Supporting Information

One-pot synthesis of benzofused heteroaryl azoles via tandem C-heteroatom coupling/C-H activation of azoles

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I. General Remarks

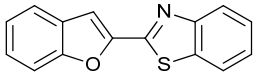
NMR spectra were obtained on a Bruker AMX-400 or a Bruker AMX-600. The ^{1}H NMR (400 MHz or 600 MHz) chemical shifts were measured relative to $CDCl_3$ as the internal reference ($CDCl_3$: δ = 7.26 ppm). The ^{13}C NMR (100 MHz or 150 MHz) chemical shifts were given using $CDCl_3$ as the internal standard ($CDCl_3$: δ = 77.16 ppm). The following abbreviations were used to designate the multiplicities: s = singlet, d = doublet, t = triplet, bs = broad signal, m = multiplet. High-resolution mass spectra (HR-MS) were obtained with a Waters-Q-TOF-Premier (ESI). Melting points were determined with XRC-1 and are uncorrected.

Unless otherwise noted, all reagents were obtained from commercial suppliers and used without further purification. 2-*gem*-dibromovinylphenols,[1] 2-*gem*-dibromovinylthiophenols,[1,2] 2-*gem*-dibromovinylanilines,[3] *n*-benzylictheophylline,[4] *n*-butyl theophylline, and 1-methylbenzimidazole[5] were prepared according to the literature procedures. Solvents were dried over CaH_2 (NMP, DMF or DMSO) or sodium (dioxane or toluene), and freshly distilled prior to use. Unless otherwise indicated, all syntheses and manipulations were carried out under N_2 atmosphere.

II. General procedure for one-pot synthesis of benzofused heteroaryl azoles

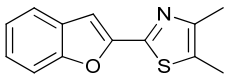
A flame-dried Schlenk test tube with a magnetic stirring bar was charged with CuI (9.5 mg, 0.05 mmol), 1,10-phenanthroline (9.0 mg, 0.05 mmol), *t*-BuOLi (120 mg, 1.5 mmol), azole (0.25 mmol), *gem*-dihaloolefin (0.5 mmol), and dioxane (1.0 mL) under N_2. The reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. The reaction mixture was then cooled to ambient temperature, diluted with 20 mL of CH_2Cl_2, filtered through a celite pad, and washed with 10-20 mL of CH_2Cl_2. The combined organic extracts were concentrated and the resulting residue was purified by column chromatography on silica gel to provide the desired product.

III. Experimental data for the described substances



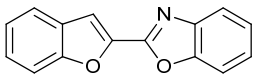
2-(Benzofuran-2-yl)-benzothiazole (3a)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 20/1, v/v) afforded the desired product as a yellow solid (83%). mp: 222-224 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.29 (t, J = 7.6 Hz, 1H), 7.39-7.44 (m, 2H), 7.51-7.54 (m, 2H), 7.61 (d, J = 8.4 Hz, 1H), 7.68 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 7.6 Hz, 1H), 8.12 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 107.7, 112.0, 121.8, 122.3, 123.6, 123.9, 125.8, 126.6, 126.8, 128.3, 134.8, 149.9, 154.0, 155.6, 157.7 ppm. HRMS (ESI): calcd for $C_{15}H_{10}NOS$ $[M+H]^+$ 252.0483, found 252.0486.



2-(Benzofuran-2-yl)-4,5-dimethylthiazole (3b)

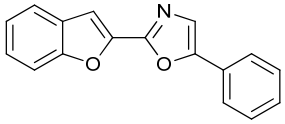
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 20/1, v/v) afforded the desired product as a yellow solid (77%). mp: 118-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.38 (s, 6H), 7.19 (s, 1H), 7.21 (d, J = 7.2 Hz, 1H), 7.27 (t, J = 7.8 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.56 (d, J = 7.6 Hz, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 11.6, 15.0, 104.0, 111.7, 121.7, 123.6, 125.5, 127.6, 128.6, 150.1, 150.4, 153.3, 155.0 ppm. HRMS (ESI): calcd for $C_{13}H_{12}NOS$ $[M+H]^+$ 230.0640, found 230.0636.



2-(Benzofuran-2-yl)-benzoxazole (3c)

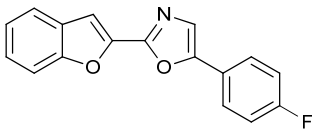
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 20/1, v/v) afforded the desired product as a yellow solid (68%). mp: 168-170 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.30 (t, J = 7.6 Hz, 1H), 7.38-7.41 (m, 2H), 7.43 (d, J = 7.6 Hz, 1H), 7.59-7.61 (m, 2H), 7.63 (d, J

= 8.4 Hz, 1H), 7.69 (d, J = 7.6 Hz, 1H), 7.80-7.82 (m, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 110.4, 110.9, 112.2, 120.6, 122.4, 124.1, 125.2, 126.0, 127.1, 127.7, 141.8, 143.8, 150.6, 155.5, 156.0 ppm. HRMS (ESI): calcd for $C_{15}H_{10}NO_2$ $[M+H]^+$ 236.0712, found 236.0709.



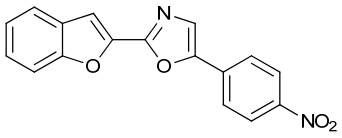
2-(Benzofuran-2-yl)-5-phenyloxazole (3d)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 10/1, v/v) afforded the desired product as a yellow solid (92%). mp: 87-89 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.28 (t, J = 7.4 Hz, 1H), 7.32-7.38 (m, 2H), 7.40-7.44 (m, 2H), 7.46 (d, J = 7.6 Hz, 1H), 7.51 (s, 1H), 7.60 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 7.6 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 107.5, 112.0, 122.0, 123.7, 123.8, 124.5, 126.3, 127.5, 127.9, 128.9, 129.1, 144.1, 151.8, 154.0, 155.5 ppm. HRMS (ESI): calcd for $C_{17}H_{12}NO_2$ $[M+H]^+$ 262.0868, found 262.0863.



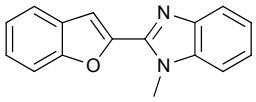
2-(Benzofuran-2-yl)-5-(4-fluorophenyl)-oxazole (3e)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 6/1, v/v) afforded the desired product as a yellow solid (91%). mp: 116-118 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.13 (t, J = 8.6 Hz, 2H), 7.28 (t, J = 7.4 Hz, 1H), 7.37-7.41 (m, 2H), 7.44 (s, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.66 (d, J = 8.0 Hz, 1H), 7.69-7.71 (m, 2H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 107.6, 112.0, 116.2, 116.4, 122.0, 123.4, 123.8, 123.88, 123.90, 126.37, 126.40, 126.5, 127.9, 144.0, 151.0, 154.0, 155.5, 162.2, 163.8 ppm. HRMS (ESI): calcd for $C_{17}H_{11}FNO_2$ $[M+H]^+$ 280.0774, found 280.0781.



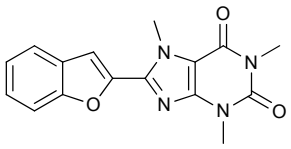
2-(Benzofuran-2-yl)-5-(4-nitrophenyl)-oxazole (3f)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether /EtOAc = 4/1, v/v) afforded the desired product as a yellow solid (72%). mp: 188-190 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.31 (t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.6 Hz, 1H), 7.52 (s, 1H), 7.62 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 8.0 Hz, 2H), 7.89 (d, J = 8.4 Hz, 2H), 8.32 (d, J = 8.4 Hz, 2H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 108.9, 112.1, 112.3, 124.1, 124.7, 124.9, 126.9, 127.2, 127.7, 133.3, 143.5, 147.5, 149.6, 155.5, 155.7 ppm. HRMS (ESI): calcd for $C_{17}H_{11}N_2O_4$ $[M+H]^+$ 307.0719, found 307.0711.



2-(Benzofuran-2-yl)-1-methylbenzoimidazole (3g)

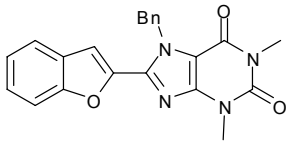
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 6/1, v/v) afforded the desired product as a white solid (68%). mp: 132-134 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.06 (s, 3H), 7.23-7.29 (m, 3H), 7.33-7.36 (m, 2H), 7.45 (s, 1H), 7.55 (d, J = 8.0 Hz, 1H), 7.63 (d, J = 8.0 Hz, 1H), 7.79-7.82 (m, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 31.9, 108.7, 109.6, 111.8, 120.2, 122.0, 123.1, 123.6, 123.8, 125.9, 128.0, 136.5, 143.1, 144.3, 147.1, 155.3 ppm. HRMS (ESI): calcd for $C_{16}H_{13}N_2O$ $[M+H]^+$ 249.1028, found 249.1033.



8-(Benzofuran-2-yl)-1,3,7-trimethylxanthine (3h)[6]

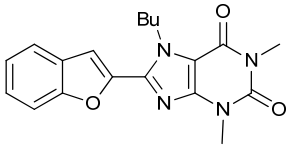
Following the general procedure, the reaction mixture was stirred for 10 min at room

temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 2/1, v/v) afforded the desired product as a yellow solid (86%). mp: 230-233 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.43 (s, 3H), 3.64 (s, 3H), 4.38 (s, 3H), 7.30 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 7.8 Hz, 1H), 7.45 (s, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 28.2, 30.0, 34.1, 108.7, 109.8, 111.9, 122.1, 124.1, 126.5, 127.6, 142.8, 145.6, 148.5, 151.7, 155.4, 155.5 ppm. HRMS (ESI): calcd for $C_{16}H_{15}N_4O_3$ $[M+H]^+$ 311.1144, found 311.1140.



8-(Benzofuran-2-yl)-7-benzyl-1,3-dimethylxanthine (3i)

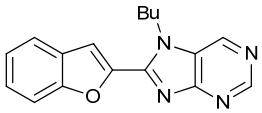
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 3/1, v/v) afforded the desired product as a yellow solid (91%). mp: >250 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.44 (s, 3H), 3.68 (s, 3H), 6.09 (s, 2H), 7.28 (m, 5H), 7.33 (t, J = 7.8 Hz, 1H), 7.40 (t, J = 7.6 Hz, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 7.6 Hz, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 28.3, 30.0, 49.9, 108.3, 110.3, 111.8, 122.2, 124.1, 126.6, 127.2, 127.6, 128.2, 129.0, 136.6, 142.6, 145.5, 148.9, 151.8, 155.2, 155.4 ppm. HRMS (ESI): calcd for $C_{22}H_{19}N_4O_3$ $[M+H]^+$ 387.1457, found 387.1460.



8-(Benzofuran-2-yl)-7-butyl-1,3-dimethylxanthine (3j)

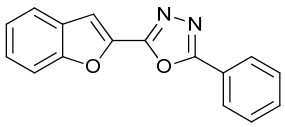
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 5/1, v/v) afforded the desired product as a yellow solid (78%). mp: 155-157 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.97 (t, J = 7.4 Hz, 3H), 1.44-1.49 (m, 2H), 1.88-1.96 (m, 2H), 3.44 (s, 3H), 3.65 (s, 3H), 4.79 (t, J =

7.6 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 1H), 7.47 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 1H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 13.8, 19.9, 28.2, 29.9, 33.4, 46.9, 108.3, 109.9, 111.7, 122.1, 124.1, 126.4, 127.6, 142.1, 145.8, 148.6, 151.7, 155.1, 155.3 ppm. HRMS (ESI): calcd for $C_{19}H_{21}N_4O_3$ $[M+H]^+$ 353.1614, found 353.1605.



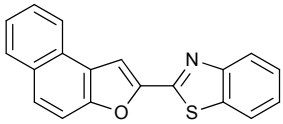
8-(Benzofuran-2-yl)-7-butylpurine (3k)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc/acetone= 4/1/1, v/v) afforded the desired product as a yellow solid (77%). mp: 92-95 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 0.97 (t, *J* = 7.4 Hz, 3H), 1.41-1.50 (m, 2H), 1.89-2.03 (m, 2H), 4.72 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.67 (s, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 9.12 (s, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.8, 20.1, 32.3, 44.1, 100.1, 110.8, 111.9, 122.4, 124.2, 126.9, 127.6, 146.1, 152.6, 152.8, 155.6 ppm. HRMS (ESI): calcd for $C_{17}H_{17}N_4O$ $[M+H]^+$ 293.1402, found 293.1403.



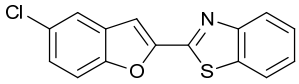
2-(Benzofuran-2-yl)-5-phenyl-1,3,4-oxadiazole (3l)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 15/1, v/v) afforded the desired product as a white solid (73%). mp: 170-172 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.32 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.53-7.57 (m, 3H), 7.59 (s, 1H), 7.64 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.0 Hz, 1H), 8.17 (d, *J* = 6.8 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 110.3, 112.3, 122.5, 123.5, 124.2, 127.2, 127.3, 127.4, 129.3, 132.2, 140.8, 155.9, 158.0, 164.8 ppm. HRMS (ESI): calcd for $C_{16}H_{11}N_2O_2$ $[M+H]^+$ 263.0821, found 263.0812.



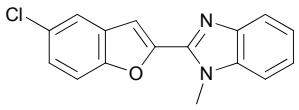
2-(Naphtho[2,1-b]furan-2-yl)-benzothiazole (4a)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 25/1, v/v) afforded the desired product as a white solid (80%). mp: 172-174 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40 (t, J = 7.6 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 9.2 Hz, 1H), 7.92 (t, J = 8.6 Hz, 2H), 8.02 (s, 1H), 8.12 (d, J = 8.4 Hz, 1H), 8.17 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 106.8, 112.5, 121.8, 123.5, 123.6, 124.1, 125.4, 125.6, 126.8, 127.2, 127.8, 127.9, 129.1, 130.7, 134.7, 149.4, 153.7, 154.0, 157.7 ppm. HRMS (ESI): calcd for $C_{19}H_{12}NOS$ $[M+H]^+$ 302.0640, found 302.0638.



2-(5-Chlorobenzofuran-2-yl)-benzothiazole (4b)

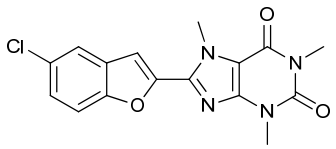
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 20/1, v/v) afforded the desired product as a yellow solid (84%). mp: 203-205 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.35 (d, J = 8.0 Hz, 1H), 7.43-7.47 (m, 2H), 7.53-7.56 (m, 2H), 7.66 (s, 1H), 7.94 (d, J = 8.0 Hz, 1H), 8.12 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 106.9, 112.4, 113.0, 121.7, 121.9, 123.8, 126.1, 126.8, 127.0, 129.6, 134.9, 151.3, 153.9, 154.0, 157.1 ppm. HRMS (ESI): calcd for $C_{15}H_9ClNOS$ $[M+H]^+$ 286.0093, found 286.0100.



2-(5-Chlorobenzofuran-2-yl)-1-methylbenzoimidazole (4c)

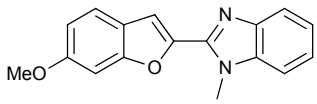
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 6/1, v/v) afforded the desired product as a

white solid (64%). mp: 108-110 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.13 (s, 3H), 7.31-7.35 (m, 3H), 7.40 (d, J = 7.2 Hz, 1H), 7.44 (s, 1H), 7.51 (d, J = 8.4 Hz, 1H), 7.65 (ds, 1H), 7.83 (d, J = 6.8 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.9, 108.0, 109.7, 112.8, 120.3, 121.4, 123.3, 123.9, 126.2, 129.3, 129.5, 136.5, 143.1, 143.7, 148.5, 153.7 ppm. HRMS (ESI): calcd for $C_{16}H_{12}ClN_2O$ $[M+H]^+$ 283.0638, found 283.0644.



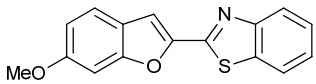
8-(5-Chlorobenzofuran-2-yl)-1,3,7-trimethylxanthine (4d)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc/acetone = 6/1/1, v/v) afforded the desired product as a yellow solid (56%). mp: >250 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.42 (s, 3H), 3.62 (s, 3H), 4.36 (s, 3H), 7.34-7.37 (m, 2H), 7.49 (d, J = 7.2 Hz, 1H), 7.63 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 28.2, 30.0, 34.1, 108.8, 109.0, 112.8, 121.5, 126.7, 128.9, 129.8, 142.1, 147.0, 148.4, 151.6, 153.7, 155.4 ppm. HRMS (ESI): calcd for $C_{16}H_{14}ClN_4O_3$ $[M+H]^+$ 345.0754, found 345.0747.



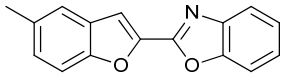
2-(6-Methoxybenzofuran-2-yl)-1-methylbenzoimidazole (4e)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 3/1, v/v) afforded the desired product as a white solid (66%). mp: 136-138 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.89 (s, 3H), 4.12 (s, 3H), 6.93 (d, J = 8.4 Hz, 1H), 7.12 (s, 1H), 7.29-7.32 (m, 2H), 7.38-7.40 (m, 1H), 7.43 (s, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.82-7.84 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.9, 55.9, 96.0, 108.7, 109.5, 113.3, 120.1, 121.3, 122.1, 123.0, 123.4, 136.5, 143.2, 144.6, 146.3, 156.5, 159.4 ppm. HRMS (ESI): calcd for $C_{17}H_{15}N_2O_2$ $[M+H]^+$ 279.1134, found 279.1138.



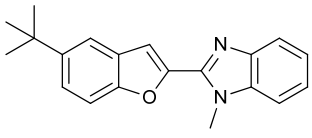
2-(6-Methoxybenzofuran-2-yl)-benzothiazole (4f)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 10/1, v/v) afforded the desired product as a white solid (81%). mp: 145-147 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.89 (s, 3H), 7.12 (s, 1H), 7.38 (t, J = 7.6 Hz, 1H), 7.45-7.49 (m, 2H), 7.51-7.55 (m, 2H), 7.90 (d, J = 8.0 Hz, 1H), 8.09 (d, J = 8.0 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 55.9, 96.0, 107.9, 112.4, 113.6, 121.6, 121.7, 122.5, 123.4, 125.5, 126.7, 134.6, 149.2, 154.0, 156.9, 159.9 ppm. HRMS (ESI): calcd for $C_{16}H_{12}NO_2S$ $[M+H]^+$ 282.0589, found 282.0587.



2-(5-Methylbenzofuran-2-yl)-benzoxazole (4g)

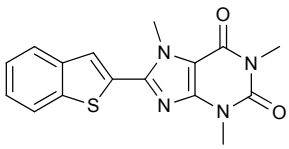
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether /EtOAc = 20/1, v/v) afforded the desired product as a white solid (74%). mp: 117-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.47 (s, 3H), 7.24 (d, J = 8.4 Hz, 1H), 7.38-7.40 (m, 2H), 7.48 (s, 1H), 7.51-7.54 (m, 2H), 7.60-7.62 (m, 1H), 7.80-7.82 (m, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.4, 110.2, 110.8, 111.7, 120.5, 122.0, 125.2, 125.9, 127.8, 128.5, 133.6, 141.8, 143.8, 150.5, 154.5, 155.6 ppm. HRMS (ESI): calcd for $C_{16}H_{12}NO_2$ $[M+H]^+$ 250.0868, found 250.0870.



2-(5-(*tert*-Butyl)benzofuran-2-yl)-1-methylbenzoimidazole (4h)

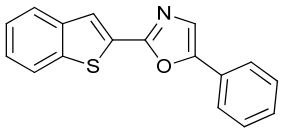
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 6/1, v/v) afforded the desired product as a

white solid (65%). mp: 119-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.41 (s, 9H), 4.15 (s, 3H), 7.32-7.34 (m, 2H), 7.40-7.42 (m, 1H), 7.46 (d, J = 8.8 Hz, 1H), 7.52-7.54 (m, 2H), 7.69 (s, 1H), 7.84 (d, J = 8.4 Hz, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 31.89, 31.92, 34.9, 109.1, 109.6, 111.1, 118.0, 120.0, 123.1, 123.5, 124.2, 127.7, 136.4, 142.9, 144.4, 146.9, 147.0, 153.6 ppm. HRMS (ESI): calcd for $C_{20}H_{21}N_2O$ $[M+H]^+$ 305.1654, found 305.1656.



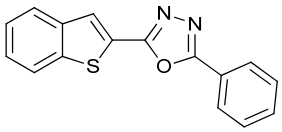
8-(Benzothiophen-2-yl)-1,3,7-trimethylxanthine (4i)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/EtOAc = 2/1, v/v) afforded the desired product as a yellow solid (63%). mp: 293-295 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.44 (s, 3H), 3.65 (s, 3H), 4.30 (s, 3H), 7.43-7.45 (m, 2H), 7.79 (s, 1H), 7.86-7.89 (m, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 28.2, 30.0, 34.0, 122.4, 124.8, 125.29, 125.33, 126.3, 130.8, 139.6, 140.7, 148.3, 151.8, 155.6 ppm. HRMS (ESI): calcd for $C_{16}H_{15}N_4O_2S$ $[M+H]^+$ 327.0916, found 327.0922.



2-(Benzothiophen-2-yl)-5-phenyloxazole (4j)

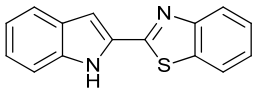
Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether/CH_2Cl_2/EtOAc = 20/2/1, v/v) afforded the desired product as a yellow solid (80%). mp: 101-103 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.37-7.42 (m, 3H), 7.47 (t, J = 7.4 Hz, 3H), 7.73 (d, J = 7.6 Hz, 2H), 7.87 (s, 2H), 7.97 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 122.7, 123.8, 124.3, 124.4, 124.7, 125.1, 126.0, 127.8, 128.8, 129.1, 129.7, 139.7, 140.6, 151.7, 157.4 ppm. HRMS (ESI): calcd for $C_{17}H_{12}NOS$ $[M+H]^+$ 278.0640, found 278.0631.



2-(Benzothiophen-2-yl)-5-phenyl-1,3,4-oxadiazole (4k)

Following the general procedure, the reaction mixture was stirred for 10 min at room temperature, and then heated at 140 °C for 30 h. Purification via silica gel column chromatography (petroleum ether /CH_2Cl_2/EtOAc = 20/2/1, v/v) afforded the desired product as a yellow solid (62%). mp: 144-146 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.43-7.49 (m, 2H), 7.55-7.57 (m, 3H), 7.90 (d, J = 7.2 Hz, 2H), 8.08 (s, 1H), 8.15 (d, J = 7.2 Hz, 2H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 122.8, 123.7, 125.1, 125.4, 126.7, 126.8, 127.2, 129.3, 132.1, 139.2, 141.1, 161.2, 164.7 ppm. HRMS (ESI): calcd for $C_{16}H_{12}N_2OS[M+H]^+$ 279.0592, found 279.0592.

IV. Procedure for one-pot synthesis of 2-(indol-2-yl)-benzothiazole 4l[7]



A flame-dried Schlenk test tube with a magnetic stirring bar was charged with $Pd(OAc)_2$ (2.8 mg, 0.0125 mmol), CuI (4.8 mg, 0.025 mmol), S-phos (10.2 mg, 0.05 mmol), *t*-BuOLi(120 mg, 1.5 mmol), benzothiazole (0.25 mmol), 2-*gem*-dibromovinylaniline (0.5 mmol), and toluene (1.0 mL) under N_2. The reaction mixture was stirred for 10 min at room temperature, and then heated at 120 ºC for 24 h. The reaction mixture was then cooled to ambient temperature, diluted with 20 mL of CH_2Cl_2, filtered through a celite pad, and washed with 10-20 mL of CH_2Cl_2. The combined organic extracts were concentrated and the resulting residue was purified by column chromatography (petroleum ether/CH_2Cl_2 = 1/1, v/v) on silica gel to afforded the desired product as a white solid (52%). mp: 144-146 °C. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 7.15 (t, J = 7.2 Hz, 2H), 7.28 (t, J = 7.8 Hz, 1H), 7.38-7.43 (m, 2H), 7.48 (t, J = 8.0 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 9.52 (s, 1H) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 105.8, 111.7, 121.0,

121.80, 121.84, 122.8, 124.9, 125.5, 126.7, 128.5, 137.2, 153.5, 166.5 ppm. HRMS (ESI): calcd for $C_{15}H_{11}N_2S$ $[M+H]^+$ 251.0643, found 251.0643.

V. References

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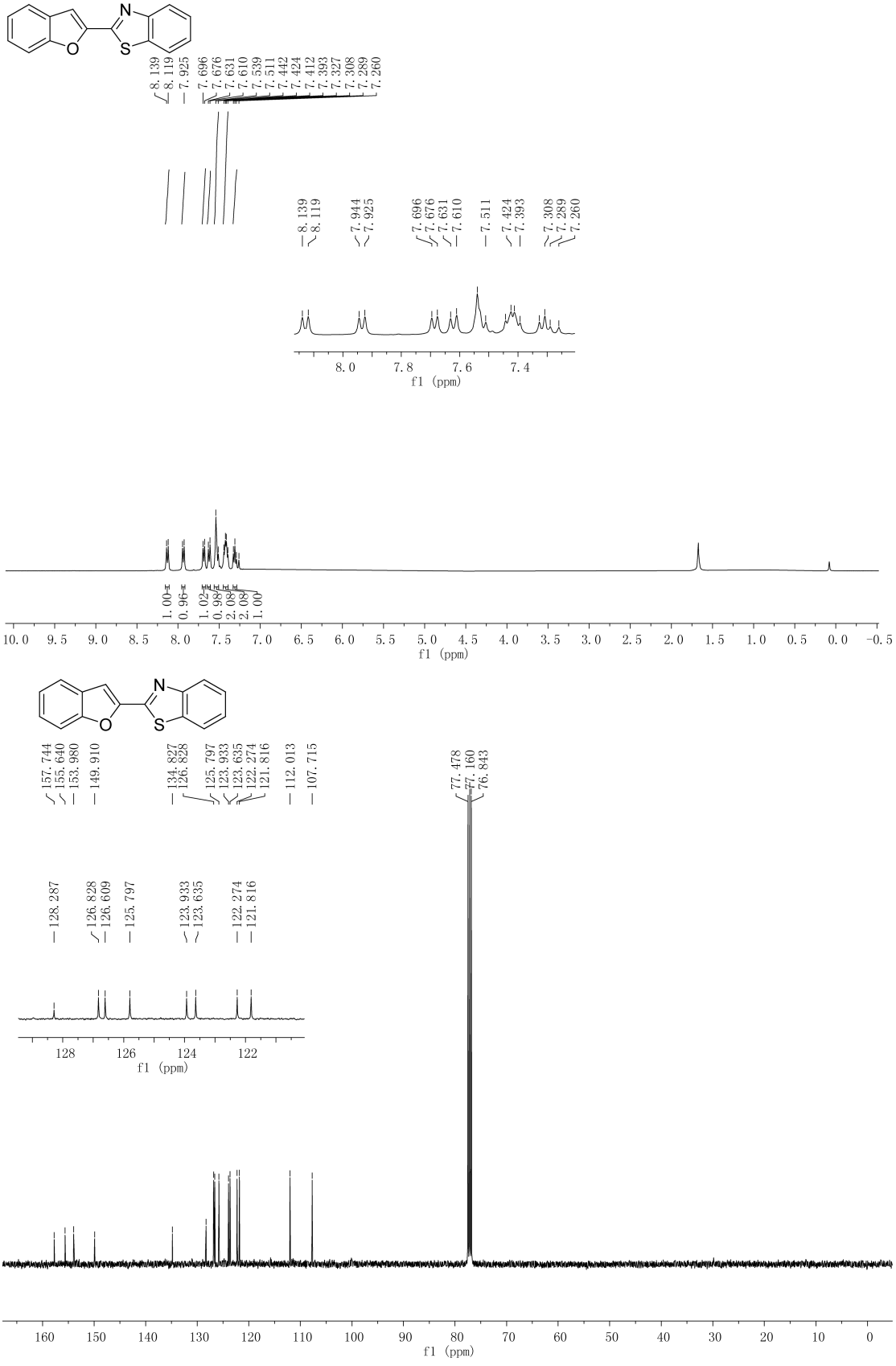
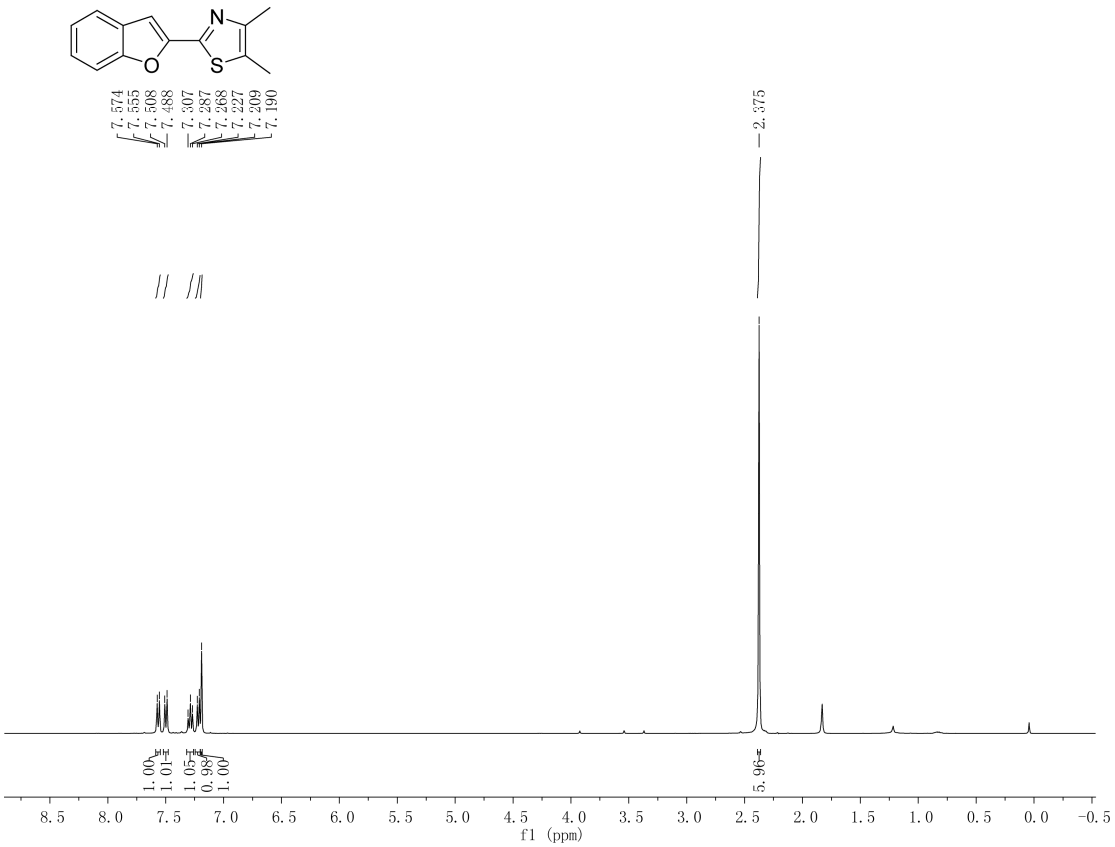
VI. Copies of ^{1}H and ^{13}C NMR spectra

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1.05
0.98
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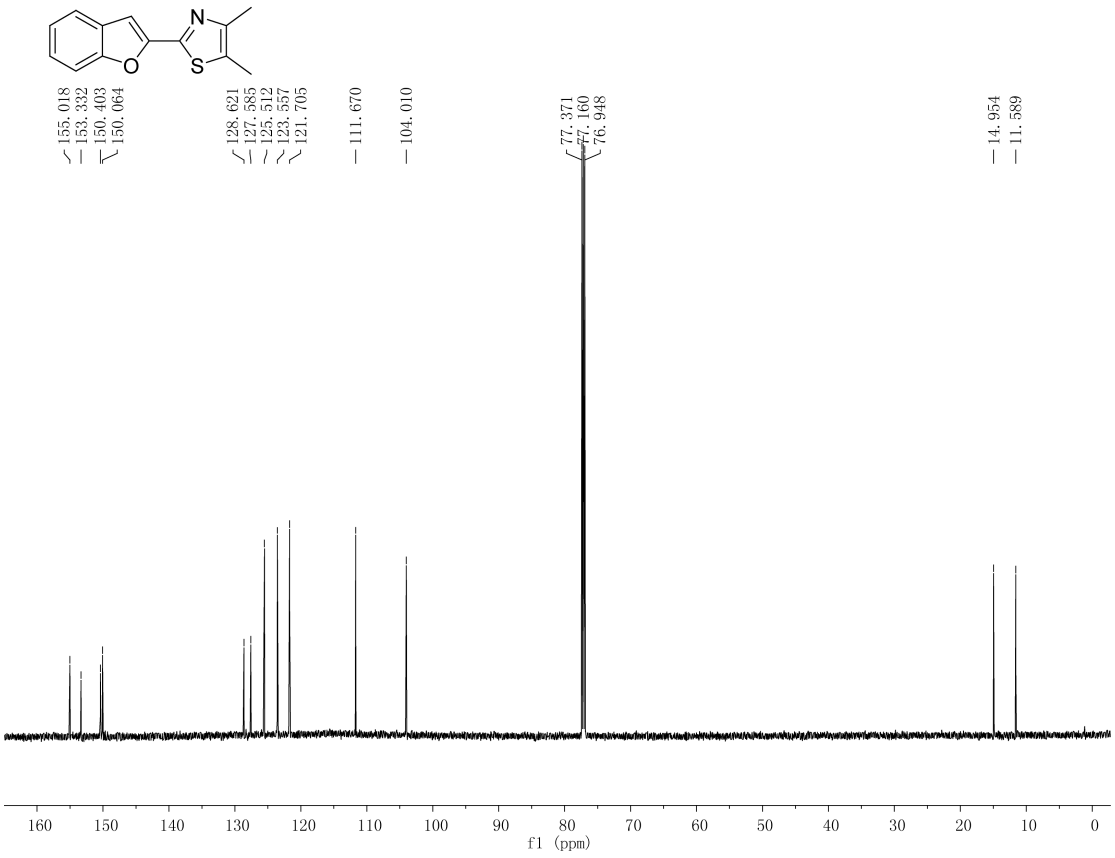
5.96
f1 (ppm)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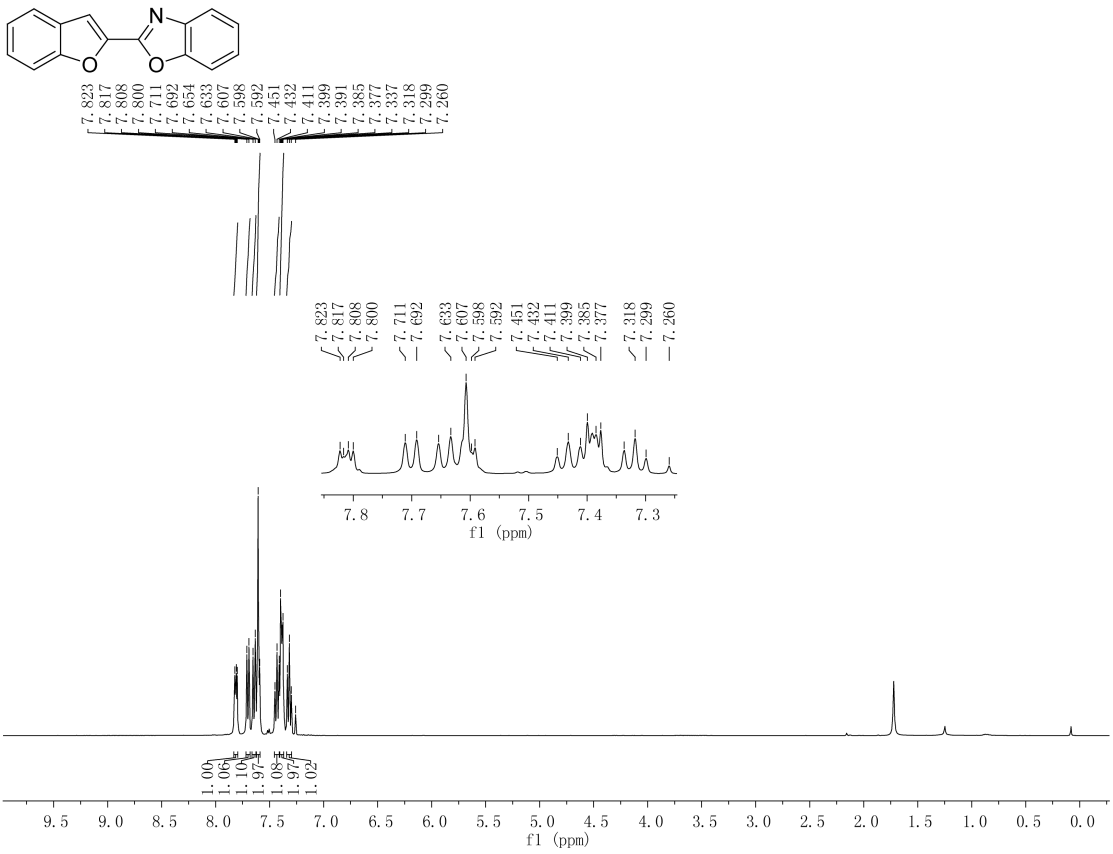
11.589
f1 (ppm)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7.411
7.399
7.391
7.385
7.377
7.337
7.318
7.299
7.260
7.8
7.7
7.6
7.5
7.4
7.3
f1 (ppm)
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1.06
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1.97
1.08
1.97
1.02
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9.0
8.5
8.0
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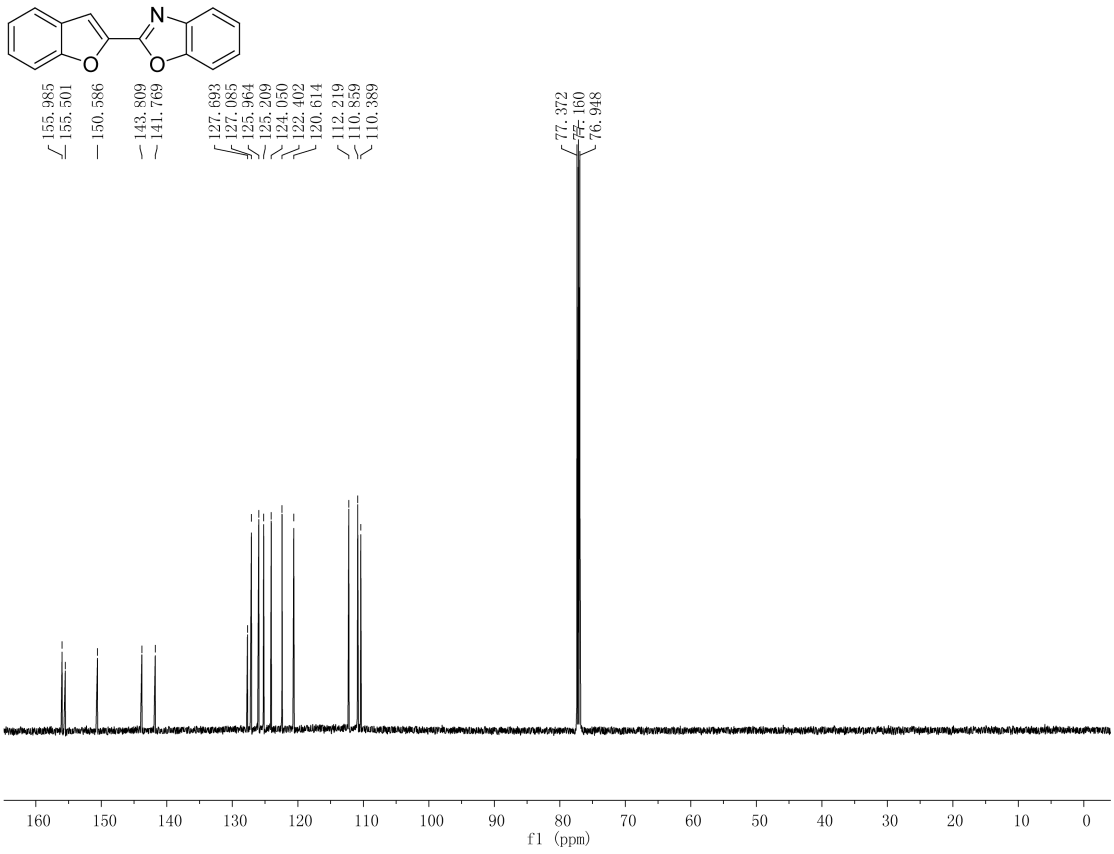
f1 (ppm)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120.614
112.219
110.859
110.389
77.372
77.160
76.948
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150
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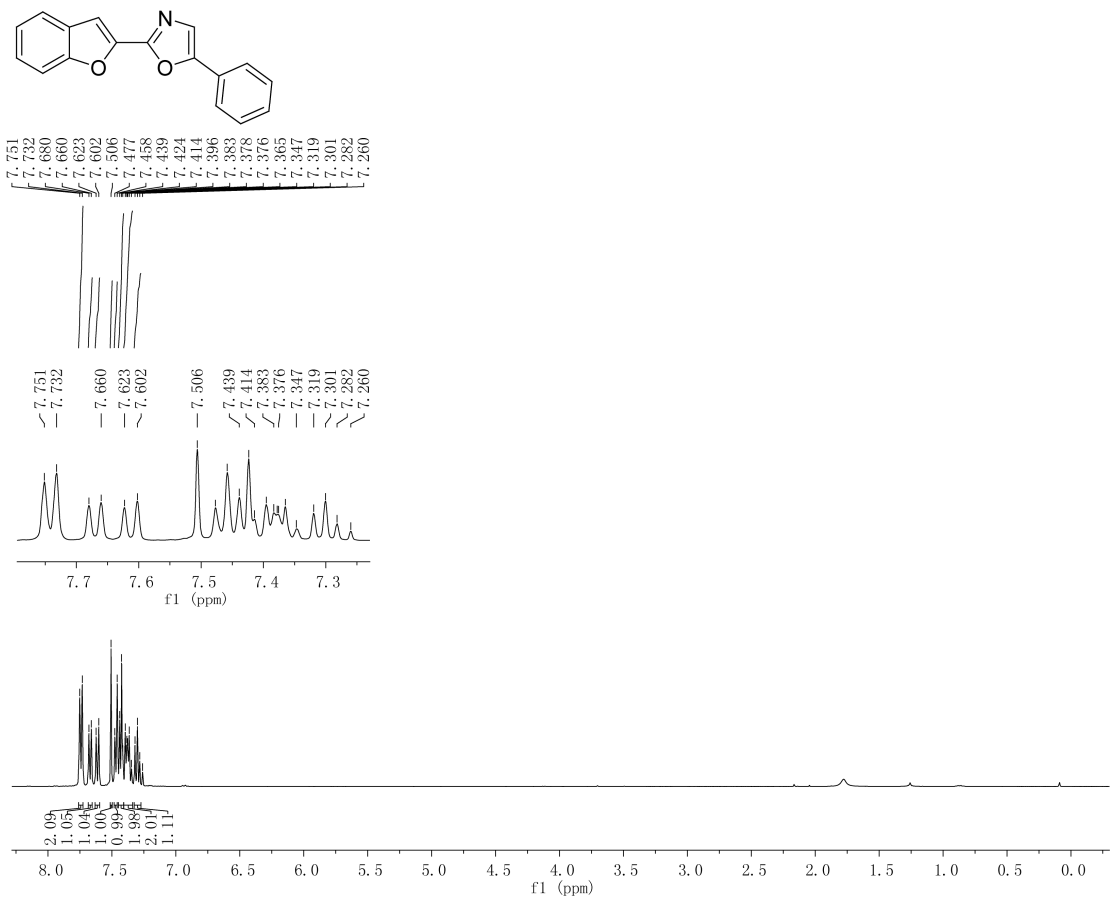
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.376
7.365
7.347
7.319
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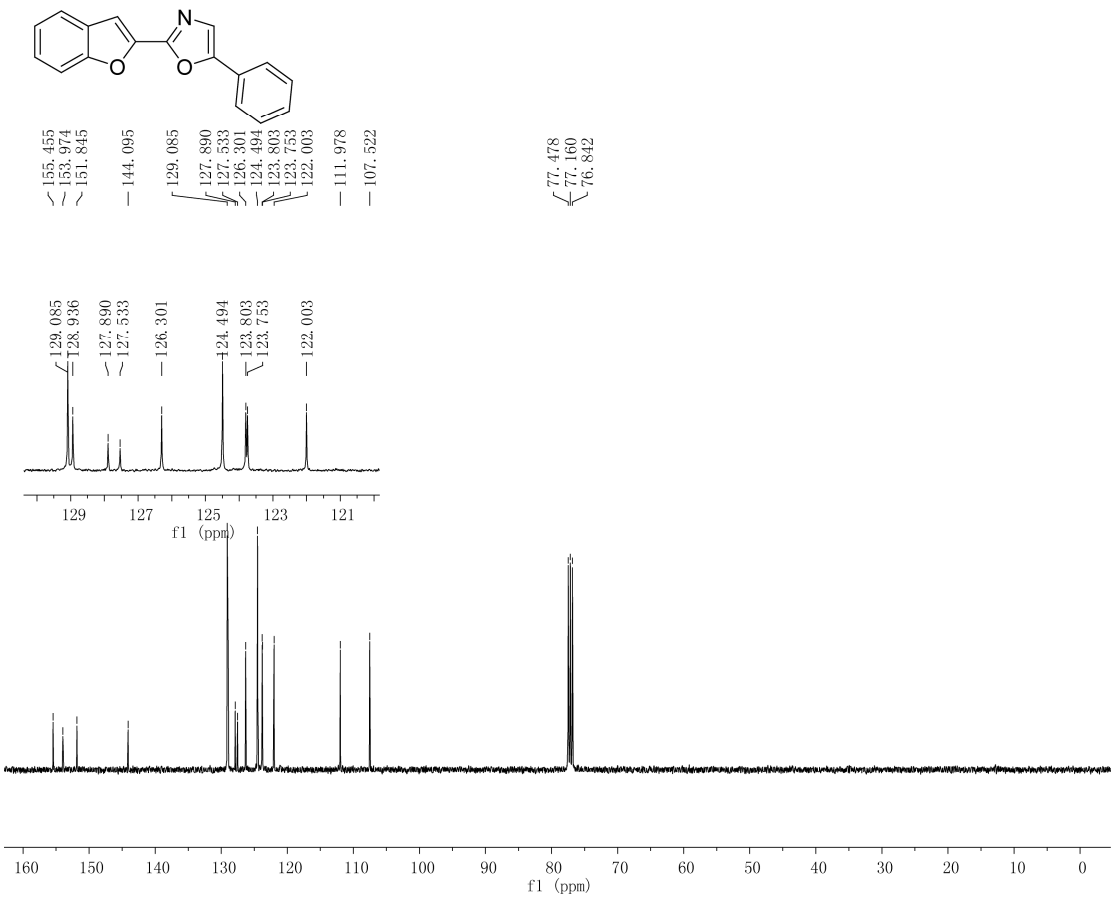
f1 (ppm)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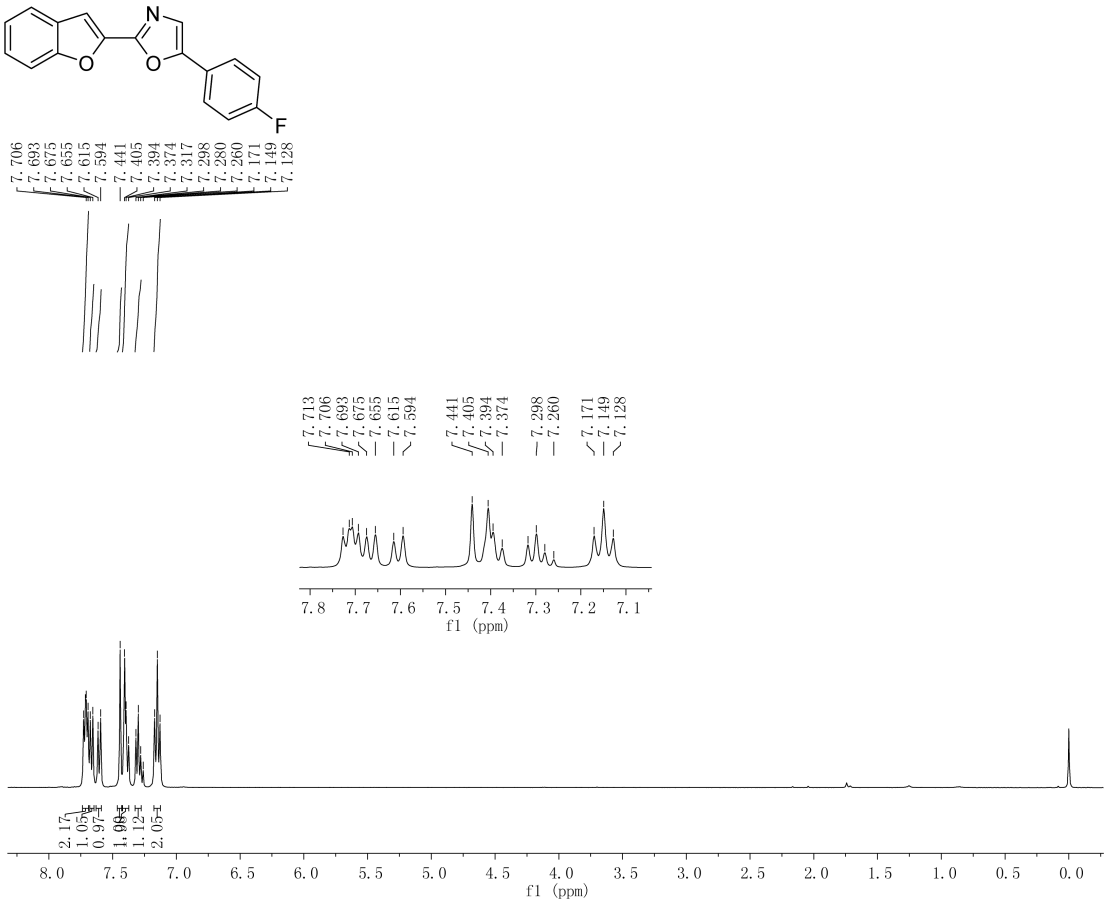
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f1 (ppm)
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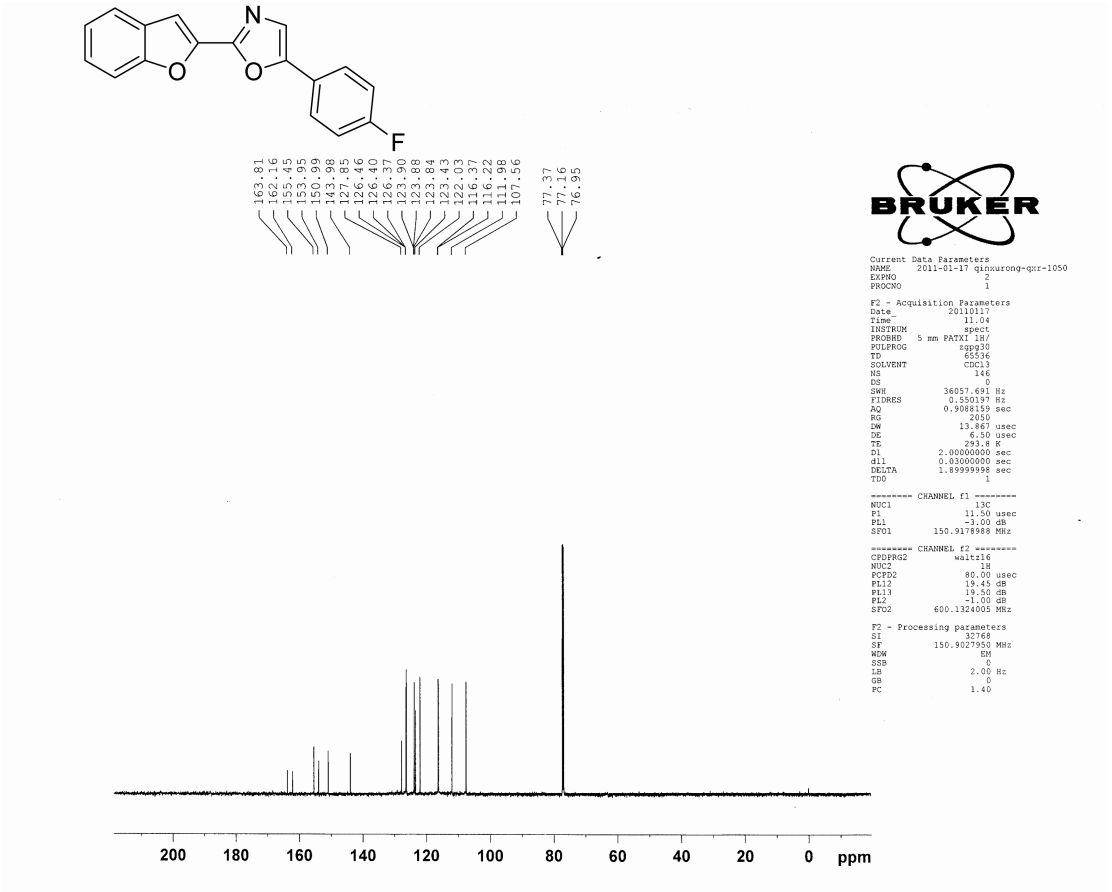
f1 (ppm)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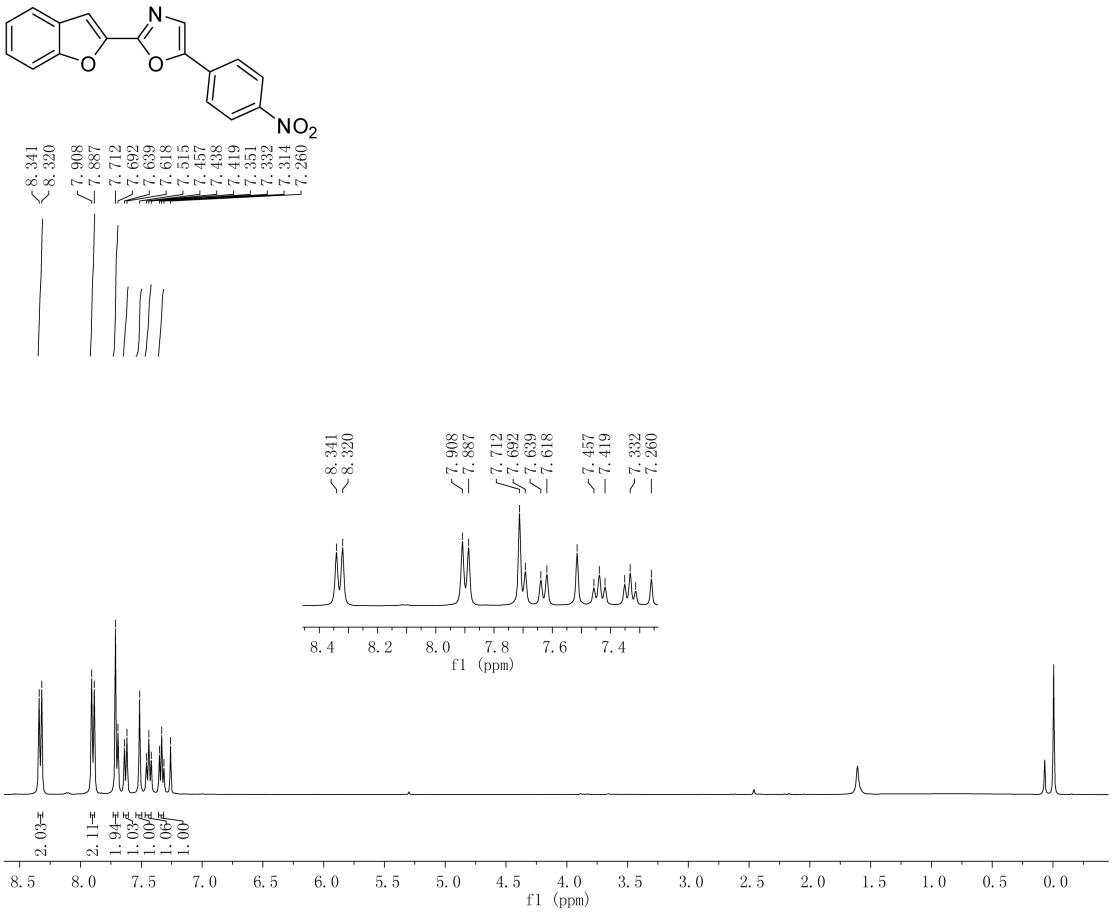
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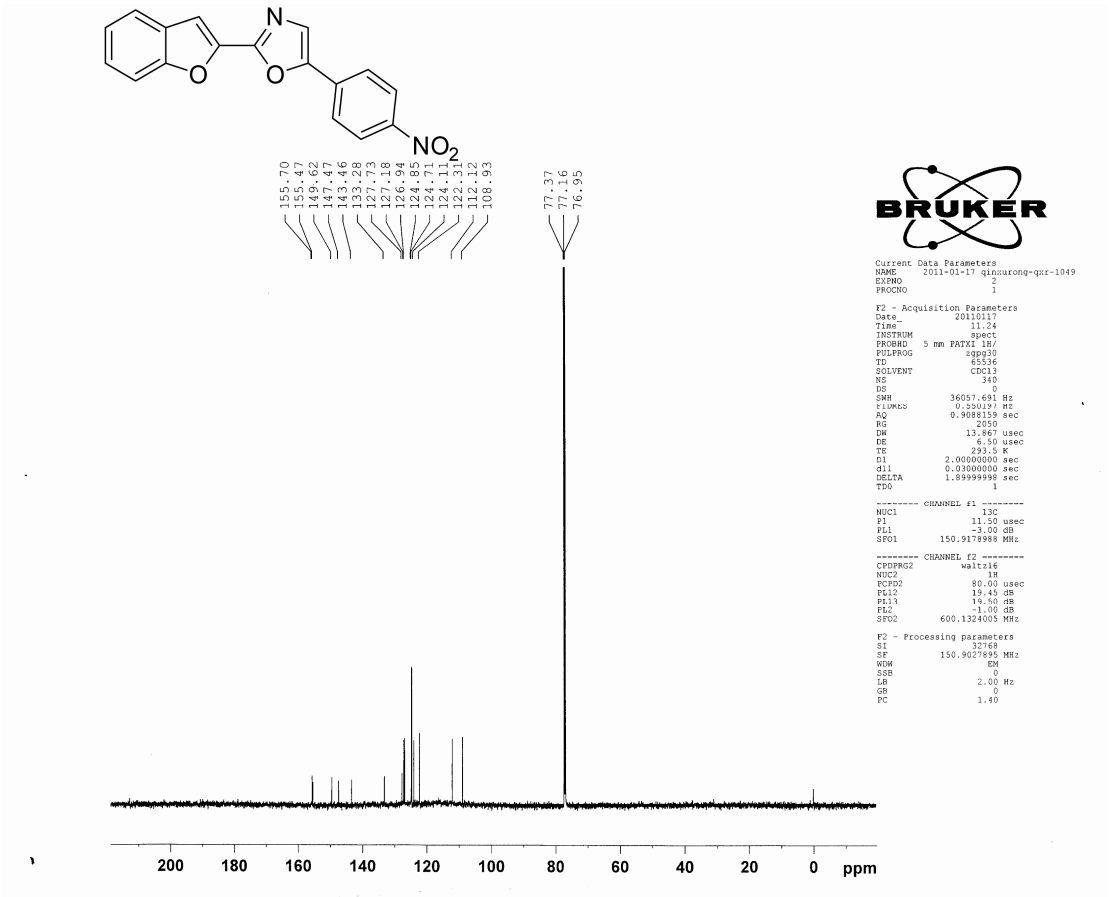
1.00
f1 (ppm)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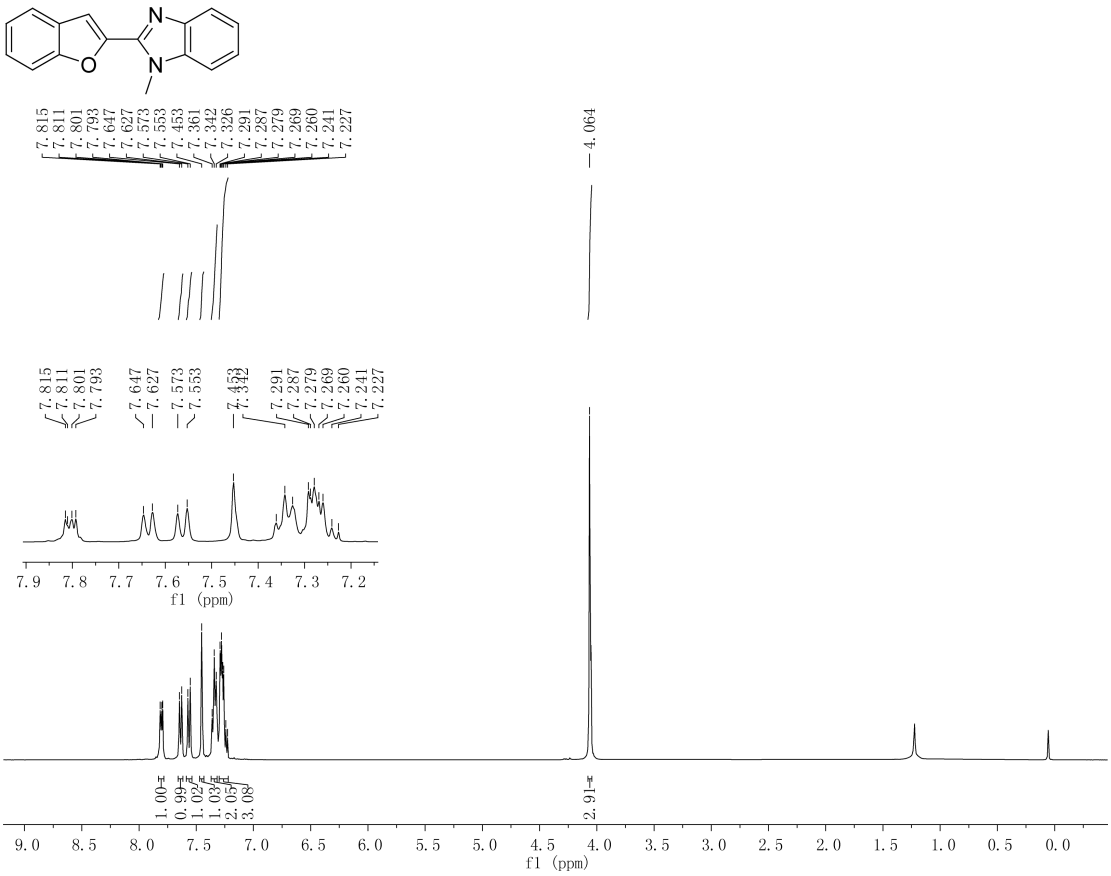
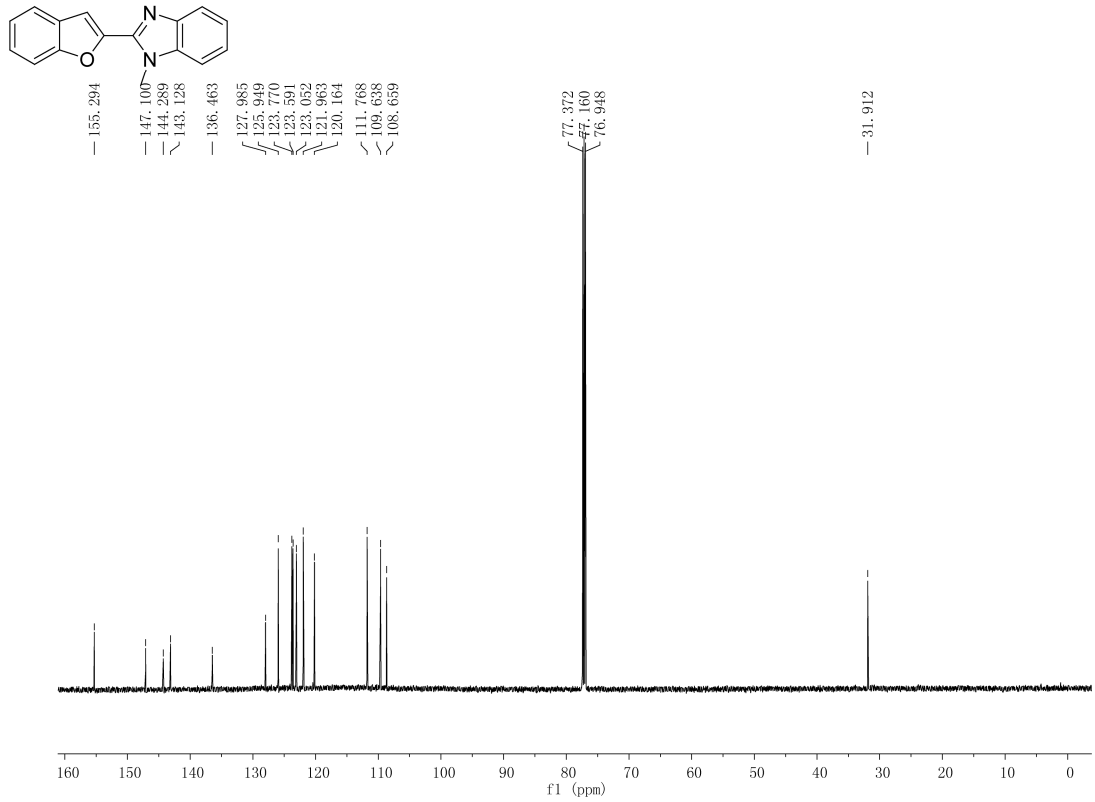
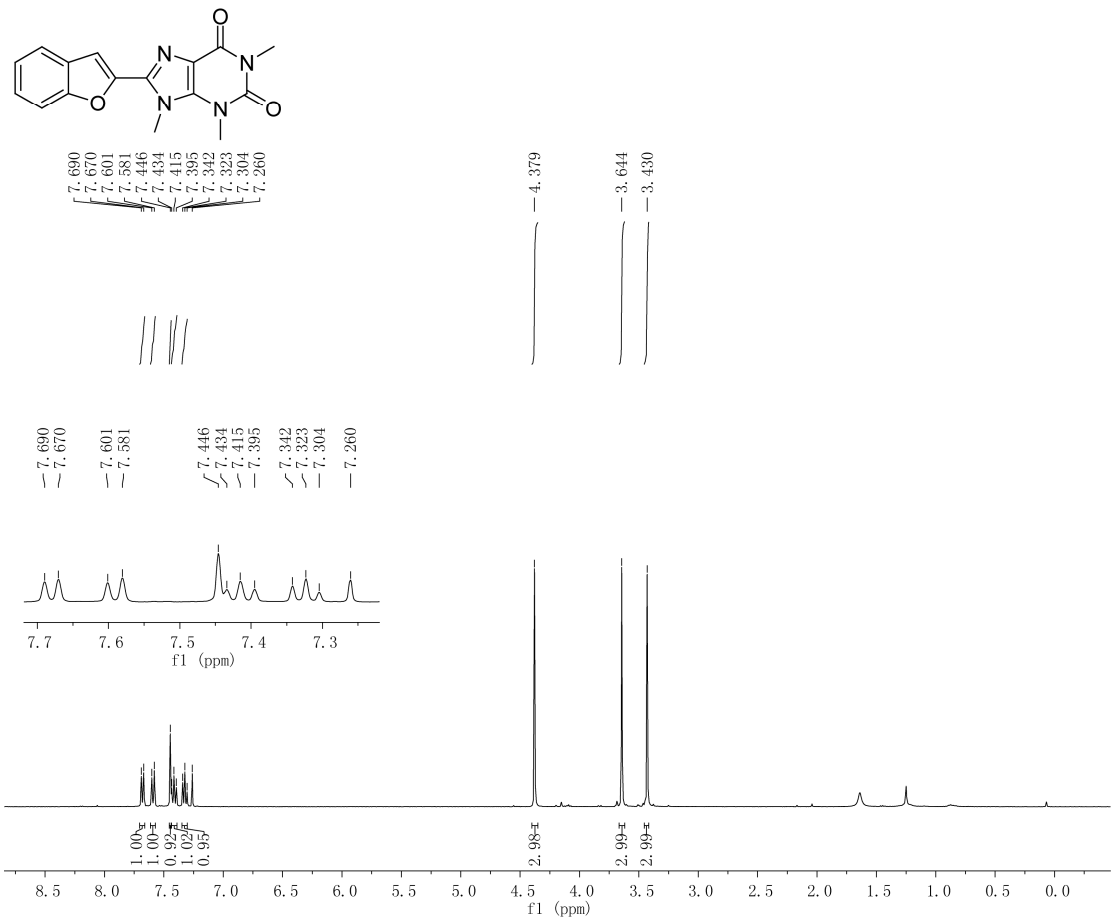
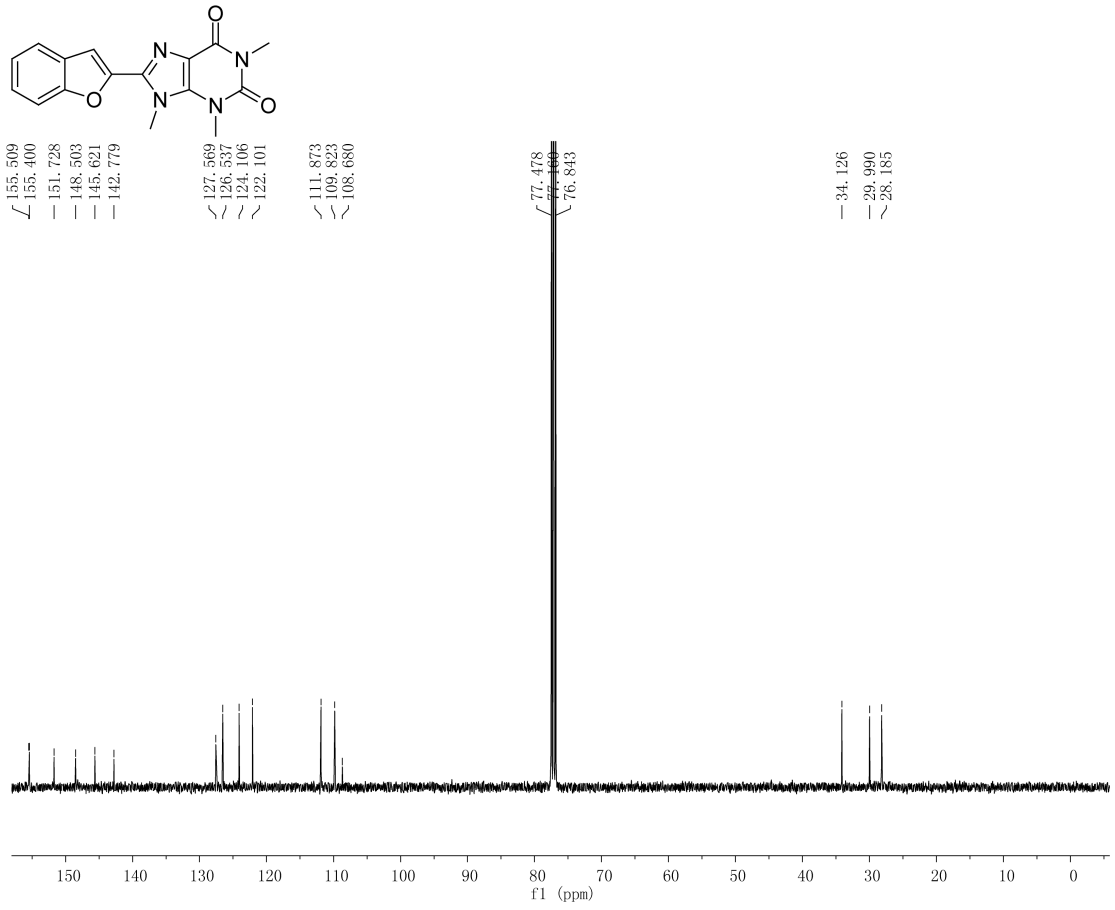
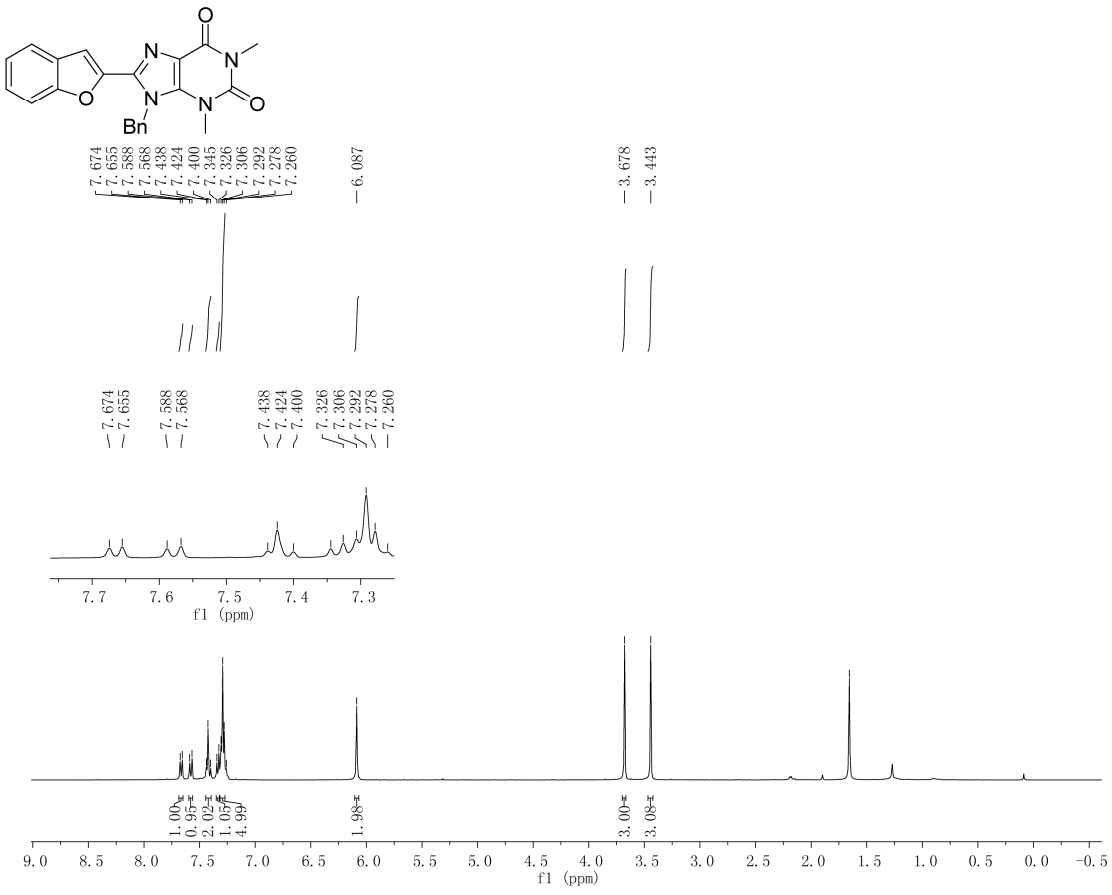
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 19.45 dB
PL13 19.50 dB
PL2 -1.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027895 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

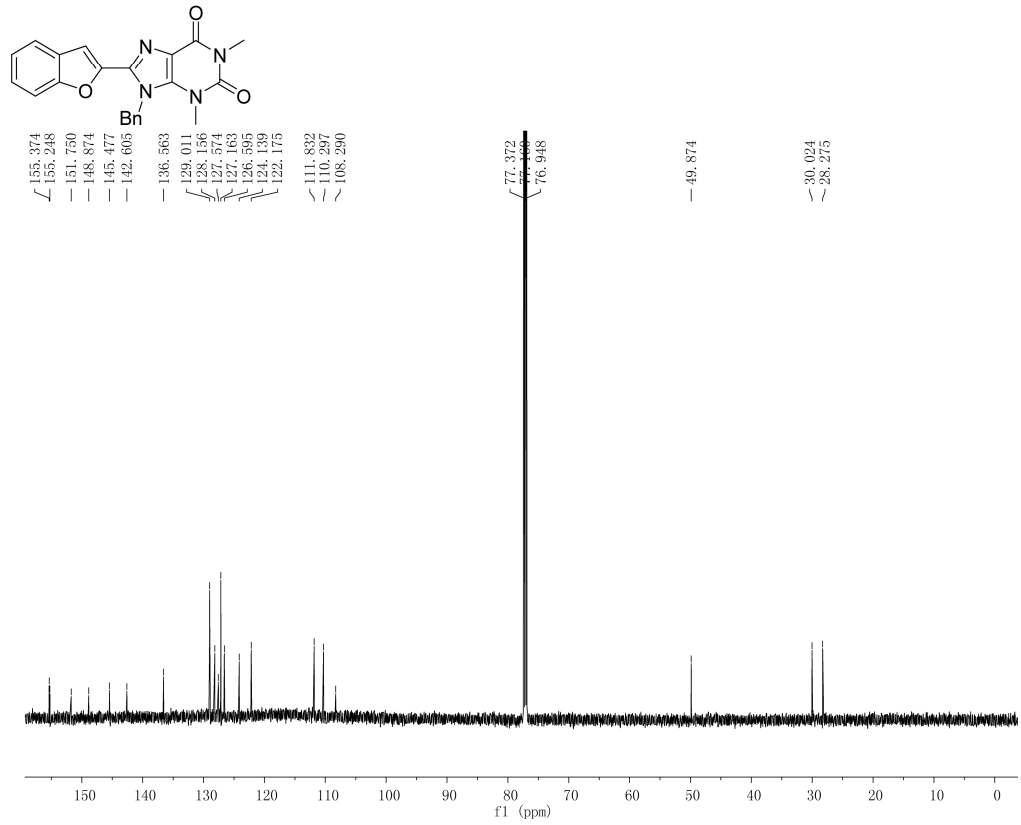

7.815
7.811
7.801
7.793
7.647
7.627
7.573
7.553
7.453
7.361
7.342
7.326
7.291
7.287
7.279
7.269
7.260
7.241
7.227
4.064
1.00
0.99
1.02
1.03
2.05
3.08
2.91
f1 (ppm)

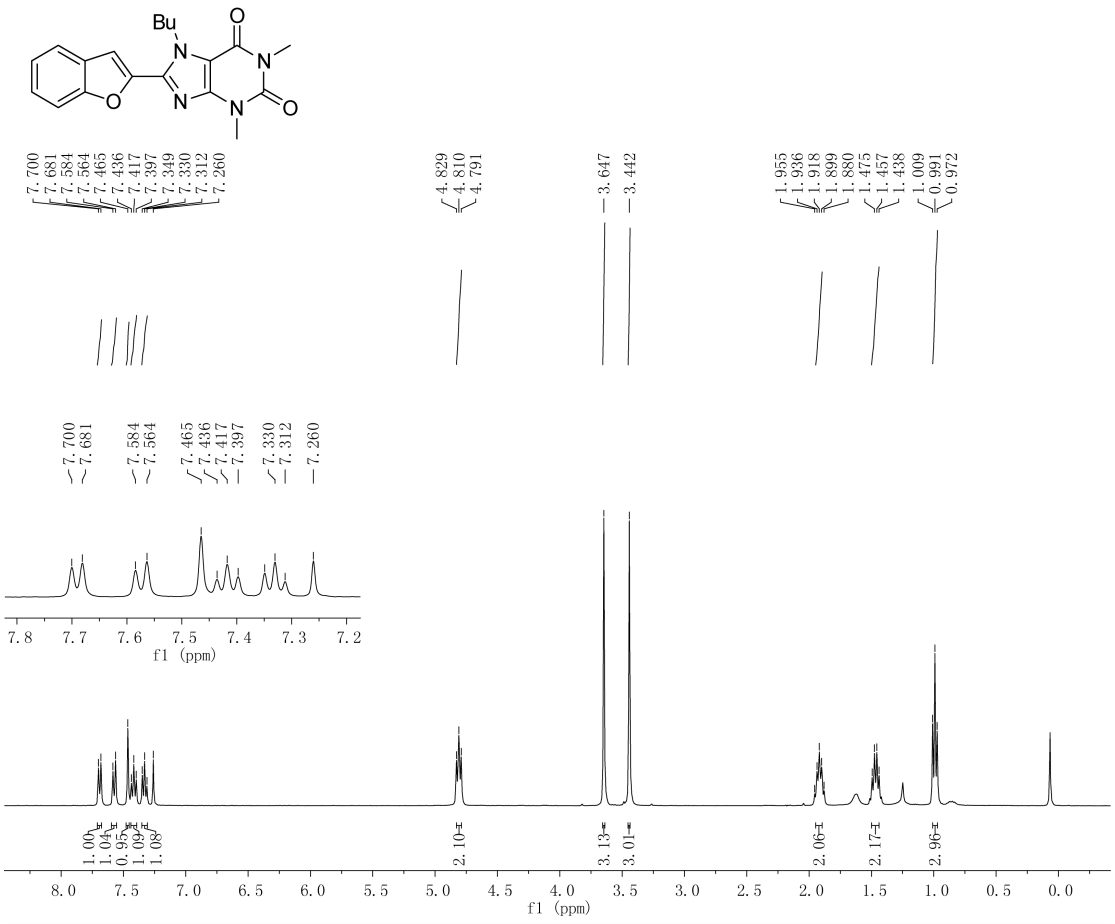

155.294
147.100
144.289
143.128
136.463
127.985
125.949
123.770
123.591
123.052
121.963
120.164
111.768
109.638
108.659
77.372
77.160
76.948
31.912
f1 (ppm)

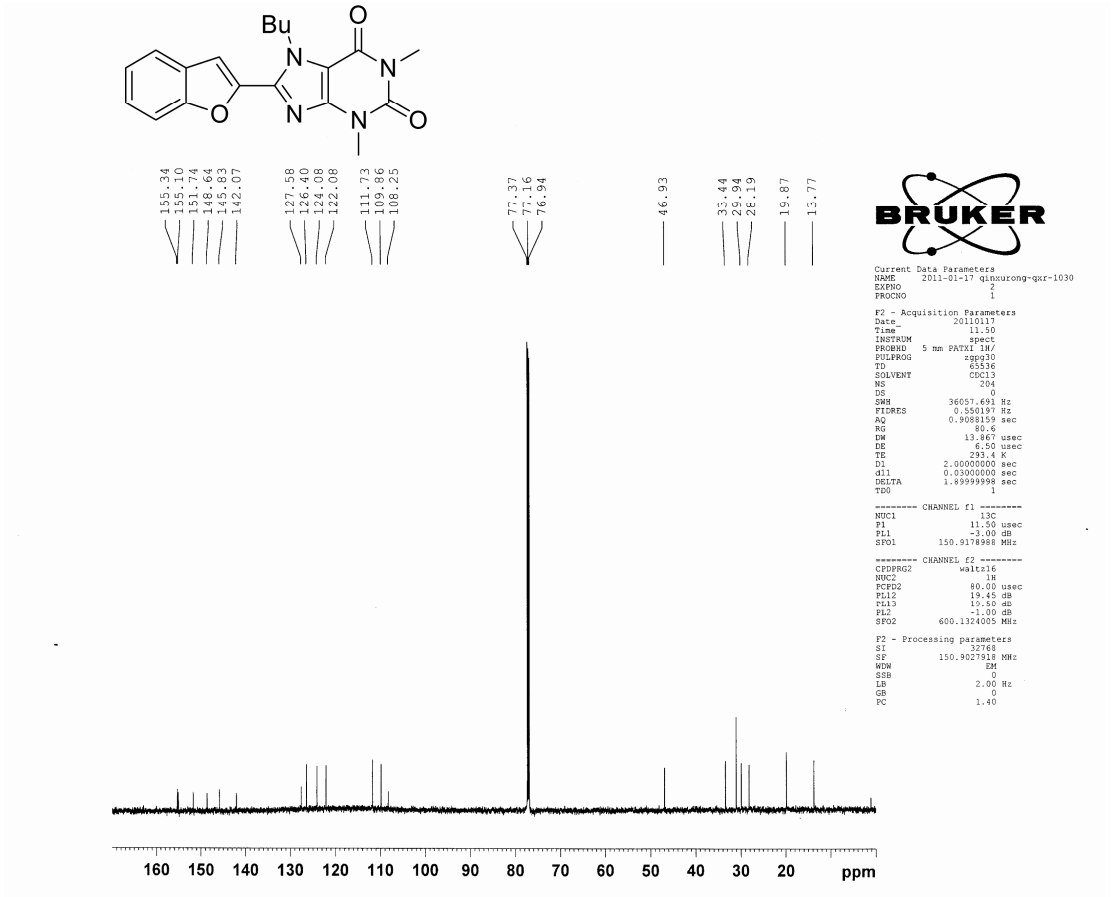

7.690
7.670
7.601
7.581
7.446
7.434
7.415
7.395
7.342
7.323
7.304
7.260
4.379
3.644
3.430
f1 (ppm)
1.00
1.00
0.92
1.02
0.95
2.98
2.99
2.99

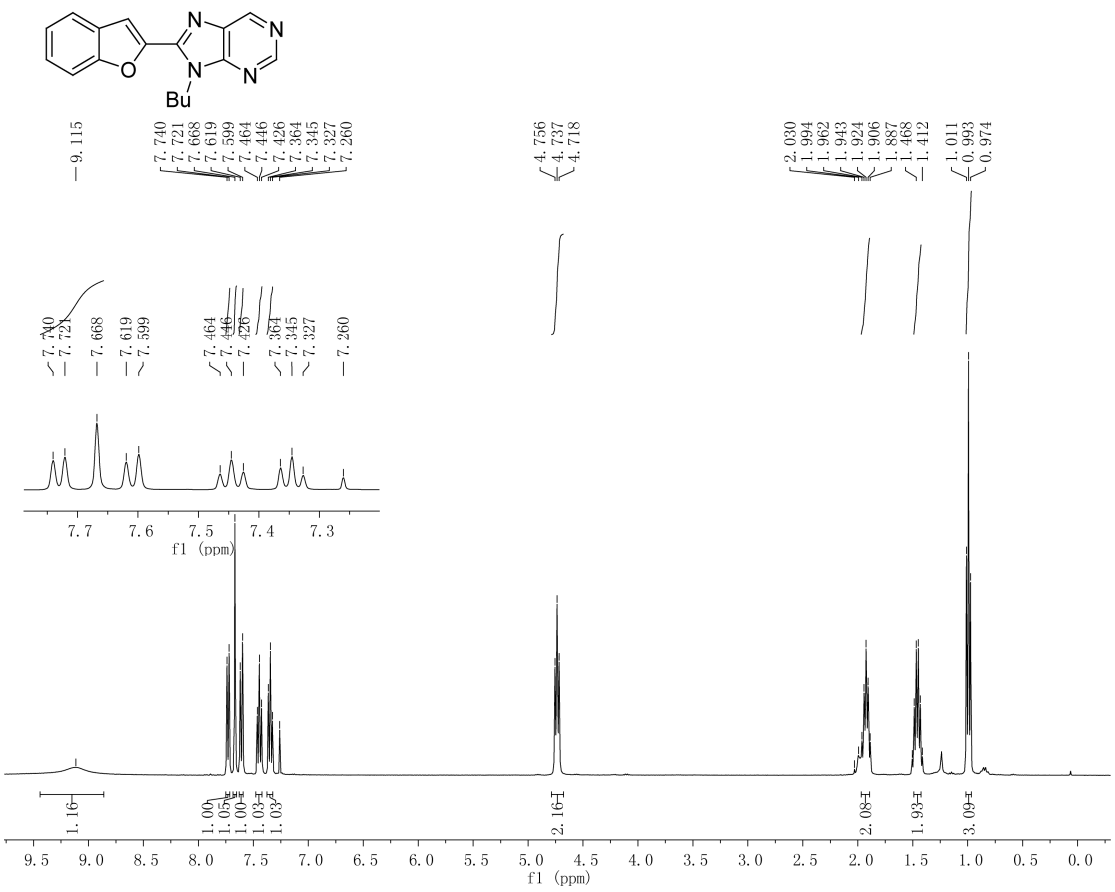

155.509
155.400
151.728
148.503
145.621
142.779
127.569
126.537
124.106
122.101
111.873
109.823
108.680
77.478
76.843
34.126
29.990
28.185
f1 (ppm)

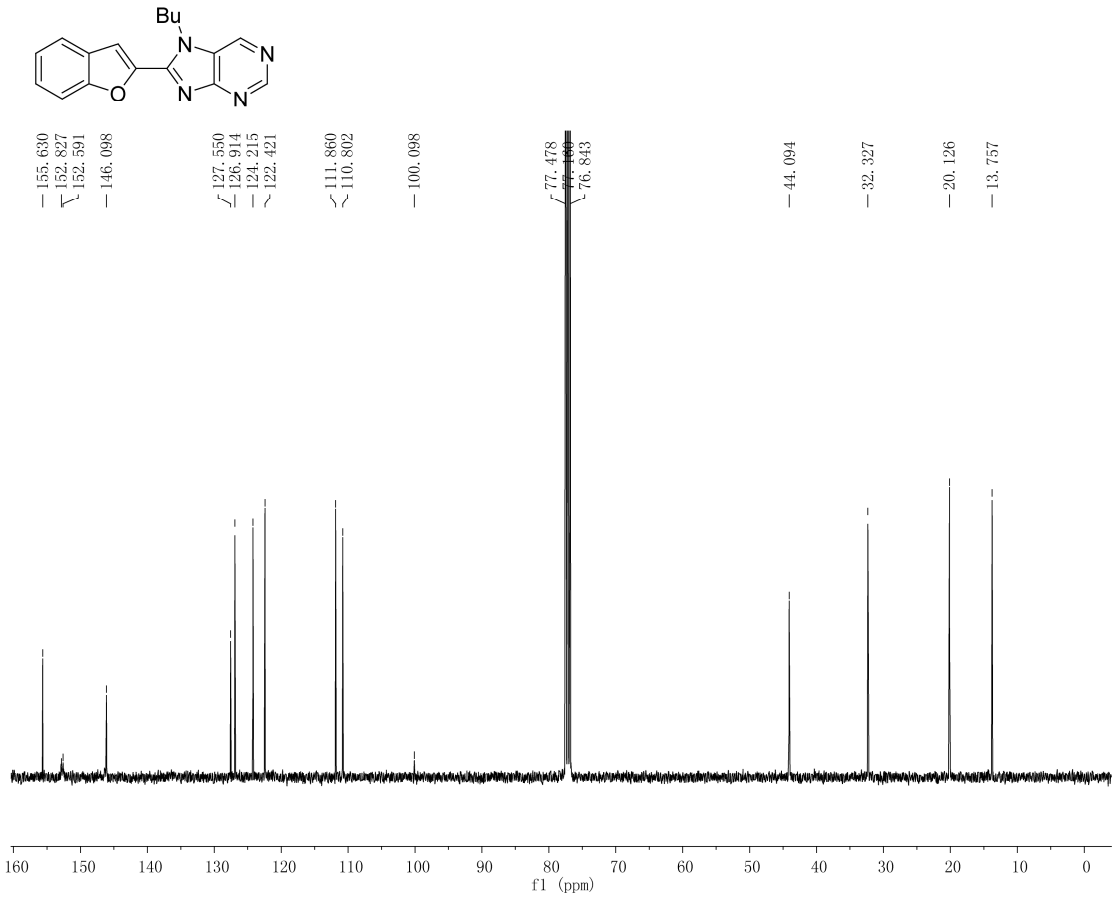

O
N
N
O
N
N
O
Bn
7.674
7.655
7.588
7.568
7.438
7.424
7.400
7.345
7.326
7.306
7.292
7.278
7.260
6.087
3.678
3.443
1.00
0.95
2.02
1.05
4.99
1.98
3.00
3.08
f1 (ppm)

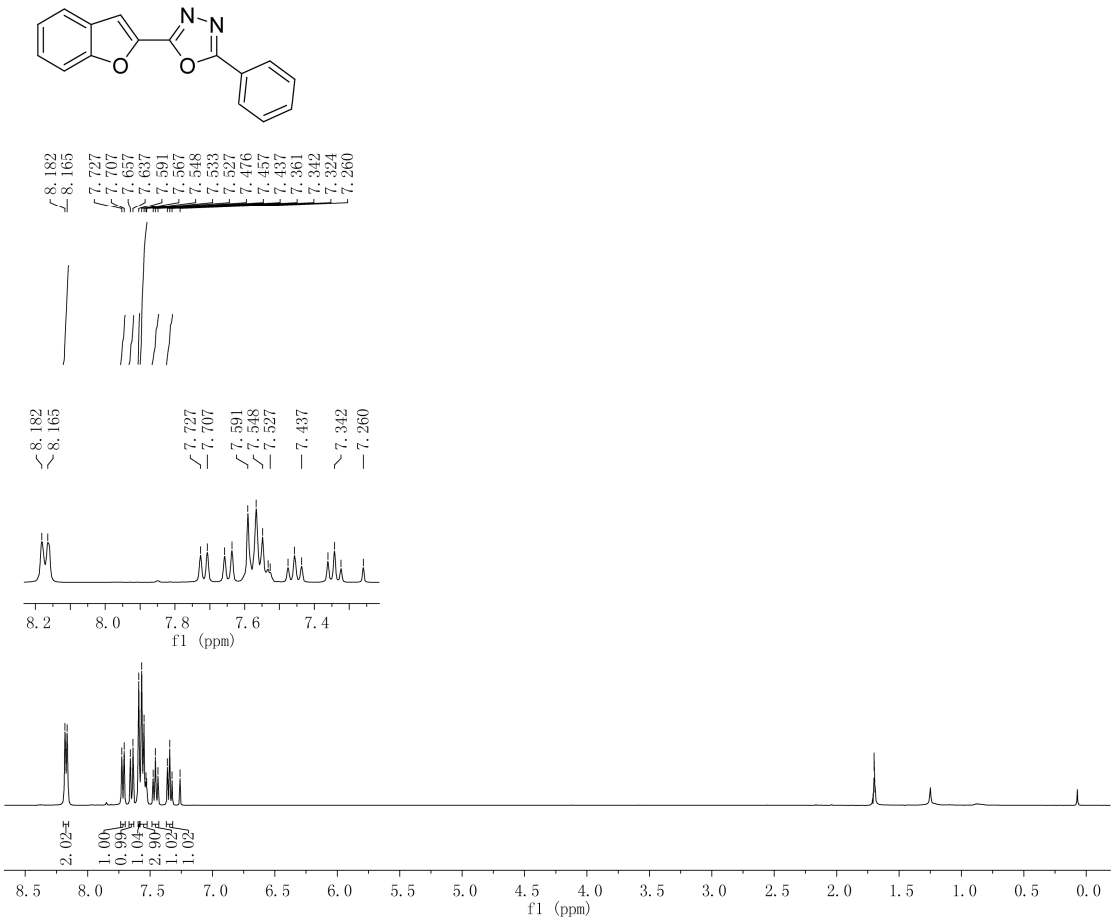

O
N
N
O
N
N
O
Bn
155.374
153.248
151.750
148.874
145.477
142.605
136.563
129.011
128.156
127.574
127.163
126.595
124.139
122.175
111.832
110.297
108.290
77.372
77.160
76.948
49.874
30.024
28.275
f1 (ppm)

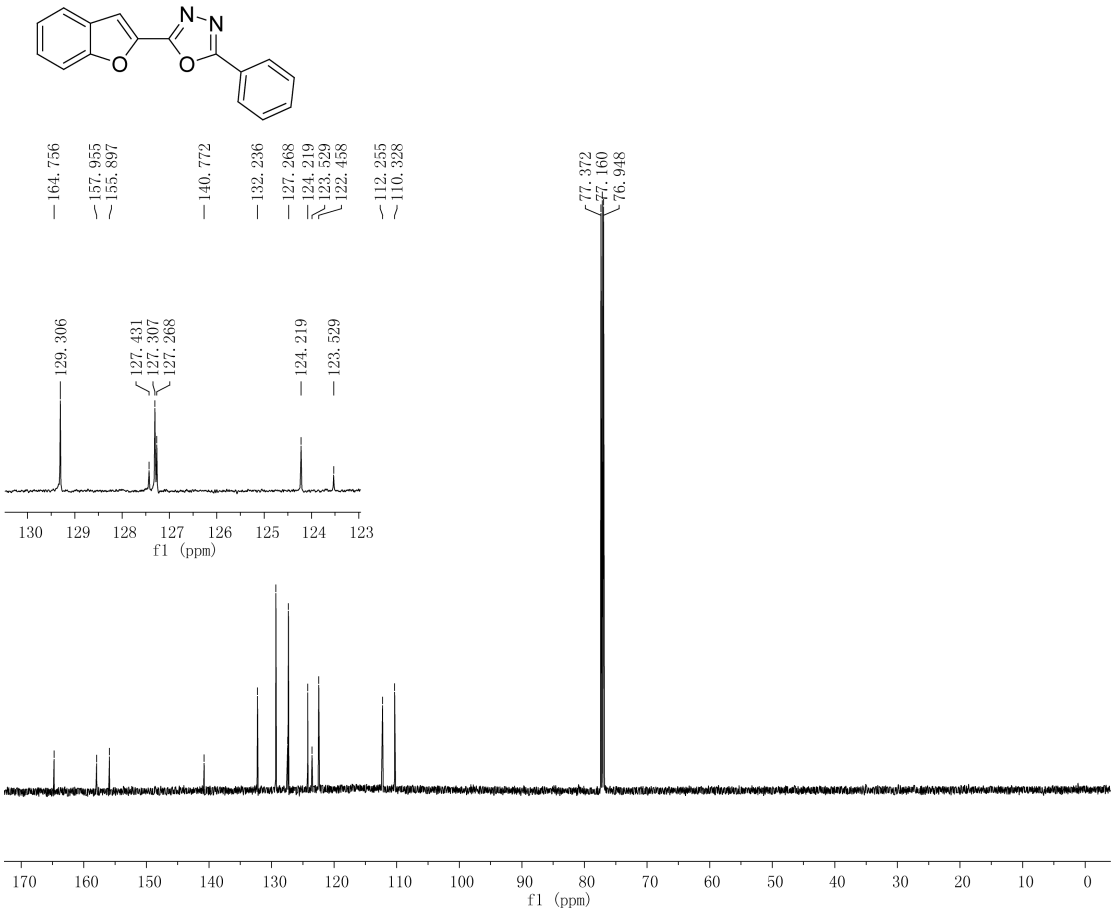

Bu
N
O
N
N
N
O
O
7.700
7.681
7.584
7.564
7.465
7.436
7.417
7.397
7.349
7.330
7.312
7.260
4.829
4.810
4.791
3.647
3.442
1.955
1.936
1.918
1.899
1.880
1.475
1.457
1.438
1.009
0.991
0.972
f1 (ppm)
1.00
1.04
0.95
1.09
1.08
2.10
3.13
3.01
2.06
2.17
2.96

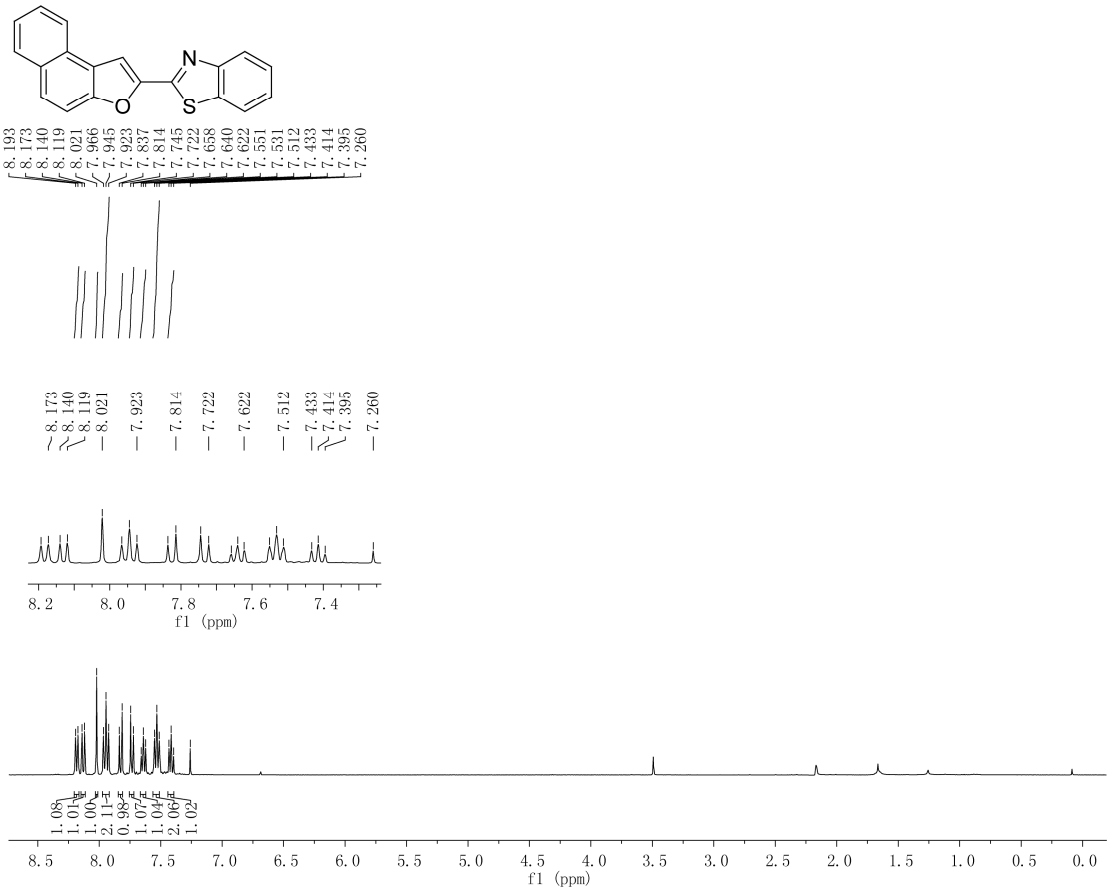

Bu
N
O
N
N
N
O
O
155.34
155.10
151.74
148.64
145.83
142.07
127.58
126.40
124.08
122.08
111.73
109.86
108.25
77.37
77.16
76.94
46.93
33.44
29.94
26.19
19.87
13.77
BRUKER
Current Data Parameters
NAME 2011-01-17 qinxurong-qxr-1030
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110117
Time_ 11.50
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 204
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
DW 13.867 usec
DE 6.50 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.50 usec
PL1 -3.00 dB
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 19.45 dB
PL13 19.50 dB
PL2 -1.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027918 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

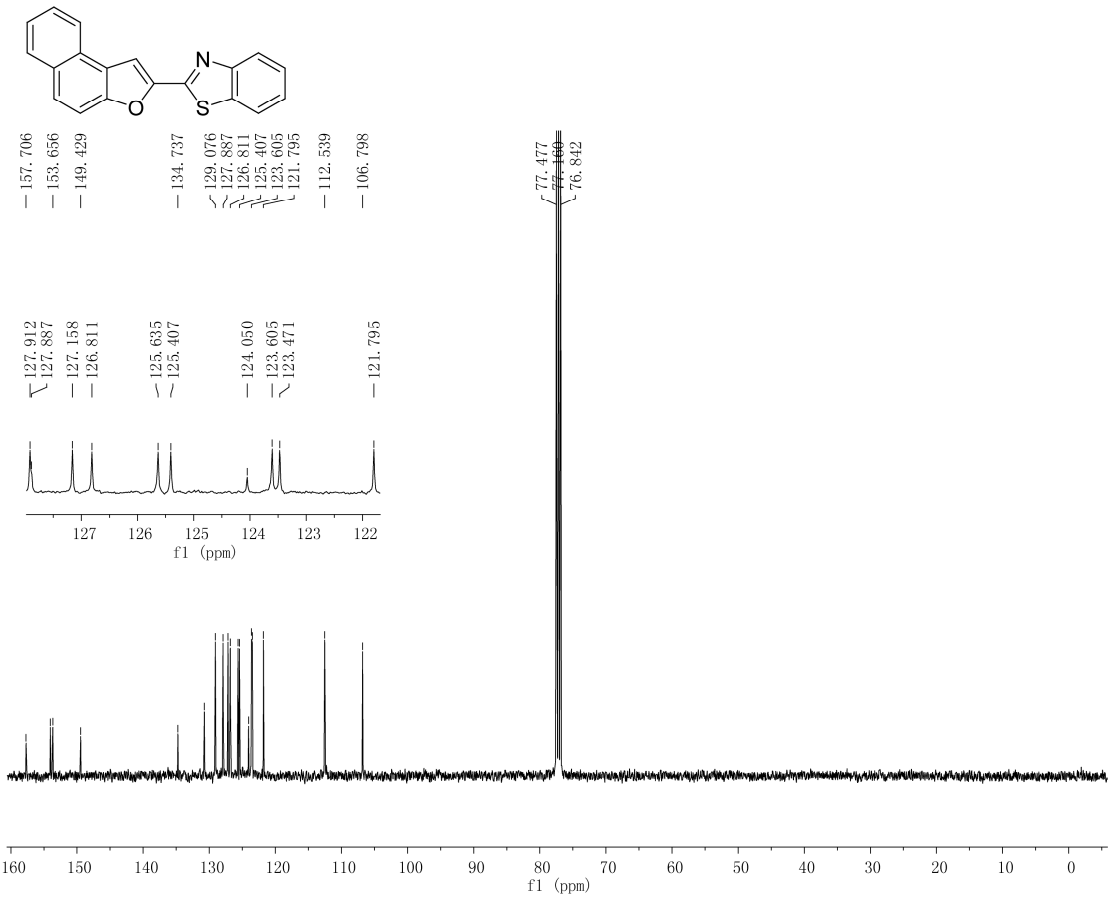

Bu
9.115
7.740
7.721
7.668
7.619
7.599
7.464
7.446
7.426
7.364
7.345
7.327
7.260
4.756
4.737
4.718
2.030
1.994
1.962
1.943
1.924
1.906
1.887
1.468
1.412
1.011
0.993
0.974
f1 (ppm)
1.16
1.00
1.05
1.00
1.03
1.03
2.16
2.08
1.93
3.09

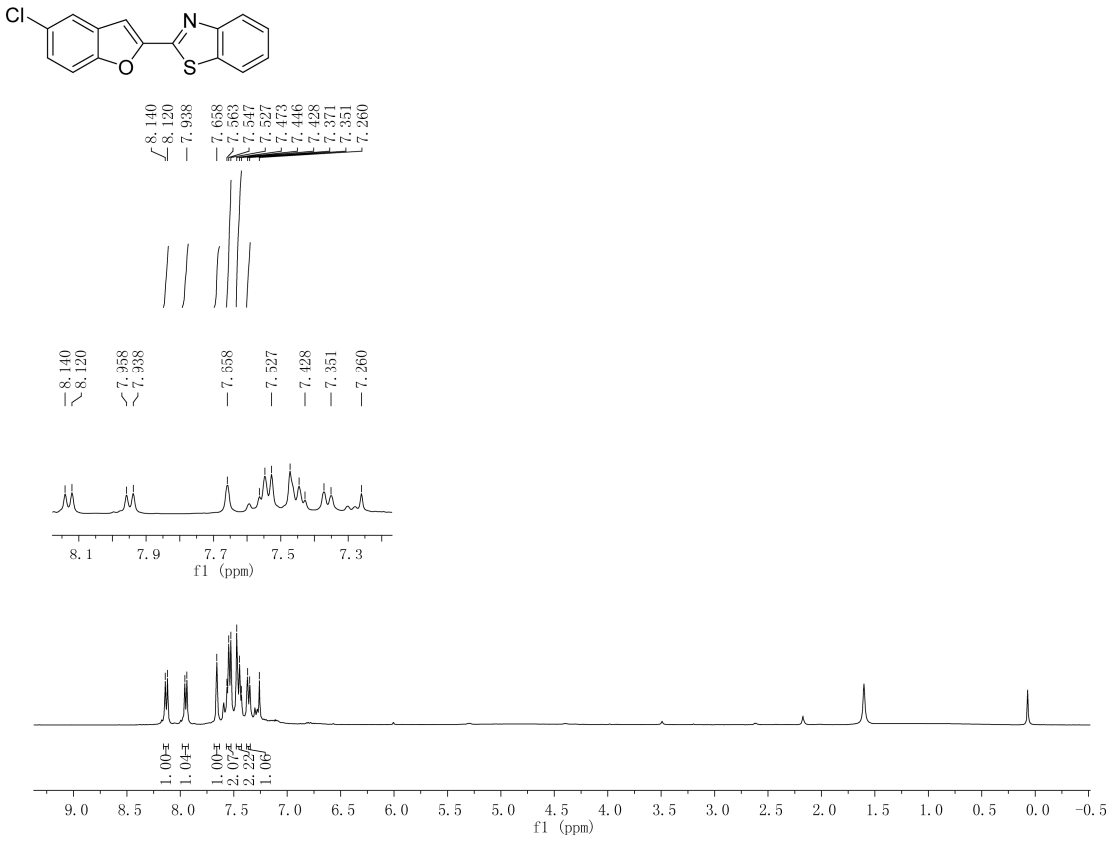

Bu
155.630
152.827
152.591
146.098
127.550
126.914
124.215
122.421
111.860
110.802
100.098
77.478
76.843
44.094
32.327
20.126
13.757
f1 (ppm)

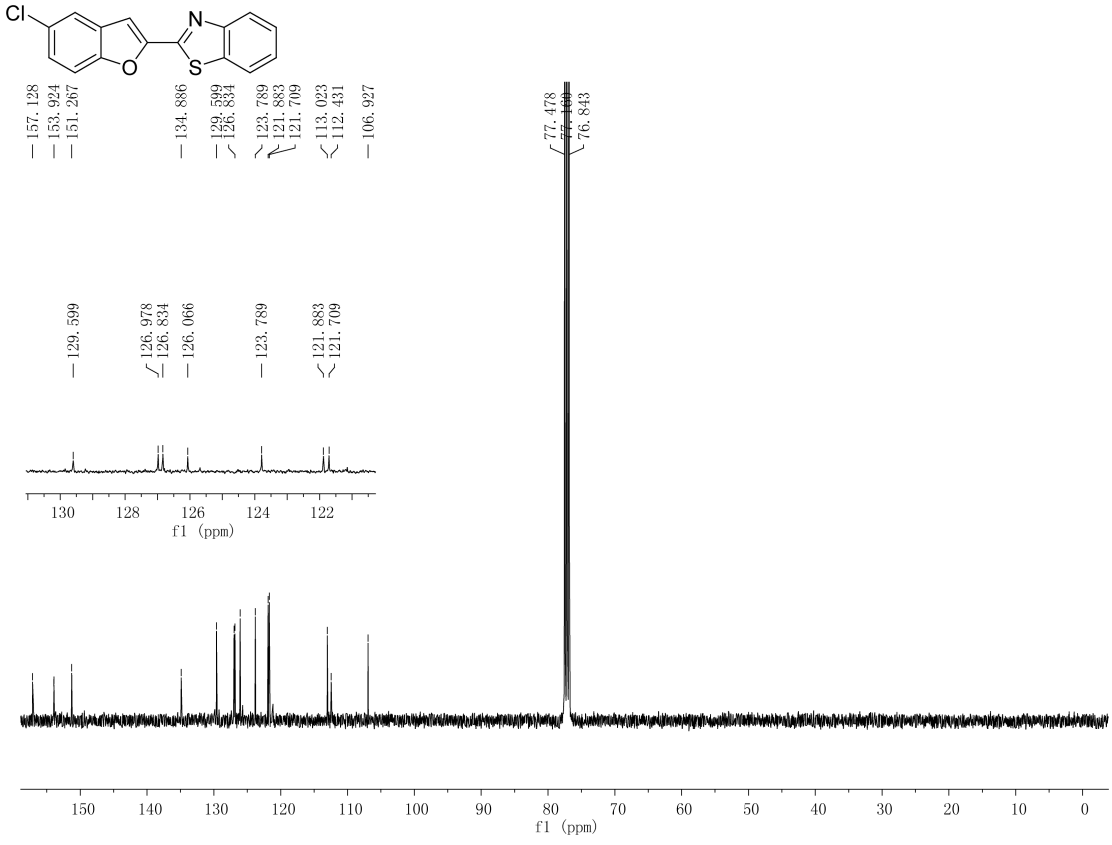

8.182
8.165
7.727
7.707
7.657
7.637
7.591
7.567
7.548
7.533
7.527
7.476
7.457
7.437
7.361
7.342
7.324
7.260
f1 (ppm)
2.02
1.00
0.99
1.04
2.90
1.02
1.02

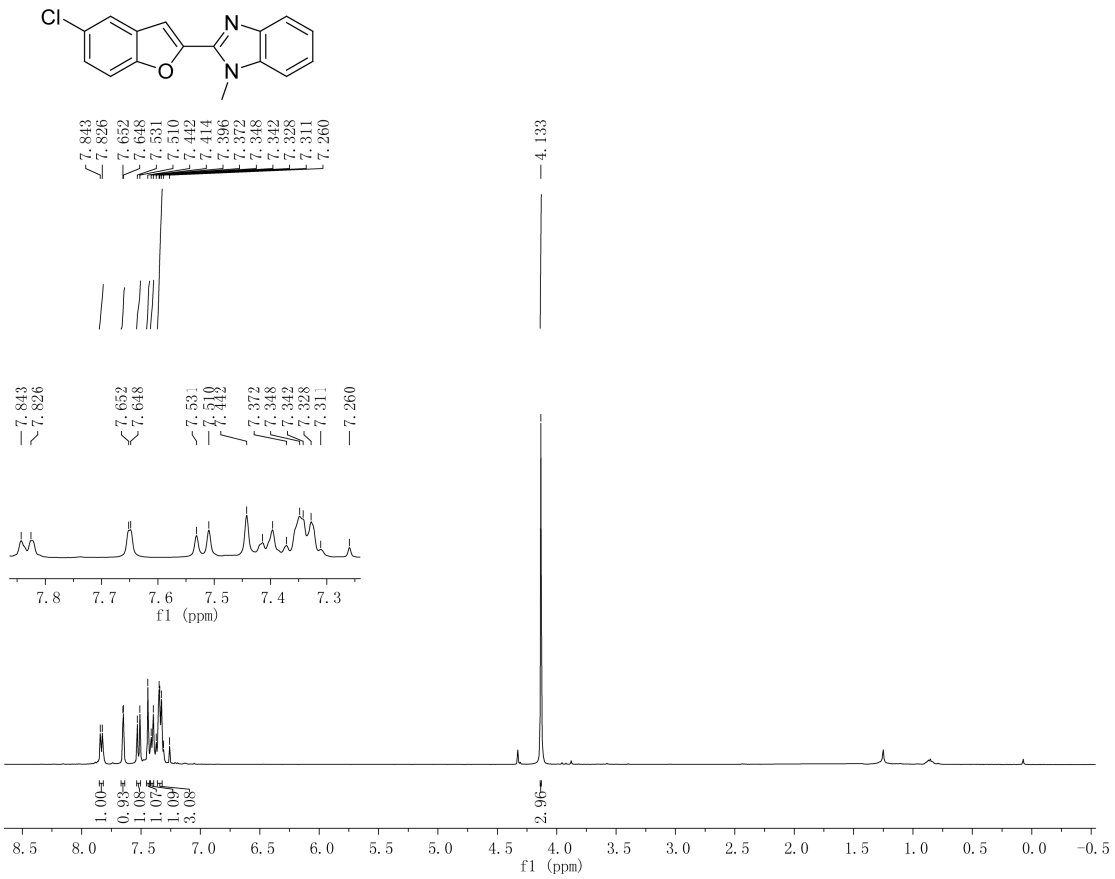

164.756
157.955
155.897
140.772
132.236
127.268
124.219
123.529
122.458
112.255
110.328
77.372
77.160
76.948
129.306
127.431
127.307
127.268
124.219
123.529
f1 (ppm)

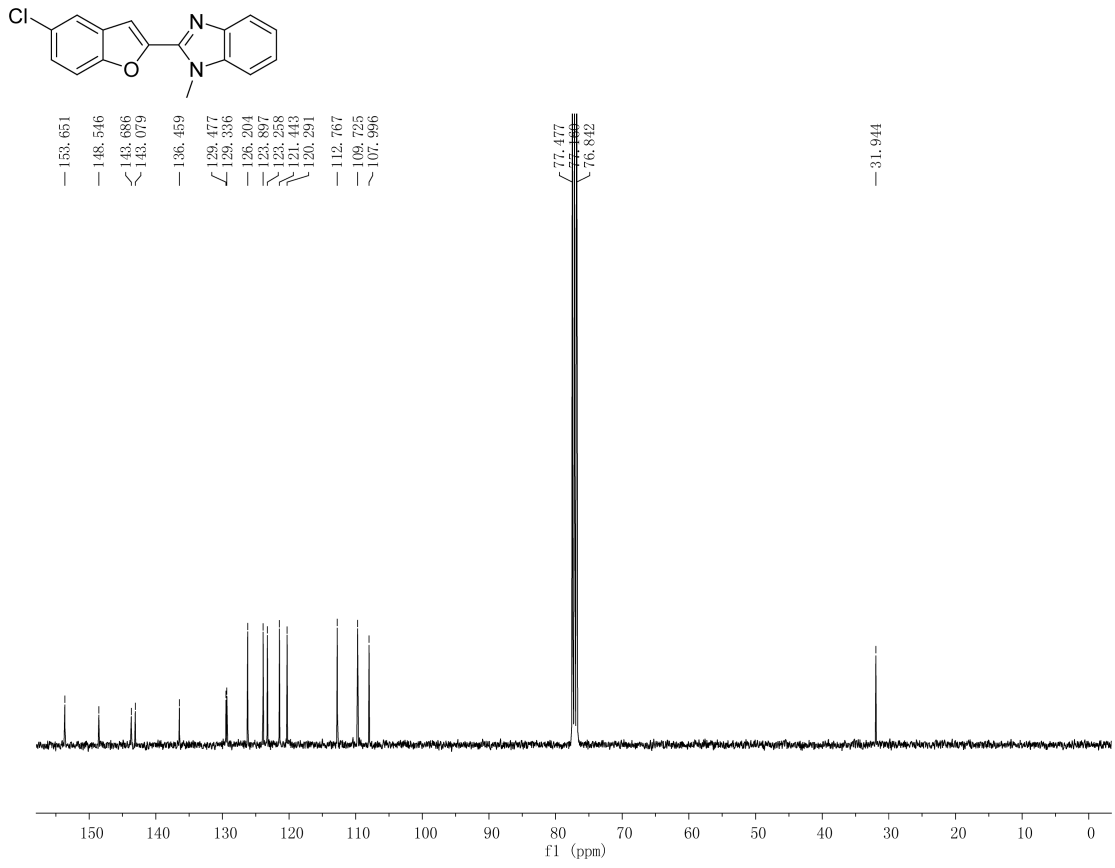

N
O
S
8.193
8.173
8.140
8.119
8.021
7.966
7.945
7.923
7.837
7.814
7.745
7.722
7.658
7.640
7.622
7.551
7.531
7.512
7.433
7.414
7.395
7.260
1.08
1.01
1.00
2.11
0.98
1.07
1.04
2.06
1.02
f1 (ppm)

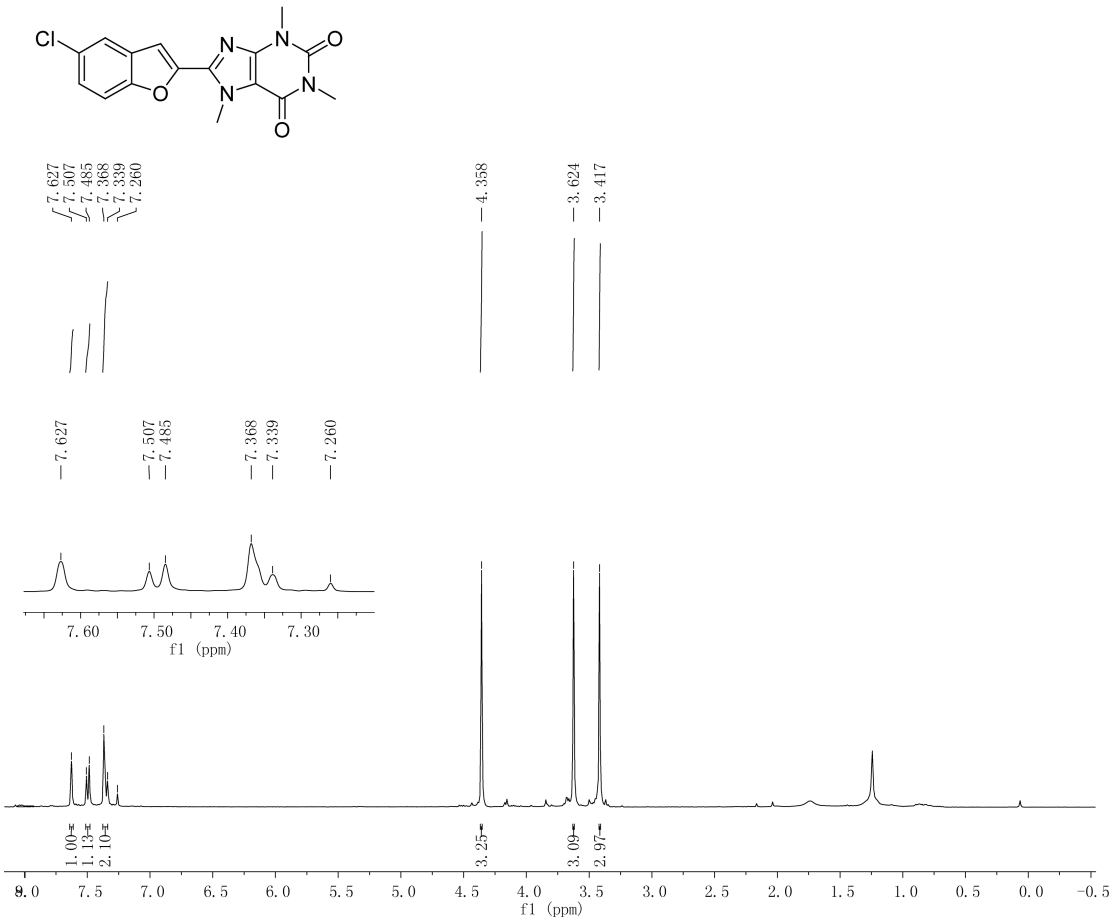

N
O
S
157.706
153.656
149.429
134.737
129.076
127.887
126.811
125.407
123.605
121.795
112.539
106.798
77.477
77.160
76.842
127.912
127.887
127.158
126.811
125.635
125.407
124.050
123.605
123.471
121.795
f1 (ppm)

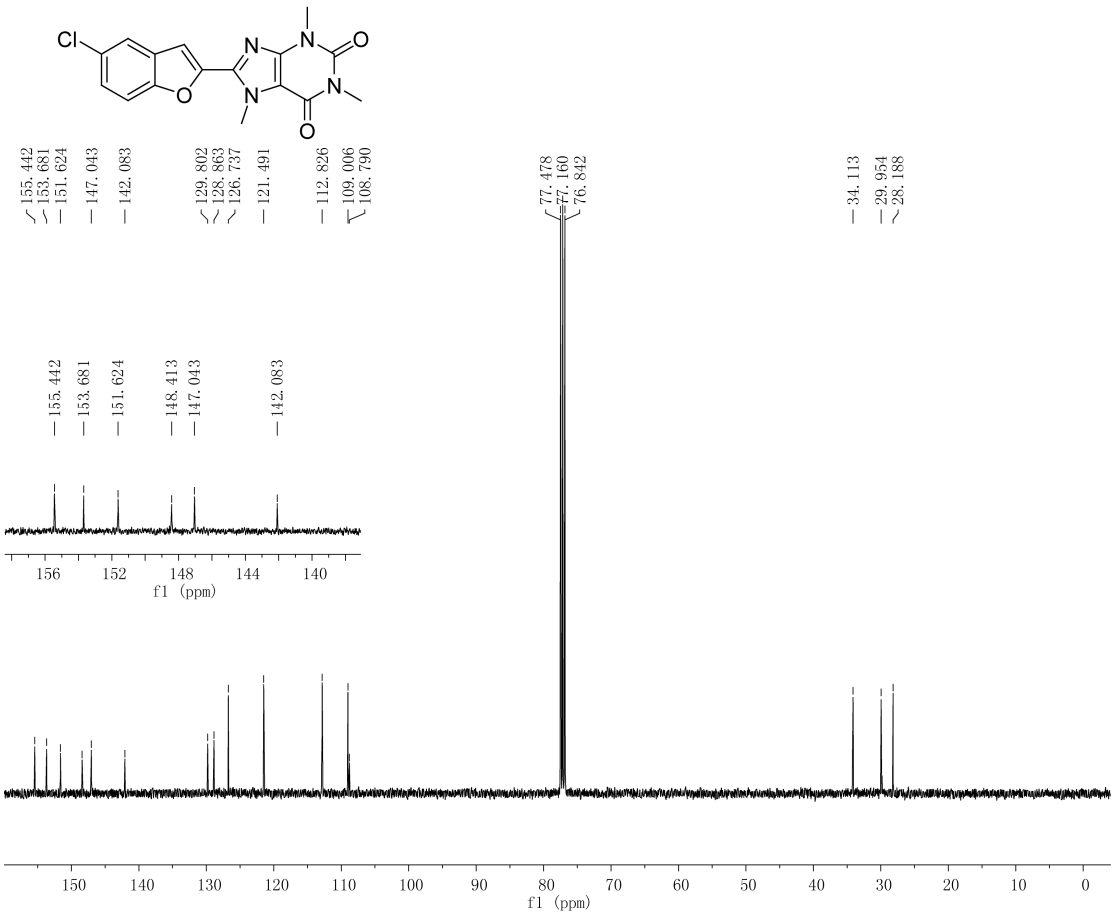

Cl
N
O
S
8.140
8.120
7.938
7.658
7.563
7.547
7.527
7.473
7.446
7.428
7.371
7.351
7.260
f1 (ppm)
1.00
1.04
1.00
2.07
2.22
1.06

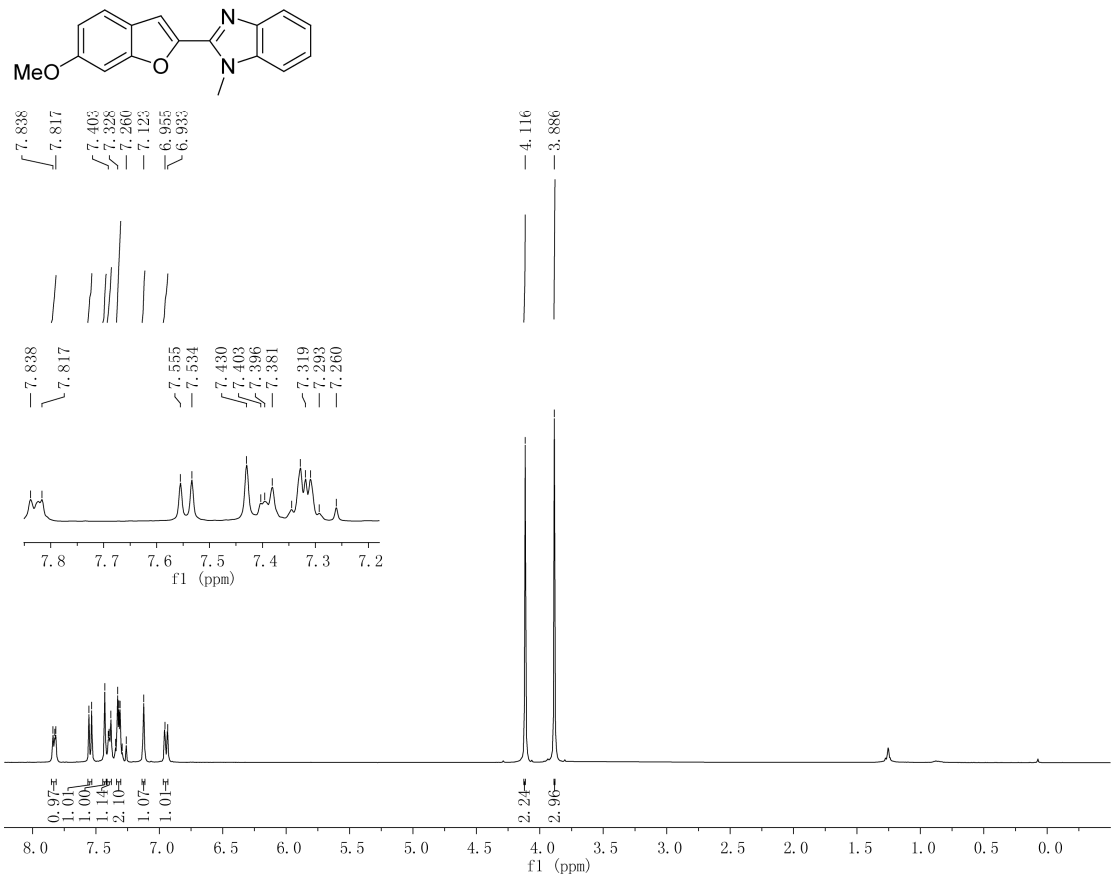

Cl
N
O
S
157.128
153.924
151.267
134.886
129.599
126.834
123.789
121.883
121.709
113.023
112.431
106.927
77.478
77.160
76.843
129.599
126.978
126.834
126.066
123.789
121.883
121.709
f1 (ppm)

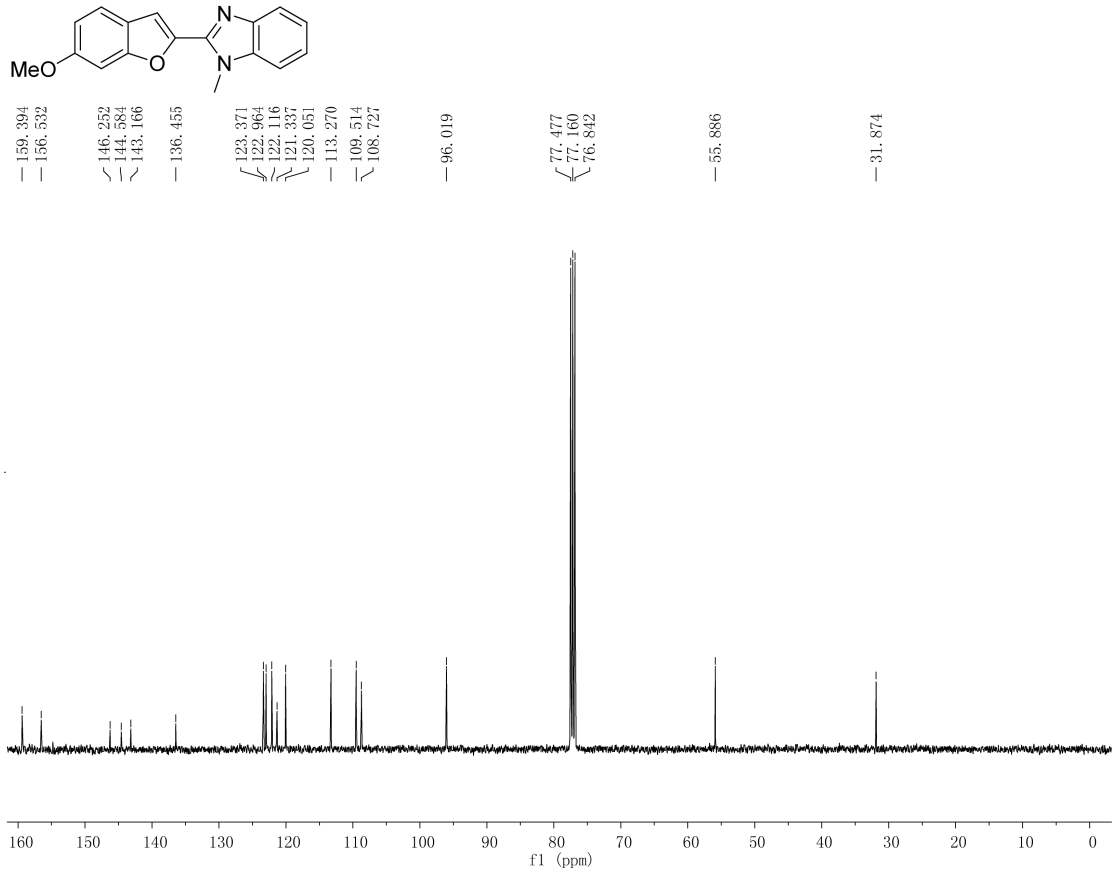

Cl
N
O
N
7.843
7.826
7.652
7.648
7.531
7.510
7.442
7.414
7.396
7.372
7.348
7.342
7.328
7.311
7.260
4.133
1.00
0.93
1.08
1.07
1.09
3.08
2.96
f1 (ppm)

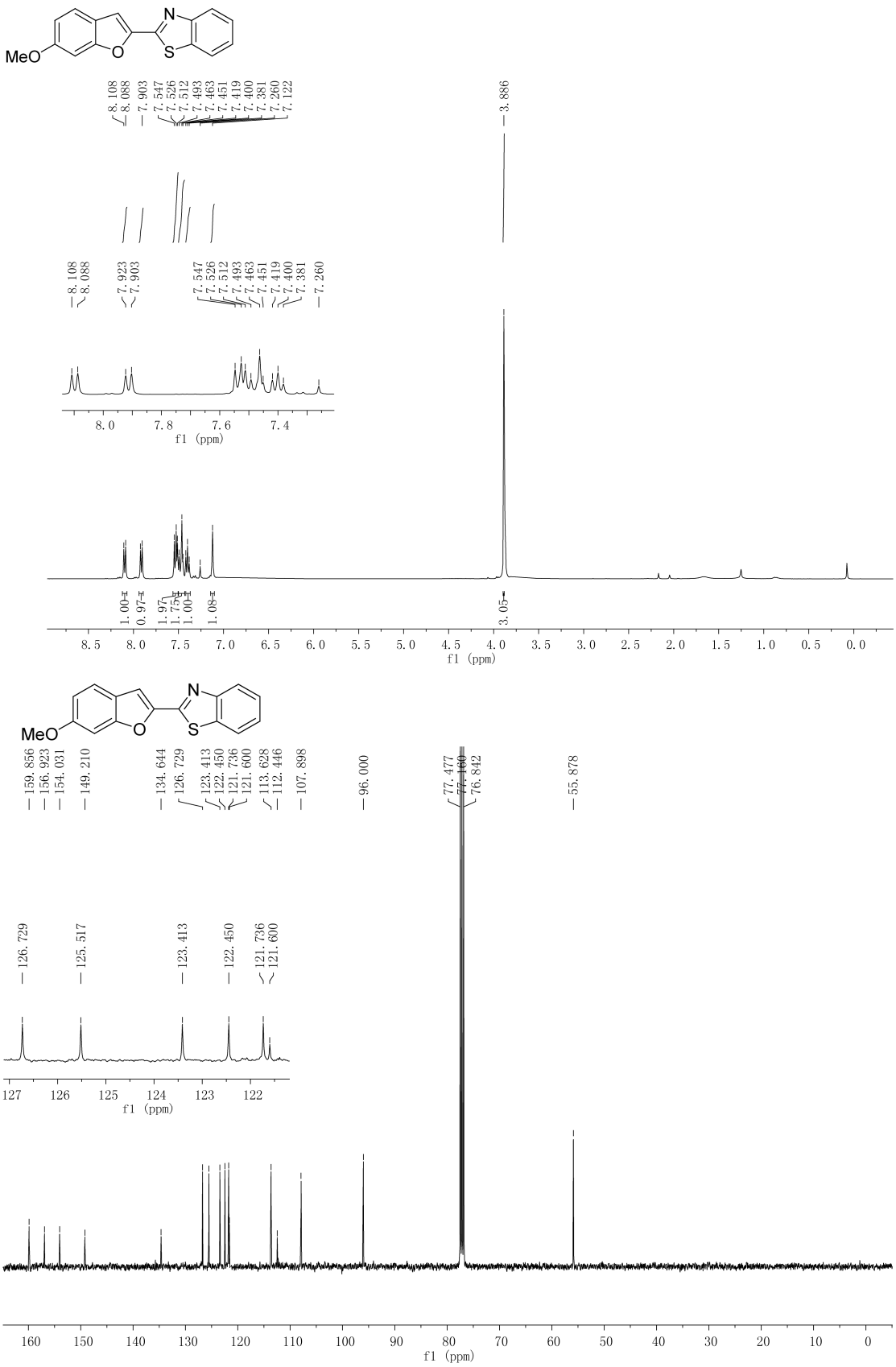

Cl
N
O
N
153.651
148.546
143.686
143.079
136.459
129.477
129.336
126.204
123.897
123.258
121.443
120.291
112.767
109.725
107.996
77.477
77.160
76.842
31.944
f1 (ppm)

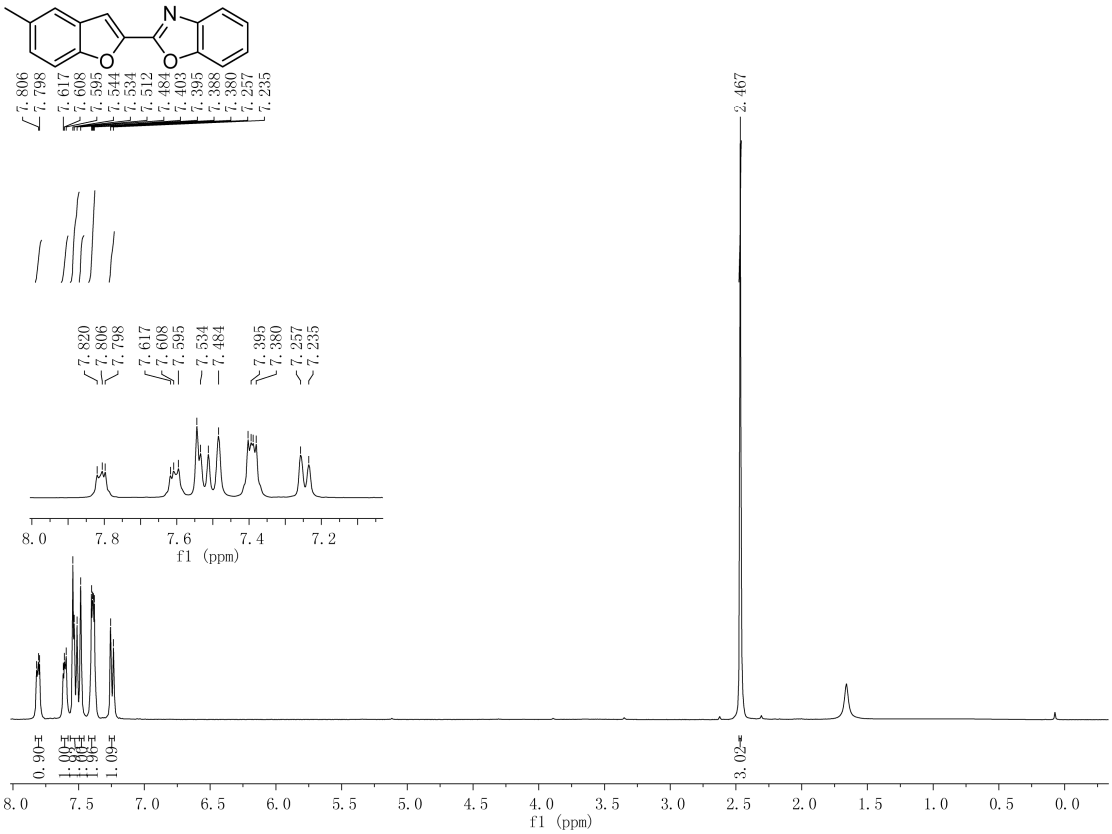

Cl
O
N
N
O
N
N
O
7.627
7.507
7.485
7.368
7.339
7.260
4.358
3.624
3.417
1.00
1.13
2.10
3.25
3.09
2.97
f1 (ppm)

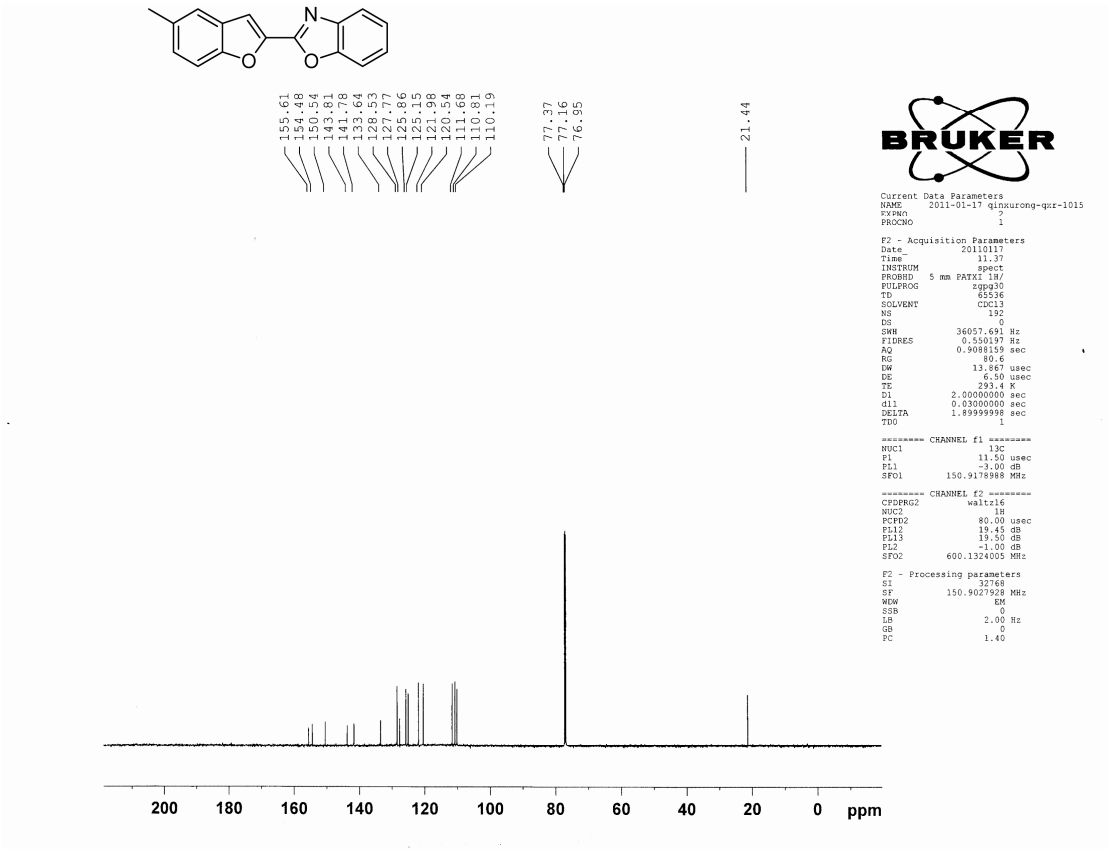

Cl
O
N
N
O
N
N
O
155.442
153.681
151.624
147.043
142.083
129.802
128.863
126.737
121.491
112.826
109.006
108.790
77.478
77.160
76.842
34.113
29.954
28.188
148.413
f1 (ppm)

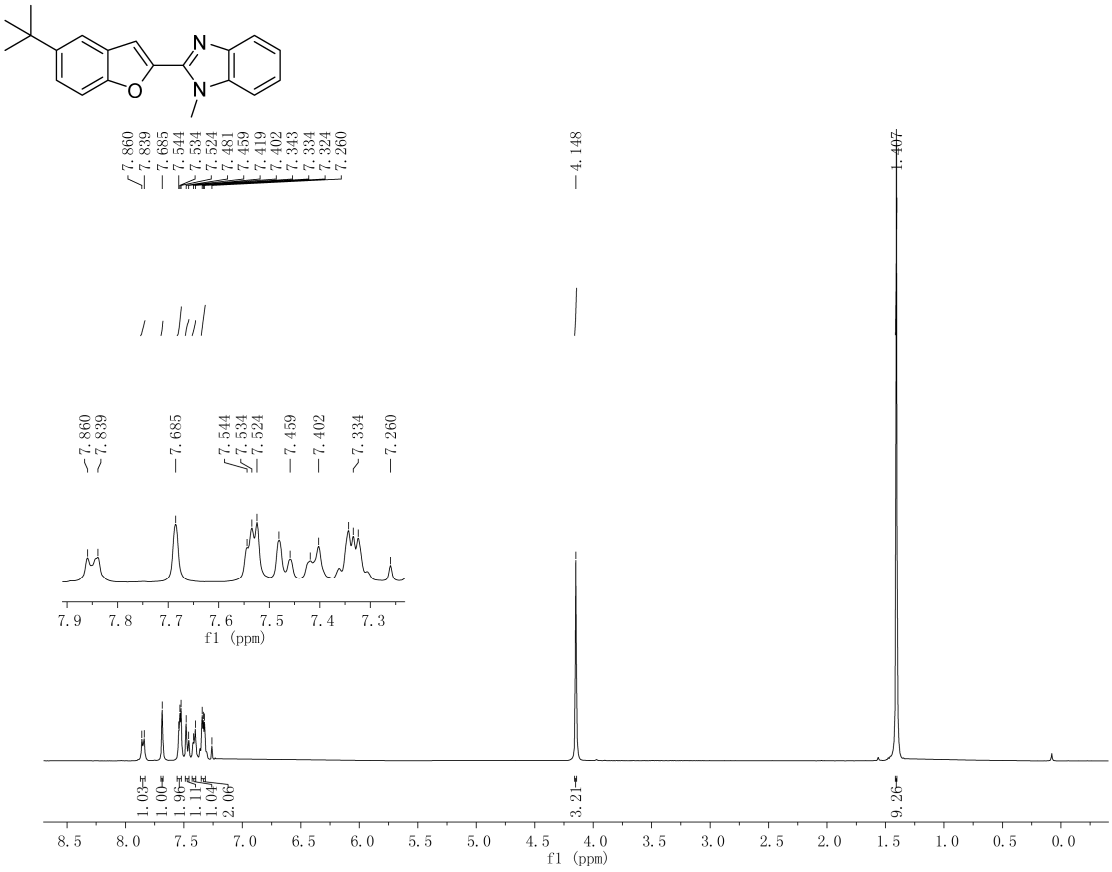

MeO
N
O
N
7.838
7.817
7.403
7.328
7.260
7.123
6.955
6.933
4.116
3.886
7.555
7.534
7.430
7.403
7.396
7.381
7.319
7.293
7.260
f1 (ppm)
0.97
1.01
1.00
1.14
2.10
1.07
1.01
2.24
2.96
f1 (ppm)

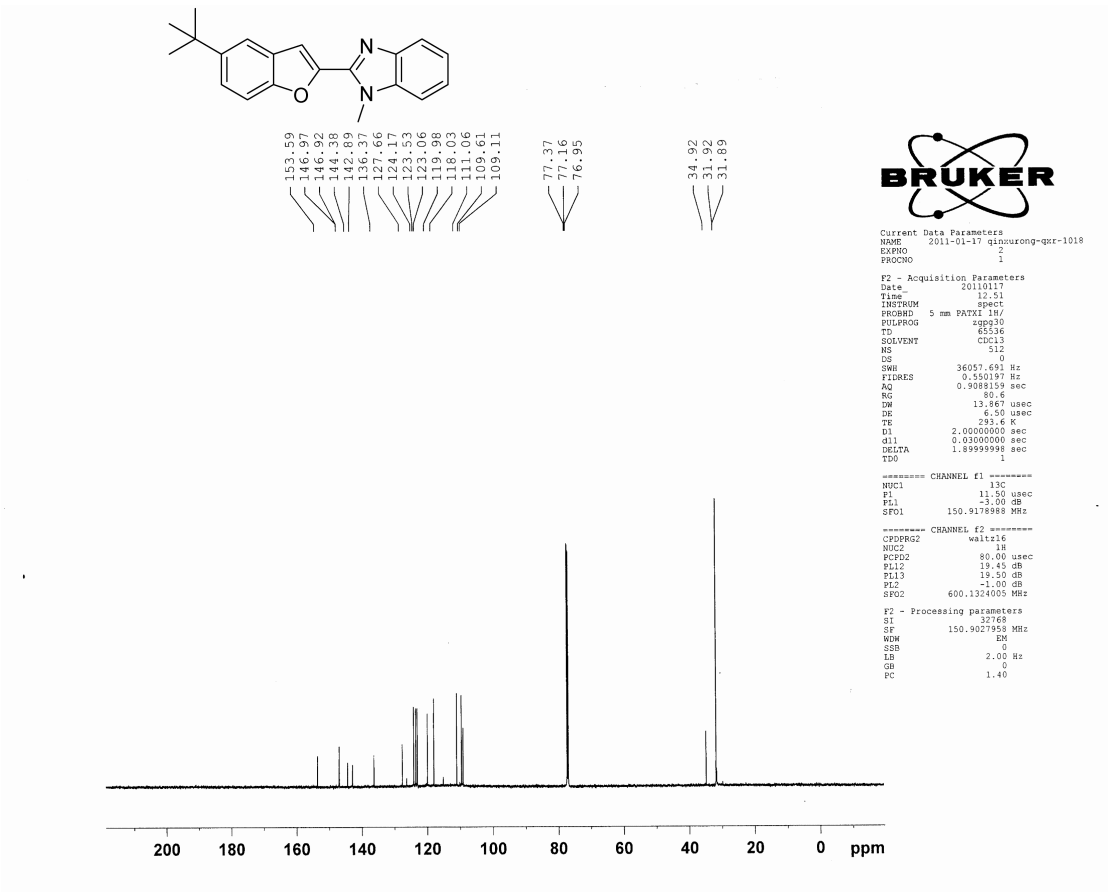

MeO
N
O
N
159.394
156.532
146.252
144.584
143.166
136.455
123.371
122.964
122.116
121.337
120.051
113.270
109.514
108.727
96.019
77.477
77.160
76.842
55.886
31.874
f1 (ppm)

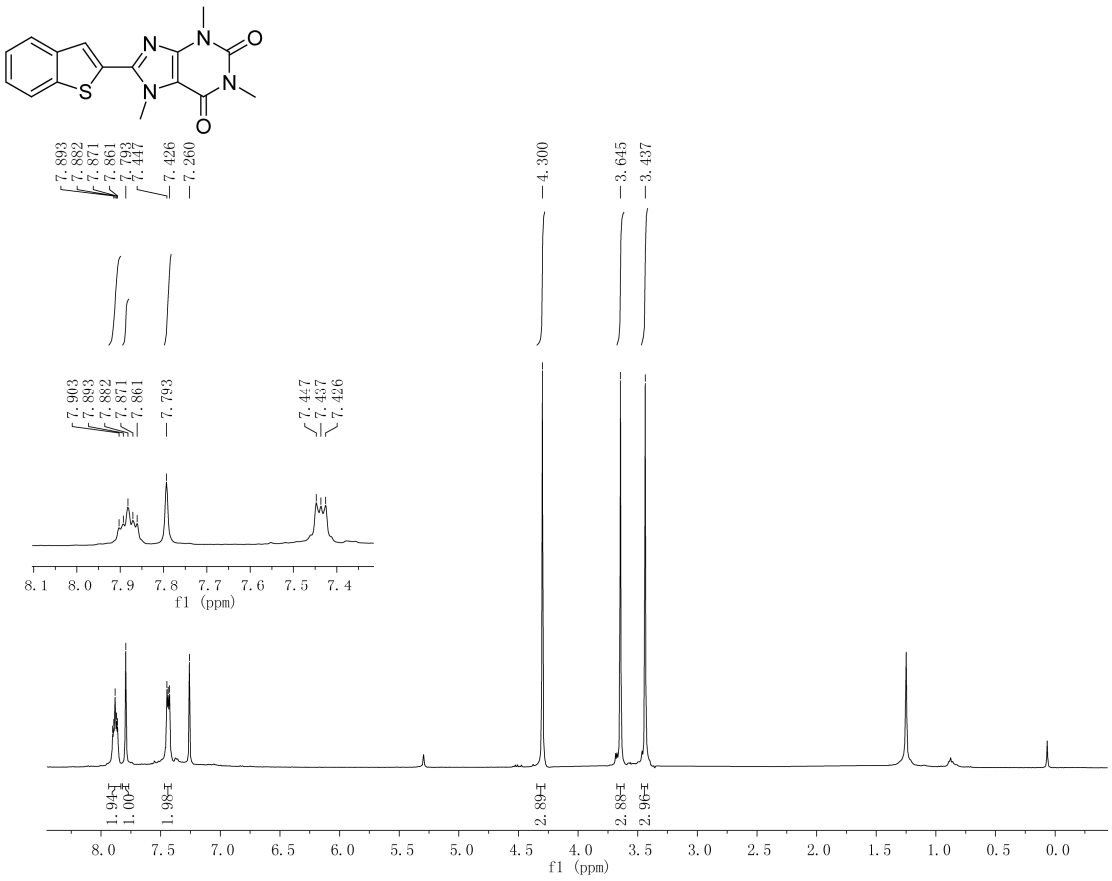

MeO
N
O
S
8.108
8.088
7.903
7.547
7.526
7.512
7.493
7.463
7.451
7.419
7.400
7.381
7.260
7.122
3.886
7.923
7.903
f1 (ppm)
1.00
0.97
1.97
1.75
1.00
1.08
3.05
f1 (ppm)
159.856
156.923
154.031
149.210
134.644
126.729
123.413
122.450
121.736
121.600
113.628
112.446
107.898
96.000
77.477
77.160
76.842
55.878
126.729
125.517
123.413
122.450
121.736
121.600
f1 (ppm)
f1 (ppm)

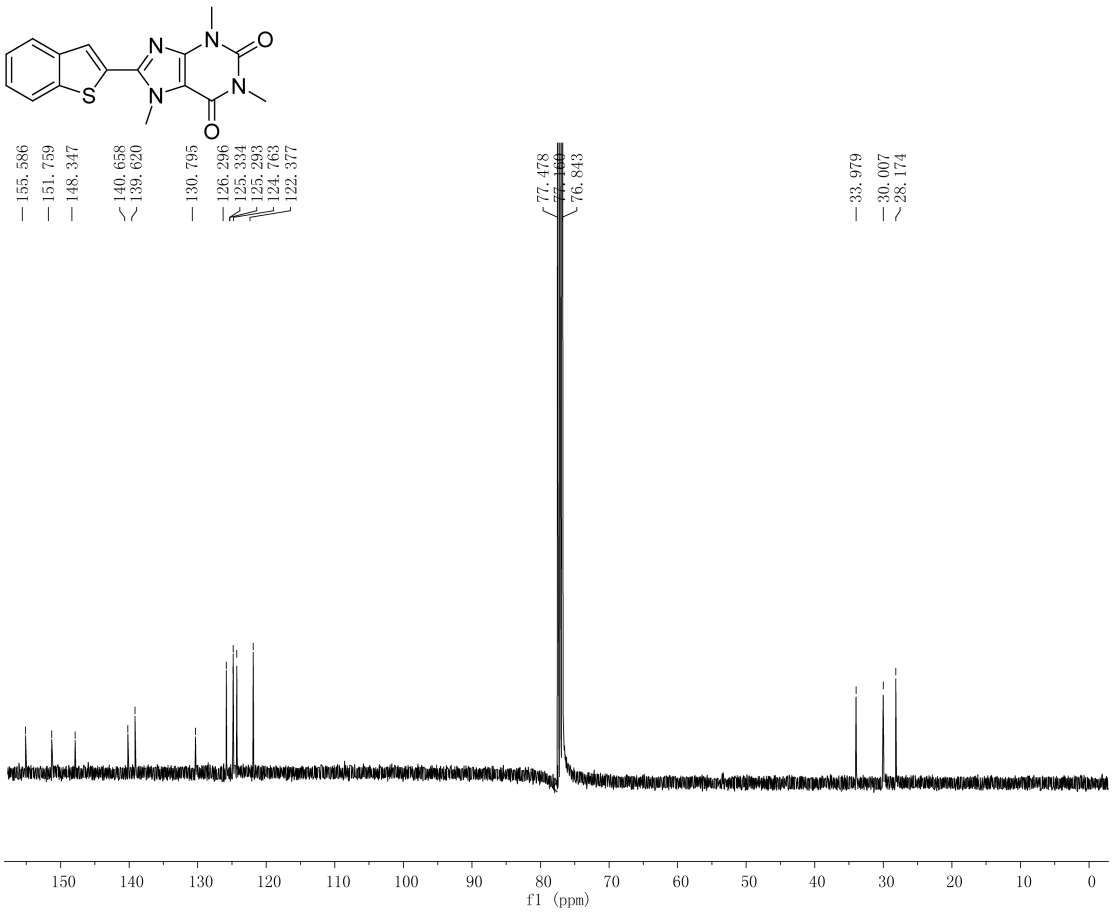

7.806
7.798
7.617
7.608
7.595
7.544
7.534
7.512
7.484
7.403
7.395
7.388
7.380
7.257
7.235
2.467
7.820
7.806
7.798
7.617
7.608
7.595
7.534
7.484
7.395
7.380
7.257
7.235
8.0
7.8
7.6
7.4
7.2
f1 (ppm)
0.90
1.00
1.00
1.96
1.09
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

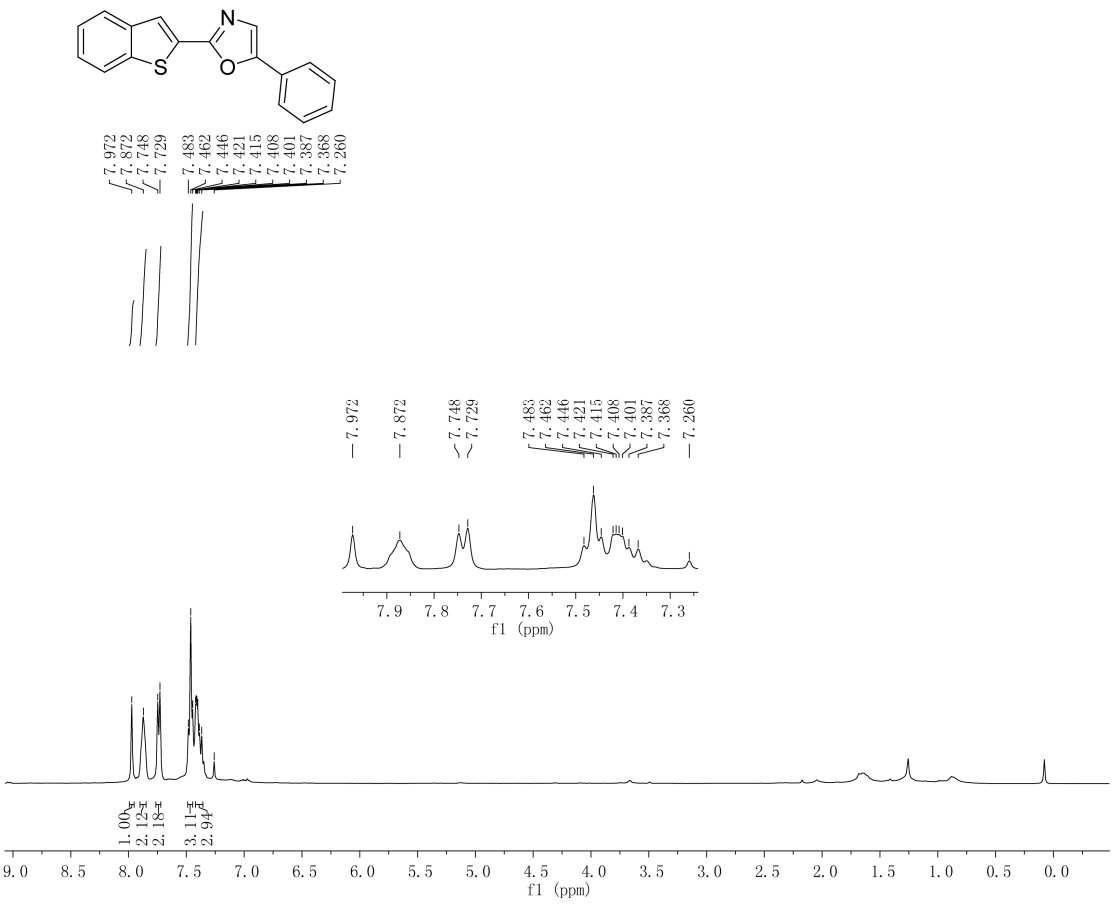

155.61
154.48
150.54
143.81
141.78
133.64
128.53
127.77
125.86
125.15
121.98
120.54
111.68
110.81
110.19
77.37
77.16
76.95
21.44
BRUKER
Current Data Parameters
NAME 2011-01-17 qinxurong-qxr-1015
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110117
Time 11.37
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 192
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
DW 13.867 usec
DE 6.50 usec
TE 293.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.50 usec
PL1 -3.00 dB
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 19.45 dB
PL13 19.50 dB
PL2 -1.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027928 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

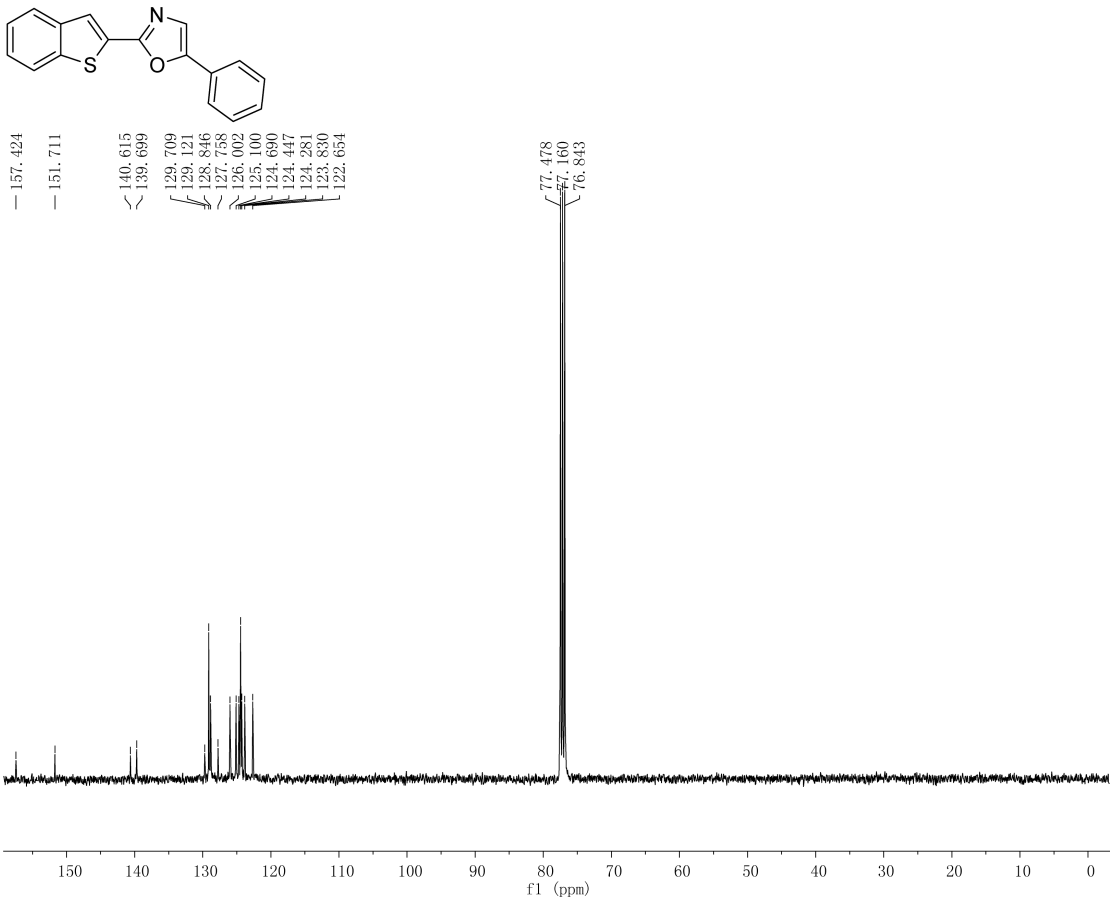

7.860
7.839
7.685
7.544
7.534
7.524
7.481
7.459
7.419
7.402
7.343
7.334
7.324
7.260
4.148
1.407
7.9 7.8 7.7 7.6 7.5 7.4 7.3
f1 (ppm)
1.03
1.00
1.96
1.11
1.04
2.06
3.21
9.26
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

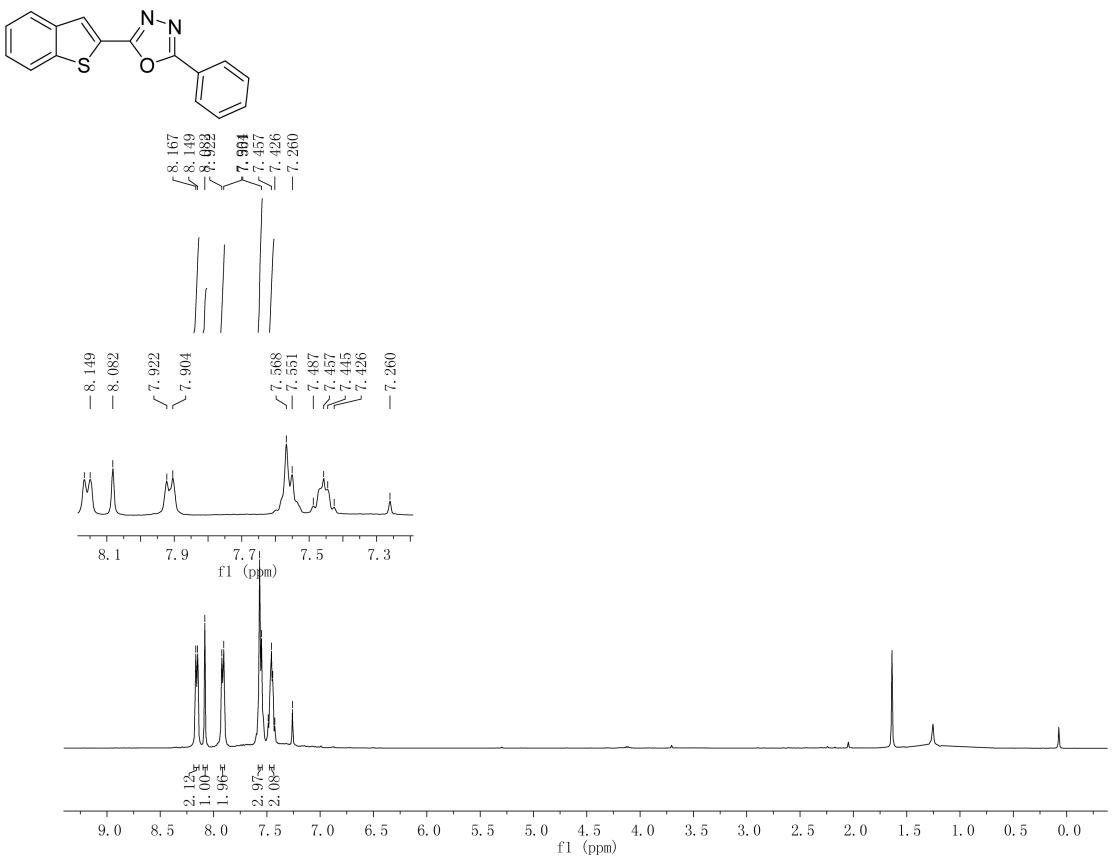

153.59
146.97
146.92
144.38
142.89
136.37
127.66
124.17
123.53
123.06
119.98
118.03
111.06
109.61
109.11
77.37
77.16
76.95
34.92
31.92
31.89
BRUKER
Current Data Parameters
NAME 2011-01-17 qinzurong-qxr-1018
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110117
Time 12.51
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 0
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9088159 sec
RG 80.6
DW 13.867 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.50 usec
PL1 -3.00 dB
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 19.45 dB
PL13 19.50 dB
PL2 -1.00 dB
SFO2 600.1324005 MHz
F2 - Processing parameters
SI 32768
SF 150.9027958 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

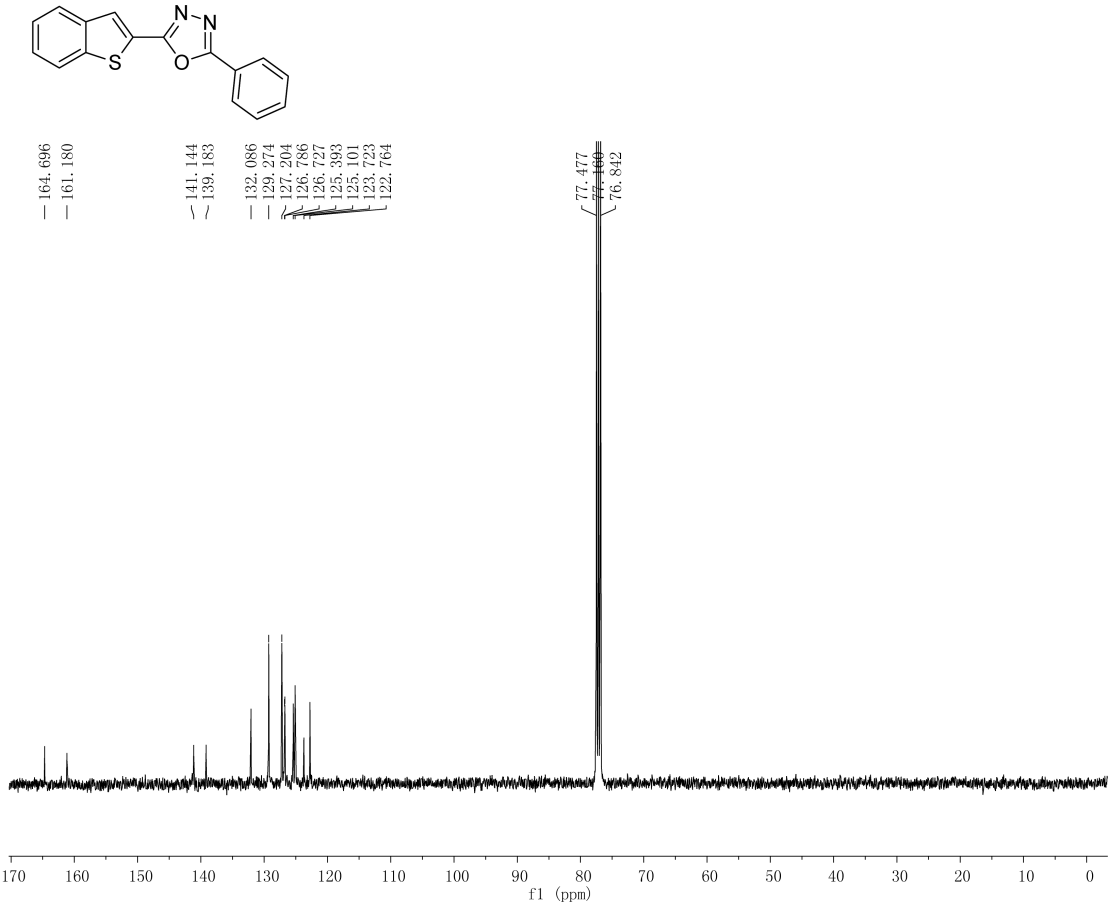

7.893
7.882
7.871
7.861
7.793
7.447
7.426
7.260
4.300
3.645
3.437
7.903
7.893
7.882
7.871
7.861
7.793
7.447
7.437
7.426
f1 (ppm)
1.94
1.00
1.98
2.89
2.88
2.96
f1 (ppm)

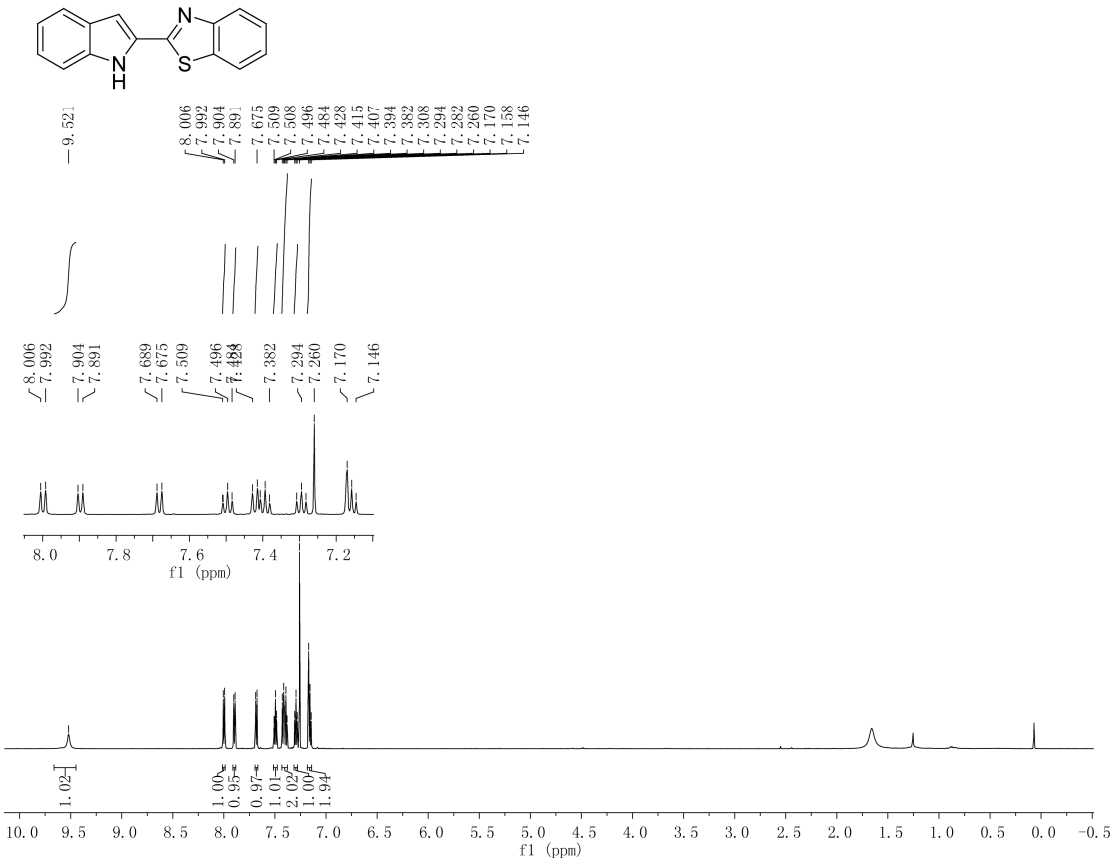

155.586
151.759
148.347
140.658
139.620
130.795
126.296
125.334
125.293
124.763
122.377
77.478
77.160
76.843
33.979
30.007
28.174
f1 (ppm)

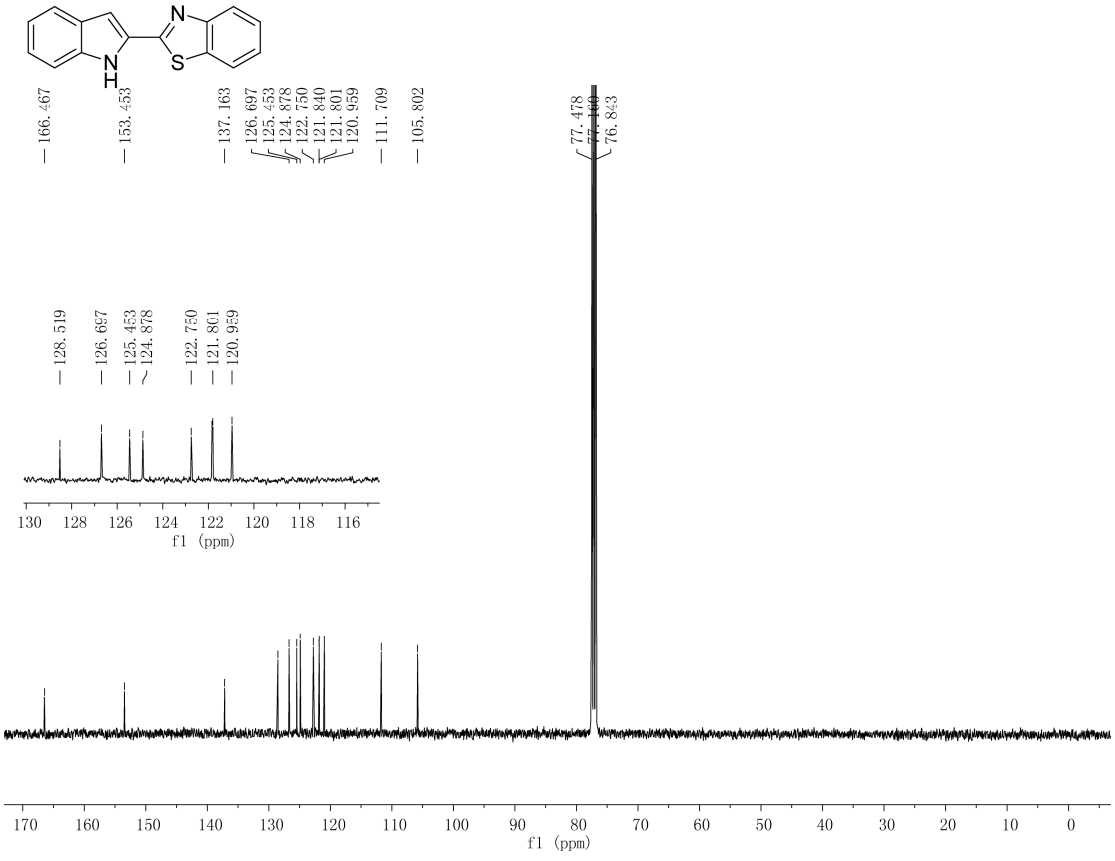

7.972
7.872
7.748
7.729
7.483
7.462
7.446
7.421
7.415
7.408
7.401
7.387
7.368
7.260
1.00
2.12
2.18
3.11
2.94
f1 (ppm)


157.424
151.711
140.615
139.699
129.709
129.121
128.846
127.758
126.002
125.100
124.690
124.447
124.281
123.830
122.654
77.478
77.160
76.843
f1 (ppm)


8.167
8.149
8.083
8.082
7.922
7.904
7.568
7.551
7.487
7.457
7.445
7.426
7.260
f1 (ppm)
2.12
1.00
1.96
2.97
2.08


164.696
161.180
141.144
139.183
132.086
129.274
127.204
126.786
126.727
125.393
125.101
123.723
122.764
77.477
76.842
f1 (ppm)


N
S
H
9.521
8.006
7.992
7.904
7.891
7.675
7.509
7.508
7.496
7.484
7.428
7.415
7.407
7.394
7.382
7.308
7.294
7.282
7.260
7.170
7.158
7.146
7.689
f1 (ppm)
1.02
1.00
0.95
0.97
1.01
2.02
1.00
1.94


N
S
H
166.467
153.453
137.163
126.697
125.453
124.878
122.750
121.840
121.801
120.959
111.709
105.802
77.478
77.160
76.843
128.519
126.697
125.453
124.878
122.750
121.801
120.959
f1 (ppm)