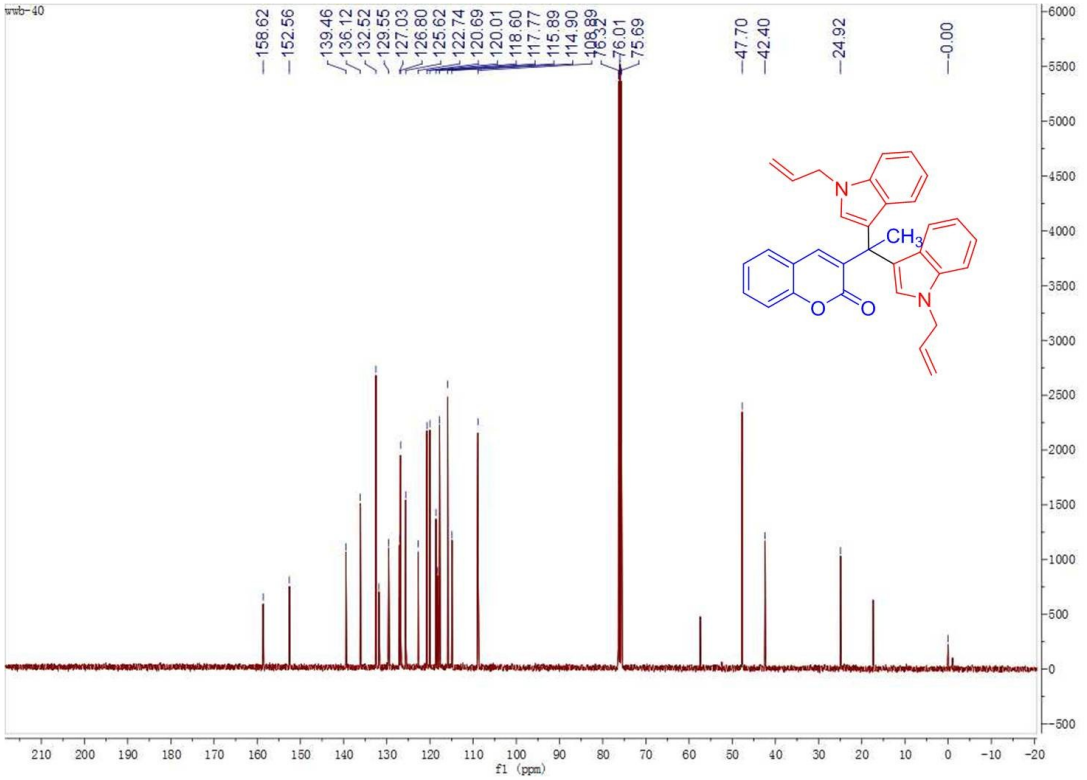
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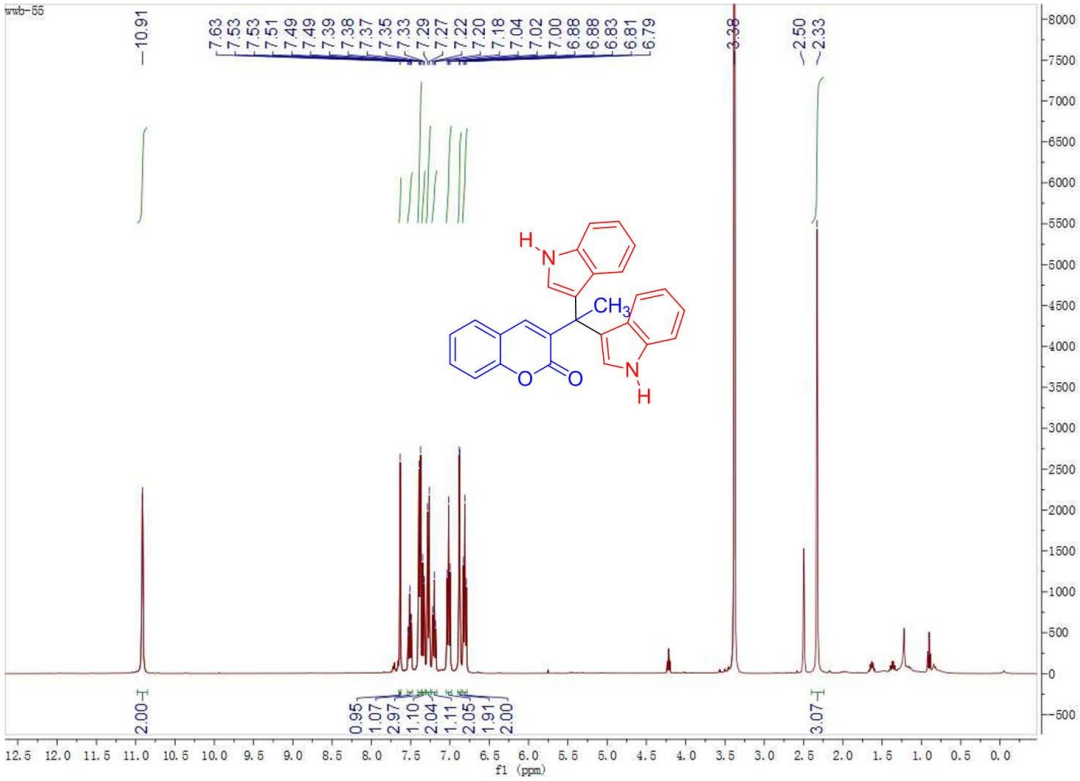
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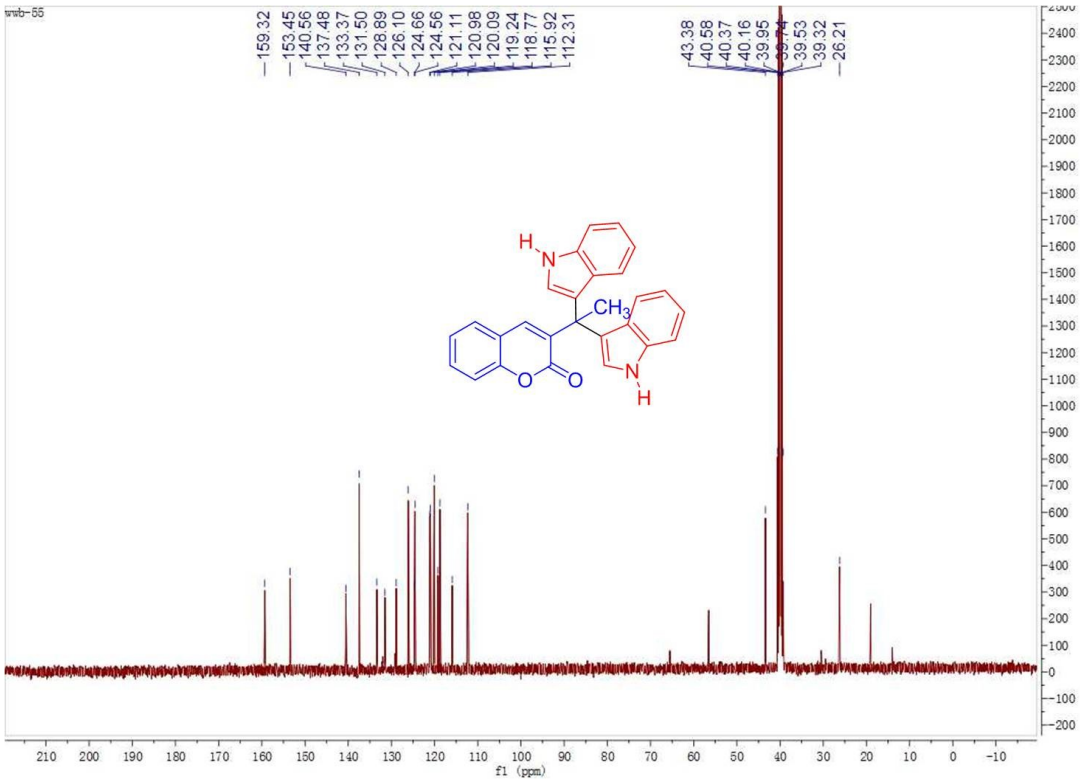
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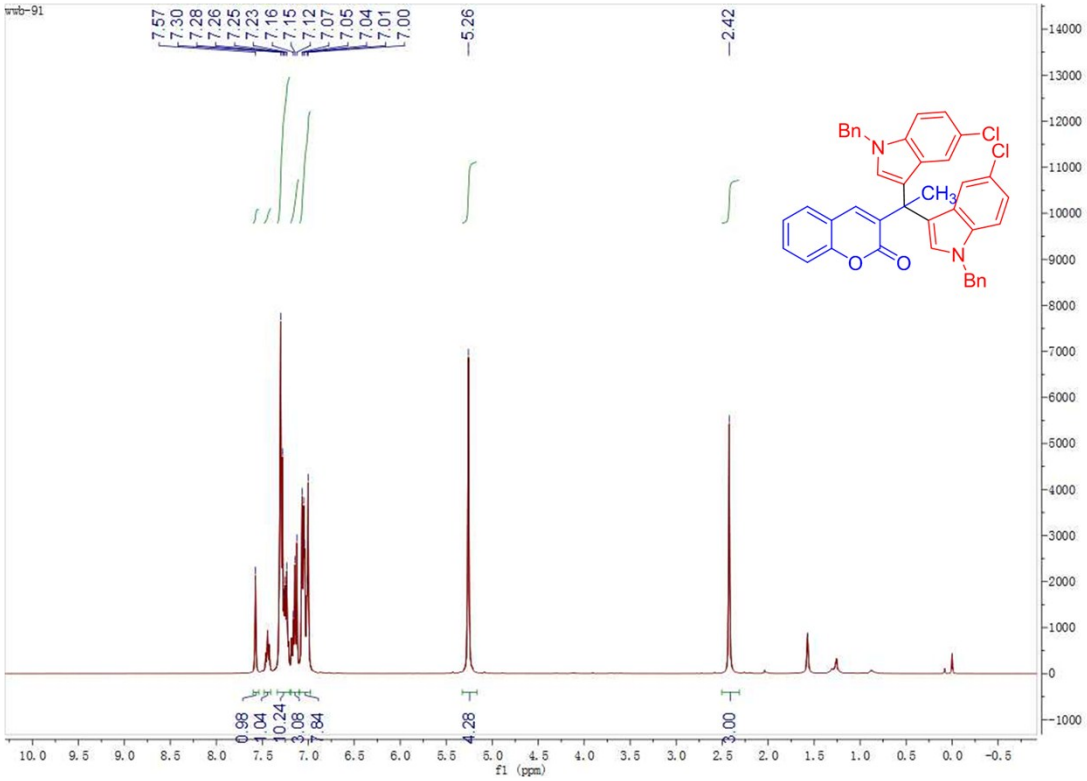
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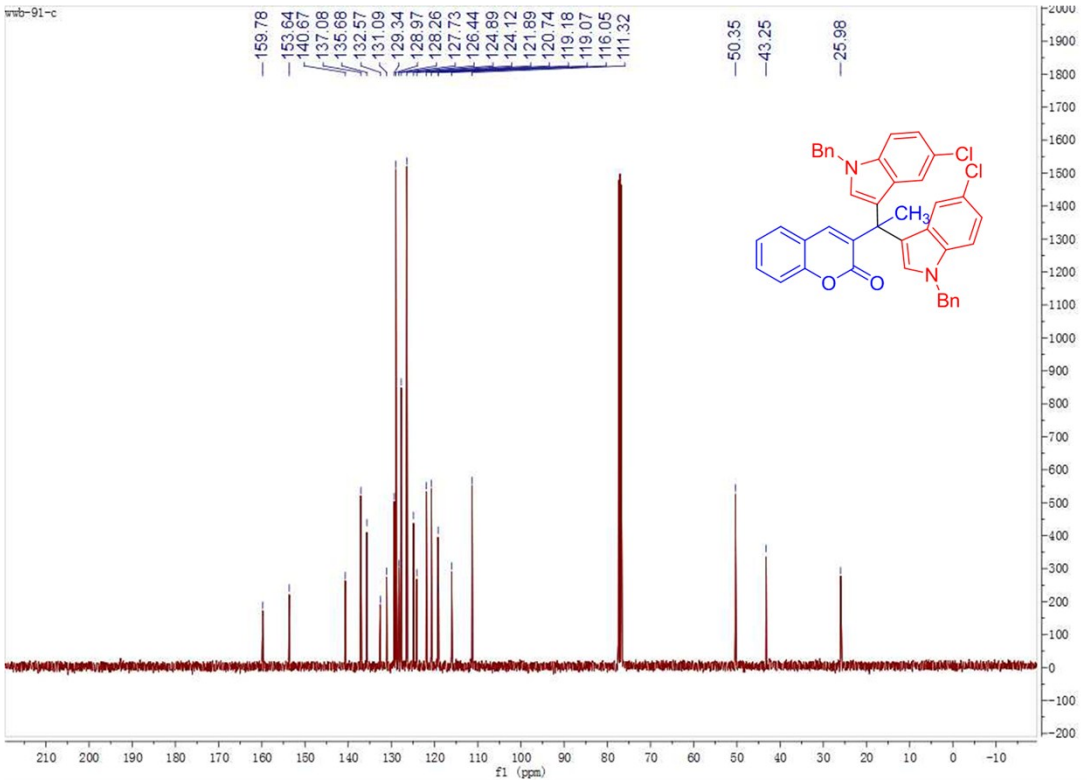
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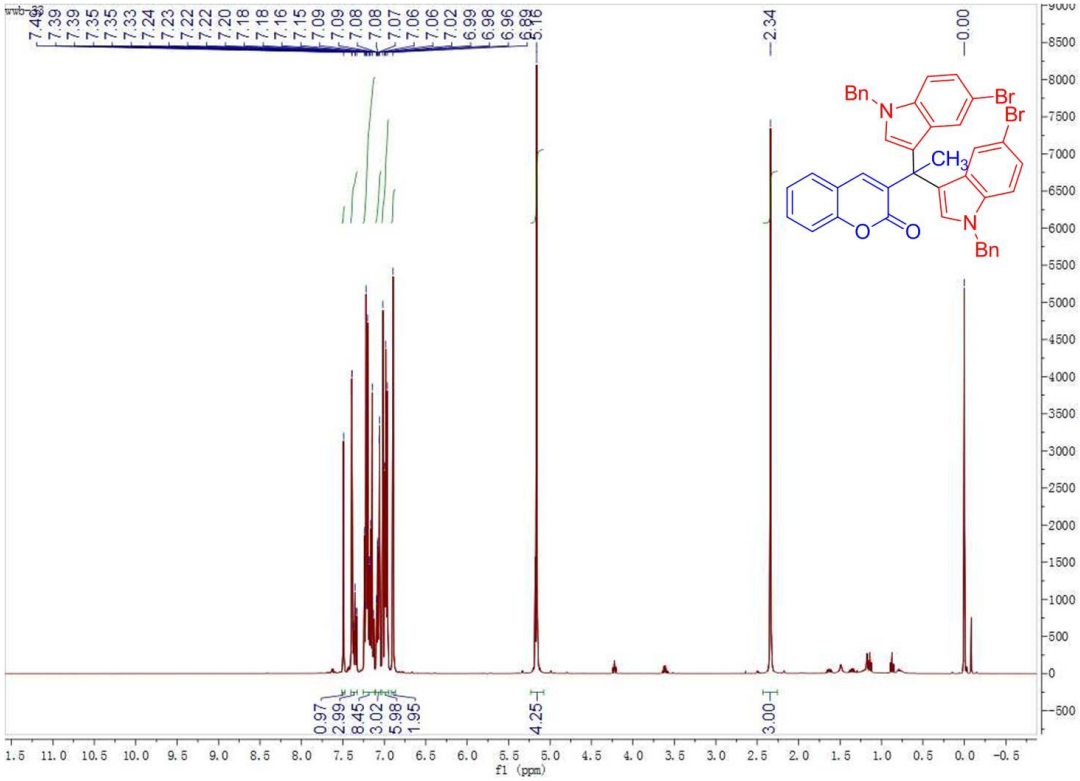
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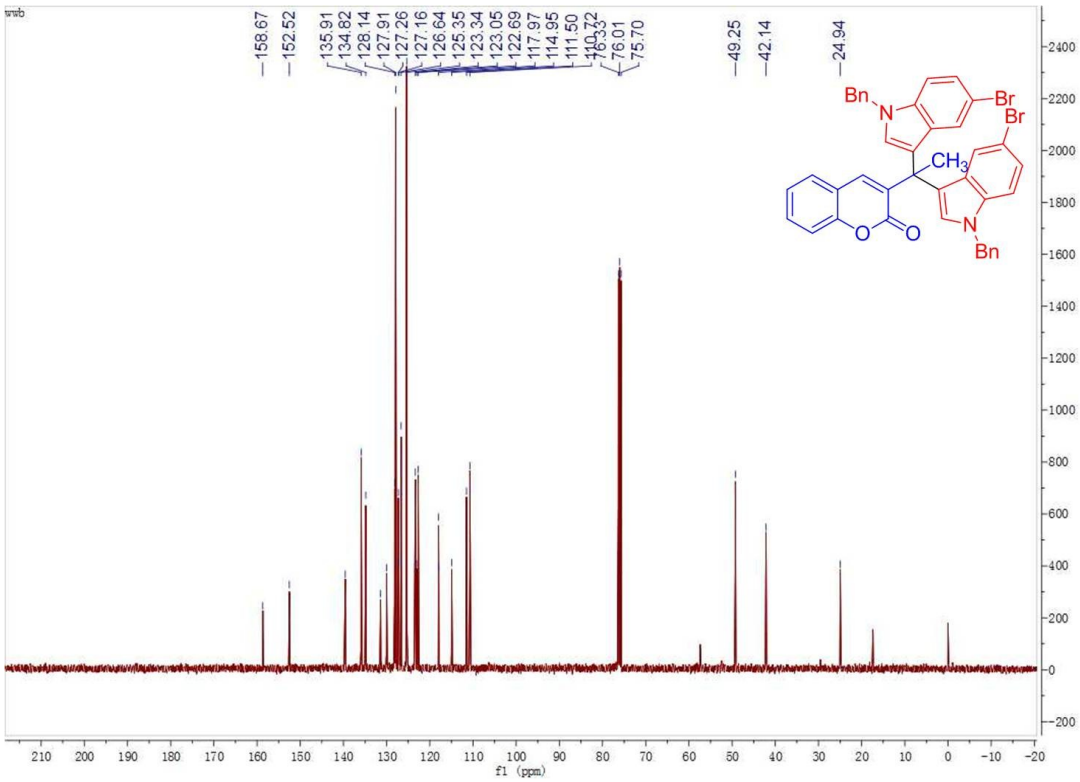
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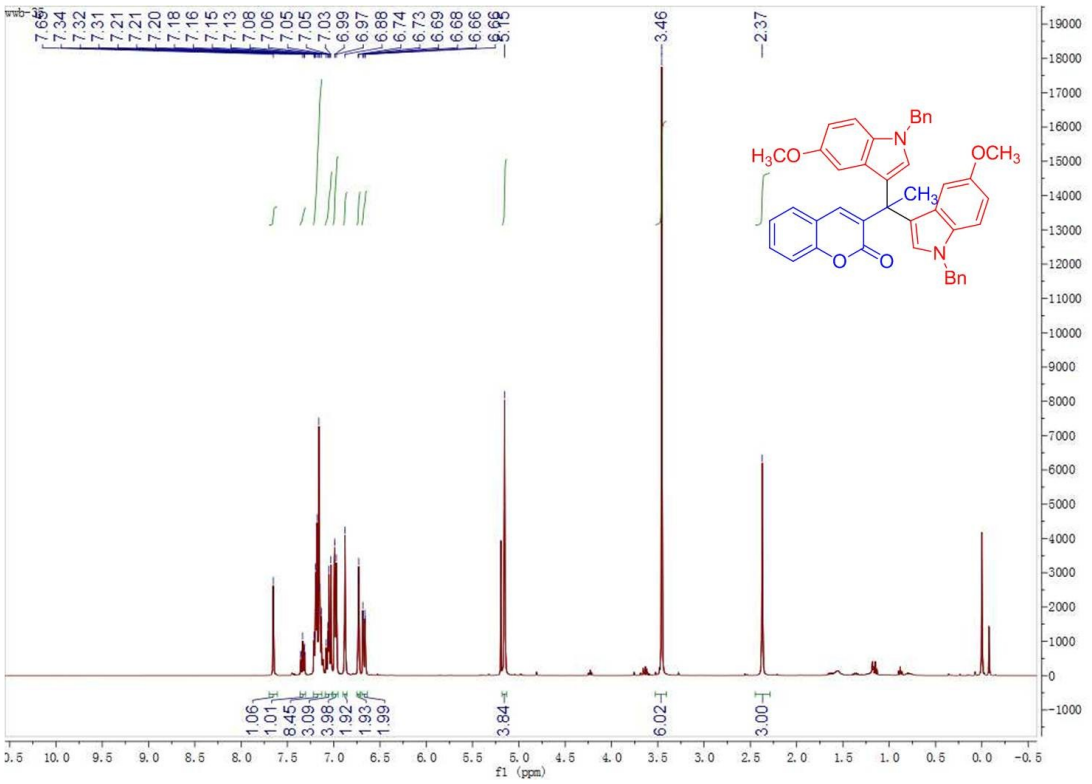
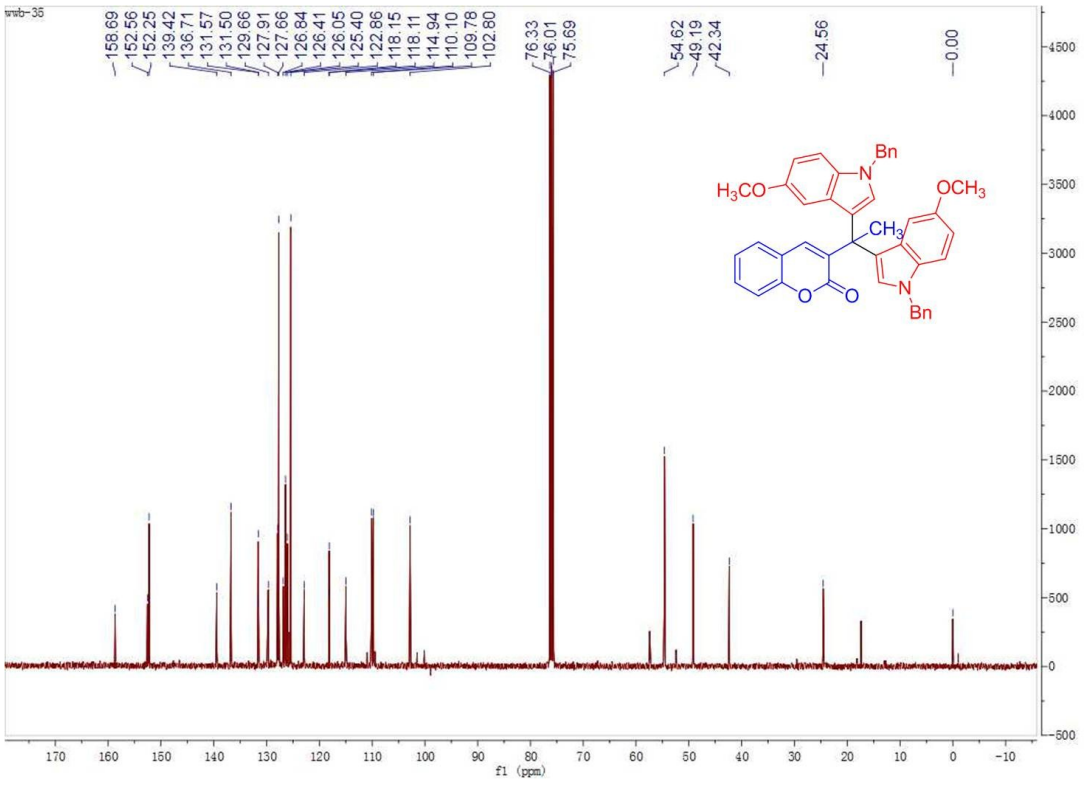
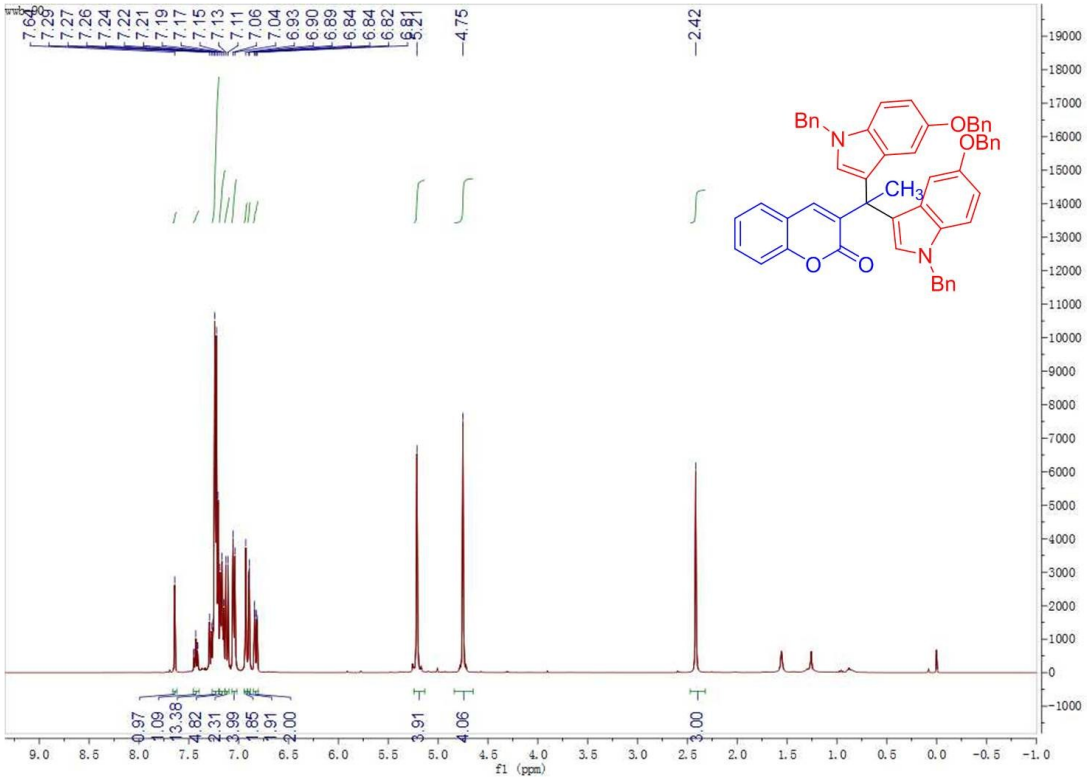
f1 (ppm)


wwb-36
7.69
7.34
7.32
7.31
7.21
7.21
7.20
7.18
7.16
7.15
7.13
7.08
7.06
7.05
7.05
7.03
6.99
6.97
6.88
6.74
6.73
6.69
6.68
6.66
6.65
3.46
2.37
Bn
H3CO
OCH3
CH3
O
O
N
Bn
1.06
1.01
8.45
3.09
3.98
1.92
1.93
1.99
3.84
6.02
3.00
f1 (ppm)


wwb-36
158.69
152.56
152.25
139.42
136.71
131.57
131.50
129.66
127.91
127.66
126.84
126.41
126.05
125.40
122.86
118.15
118.11
114.94
110.10
109.78
102.80
76.33
76.01
75.69
54.62
49.19
42.34
24.56
0.00
Bn
H3CO
OCH3
CH3
O
O
N
Bn
f1 (ppm)


wwb-90
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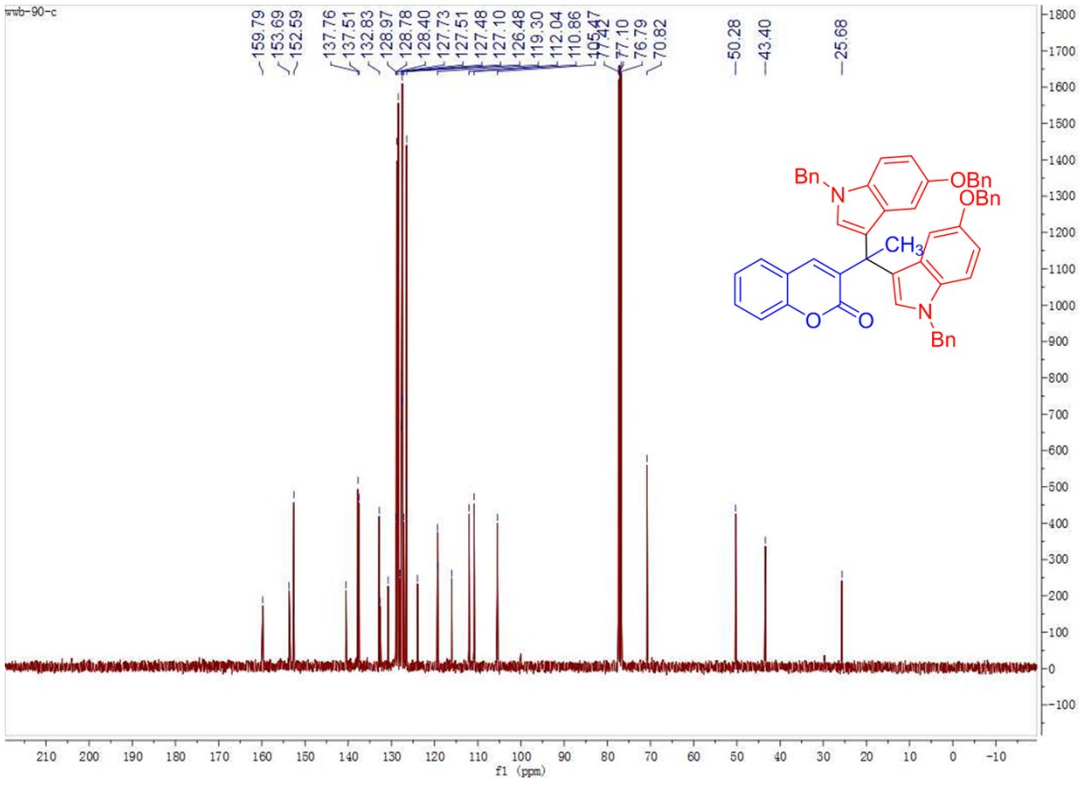
7.29
7.27
7.26
7.24
7.22
7.21
7.19
7.17
7.15
7.13
7.11
7.06
7.04
6.93
6.90
6.89
6.84
6.84
6.82
6.81
5.21
4.75
2.42
Bn
N
OBn
OBn
CH3
O
O
N
Bn
0.97
1.09
13.38
4.82
2.31
3.99
1.85
1.91
2.00
3.91
4.06
3.00
f1 (ppm)


wwb-90-c
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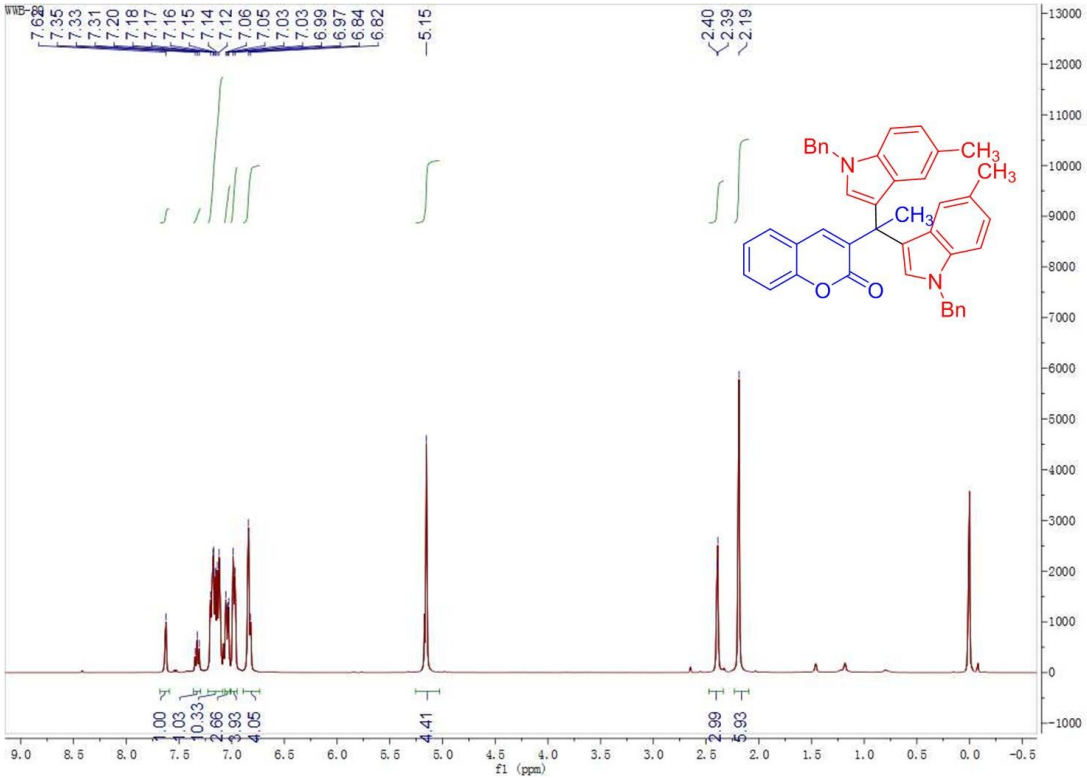
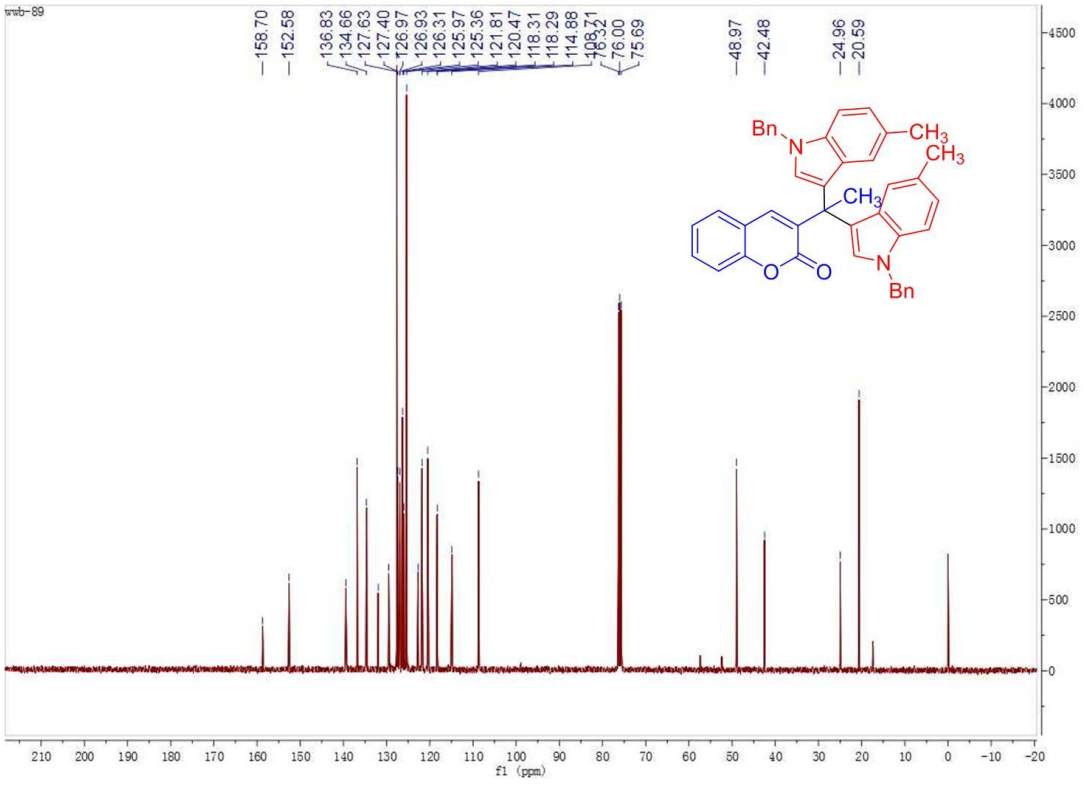
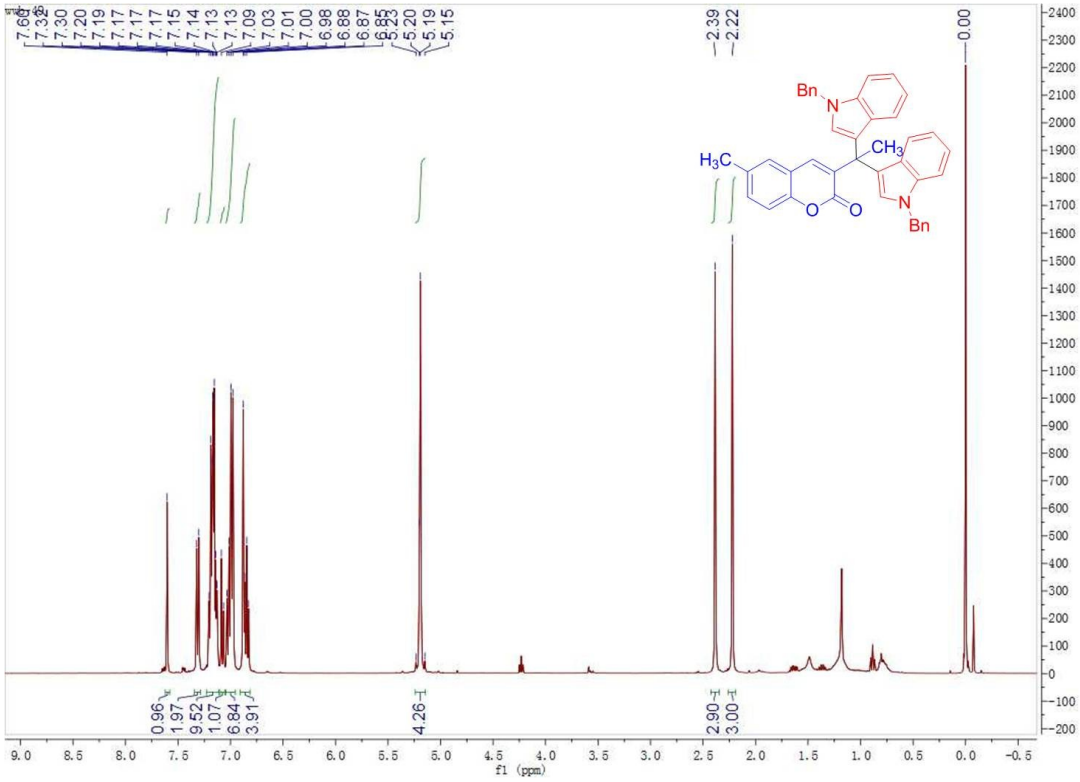
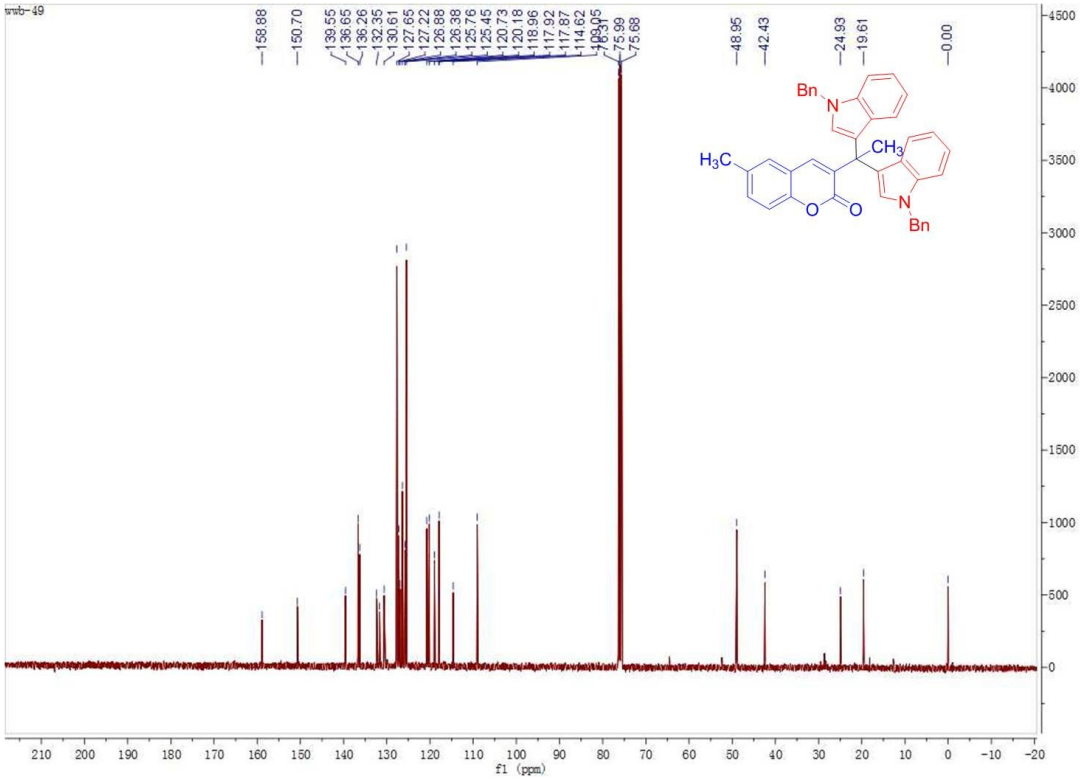
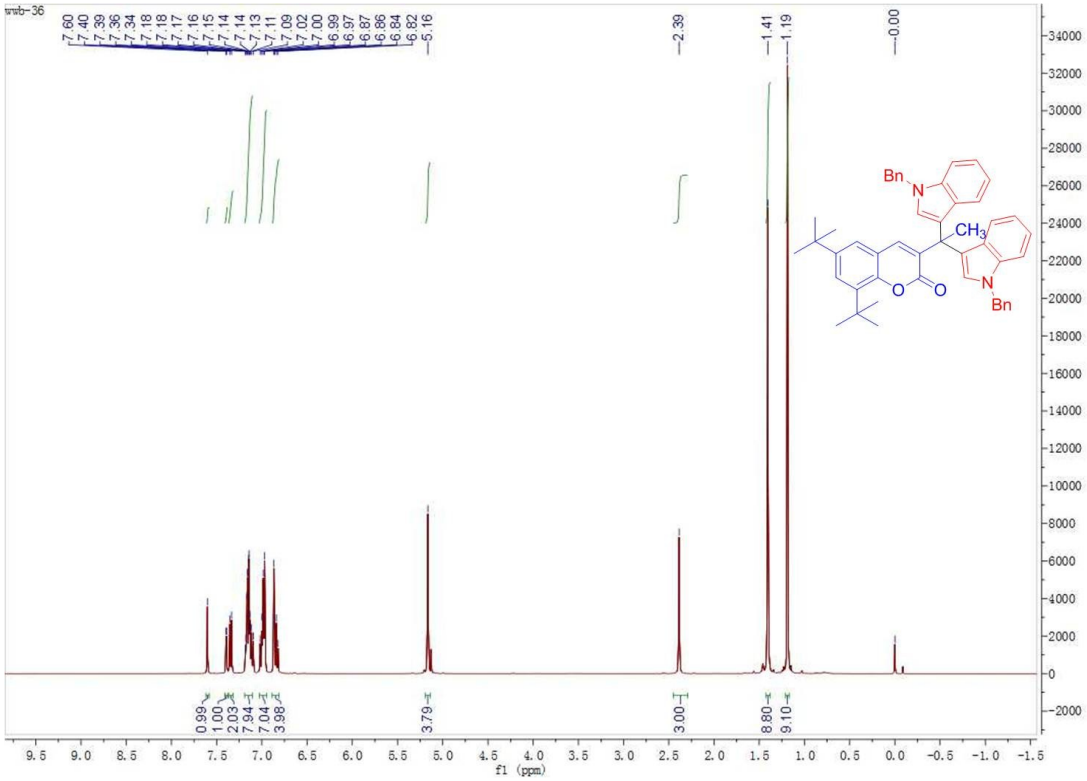
152.59
137.76
137.51
132.83
128.97
128.78
128.40
127.73
127.51
127.48
127.10
126.48
119.30
112.04
110.86
77.42
77.10
76.79
70.82
50.28
43.40
25.68
Bn
N
OBn
OBn
CH3
O
O
N
Bn
f1 (ppm)

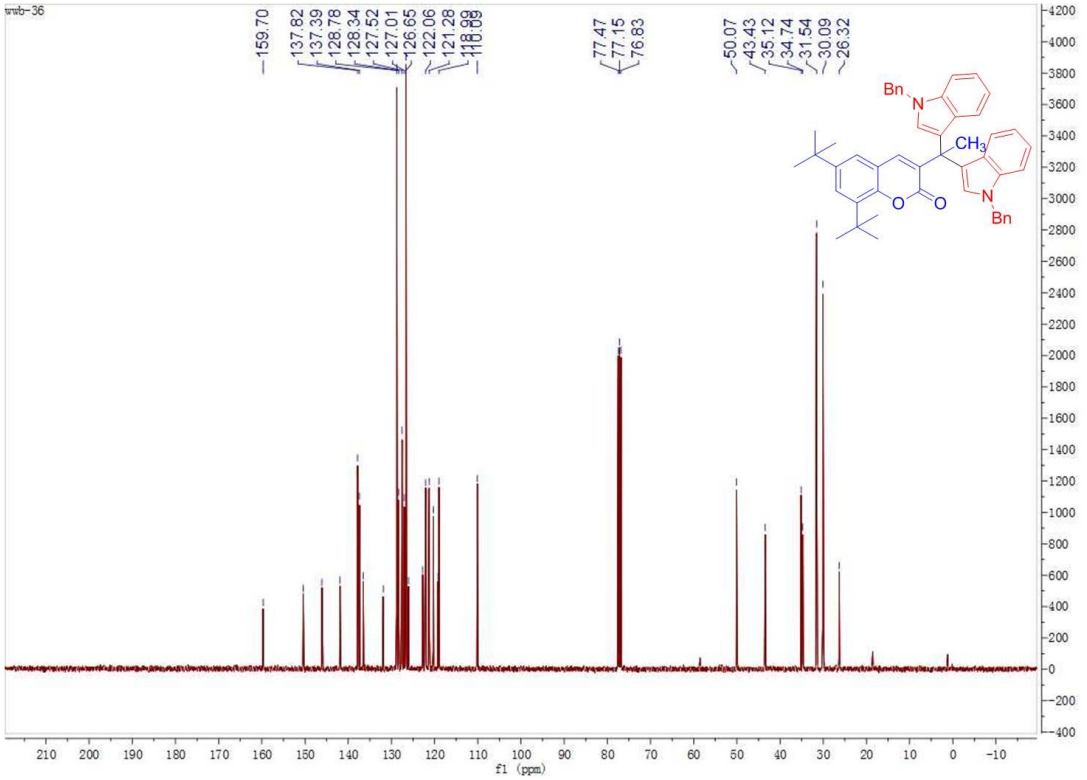

WWB-89
7.62
7.35
7.33
7.31
7.20
7.18
7.17
7.16
7.15
7.14
7.12
7.06
7.05
7.03
6.99
6.97
6.84
6.82
5.15
2.40
2.39
2.19
Bn
N
CH3
CH3
CH3
O
O
N
Bn
1.00
1.03
10.33
2.66
3.93
4.05
4.41
2.99
5.93
f1 (ppm)


wwb-89
158.70
152.58
136.83
134.66
127.63
127.40
126.97
126.93
126.31
125.97
125.36
121.81
120.47
118.31
118.29
114.88
108.71
108.21
76.00
75.69
48.97
42.48
24.96
20.59
Bn
N
CH3
CH3
CH3
O
O
N
Bn
f1 (ppm)


Bn
N
CH3
H3C
O
O
N
Bn


wwb-49
Bn
N
CH3
H3C
O
O
N
Bn


wwb-36
7.60
7.40
7.39
7.36
7.34
7.18
7.18
7.17
7.16
7.15
7.14
7.14
7.13
7.11
7.09
7.02
7.00
6.99
6.97
6.87
6.86
6.84
6.82
5.16
2.39
1.41
1.19
0.00
Bn
N
CH3
N
Bn
O
O
0.99
1.00
2.03
7.94
7.04
3.98
3.79
3.00
8.80
9.10
f1 (ppm)


wwb-36
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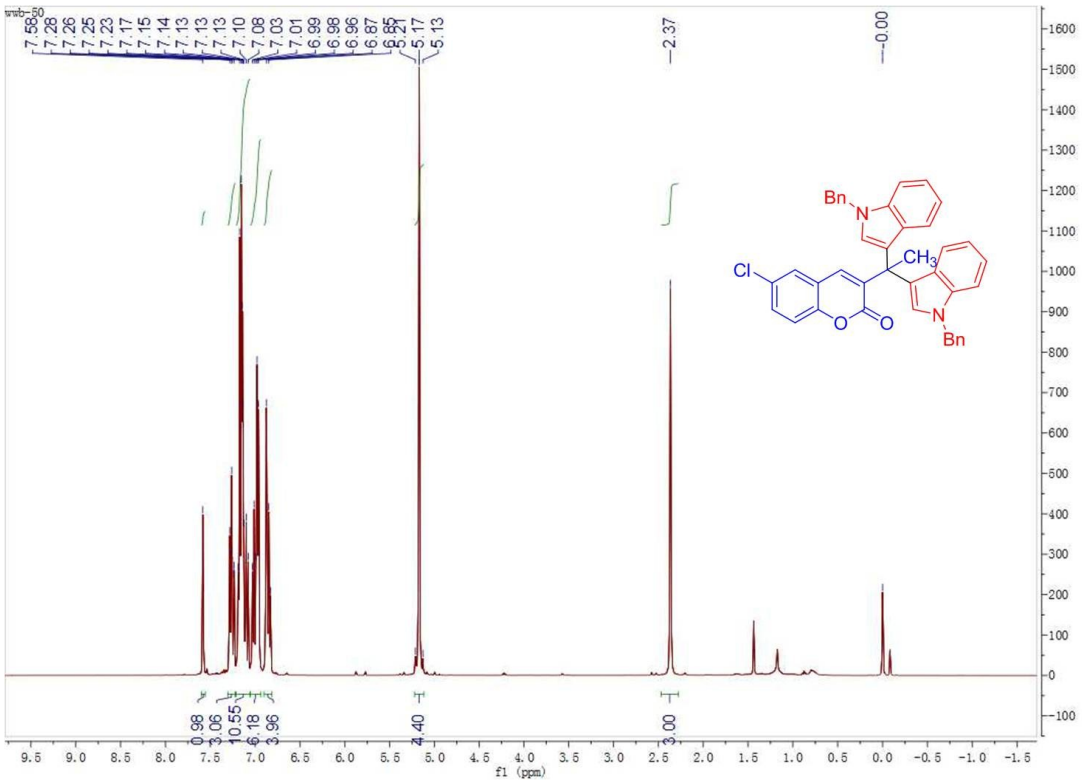
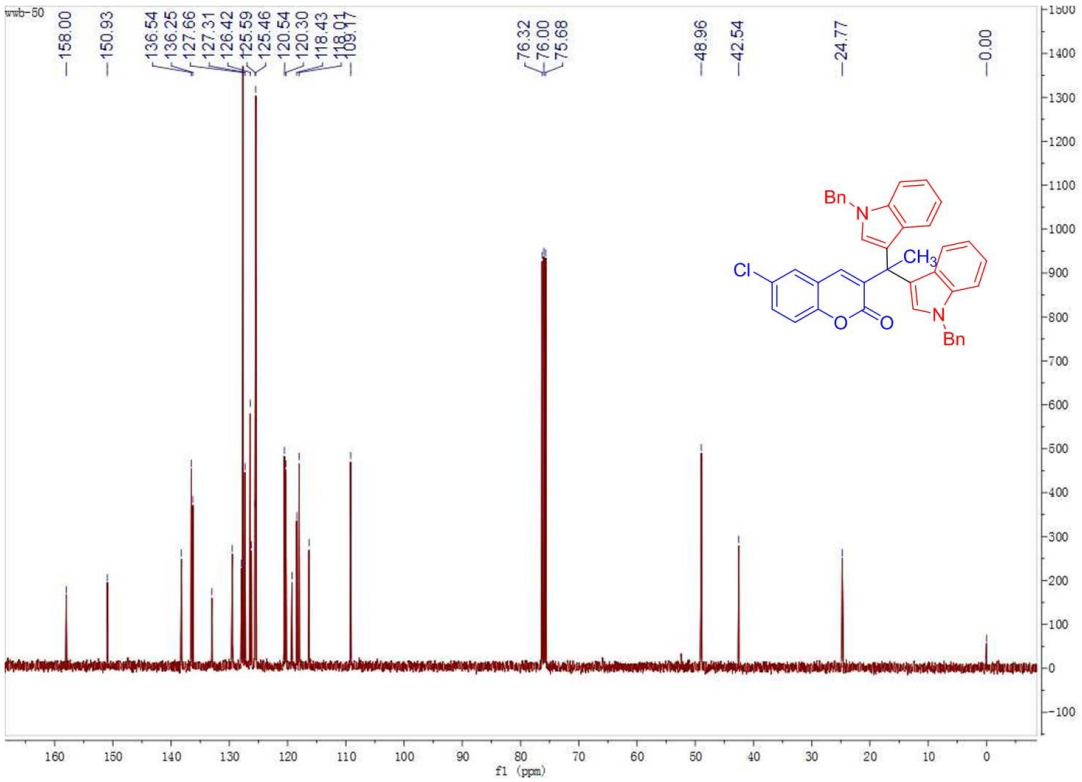
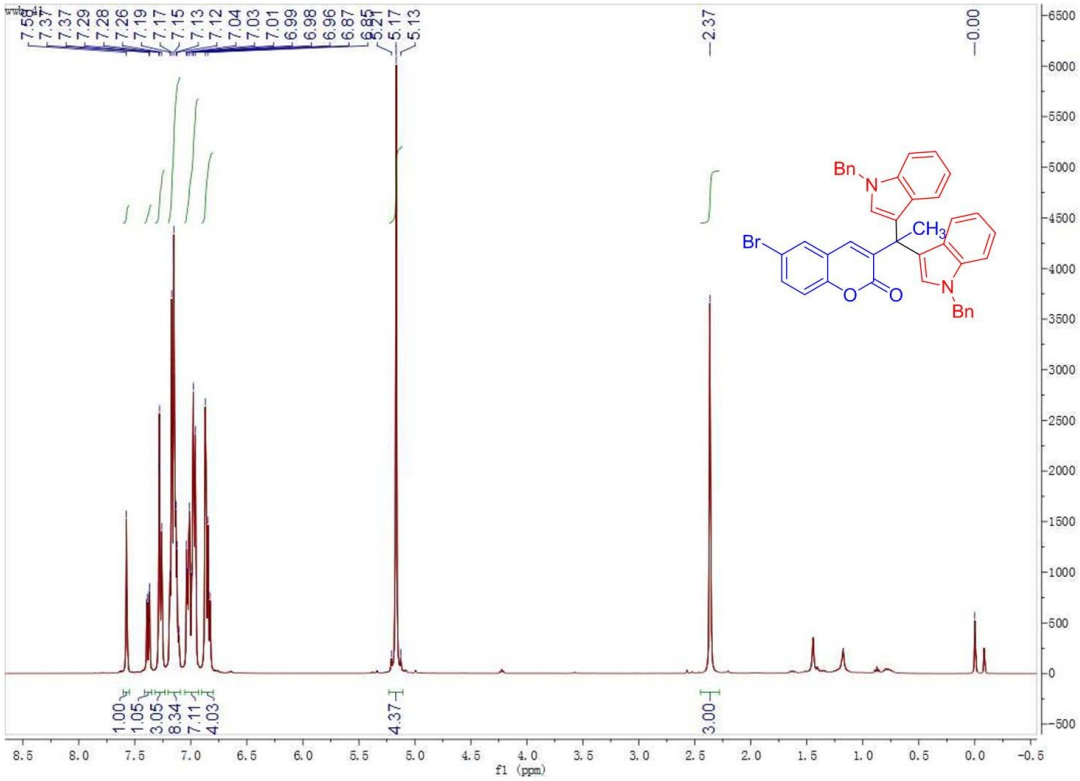
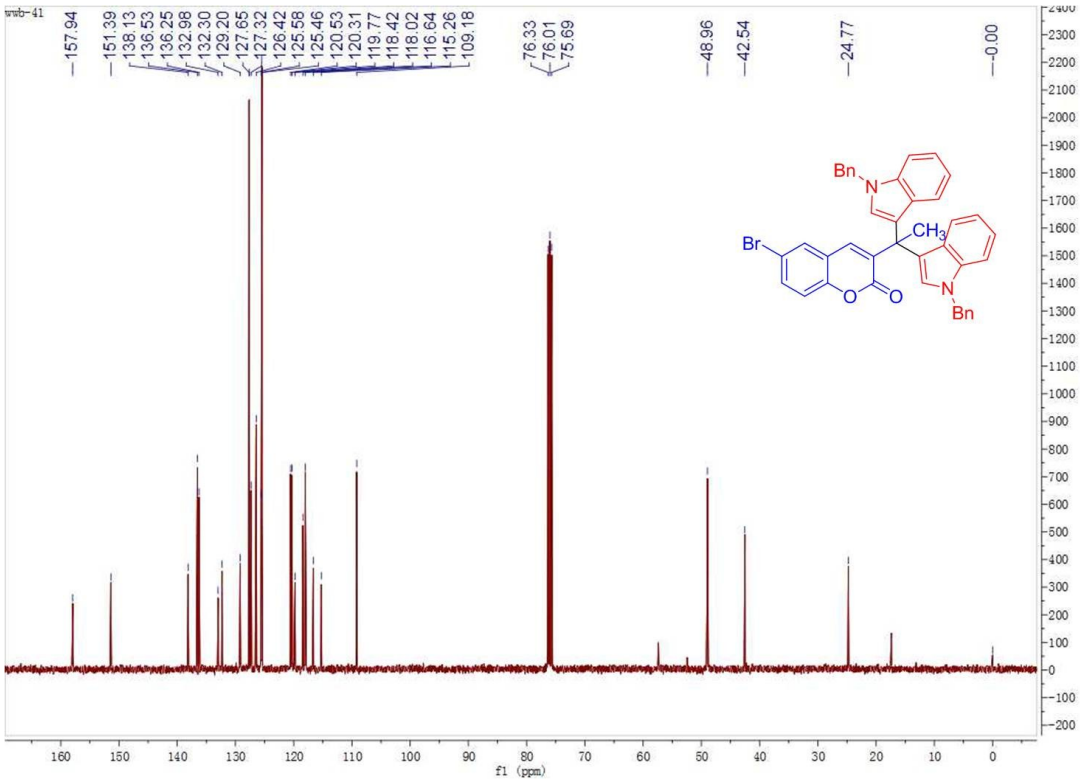
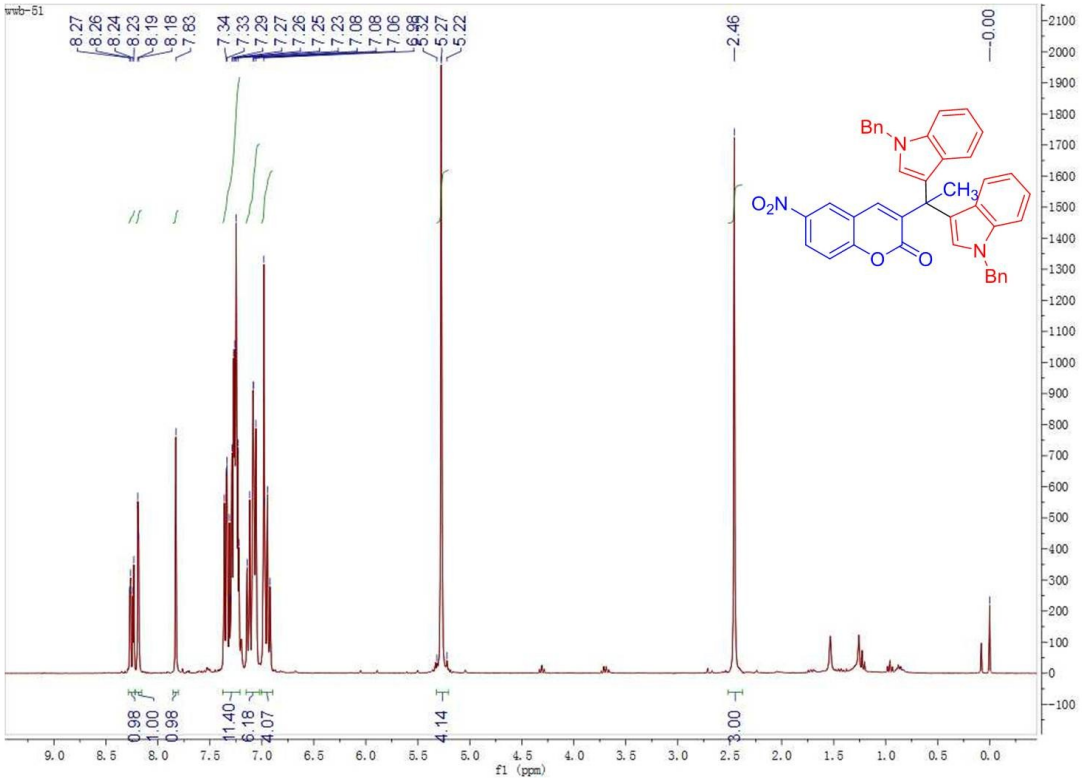
137.82
137.39
128.78
128.34
127.52
127.01
126.65
122.06
121.28
118.09
118.09
77.47
77.15
76.83
50.07
43.43
35.12
34.74
31.54
30.09
26.32
Bn
N
CH3
N
Bn
O
O
f1 (ppm)

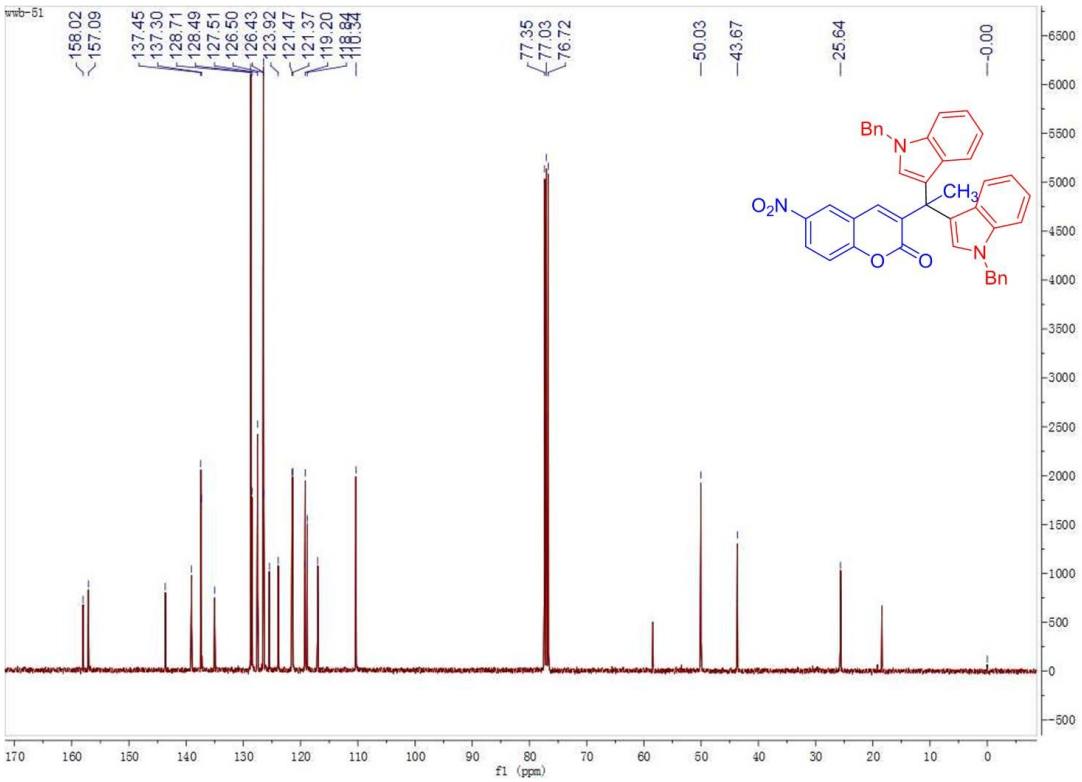

wwb-50
7.58
7.28
7.26
7.25
7.23
7.17
7.15
7.14
7.13
7.13
7.13
7.10
7.08
7.03
7.01
6.99
6.98
6.96
6.87
6.85
5.21
5.17
5.13
2.37
0.00
Bn
N
CH3
Cl
O
O
N
Bn
0.98
3.06
10.55
6.18
3.96
4.40
3.00
f1 (ppm)

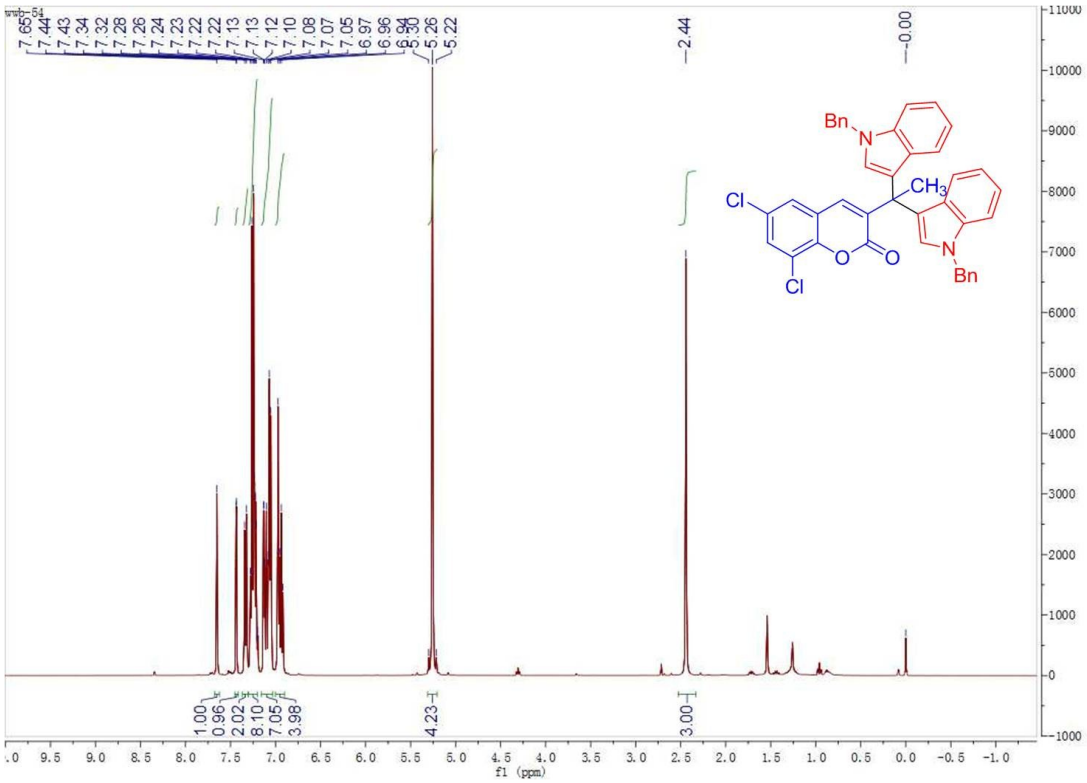

wwb-50
158.00
150.93
136.54
136.25
127.66
127.31
126.42
125.59
125.46
120.54
120.30
118.43
108.97
108.17
76.32
76.00
75.68
48.96
42.54
24.77
0.00
Bn
N
CH3
Cl
O
O
N
Bn
f1 (ppm)


7.50
7.37
7.37
7.29
7.28
7.26
7.19
7.17
7.15
7.13
7.12
7.04
7.03
7.01
6.99
6.98
6.96
6.87
5.17
5.13
2.37
0.00
Bn
N
CH3
Br
O
O
N
Bn
1.00
1.05
3.05
8.34
7.11
4.03
4.37
3.00
f1 (ppm)


wwb-41
157.94
151.39
138.13
136.53
136.25
132.98
132.30
129.20
127.65
127.32
126.42
125.58
125.46
120.53
120.31
119.77
118.42
118.02
116.64
115.26
109.18
76.33
76.01
75.69
48.96
42.54
24.77
0.00
Bn
N
CH3
Br
O
O
N
Bn
f1 (ppm)


wwb-51
8.27
8.26
8.24
8.23
8.19
8.18
7.83
7.34
7.33
7.29
7.27
7.26
7.25
7.23
7.08
7.06
5.27
5.22
2.46
0.00
Bn
N
CH3
O2N
O
O
N
Bn
0.98
1.00
0.98
11.40
6.18
4.07
4.14
3.00
f1 (ppm)


wwb-51
158.02
157.09
137.45
137.30
128.71
128.49
127.51
126.50
126.43
123.92
121.47
121.37
119.20
77.35
77.03
76.72
50.03
43.67
25.64
0.00
Bn
N
CH3
O2N
O
O
N
Bn
f1 (ppm)


wwb-54
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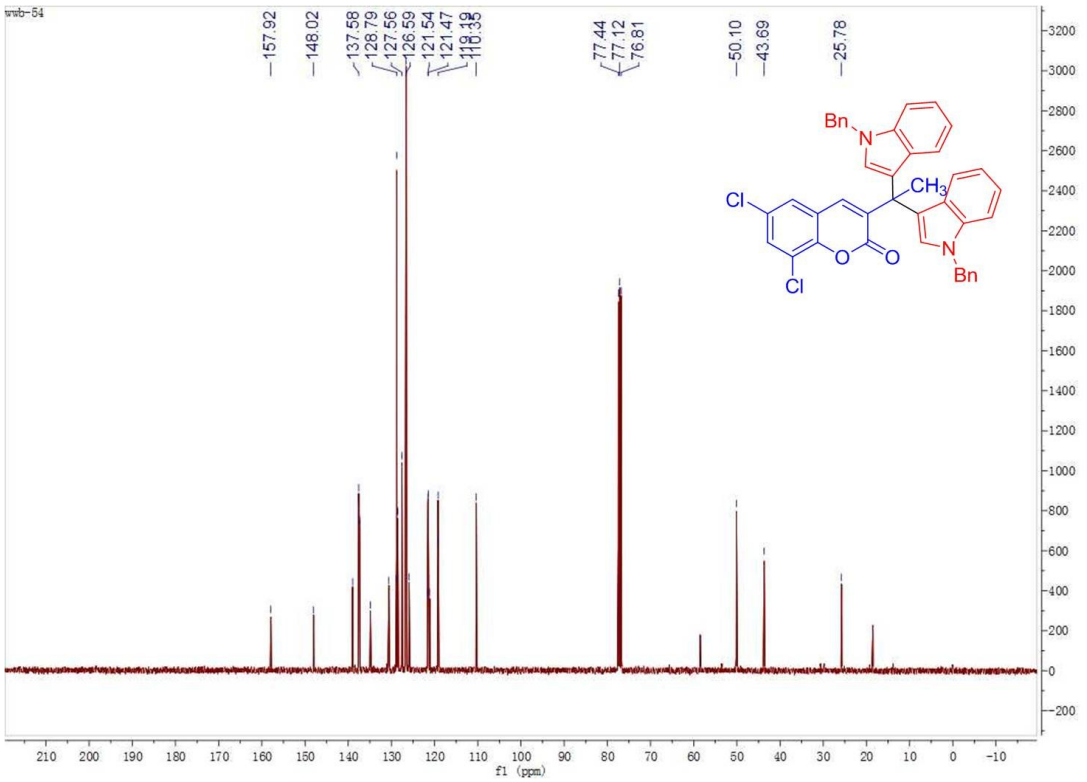
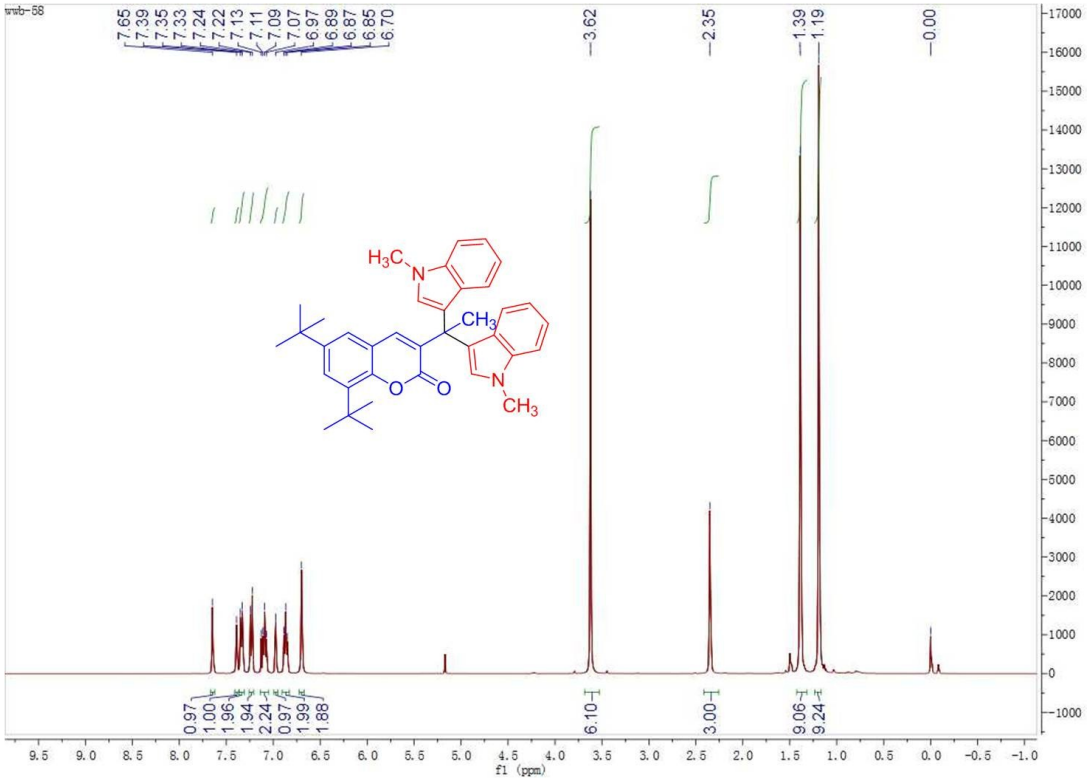
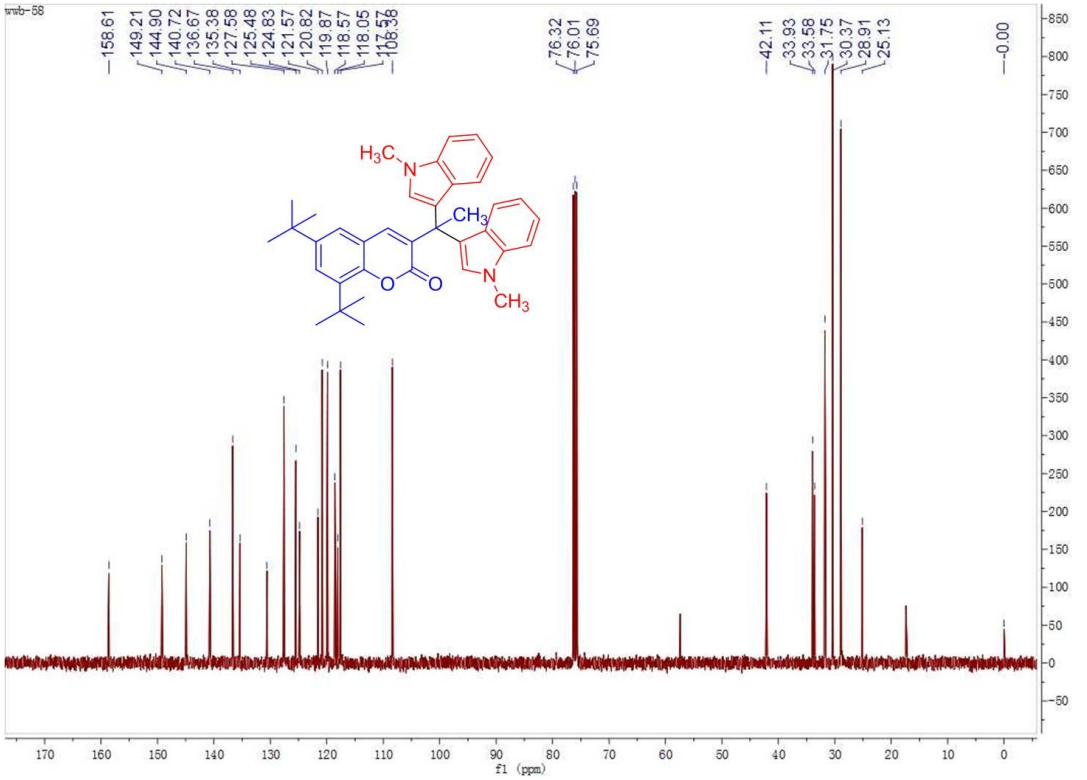
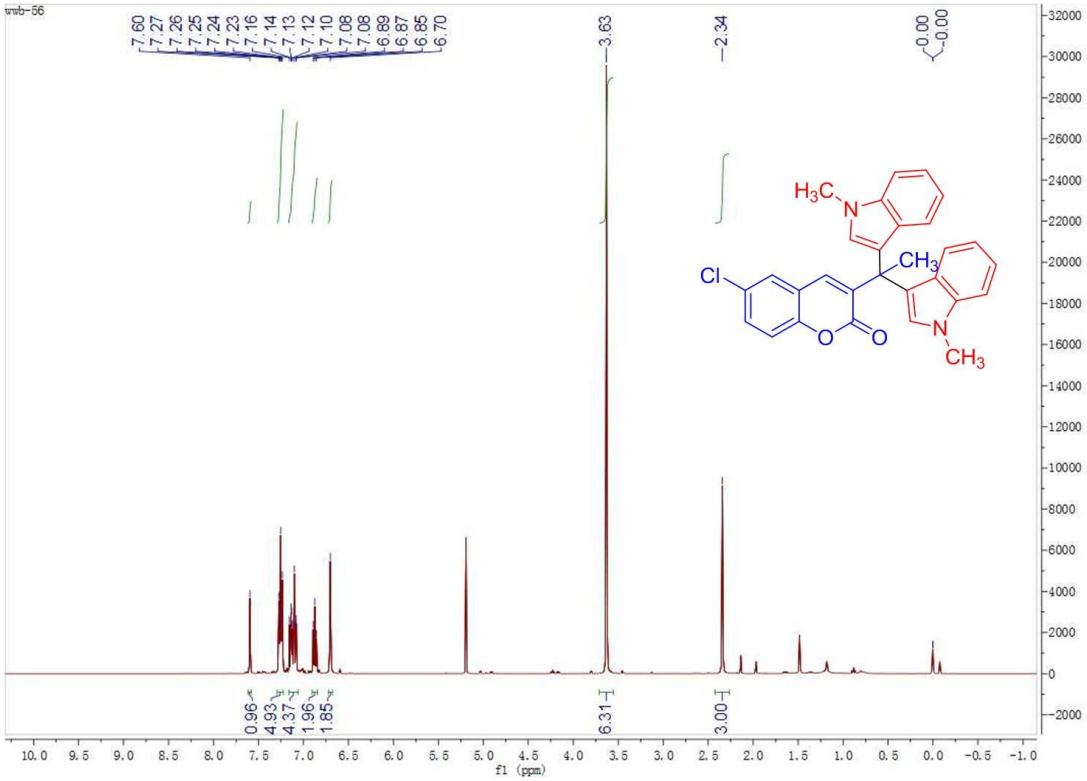
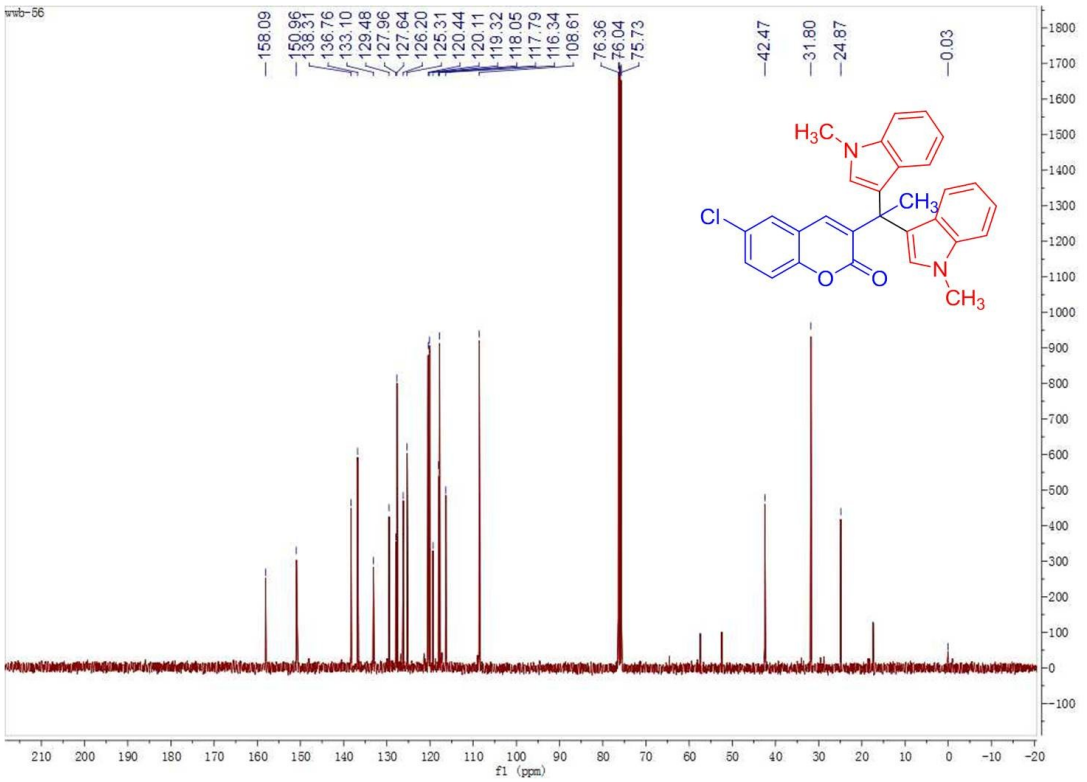
7.44
7.43
7.34
7.32
7.28
7.26
7.24
7.23
7.22
7.22
7.13
7.13
7.12
7.10
7.08
7.07
7.05
6.97
6.96
6.94
5.30
5.26
5.22
2.44
0.00
Bn
N
CH3
Cl
O
O
N
Bn
Cl
1.00
0.96
2.02
8.10
7.05
3.98
4.23
3.00
f1 (ppm)

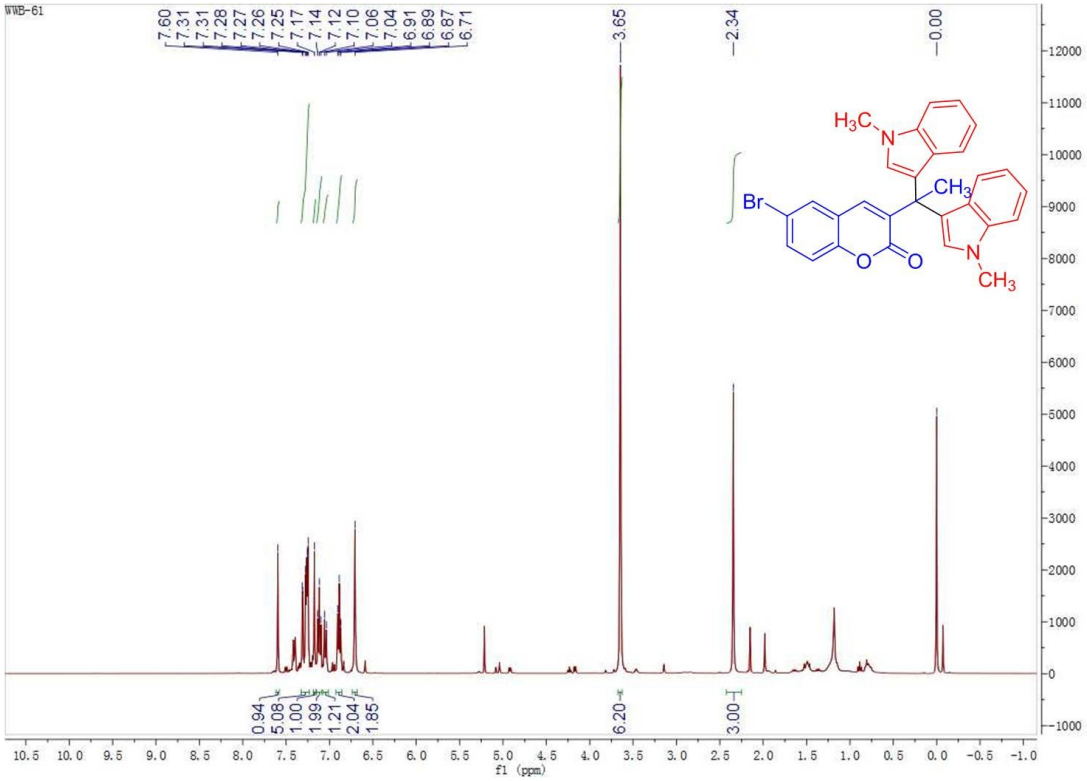

wwb-54
157.92
148.02
137.58
128.79
127.56
126.59
121.54
121.47
77.44
77.12
76.81
50.10
43.69
25.78
Bn
N
CH3
Cl
O
O
N
Bn
Cl
f1 (ppm)

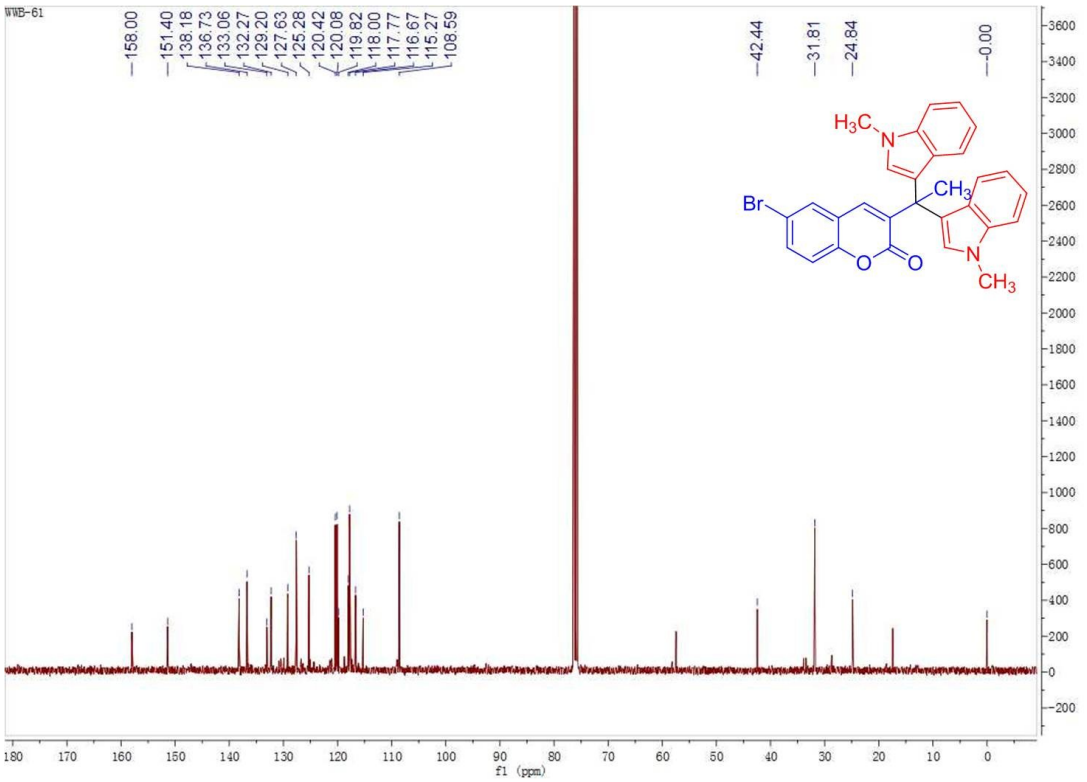

wwb-58
7.65
7.39
7.35
7.33
7.24
7.22
7.13
7.11
7.09
7.07
6.97
6.89
6.87
6.85
6.70
3.62
2.35
1.39
1.19
0.00
0.97
1.00
1.96
1.94
2.24
0.97
1.99
1.88
6.10
3.00
9.06
9.24
f1 (ppm)


wwb-58
158.61
149.21
144.90
140.72
136.67
135.38
127.58
125.48
124.83
121.57
120.82
119.87
118.57
118.05
76.32
76.01
75.69
42.11
33.93
33.58
31.75
30.37
28.91
25.13
0.00
f1 (ppm)


wwb-56
7.60
7.27
7.26
7.25
7.24
7.23
7.16
7.14
7.13
7.12
7.10
7.08
7.08
6.89
6.87
6.85
6.70
3.63
2.34
0.00
0.00
0.96
4.93
4.37
1.96
1.85
6.31
3.00
f1 (ppm)


wwb-56
158.09
150.96
138.31
136.76
133.10
129.48
127.96
127.64
126.20
125.31
120.44
120.11
119.32
118.05
117.79
116.34
108.61
76.36
76.04
75.73
42.47
31.80
24.87
0.03
f1 (ppm)


WWB-61
7.60
7.31
7.31
7.28
7.27
7.26
7.25
7.17
7.14
7.12
7.10
7.06
7.04
6.91
6.89
6.87
6.71
3.65
2.34
0.00
0.94
5.08
1.00
1.99
1.21
2.04
1.85
6.20
3.00
f1 (ppm)


WWB-61
158.00
151.40
138.18
136.73
133.06
132.27
129.20
127.63
125.28
120.42
120.08
119.82
118.00
117.77
116.67
115.27
108.59
42.44
31.81
24.84
0.00
f1 (ppm)