Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Three-component synthesis of 2-heteroaryl-benzothiazoles under metal-free conditions

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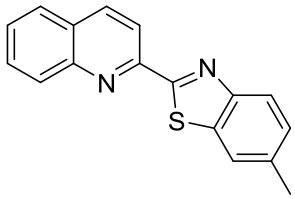
General information

All reactions were carried out under an atmosphere of air. Column chromatography was performed using silica gel 48-75 μm. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at the Institute of Chemistry, Chinese Academy of Sciences. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Most reagents were obtained from commercial suppliers and used without further purification.

General procedure for benzothiazole synthesis

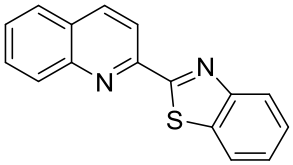
Ammonium iodide (29 mg, 0.2 mmol), *p*-toluidine (**1a**, 54 mg, 0.6 mmol), sulfur (32 mg, 1 mmol), 2-methylquinoline (**2a**, 27 μL , 0.2 mmol) , 1-methyl-2-pyrrolidinone (0.6 mL) were added to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred at 160 ^{o}C for 40 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layer was dried over magnesium sulfate and the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3a** as white solid (35.9 mg, 65% yield), mp 232-233 ^{o}C.

6-Methyl-2-(quinolin-2-yl)benzo[d]thiazole (3a, CAS: 103042-07-5)[1]



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 8.6 Hz, 1H), 8.30 (d, J = 8.5 Hz, 1H), 8.21 (d, J = 8.4 Hz, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.87 (d, J = 8.0 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.63 – 7.57 (m, 1H), 7.37 – 7.32 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 152.5, 151.5, 147.9, 137.0, 136.7, 136.2, 130.0, 129.7, 128.9, 128.0, 127.7, 127.5, 123.3, 121.7, 118.3, 21.6.

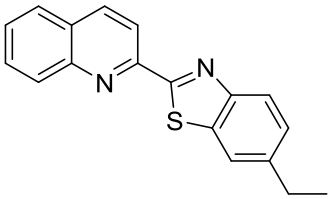
2-(Quinolin-2-yl)benzo[d]thiazole (3b, CAS: 24613-99-8)[1]



The reaction was conducted with aniline (**1b**, 55 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 25:1) to yield the desired product **3b** as white solid (29.3 mg, 56% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (d, J = 8.5 Hz, 1H), 8.30 (d, J = 8.5 Hz, 1H), 8.20 (d, J = 8.5 Hz, 1H), 8.14 (d, J = 8.1 Hz, 1H), 7.99 (d, J = 7.5 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.63 – 7.56 (m, 1H), 7.55 – 7.49 (m, 1H), 7.47 – 7.41 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 154.3, 151.3, 147.9, 137.0, 136.5, 130.1, 129.7, 129.0, 127.7, 127.6, 126.3, 125.9, 123.8, 122.0, 118.3.

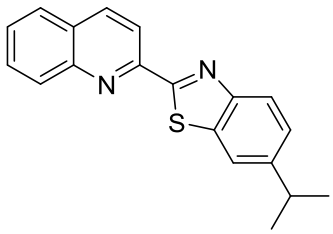
6-Ethyl-2-(quinolin-2-yl)benzo[d]thiazole (3c)



The reaction was conducted with 4-ethylaniline (**1c**, 73 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3c** as white solid (36.5 mg, 63% yield), mp173-174 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 – 8.44 (m, 1H), 8.30 – 8.24 (m, 1H), 8.19 (d, J = 8.5 Hz, 1H), 8.04 (d, J = 8.4 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.80 – 7.72 (m, 2H), 7.61 – 7.54 (m, 1H), 7.39 – 7.33 (m, 1H), 2.81 (m, 2H), 1.33 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.8, 152.6, 151.4, 147.8, 142.6, 136.9, 136.6, 130.0, 129.6, 128.9, 127.7, 127.4, 126.9, 123.3, 120.5, 118.28, 29.0, 15.7; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09497.

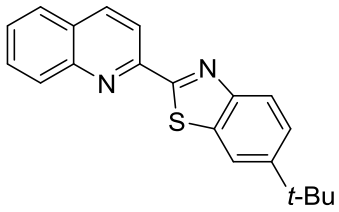
6-Isopropyl-2-(quinolin-2-yl)benzo[d]thiazole (3d)



The reaction was conducted with 4-isopropylaniline (**1d**, 81 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3d** as white solid (43.8 mg, 72% yield), mp 138-140 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 8.5 Hz, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.22 (d, J = 8.5 Hz, 1H), 8.06 (d, J = 8.5 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.83 (d, J = 1.5 Hz, 1H), 7.80 – 7.75 (m, 1H), 7.63 – 7.57 (m, 1H), 7.44 – 7.39 (m, 1H), 3.14 – 3.04 (m, 1H), 1.36 (d, J = 6.9 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 152.7, 151.4, 147.8, 147.2, 136.9, 136.6, 130.0, 129.6, 128.8, 127.7, 127.4, 125.6, 123.4, 119.1, 118.3, 34.3, 24.1; HRMS (ESI) m/z calcd. for $C_{19}H_{17}N_2S^+$ $(M+H)^+$ 305.11070, found 305.11060.

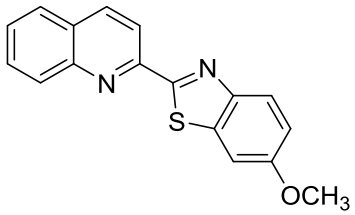
6-(*tert*-Butyl)-2-(quinolin-2-yl)benzo[d]thiazole (3e)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3e** as white solid (49.6 mg, 78% yield), mp 248-249 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 8.6 Hz, 1H), 8.32 (d, J = 8.6 Hz, 1H), 8.24 (d, J = 8.5 Hz, 1H), 8.08 (d, J = 8.7 Hz, 1H), 7.98 (d, J = 1.8 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.64 – 7.58 (m, 2H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.1, 152.2, 151.4, 149.4, 147.8, 136.9, 136.5, 130.0, 129.6, 128.8, 127.7, 127.4, 124.6, 123.0, 118.3, 118.0, 35.1, 31.5; HRMS (ESI) m/z calcd. for $C_{20}H_{19}N_2S^+$ $(M+H)^+$ 319.12635, found 319.12628.

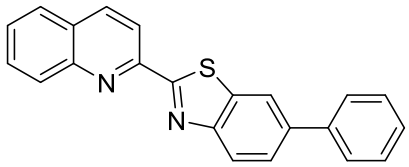
6-Methoxy-2-(quinolin-2-yl)benzo[d]thiazole (3f, CAS:107524-00-5)[1]



The reaction was conducted with *p*-anisidine (**1f**, 74 mg, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3f** as yellow solid (35.6 mg, 61% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, J = 8.6 Hz, 1H), 8.29 (d, J = 8.6 Hz, 1H), 8.21 (d, J = 8.5 Hz, 1H), 8.02 (d, J = 9.0 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.80 – 7.74 (m, 1H), 7.62 – 7.56 (m, 1H), 7.43 (d, J = 2.5 Hz, 1H), 7.16 – 7.10 (m, 1H), 3.93 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.2, 158.3, 151.4, 148.9, 147.8, 138.0, 136.9, 130.0, 129.6, 128.8, 127.7, 127.4, 124.3, 118.1, 116.1, 104.1, 55.8.

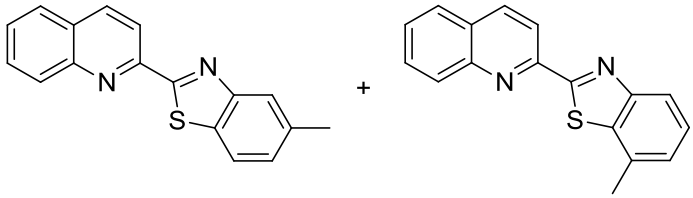
6-Phenyl-2-(quinolin-2-yl)benzo[d]thiazole (3g)



The reaction was conducted with 4-aminobiphenyl (**1g**, 102 mg, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 45:1) to yield the desired product **3g** as white solid (36.5 mg, 54% yield), mp 182-183 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 8.5 Hz, 1H), 8.32 (d, J = 8.5 Hz, 1H), 8.25 – 8.16 (m, 3H), 7.88 (d, J = 8.1 Hz, 1H), 7.82 – 7.74 (m, 2H), 7.72 – 7.67 (m, 2H), 7.61 (t, J = 7.5 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.44 – 7.37 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 153.6, 151.2, 147.9, 140.5, 139.3, 137.2, 137.1, 120.3, 118.4, 77.3, 77.00, 76.7; HRMS (ESI) m/z calcd. for $C_{22}H_{15}N_2S^+$ $(M+H)^+$ 339.09505, found 339.09512.

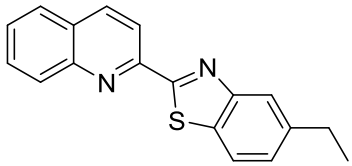
5-Methyl-2-(quinolin-2-yl)benzo[d]thiazole (3h+3h')[2]



The reaction was conducted with 3- toluidine (**1h**, 64 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 70:1) to yield the desired product **3h+3h'** as white solid (30.8 mg, 56% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 – 8.46 (m, 1H), 8.33 – 8.26 (m, 1H), 8.20 (d, J = 8.4 Hz, 1H), 7.99 (d, J = 8.2 Hz, 1H), 7.94 (s, 1H), 7.89 – 7.81 (m, 1H), 7.80 – 7.73 (m, 1H), 7.59 (t, J = 7.4 Hz, 1H), 7.45 (t, J = 7.7 Hz, 1H), 7.30 – 7.22 (m, 1H), 2.66 (s, 2H), 2.54 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 169.3, 166.7, 154.8, 154.3, 152.9, 151.4, 150.0, 148.0, 146.2, 137.0, 137.0, 136.4, 133.5, 132.3, 132.2, 130.1, 130.1, 129.7, 129.7, 129.0, 1289.0, 127.7, 127.7, 127.6, 127.5, 127.5, 126.5, 126.0, 123.7, 121.5, 121.2, 118.4, 118.3, 77.3, 77.2, 77.0, 76.7, 21.5, 21.3.

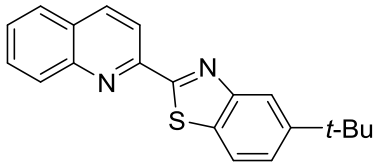
5-Ethyl-2-(quinolin-2-yl)benzo[d]thiazole (3i)



The reaction was conducted with 3-ethylaniline (**1i**, 73 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3i** as white solid (35.4 mg, 61% yield), mp 182-184 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 8.5 Hz, 1H), 8.31 (d, J = 8.5 Hz, 1H), 8.21 (d, J = 8.5 Hz, 1H), 7.99 (s, 1H), 7.88 (t, J = 7.6 Hz, 2H), 7.77 (d, J = 8.2 Hz, 1H), 7.61 (d, J = 7.2 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 2.90 – 2.79 (m, 2H), 1.35 (t, J = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 154.6, 151.3, 147.8, 142.9, 137.0, 133.6, 130.1, 129.7, 128.9, 127.7, 127.5, 126.7, 122.4, 121.6, 118.3, 77.3, 77.0, 76.7, 28.8, 29.0, 15.8; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09485.

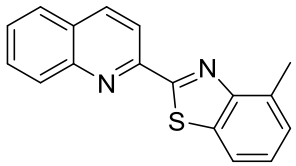
5-(tert-Butyl)-2-(quinolin-2-yl)benzo[d]thiazole (3j)



The reaction was conducted with 3-tert-butylaniline (**1j**, 95.6 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3j** as white solid (52.2 mg, 82% yield), mp 173-174 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 8.5 Hz, 1H), 8.32 (d, J = 8.6 Hz, 1H), 8.25 – 8.16 (m, 2H), 7.92 (d, J = 8.5 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.78 (t, J = 7.7 Hz, 1H), 7.61 (t, J = 7.5 Hz, 1H), 7.57 – 7.52 (m, 1H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.9, 154.6, 151.4, 150.0, 147.9, 137.0, 133.4, 130.0, 129.7, 128.9, 127.7, 127.5, 124.2, 121.3, 120.1, 118.2, 77.3, 77.0, 76.7, 34.9, 31.5; HRMS (ESI) m/z calcd. for $C_{20}H_{19}N_2S^+$ $(M+H)^+$ 319.12635, found 319.12604.

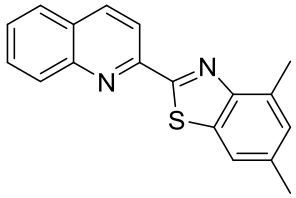
4-Methyl-2-(quinolin-2-yl)benzo[d]thiazole (3k)[1]



The reaction was conducted with 2-toluidine (**1k**, 64.2 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 60:1) to yield the desired product **3k** as white solid (20.2 mg, 37% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, J = 8.5 Hz, 1H), 8.27 (d, J = 8.5 Hz, 1H), 8.20 (d, J = 8.5 Hz, 1H), 7.85 (d, J = 8.1 Hz, 1H), 7.83 – 7.78 (m, 1H), 7.76 (t, J = 7.6 Hz, 1H), 7.58 (t, J = 7.5 Hz, 1H), 7.36 – 7.27 (m, 2H), 2.84 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.2, 153.8, 151.6, 147.8, 136.8, 136.4, 133.9, 130.0, 129.6, 128.9, 127.7, 127.4, 126.6, 125.8, 119.3, 118.5, 77.3, 77.0, 76.7, 18.2.

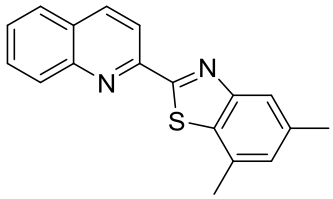
4,6-Dimethyl-2-(quinolin-2-yl)benzo[d]thiazole(3l)



The reaction was conducted with 2,4-dimethylaniline (**1l**, 73 mg, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3l** as white solid (33.2 mg, 56% yield), mp 161-162 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 8.5 Hz, 1H), 8.26 (d, J = 8.5 Hz, 1H), 8.19 (d, J = 8.5 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.75 (t, J = 7.5 Hz, 1H), 7.64 – 7.53 (m, 2H), 7.12 (s, 1H), 2.80 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 152.0, 151.8, 147.8, 136.7, 136.6, 136.0, 133.3, 129.9, 129.6, 128.8, 128.4, 127.7, 127.3, 119.1, 118.4, 77.3, 77.0, 76.7, 21.6, 18.1; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09494.

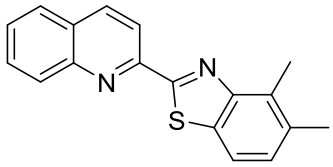
5,7-Dimethyl-2-(quinolin-2-yl)benzo[d]thiazole (3m)



The reaction was conducted with 3,5-dimethylaniline (**1m**, 72.6 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3m** as white solid (31.8 mg, 55% yield), mp 184-185 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 8.5 Hz, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.20 (d, J = 8.5 Hz, 1H), 7.87 (d, J = 8.1 Hz, 1H), 7.81 – 7.73 (m, 2H), 7.62 – 7.56 (m, 1H), 7.09 (s, 1H), 2.62 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 154.34, 151.34, 147.9, 137.0, 136.6, 133.9, 131.5, 130.1, 129.6, 128.9, 127.9, 127.7, 127.5, 121.1, 118.3, 77.3, 77.0, 76.7, 21.5, 21.2; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09518.

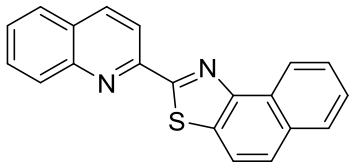
4,5-Dimethyl-2-(quinolin-2-yl)benzo[d]thiazole (3n)



The reaction was conducted with 2,3-dimethylaniline (**1n**, 74.1 μL, 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3n** as white solid (41.2 mg, 71% yield), mp 253-255 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 – 8.54 (m, 1H), 8.36 – 8.25 (m, 2H), 7.92 – 7.84 (m, 1H), 7.82 – 7.74 (m, 1H), 7.74 – 7.65 (m, 1H), 7.64 – 7.56 (m, 1H), 7.29 – 7.22 (m, 2H), 2.85 – 2.74 (m, 3H), 2.49 – 2.41 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 154.2, 151.8, 147.9, 136.7, 134.0, 133.7, 132.0, 129.9, 129.6, 128.9, 128.1, 127.7, 127.3, 118.5, 77.3, 77.0, 76.7, 19.6, 14.8; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09506.

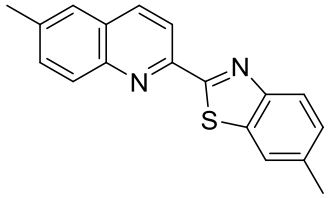
2-(Quinolin-2-yl)naphtho[1,2-d]thiazole (3o)[3]



The reaction was conducted with 1-aminonaphthalene (**1o**, 86.1 mg 0.6 mmol) and 2-methylquinoline (**2a**, 27 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 70:1) yield the desired product **3o** as green solid (38.7 mg, 62% yield), mp 243-245 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.97 (d, J = 8.3 Hz, 1H), 8.70 (d, J = 8.5 Hz, 1H), 8.37 (d, J = 8.5 Hz, 1H), 8.31 (d, J = 8.7 Hz, 1H), 8.00 (t, J = 8.8 Hz, 2H), 7.89 (t, J = 8.8 Hz, 2H), 7.82 – 7.78 (m, 1H), 7.77 – 7.71 (m, 1H), 7.65 – 7.59 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 151.7, 150.7, 147.9, 137.0, 133.7, 132.0, 130.1, 129.6, 129.0, 128.9, 128.2, 127.7, 127.4, 127.1, 126.7, 126.2, 123.7, 119.4, 118.5, 77.3, 77.0, 76.7; HRMS (ESI) m/z calcd. for $C_{20}H_{13}N_2S^+$ $(M+H)^+$ 313.07940, found 313.07916.

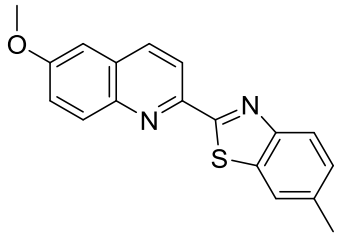
6-Methyl-2-(6-methylquinolin-2-yl)benzo[d]thiazole (3p)



The reaction was conducted with *p*-toluidine (**1b**, 64 mg, 0.6 mmol) and 2,6-dimethylquinoline (**2b** 31.4 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to yield the desired product **3p** as white solid (37.8 mg, 65% yield), mp 211-213 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43 (d, J = 8.5 Hz, 1H), 8.19 (d, J = 8.4 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.01 (d, J = 8.3 Hz, 1H), 7.77 (s, 1H), 7.60 (d, J = 12.8 Hz, 2H), 7.33 (d, J = 8.3 Hz, 1H), 2.56 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 152.4, 150.5, 146.4, 137.7, 136.5, 136.3, 136.1, 132.4, 129.3, 128.9, 127.9, 126.6, 123.1, 121.7, 118.3, 77.3, 77.0, 76.7, 21.7, 21.6; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2S^+$ $(M+H)^+$ 291.09505, found 291.09479.

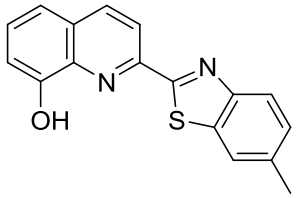
2-(6-Methoxyquinolin-2-yl)-6-methylbenzo[d]thiazole (3q)



The reaction was conducted with *p*-toluidine (**1a**, 64 mg, 0.6 mmol) and 6-methoxy-2-methylquinoline (**2c**, 37 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to yield the desired product **3q** as white solid (41.6 mg, 68% yield), mp 215-217 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, J = 8.5 Hz, 1H), 8.17 (d, J = 8.6 Hz, 1H), 8.09 (d, J = 9.2 Hz, 1H), 8.00 (d, J = 8.4 Hz, 1H), 7.76 (s, 1H), 7.44 – 7.38 (m, 1H), 7.33 (d, J = 8.4 Hz, 1H), 7.11 (s, 1H), 3.96 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.9, 158.6, 152.3, 149.1, 143.9, 136.4, 136.0, 135.6, 131.1, 130.2, 127.9, 123.0, 123.0, 121.7, 118.7, 105.2, 77.3, 77.0, 76.7, 55.6, 21.6; HRMS (ESI) m/z calcd. for $C_{18}H_{15}N_2OS^+$ $(M+H)^+$ 307.08996, found 307.09088.

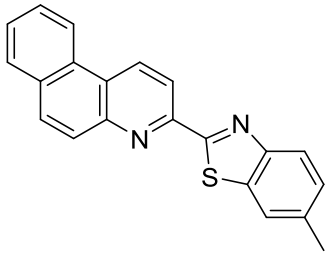
2-(6-Methylbenzo[d]thiazol-2-yl)quinolin-8-ol (3r)



The reaction was conducted with and *p*-toluidine (**1a**, 64 mg, 0.6 mmol) and 2-methylquinolin-8-ol (**2d**, 32 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to yield the desired product **3r** as canary yellow solid (40.1 mg, 68% yield), mp 205-206 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (d, J = 8.6 Hz, 1H), 8.30 (d, J = 8.6 Hz, 1H), 8.08 (s, 1H), 8.02 (d, J = 8.4 Hz, 1H), 7.77 (s, 1H), 7.51 (t, J = 7.9 Hz, 1H), 7.41 – 7.32 (m, 2H), 7.28 – 7.21 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.6, 152.4, 152.1, 149.3, 137.6, 137.2, 136.5, 136.4, 129.1, 128.9, 128.2, 123.3, 121.7, 119.0, 118.1, 110.9, 77.3, 77.0, 76.7, 21.7; HRMS (ESI) m/z calcd. for $C_{17}H_{13}N_2OS^+$ $(M+H)^+$ 293.07431, found 293.07465.

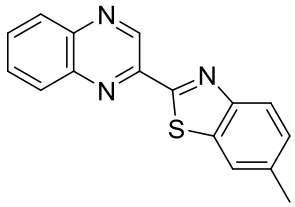
2-(Benzo[f]quinolin-3-yl)-6-methylbenzo[d]thiazole (3s)



The reaction was conducted with *p*-toluidine (**1a**, 64 mg, 0.6 mmol) and 3-methylbenzo[f]quinoline (**2e**, 39 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **3s** as white solid (35.9 mg, 55% yield), mp 233-234 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (d, J = 8.6 Hz, 1H), 8.72 – 8.63 (m, 2H), 8.13 – 8.03 (m, 3H), 7.97 (d, J = 7.5 Hz, 1H), 7.80 (s, 1H), 7.78 – 7.67 (m, 2H), 7.36 (d, J = 8.2 Hz, 1H), 2.54 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 152.5, 150.9, 148.0, 136.6, 136.1, 132.0, 131.6, 131.5, 129.5, 128.8, 128.1, 128.0, 127.8, 127.3, 126.4, 123.2, 123.0, 121.7, 118.4, 77.3, 77.0, 76.7, 21.6; HRMS (ESI) m/z calcd. for $C_{21}H_{15}N_2S^+$ $(M+H)^+$ 327.09505, found 327.09518.

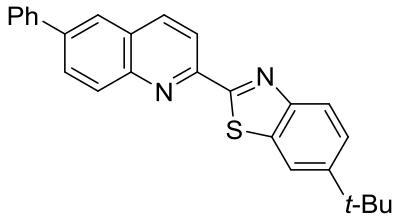
6-Methyl-2-(quinoxalin-2-yl)benzo[d]thiazole (3t)



The reaction was conducted with and *p*-tluidine (**1a**, 64 mg, 0.6 mmol) and 6-methyl-2-(quinoxalin-2-yl)benzo[d]thiazole (**2f**, 29 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 10:1) to yield the desired product **3t** as yellow solid (34.9 mg, 63% yield), mp 223-225 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.19 – 8.14 (m, 2H), 8.04 (d, J = 8.4 Hz, 1H), 7.84 – 7.79 (m, 2H), 7.77 (s, 1H), 7.35 (d, J = 8.3 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.0, 152.5, 146.1, 143.1, 142.9, 141.8, 136.8, 136.4, 130.7, 130.6, 129.5, 129.4, 128.3, 123.6, 121.7, 77.3, 77.0, 76.7, 21.7; HRMS (ESI) m/z calcd. for $C_{16}H_{12}N_3S^+$ $(M+H)^+$ 278.07464, found 278.07452.

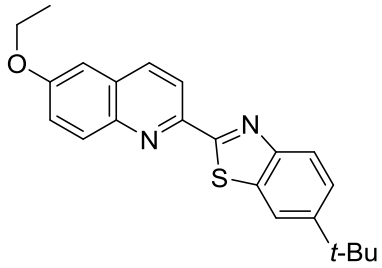
6-(*tert*-Butyl)-2-(6-phenylquinolin-2-yl)benzo[d]thiazole (3u)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL , 0.6 mmol) and 2-methyl-6-phenylquinoline (**2g**, 43 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **3u** as white solid (57.5 mg, 73% yield), mp 203-205 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (d, J = 8.6 Hz, 1H), 8.40 – 8.31 (m, 2H), 8.11 (d, J = 8.8 Hz, 1H), 8.07 (s, 2H), 7.98 (s, 1H), 7.76 (d, J = 7.6 Hz, 2H), 7.62 (d, J = 8.8 Hz, 1H), 7.53 (t, J = 7.4 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H), 1.44 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.0, 152.3, 151.3, 149.5, 147.2, 140.1, 140.0, 137.0, 136.5, 130.0, 129.7, 129.1, 129.0, 127.9, 127.4, 125.3, 124.6, 123.0, 118.7, 118.0, 77.3, 77.0, 76.7, 35.1, 31.5; HRMS (ESI) m/z calcd. for $C_{26}H_{23}N_2S^+$ $(M+H)^+$ 395.15765, found 395.15747.

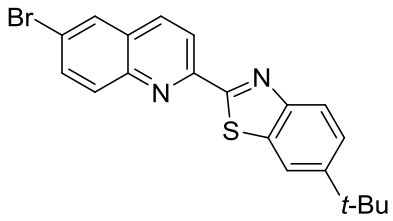
6-(*tert*-Butyl)-2-(6-ethoxyquinolin-2-yl)benzo[d]thiazole (3v)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL, 0.6 mmol) and 6-ethoxy-2-methylquinoline (**2h**, 37.4 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **3v** as white solid (63 mg, 87% yield), mp 192-193 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 8.4 Hz, 1H), 8.14 – 8.00 (m, 3H), 7.95 (s, 1H), 7.56 (d, J = 8.7 Hz, 1H), 7.38 (d, J = 9.2 Hz, 1H), 7.06 (s, 1H), 4.18 – 4.10 (m, 2H), 1.48 (t, J = 6.8 Hz, 3H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.4, 157.9, 152.3, 149.2, 149.1, 143.8, 136.3, 135.4, 131.1, 130.2, 124.4, 123.1, 122.8, 118.6, 117.9, 105.8, 77.3, 77.0, 76.7, 63.8, 35.1, 31.5, 14.7; HRMS (ESI) m/z calcd. for $C_{22}H_{23}N_2OS^+$ $(M+H)^+$ 363.15256, found 363.15262.

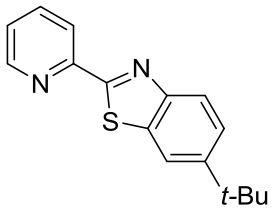
2-(6-Bromoquinolin-2-yl)-6-(*tert*-butyl)benzo[d]thiazole (3w)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL, 0.6 mmol) and 6-bromo-2-methylquinoline (**2i**, 44 mg, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **3w** as canary yellow solid (24.5 mg, 31% yield), mp 181-182 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 8.6 Hz, 1H), 8.17 (d, J = 8.6 Hz, 1H), 8.06 (s, 1H), 8.04 (s, 1H), 8.00 (d, J = 2.1 Hz, 1H), 7.96 (d, J = 1.8 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.59 (m, J = 8.7, 1.9 Hz, 1H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 152.2, 151.8, 149.7, 146.4, 136.5, 135.8, 133.5, 131.3, 129.9, 129.8, 124.7, 123.1, 121.4, 119.2, 118.0, 77.3, 77.0, 76.7, 35.2, 31.5; HRMS (ESI) m/z calcd. for $C_{20}H_{18}BrN_2S^+$ $(M+H)^+$ 397.03686, found 397.03690.

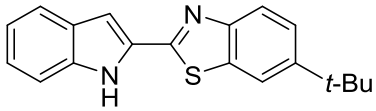
6-(*tert*-Butyl)-2-(pyridin-2-yl)benzo[d]thiazole (3x)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL, 0.6 mmol) and 2-methylpyridine (**2j**, 19 μL, 0.2 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3x** as yellow liquid (38 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 – 8.66 (m, 1H), 8.38 – 8.34 (m, 1H), 8.02 (d, J = 8.7 Hz, 1H), 7.95 (d, J = 1.7 Hz, 1H), 7.86 – 7.80 (m, 1H), 7.59 – 7.55 (m, 1H), 7.40 – 7.34 (m, 1H), 1.41 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 152.2, 151.5, 149.6, 149.2, 137.0, 136.1, 125.0, 124.6, 122.8, 120.6, 118.0, 77.3, 77.0, 76.7, 35.1, 31.5; HRMS (ESI) m/z calcd. for $C_{16}H_{17}N_2S^+$ $(M+H)^+$ 269.11070, found 269.11084.

6-(*tert*-Butyl)-2-(1H-indol-2-yl)benzo[d]thiazole (3y)



The reaction was conducted with 4-*tert*-butylaniline (**1e**, 95.6 μL , 0.6 mmol), 2-methyl-1H-indole (**2k**, 26.5 mg, 0.2 mmol) for 72 h. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3y** as yellow solid (27.5 mg, 45% yield), mp 181-183 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.10 (s, 1H), 7.90 – 7.86 (m, 2H), 7.66 (d, J = 7.9 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.32 – 7.28 (m, 1H), 7.26 – 7.20 (m, 1H), 7.16 – 7.10 (m, 2H), 1.40 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 151.1, 148.9, 137.1, 134.6, 131.4, 128.3, 124.7, 124.5, 121.8, 121.5, 120.6, 117.8, 111.6, 105.4, 77.3, 77.0, 76.7, 35.1, 31.5; HRMS (ESI) m/z calcd. for $C_{19}H_{19}N_2S^+$ $(M+H)^+$ 307.12635, found 307.12628.

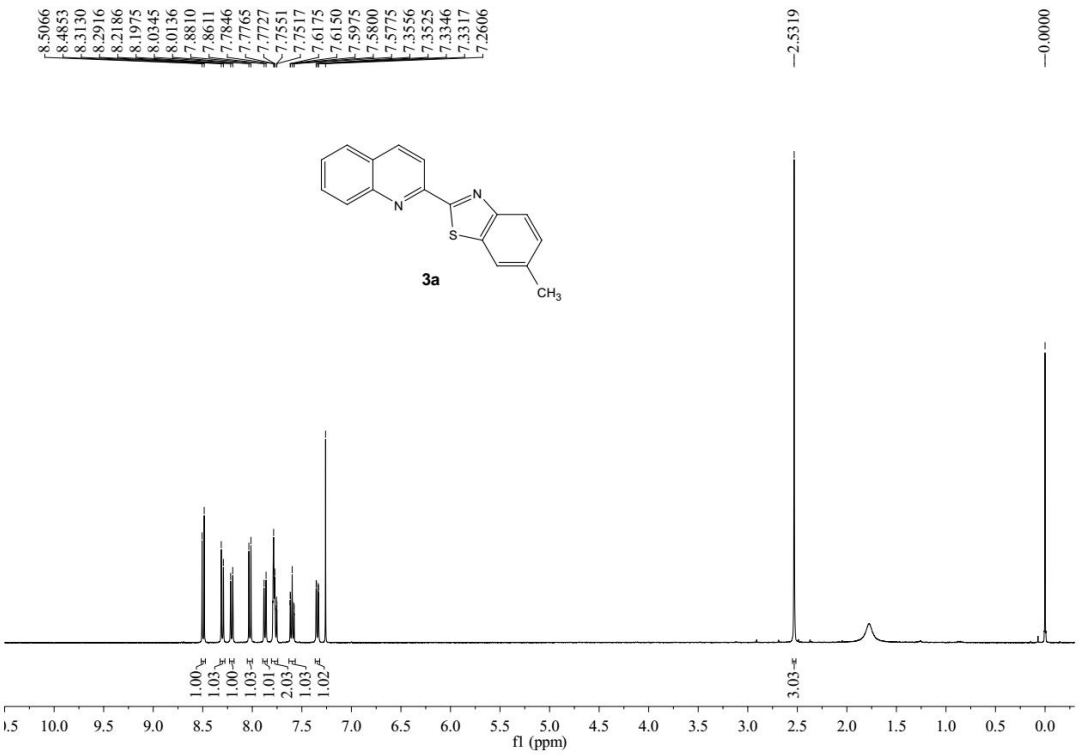
References

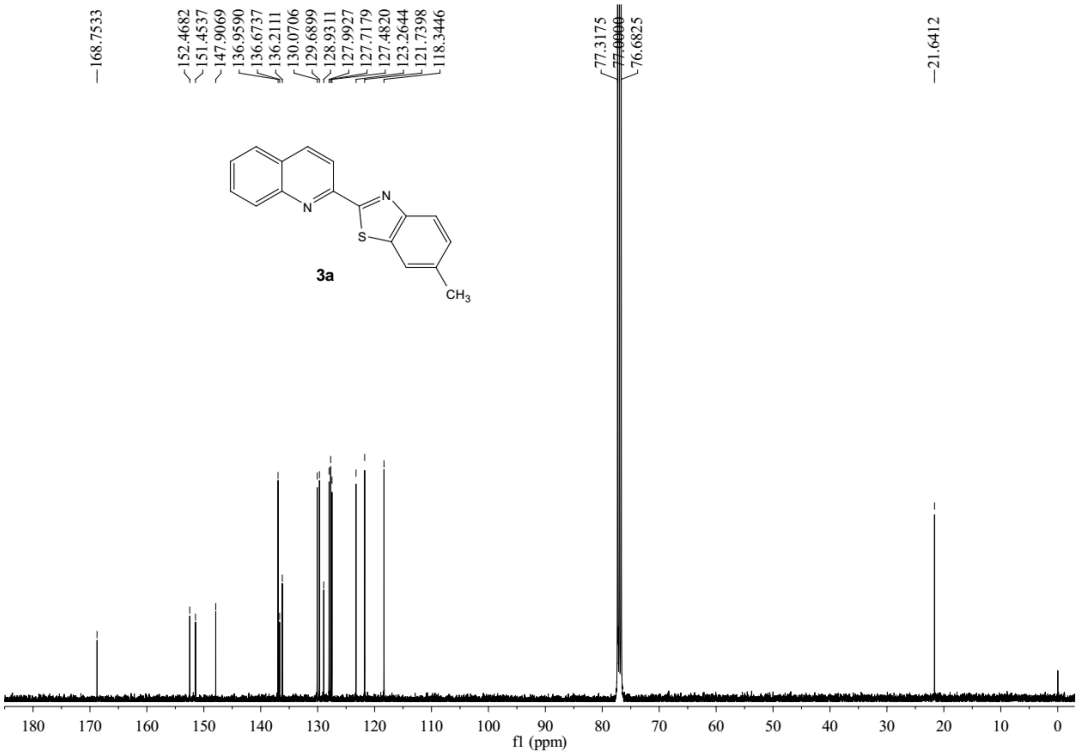
[1] X. L. Chu, T. T. Duan, X. Liu, L. Feng, J. Jia, C. Ma, *Org. Biomol. Chem.* **2017**, *15*, 1606.

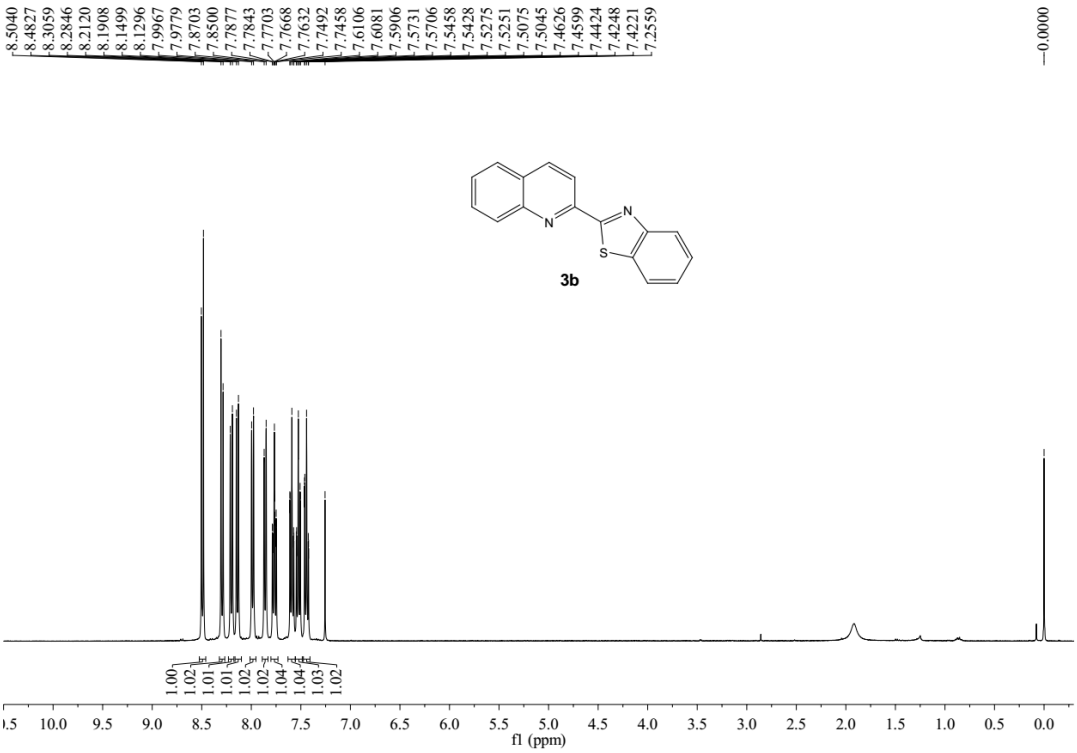
[2] T. Hisano, M. Ichikawa, *Chem. Pharm. Bull*.**1974**, *22*, 2051.

[3] M. Z. Jonaghani, H. Zali-Boeini, R. Taheri, H. A. Rudbari, B. Askari, *RSC Adv.* **2016**, *41*, 34940.

^{1}H and ^{13}C NMR spectra for all products



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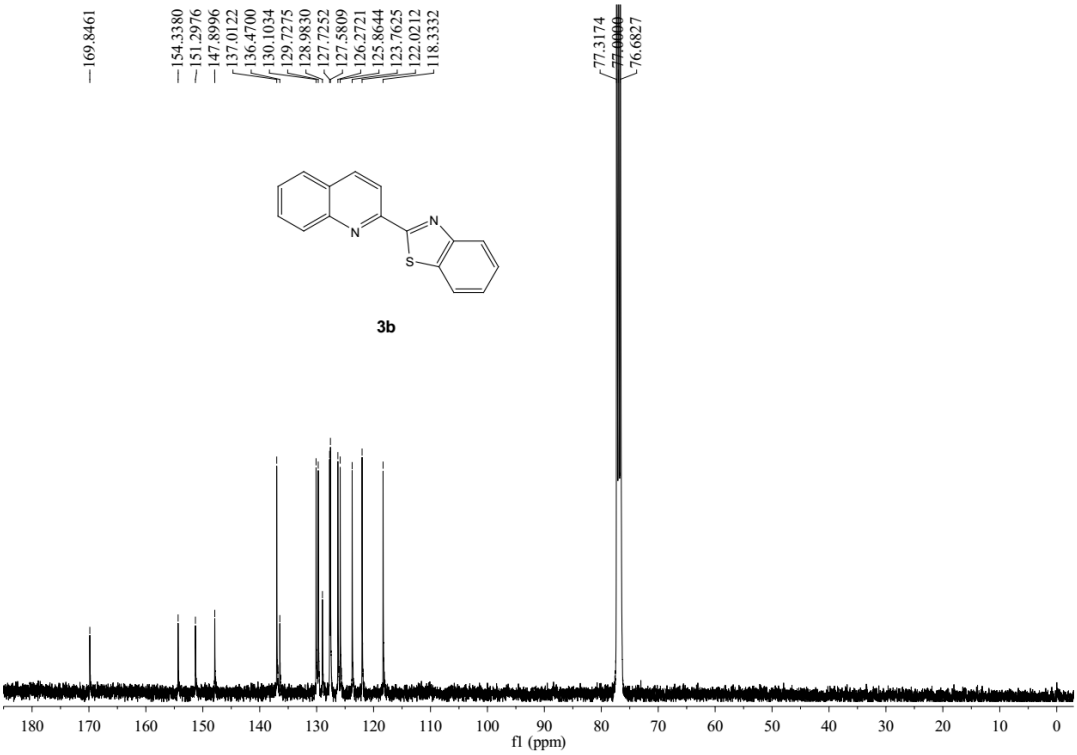
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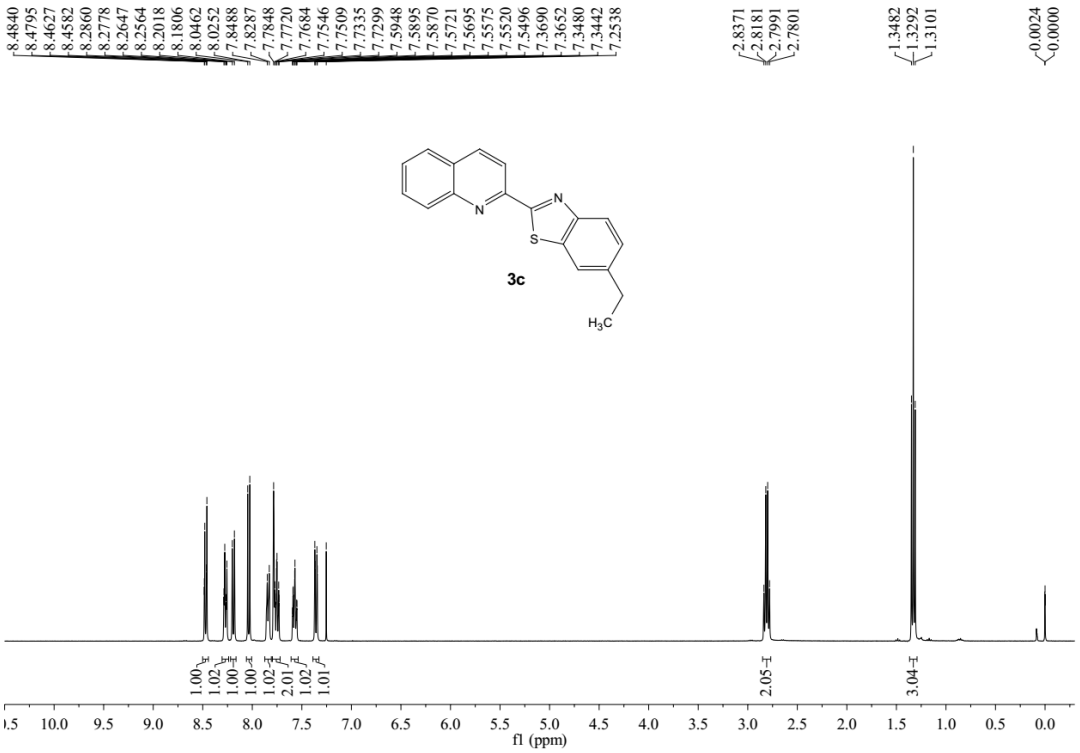
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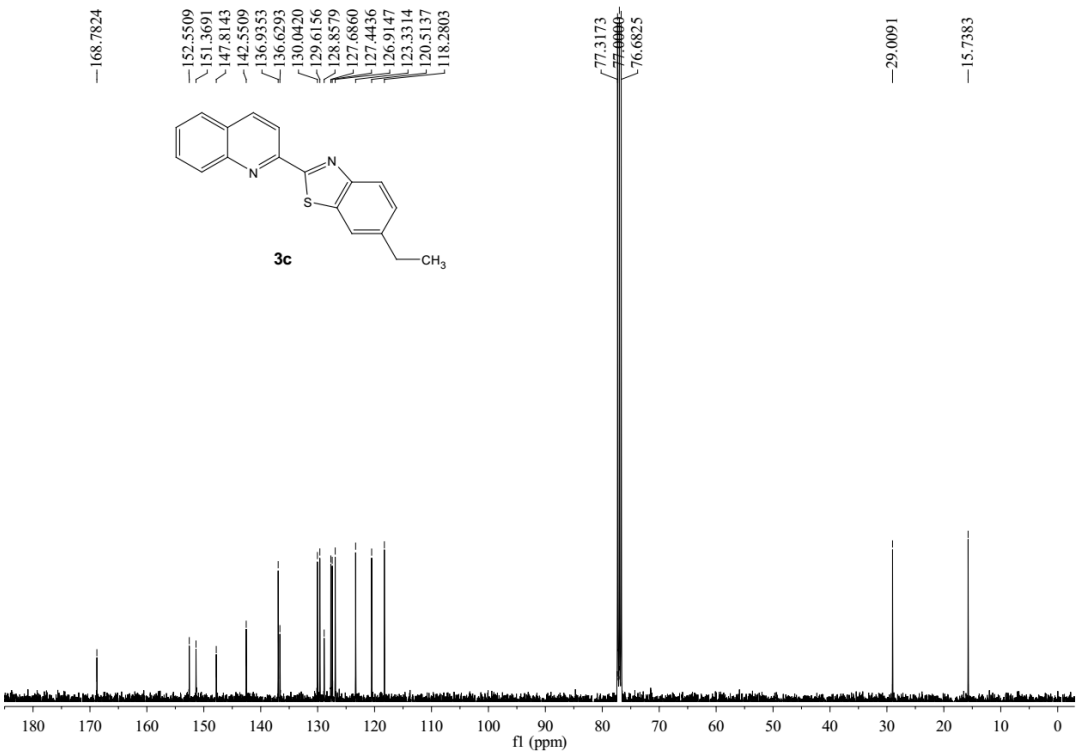
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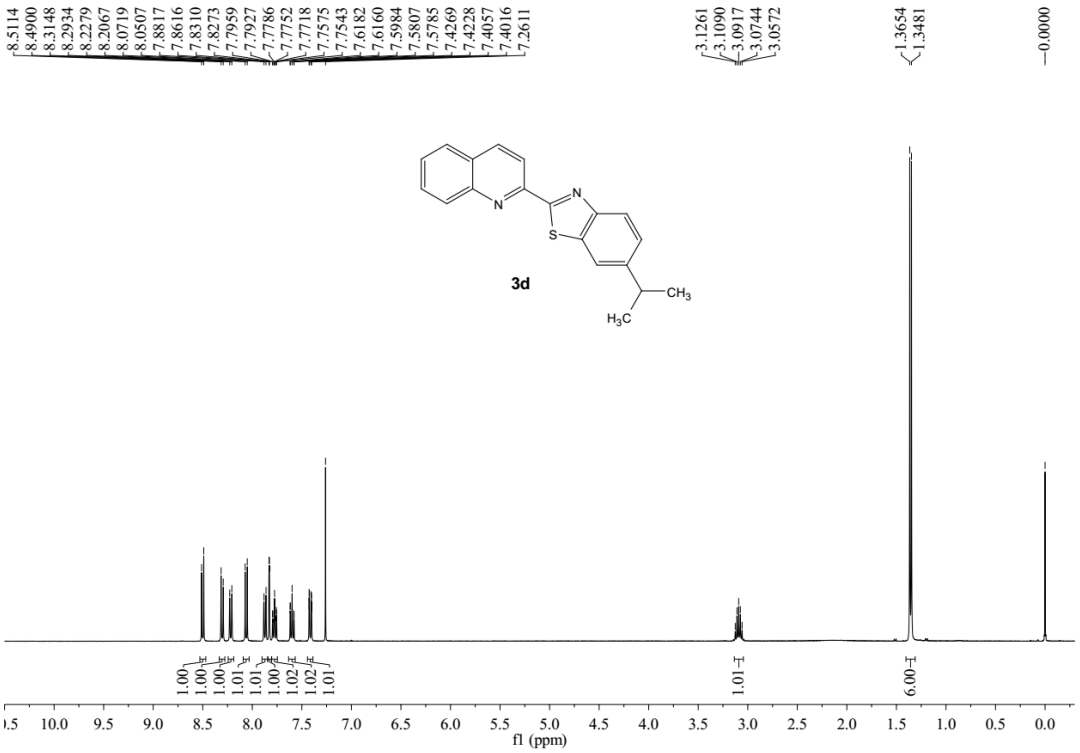
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1.02
1.01
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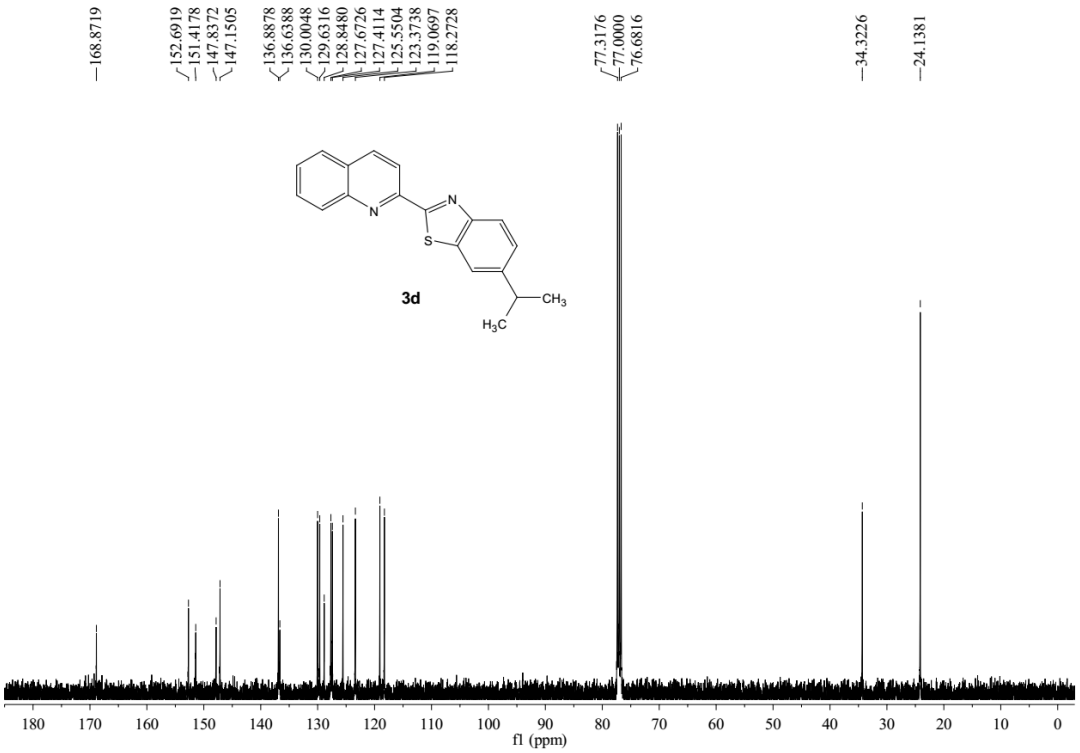
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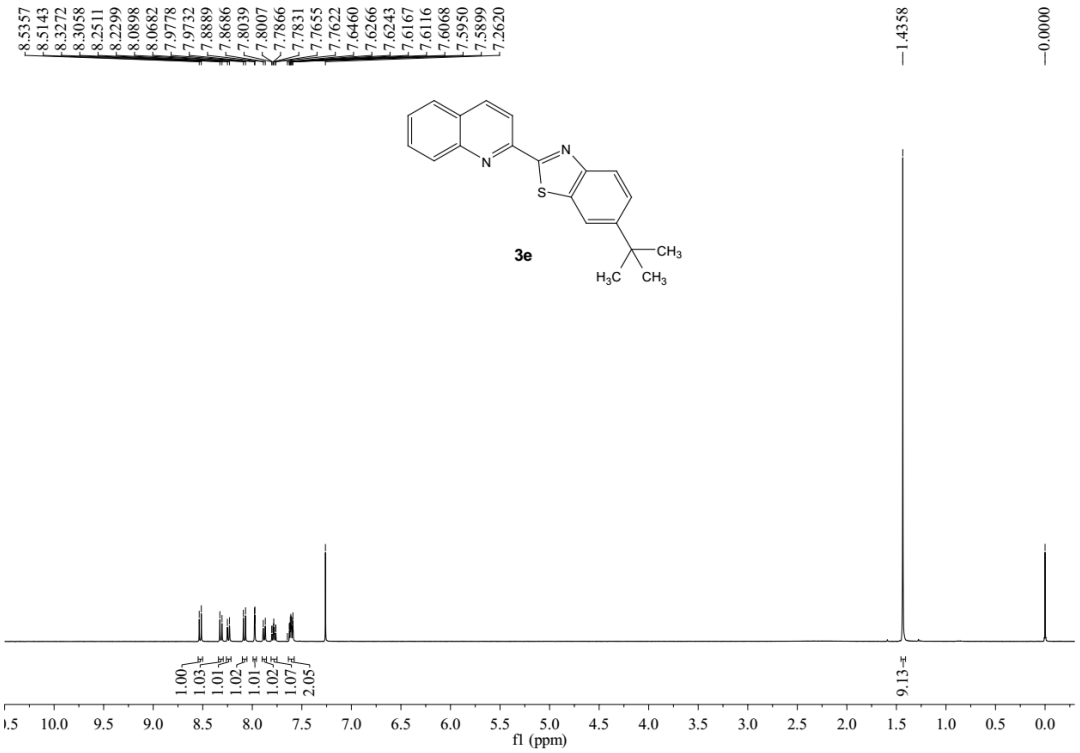
f1 (ppm)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7.8686
7.8039
7.8007
7.7866
7.7831
7.7655
7.7622
7.6460
7.6266
7.6243
7.6167
7.6116
7.6068
7.5950
7.5899
7.2620
1.4358
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S
N
CH3
H3C
CH3
3e
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1.03
1.01
1.02
1.01
1.02
1.07
2.05
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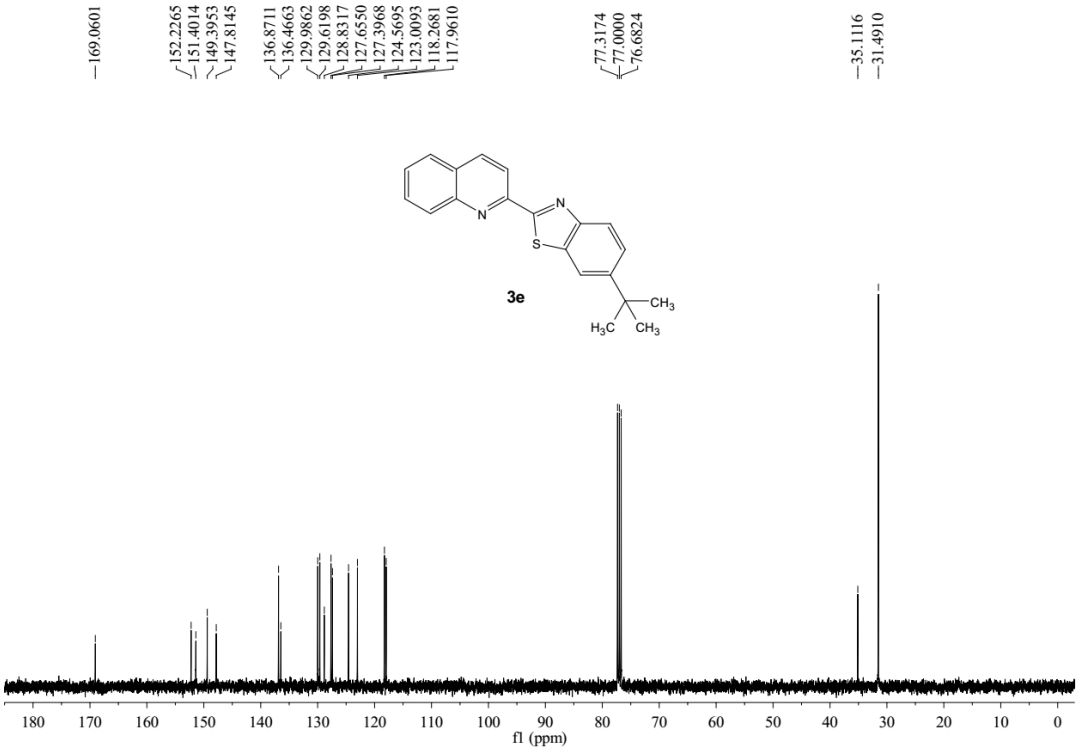
f1 (ppm)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124.5695
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117.9610
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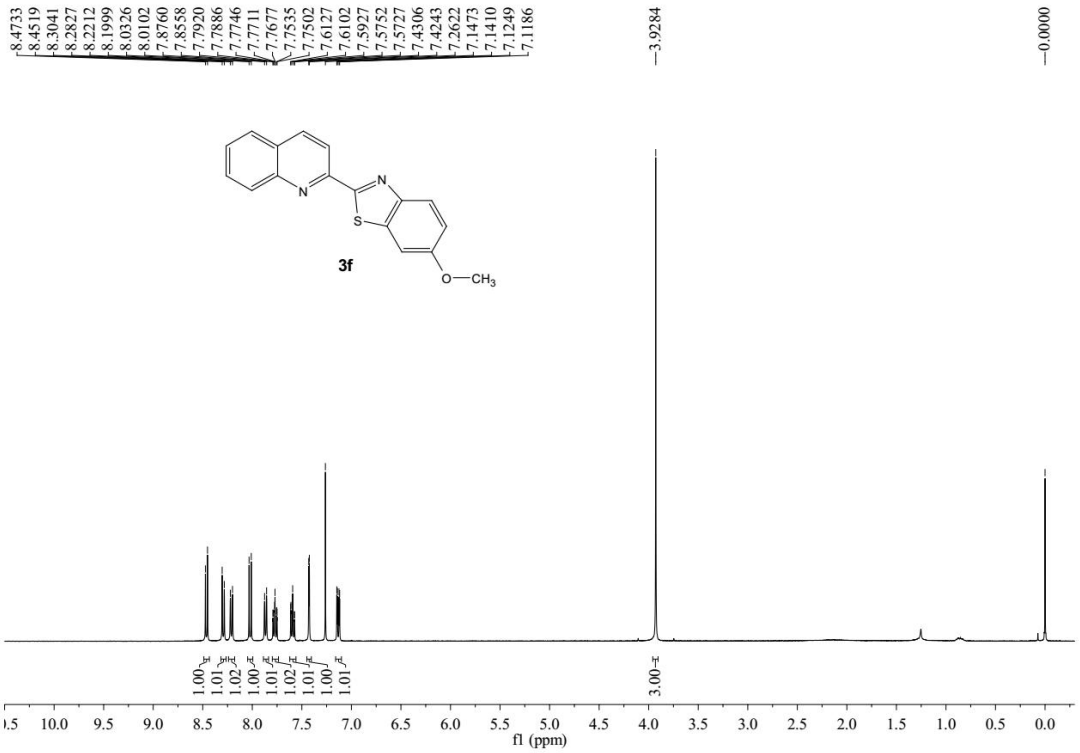
S
N
CH3
H3C
CH3
3e
f1 (ppm)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7.7746
7.7711
7.7677
7.7535
7.7502
7.6127
7.6102
7.5927
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7.5727
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7.4243
7.2622
7.1473
7.1410
7.1249
7.1186
3.9284
0.0000
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1.02
1.00
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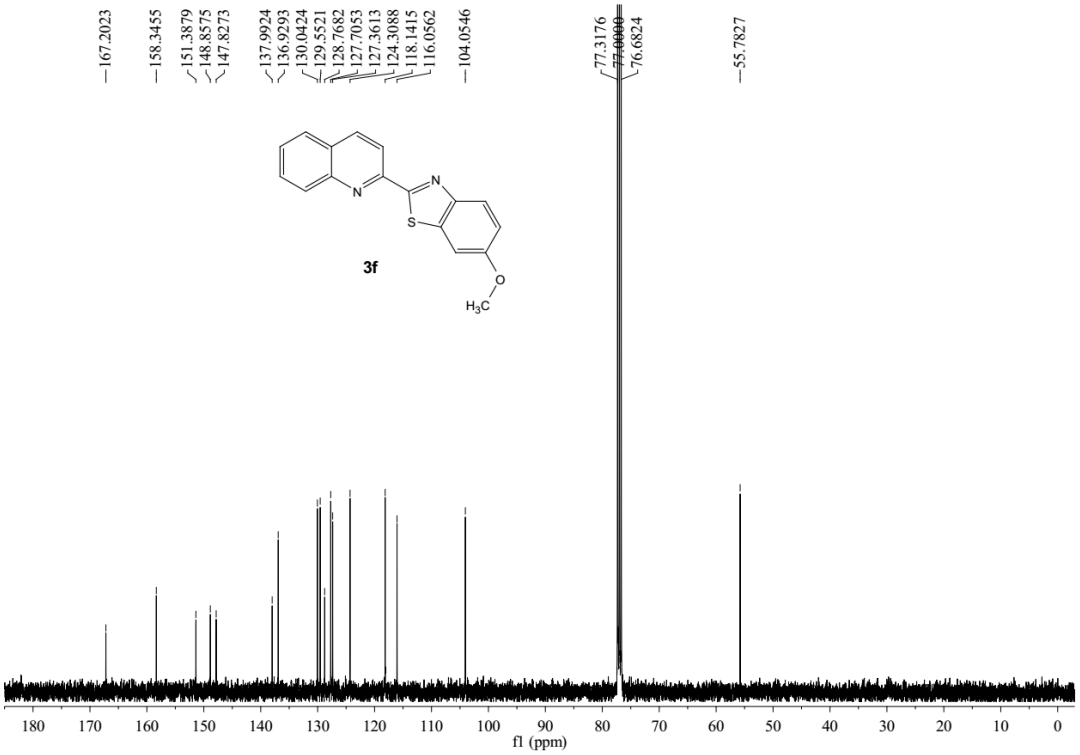
fl (ppm)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127.7053
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104.0546
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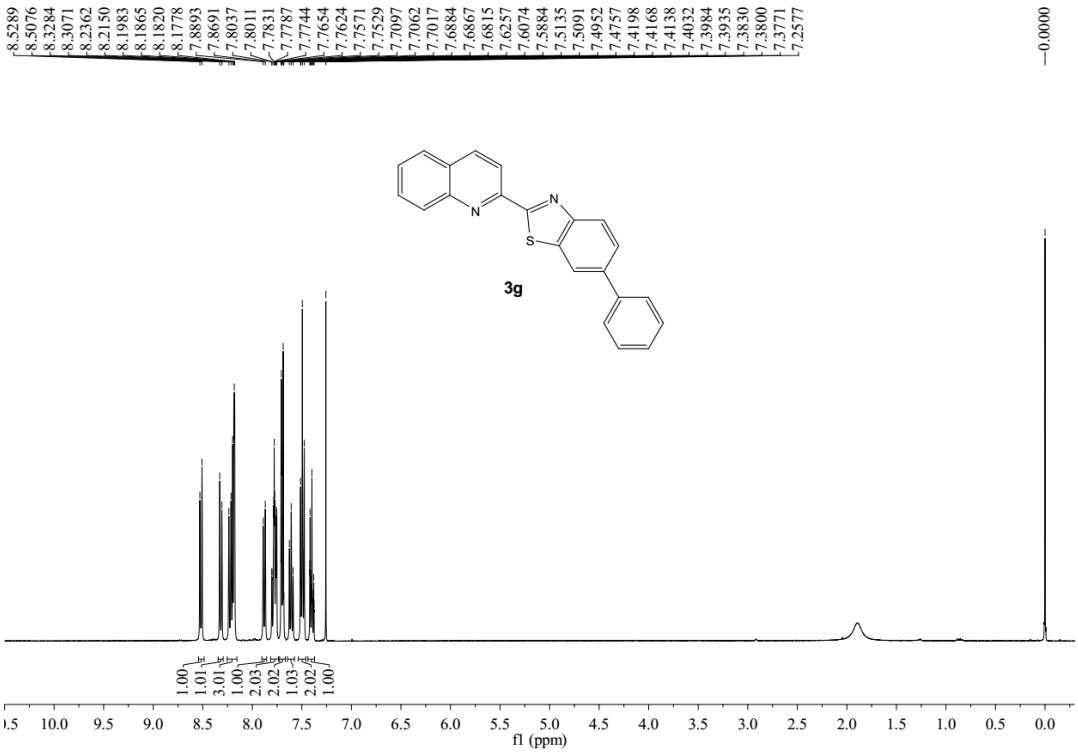
fl (ppm)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7.8037
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7.7744
7.7654
7.7624
7.7571
7.7529
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7.7062
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7.3830
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7.3771
7.2577
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3.01
1.00
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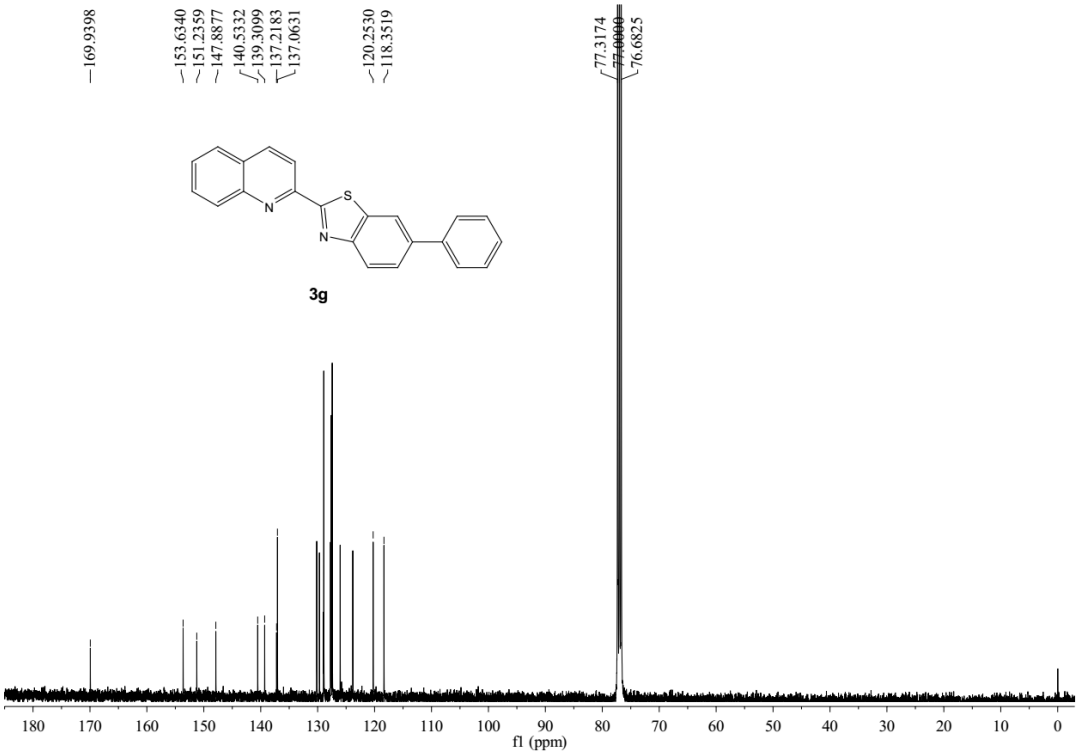
2.02
1.03
2.02
1.00
f1 (ppm)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120.2530
118.3519
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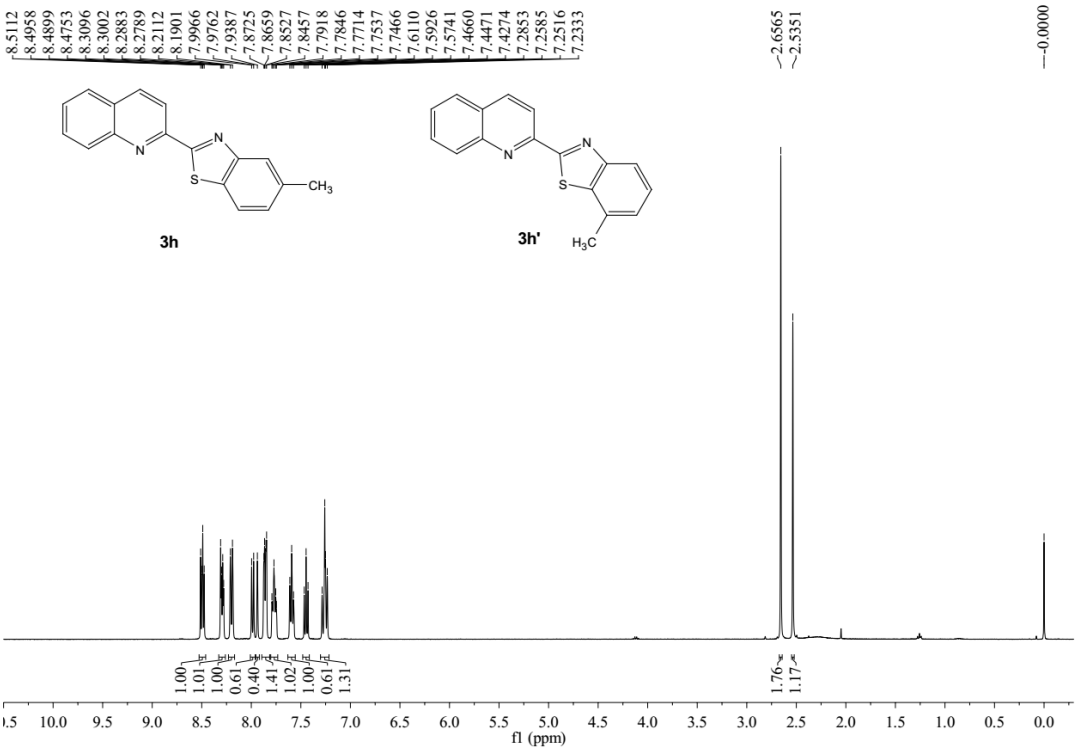
77.0000
76.6825
3g
f1 (ppm)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8.4899
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8.3096
8.3002
8.2883
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8.2112
8.1901
7.9966
7.9762
7.9387
7.8725
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7.8527
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7.7918
7.7846
7.7714
7.7537
7.7466
7.6110
7.5926
7.5741
7.4660
7.4471
7.4274
7.2853
7.2585
7.2516
7.2333
2.6565
2.5351
0.0000
3h
3h'
1.00
1.01
1.00
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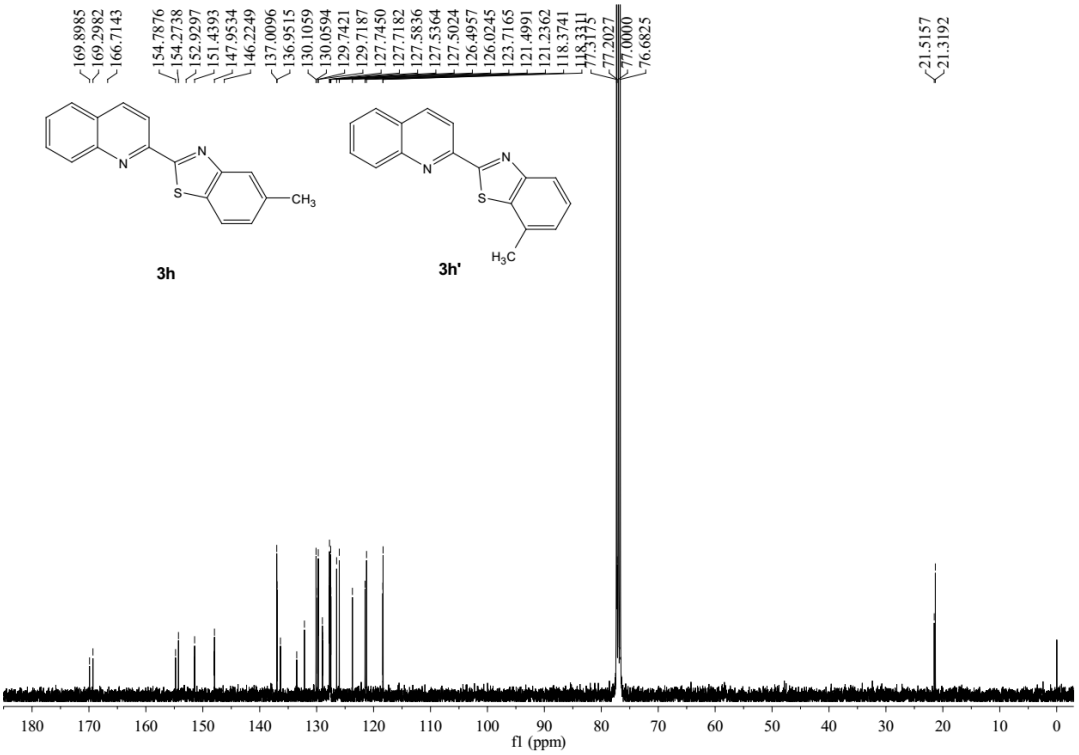
0.40
1.41
1.02
1.00
0.61
1.31
1.76
1.17
f1 (ppm)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127.7450
127.7182
127.5836
127.5364
127.5024
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121.4991
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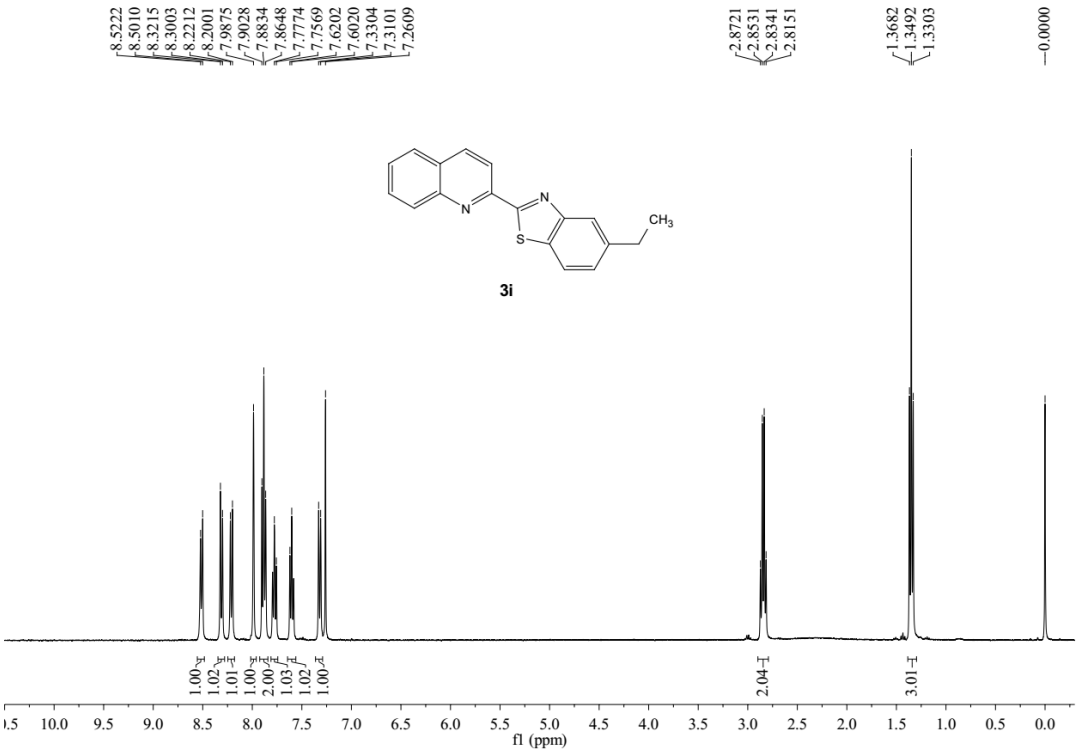
21.3192
3h
3h'
f1 (ppm)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8.2212
8.2001
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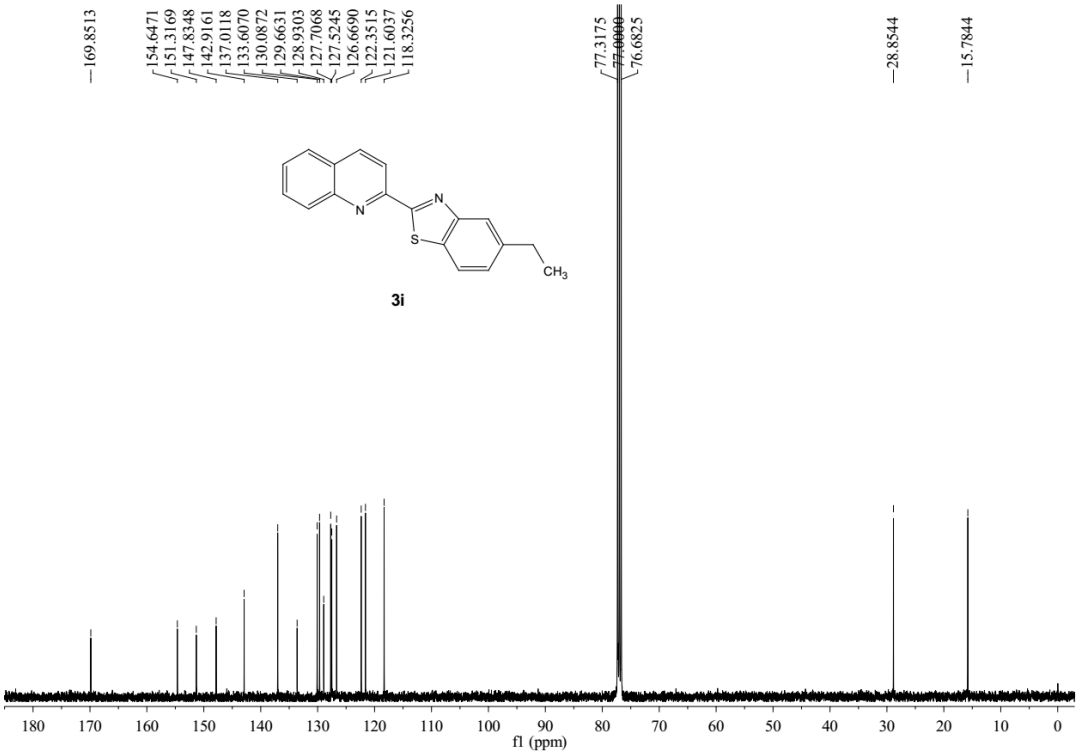
7.7569
7.6202
7.6020
7.3304
7.3101
7.2609
2.8721
2.8531
2.8341
2.8151
1.3682
1.3492
1.3303
0.0000
N
S
N
CH3
3i
1.00
1.02
1.01
1.00
2.00
1.03
1.02
1.00
2.04
3.01
fl (ppm)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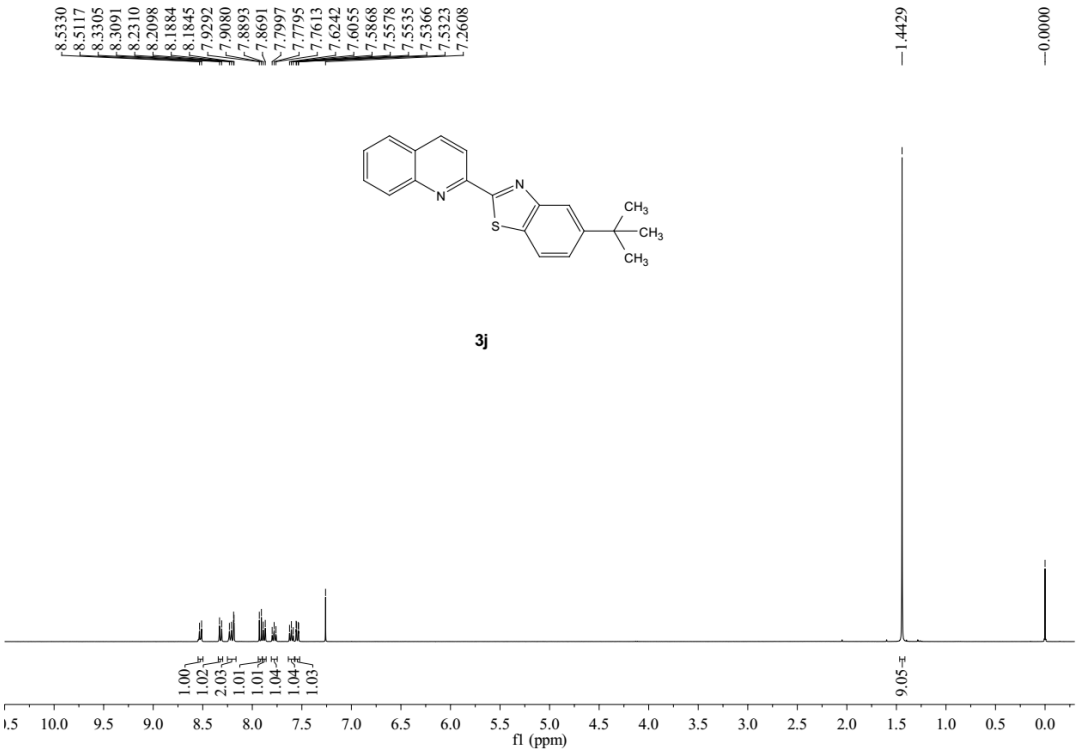
S
N
CH3
3i
fl (ppm)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7.7613
7.6242
7.6055
7.5868
7.5578
7.5535
7.5366
7.5323
7.2608
1.4429
0.0000
N
S
CH3
CH3
CH3
1.00
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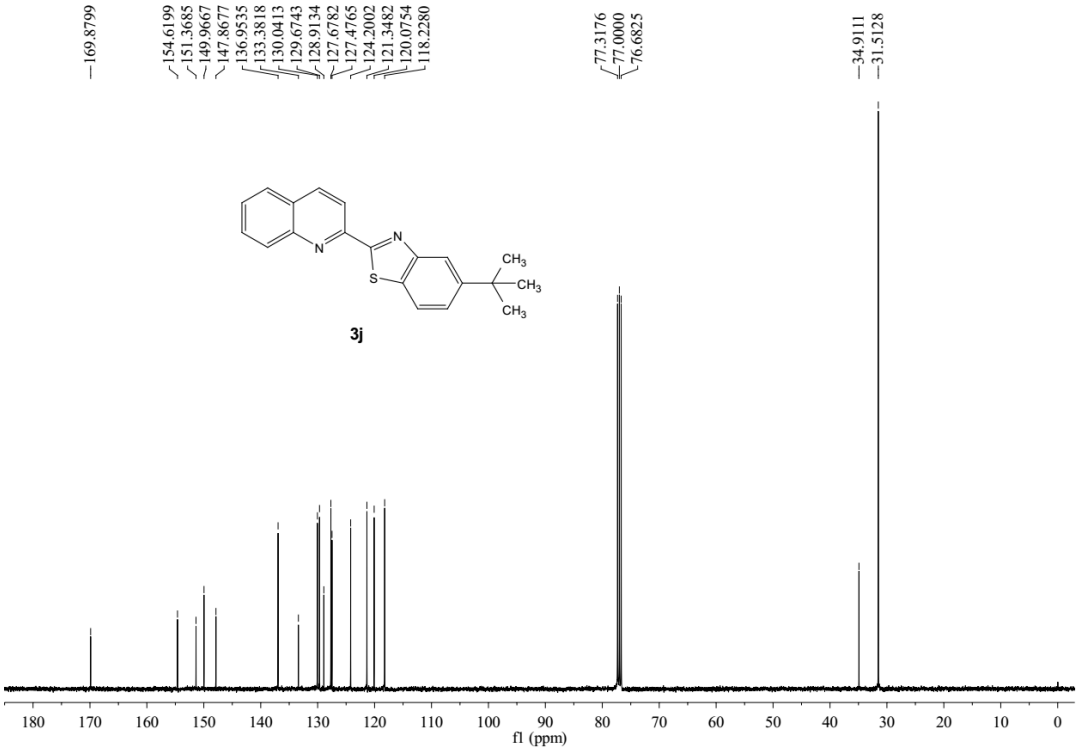
2.03
1.01
1.01
1.04
1.04
1.03
9.05
f1 (ppm)

3j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127.4765
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121.3482
120.0754
118.2280
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31.5128
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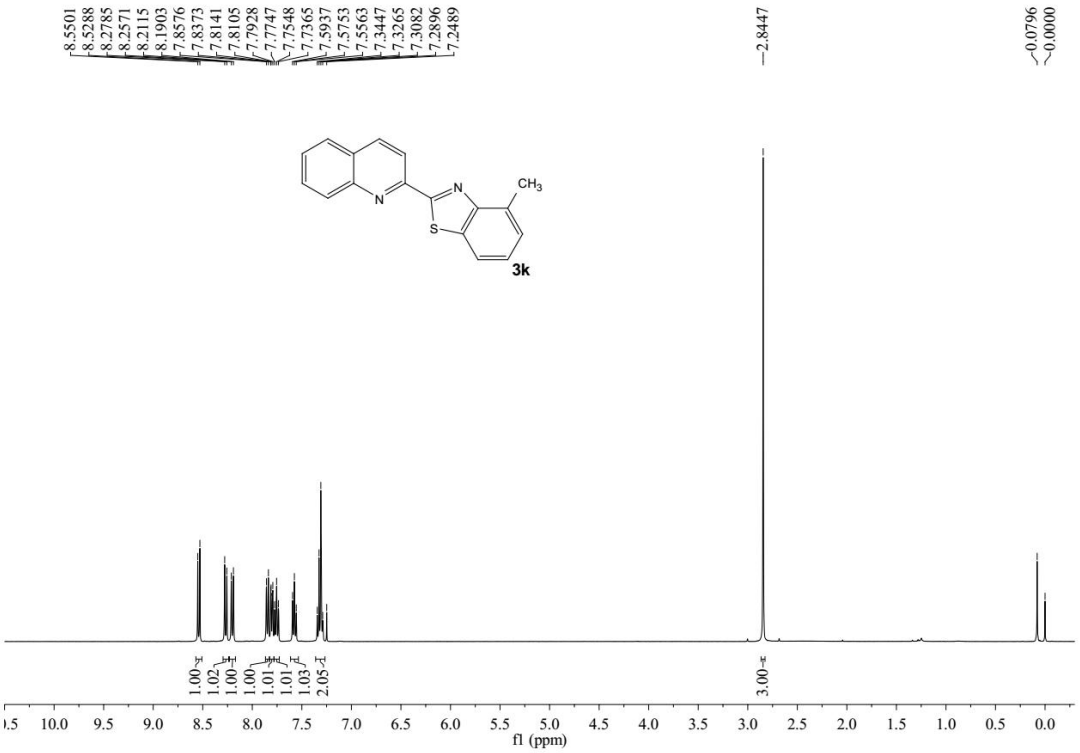
S
CH3
CH3
CH3
f1 (ppm)

3j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7.7365
7.5937
7.5753
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7.3447
7.3265
7.3082
7.2896
7.2489
2.8447
0.0796
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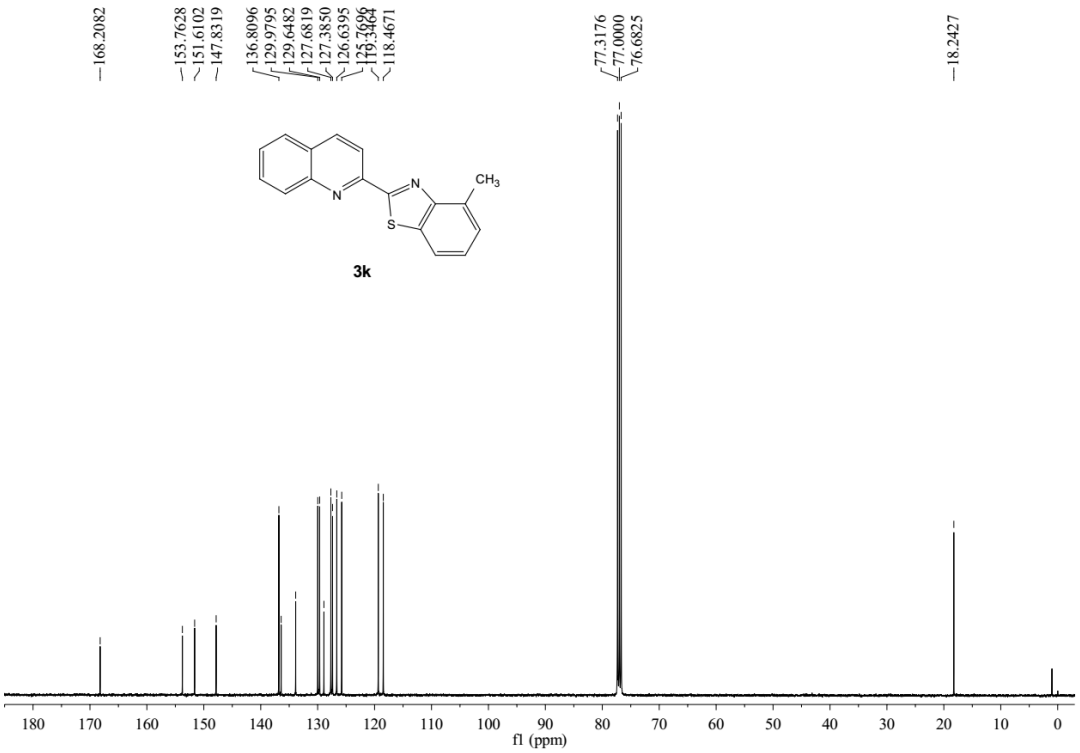
1.02
1.00
1.00
1.01
1.01
1.03
2.05
3.00
fl (ppm)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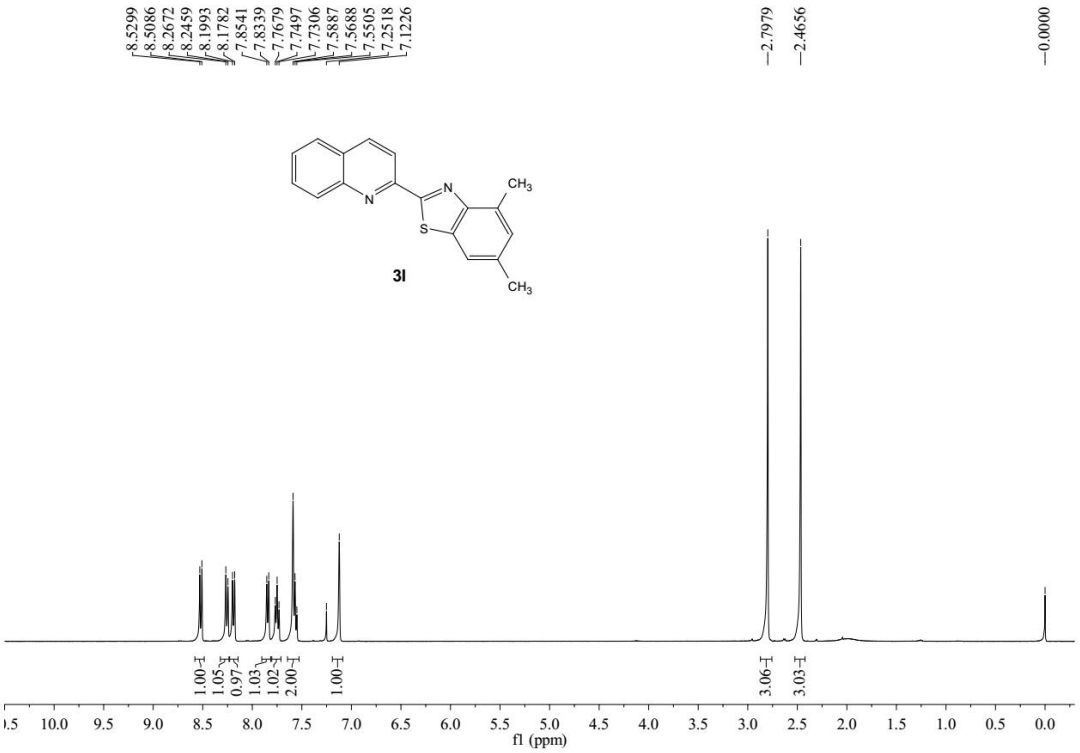
fl (ppm)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7.5688
7.5505
7.2518
7.1226
2.7979
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0.97
1.03
1.02
2.00
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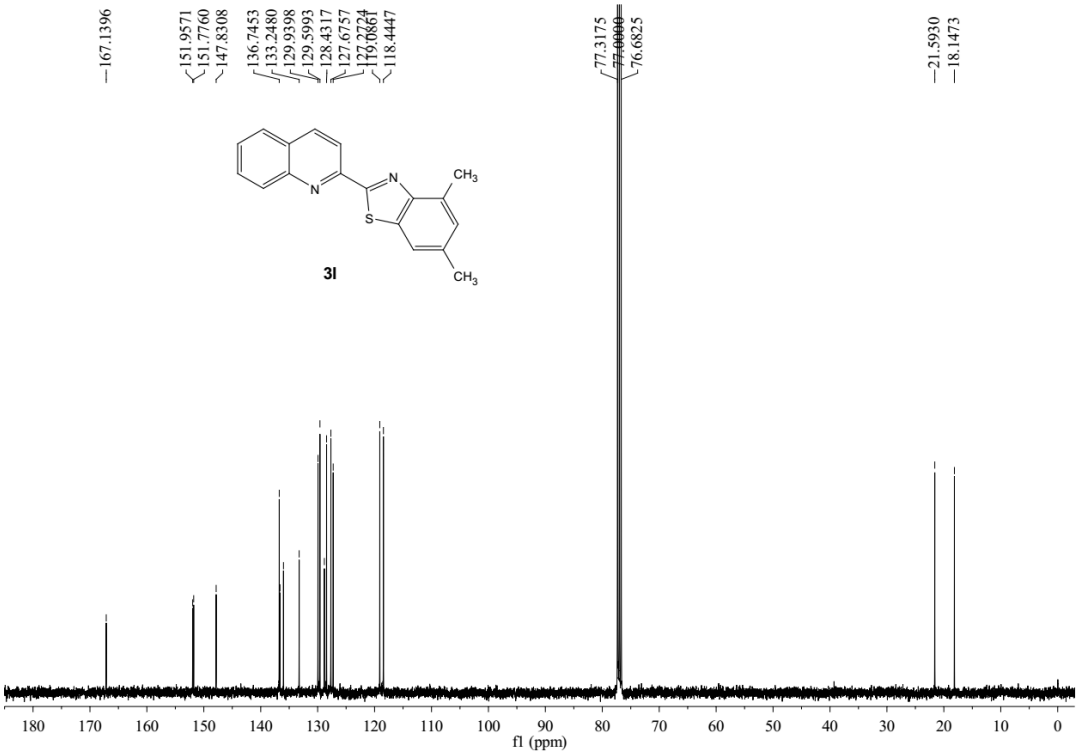
3.03
fl (ppm)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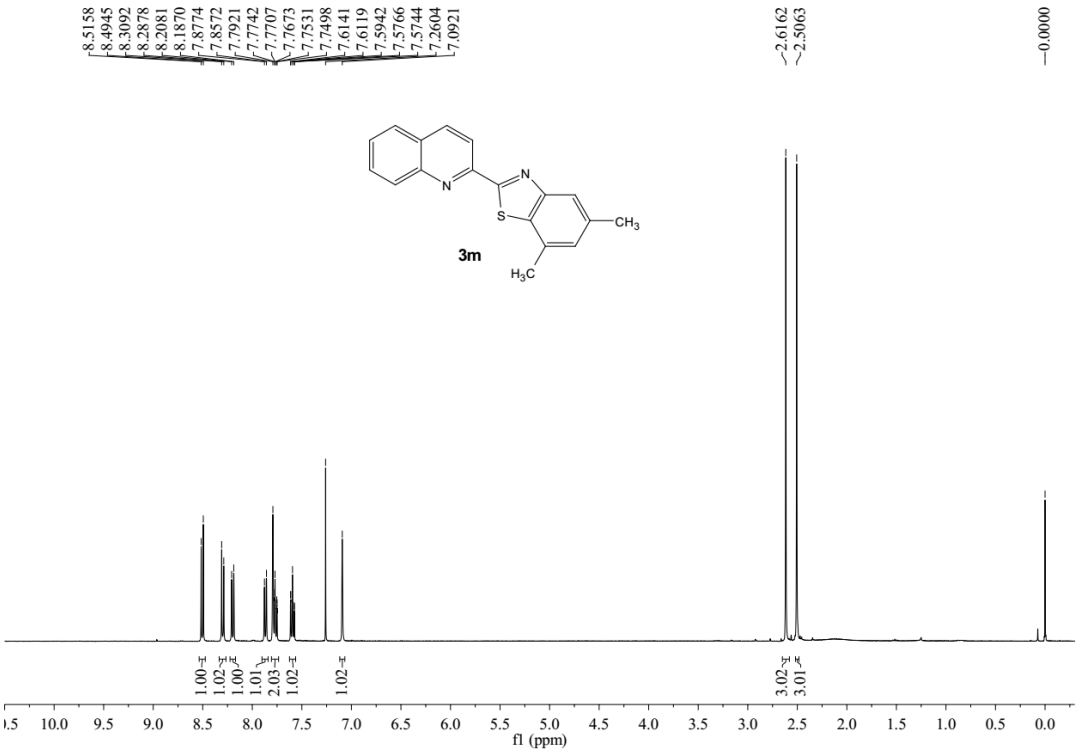
fl (ppm)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7.7921
7.7742
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7.7673
7.7531
7.7498
7.6141
7.6119
7.5942
7.5766
7.5744
7.2604
7.0921
2.6162
2.5063
0.0000
N
S
N
CH3
H3C
3m
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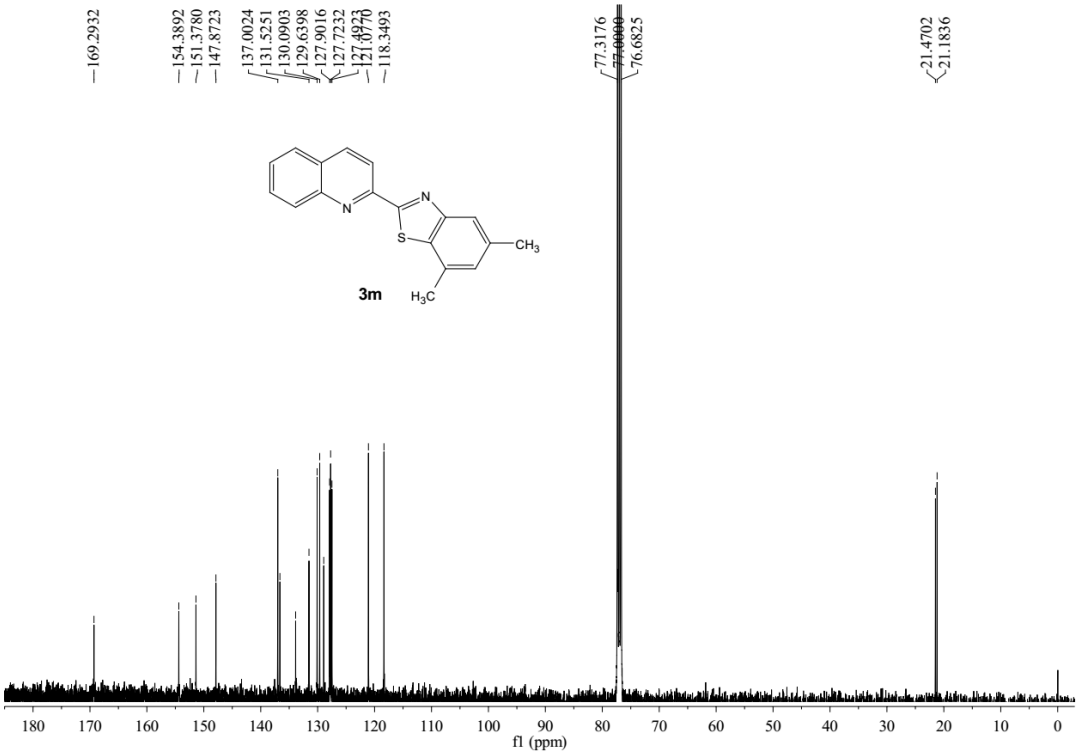
1.02
1.00
1.01
2.03
1.02
1.02
3.02
3.01
fl (ppm)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121.0770
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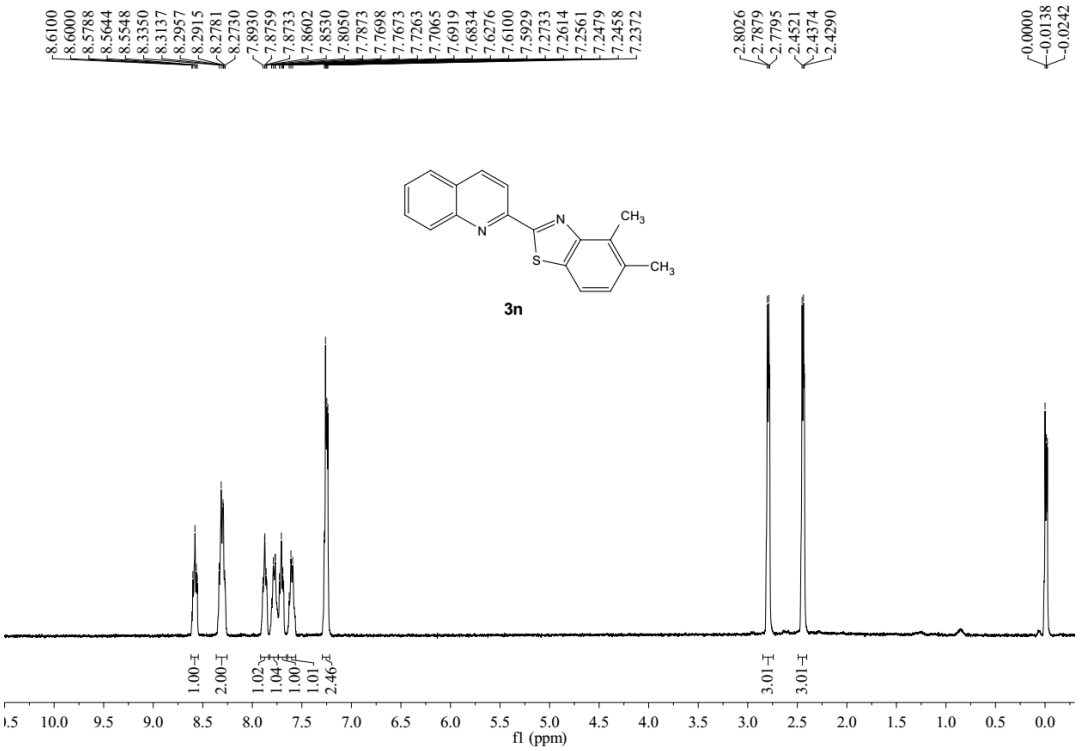
S
N
CH3
H3C
3m
fl (ppm)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7.8930
7.8759
7.8733
7.8602
7.8530
7.8050
7.7873
7.7698
7.7673
7.7263
7.7065
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7.2479
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7.2372
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CH3
CH3
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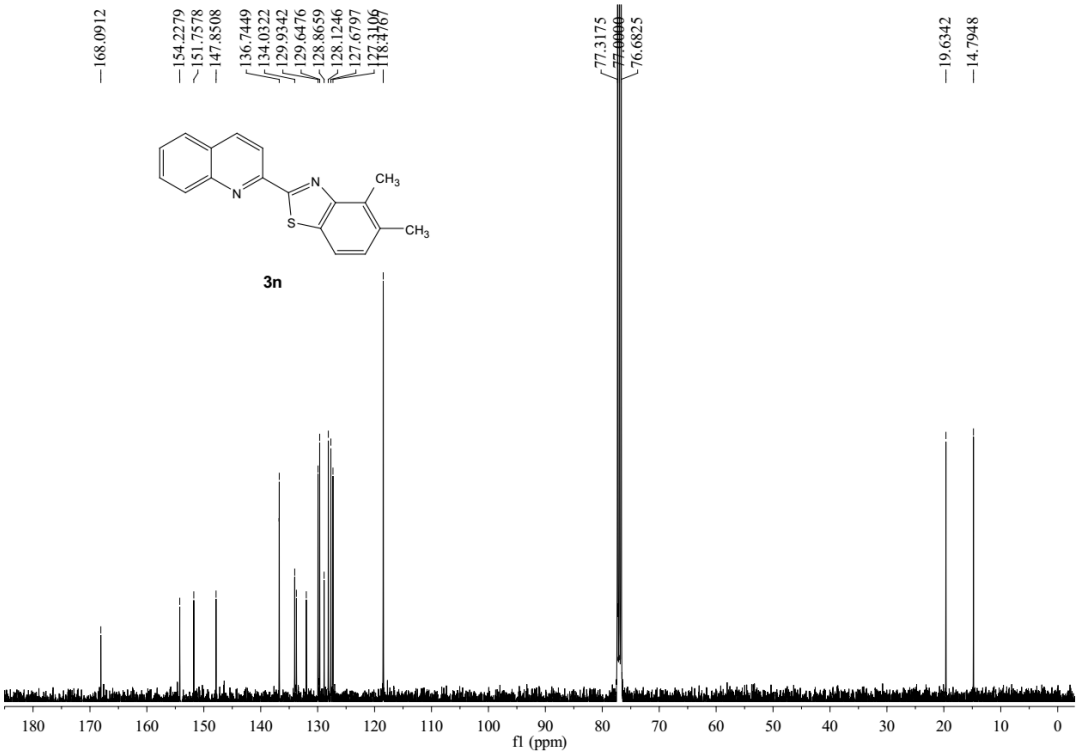
f1 (ppm)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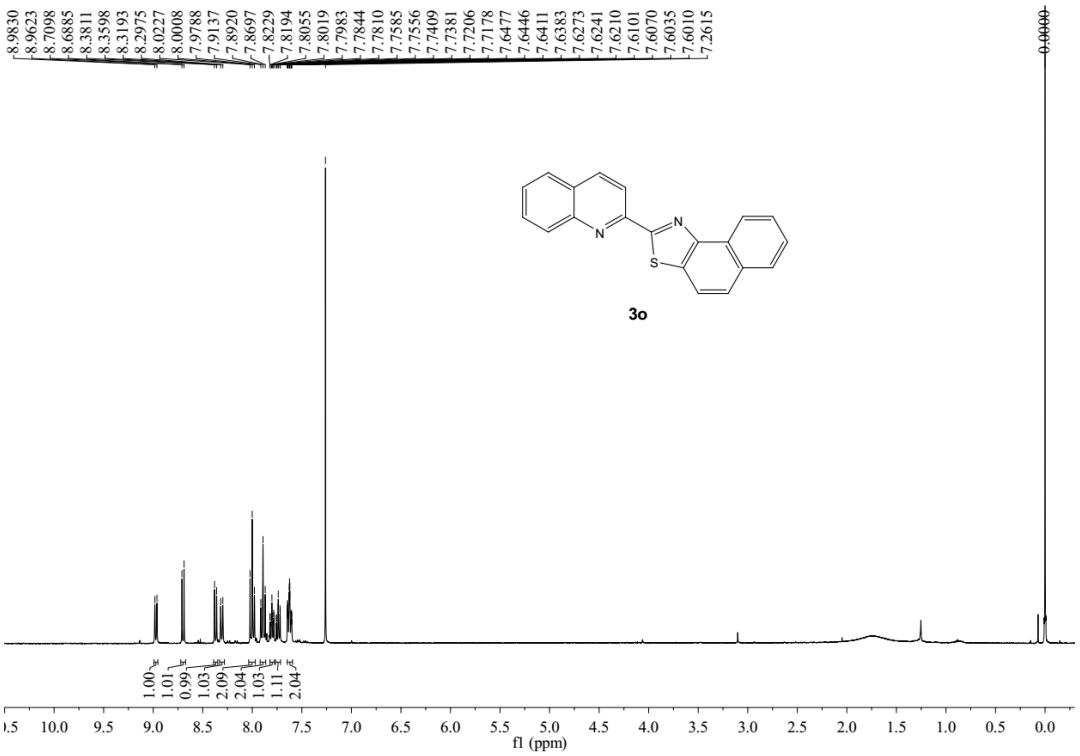
19.6342
14.7948
CH3
CH3
N
S
3n
f1 (ppm)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7.6210
7.6101
7.6070
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7.6010
7.2615
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0.99
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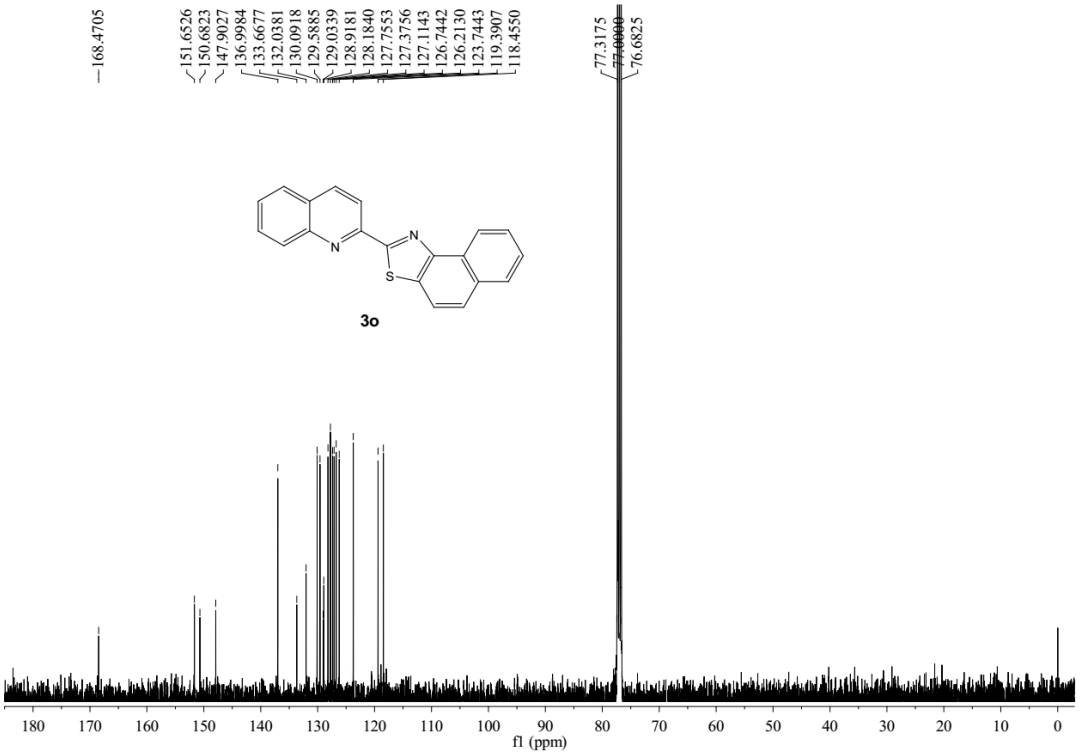
2.09
2.04
1.03
1.11
2.04
f1 (ppm)

3o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127.7553
127.3756
127.1143
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123.7443
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118.4550
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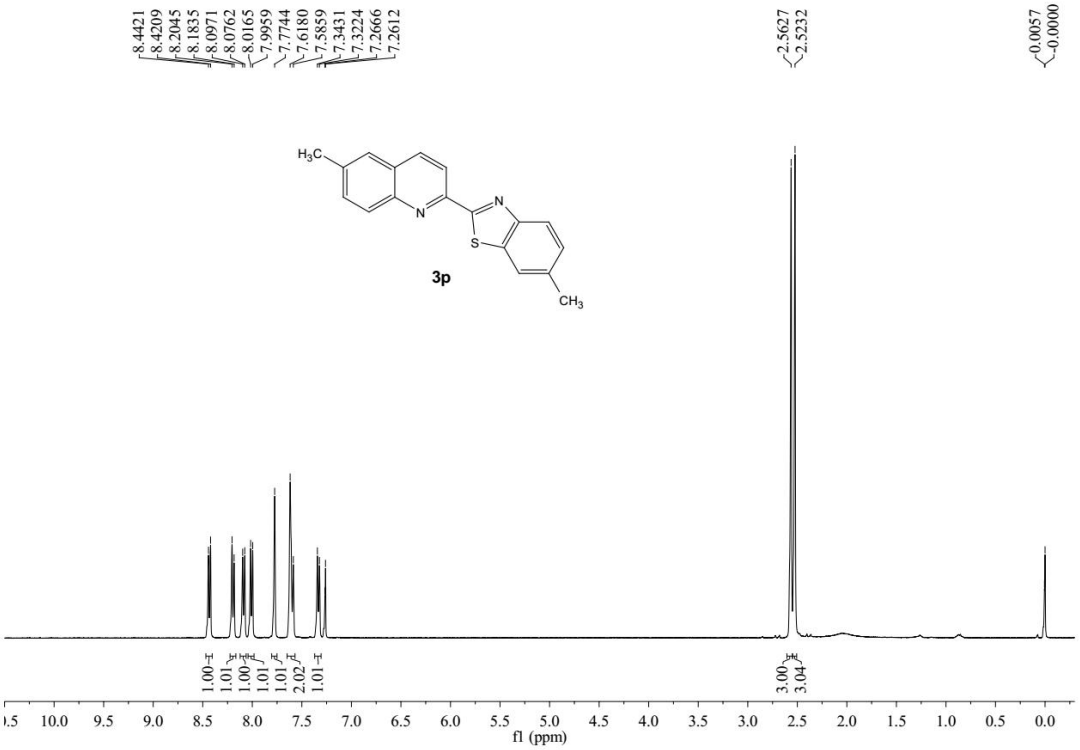
77.0000
76.6825
f1 (ppm)

3o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7.3431
7.3224
7.2666
7.2612
2.5627
2.5232
0.0057
-0.0000
3p
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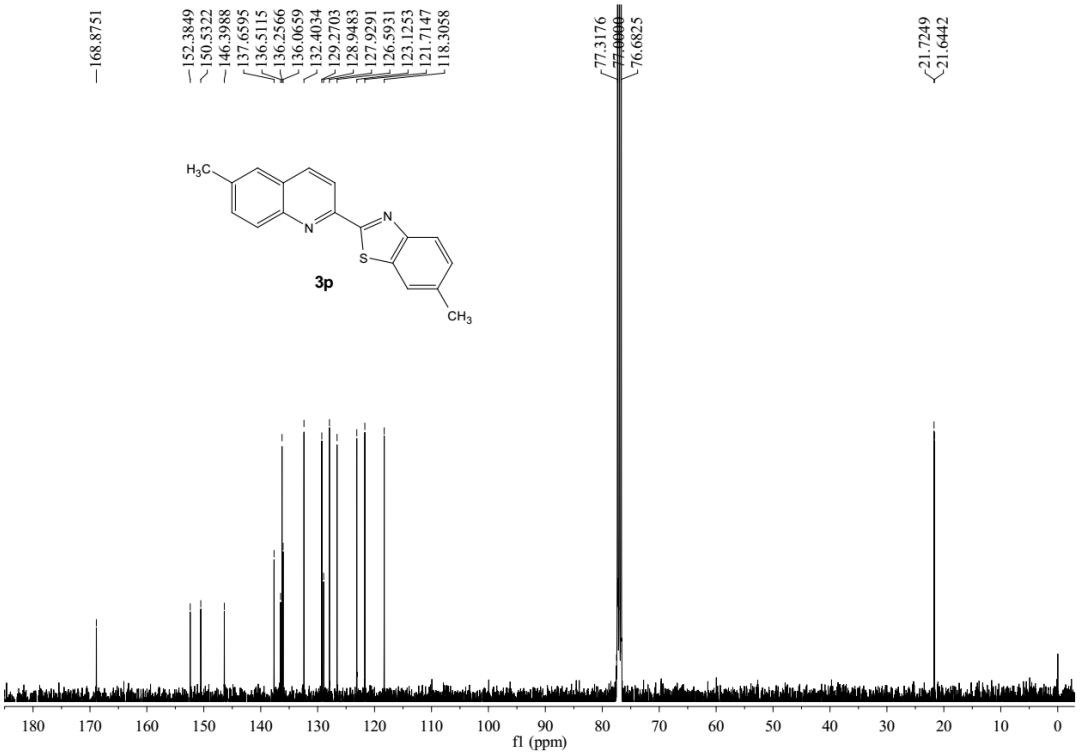
1.01
1.00
1.01
1.01
2.02
1.01
3.00
3.04
f1 (ppm)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127.9291
126.5931
123.1253
121.7147
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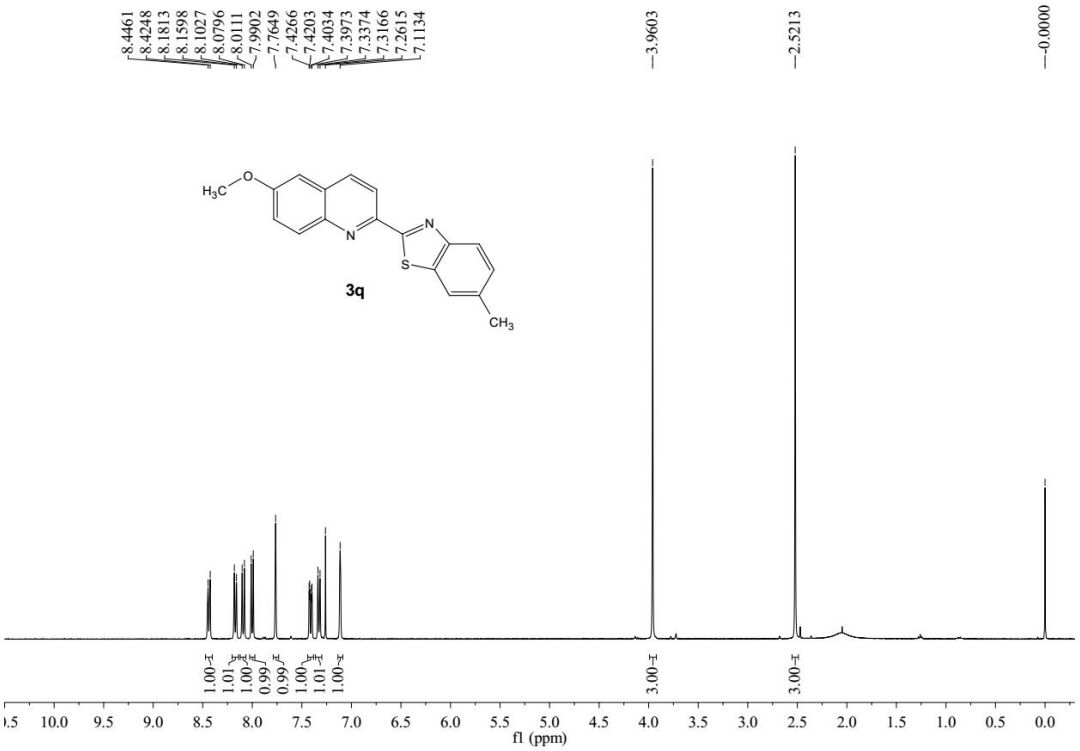
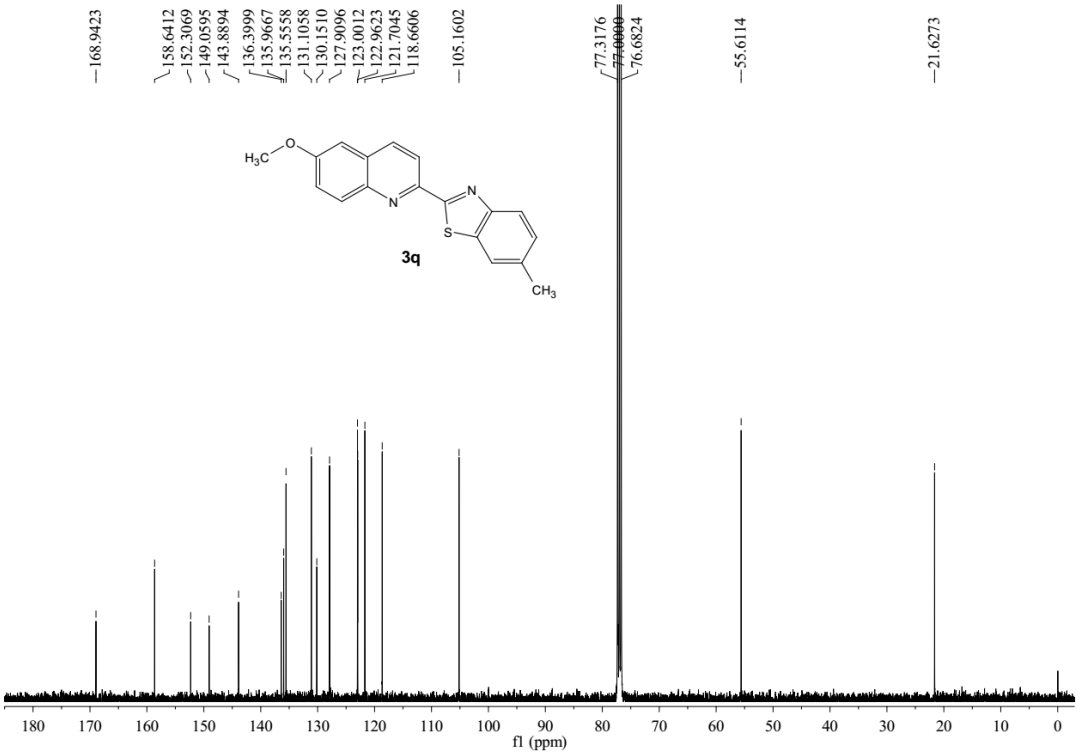
77.0000
76.6825
21.7249
21.6442
3p
f1 (ppm)


8.4461
8.4248
8.1813
8.1598
8.1027
8.0796
8.0111
7.9902
7.7649
7.4266
7.4203
7.4034
7.3973
7.3374
7.3166
7.2615
7.1134
3.9603
2.5213
0.0000
3q
1.00
1.01
1.00
0.99
1.00
1.01
1.00
3.00
3.00
f1 (ppm)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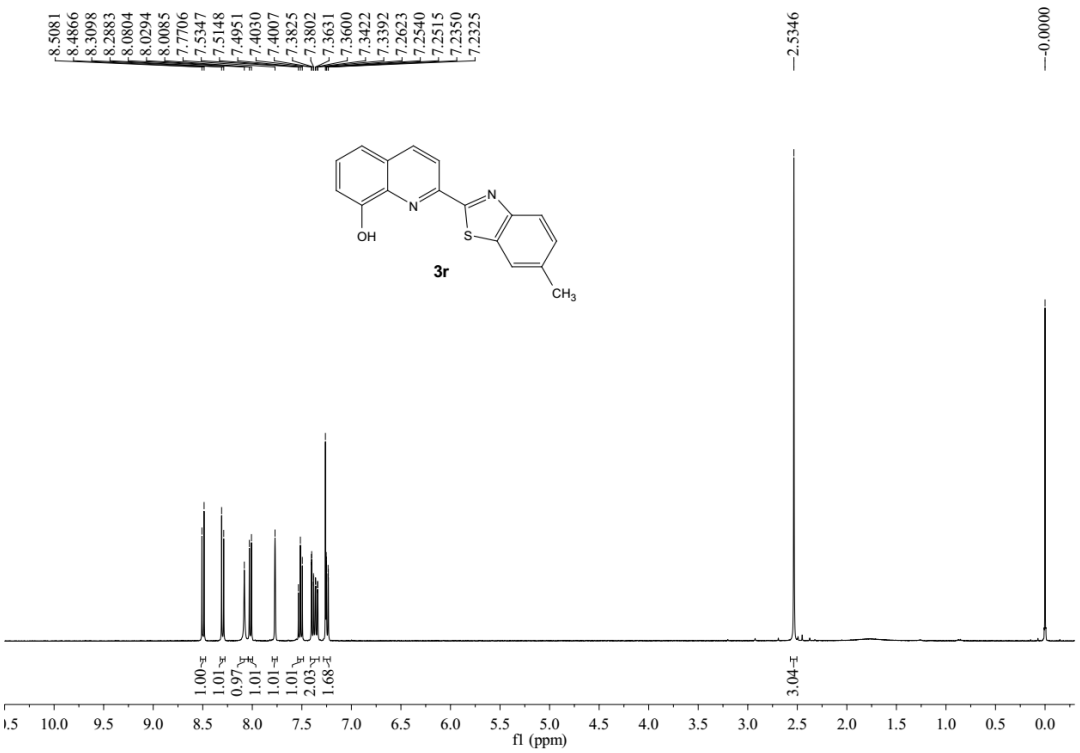
152.3069
149.0595
143.8894
136.3999
135.9667
135.5558
131.1058
130.1510
127.9096
123.0012
122.9623
121.7045
118.6606
105.1602
77.3176
77.0000
76.6824
55.6114
21.6273
3q
f1 (ppm)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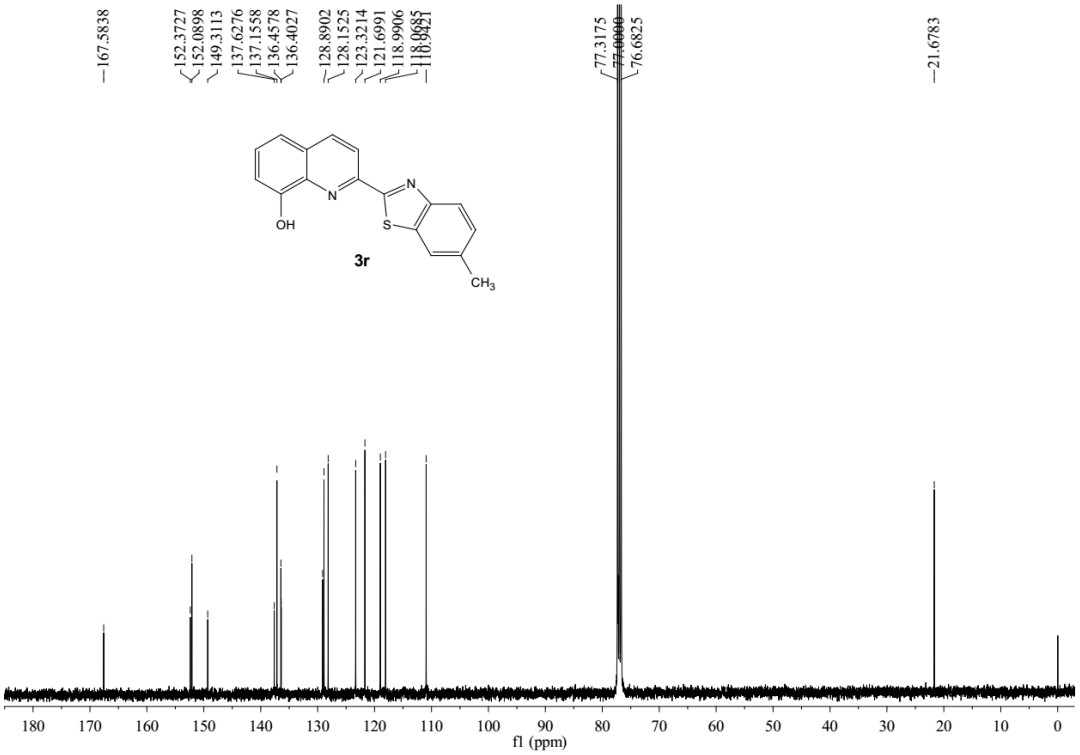
8.3098
8.2883
8.0804
8.0294
8.0085
7.7706
7.5347
7.5148
7.4951
7.4030
7.4007
7.3825
7.3802
7.3631
7.3600
7.3422
7.3392
7.2623
7.2540
7.2515
7.2350
7.2325
2.5346
0.0000
OH
N
S
N
CH3
3r
1.00
1.01
0.97
1.01
1.01
1.01
2.03
1.68
3.04
fl (ppm)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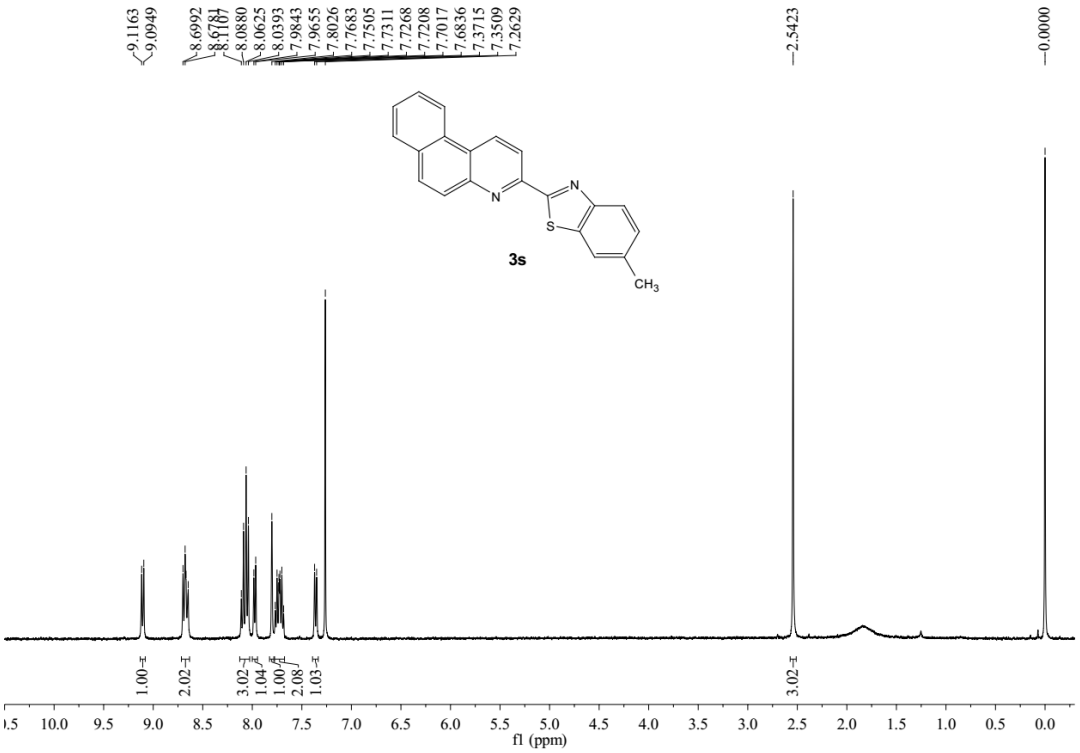
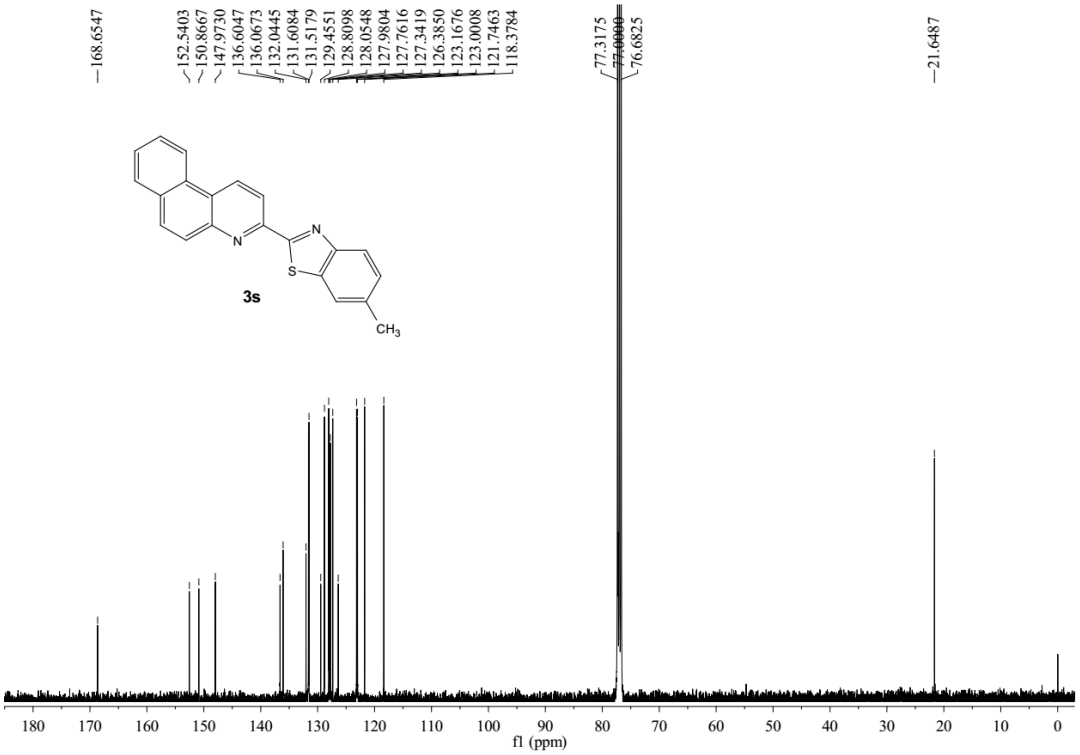
152.3727
152.0898
149.3113
137.6276
137.1558
136.4578
136.4027
128.8902
128.1525
123.3214
121.6991
118.9906
77.3175
77.0000
76.6825
21.6783
OH
N
S
N
CH3
3r
fl (ppm)


9.1163
9.0949
8.6992
8.6781
8.1107
8.0880
8.0625
8.0393
7.9843
7.9655
7.8026
7.7683
7.7505
7.7311
7.7268
7.7208
7.7017
7.6836
7.3715
7.3509
7.2629
2.5423
0.0000
3s
CH3
1.00
2.02
3.02
1.04
1.00
2.08
1.03
3.02
f1 (ppm)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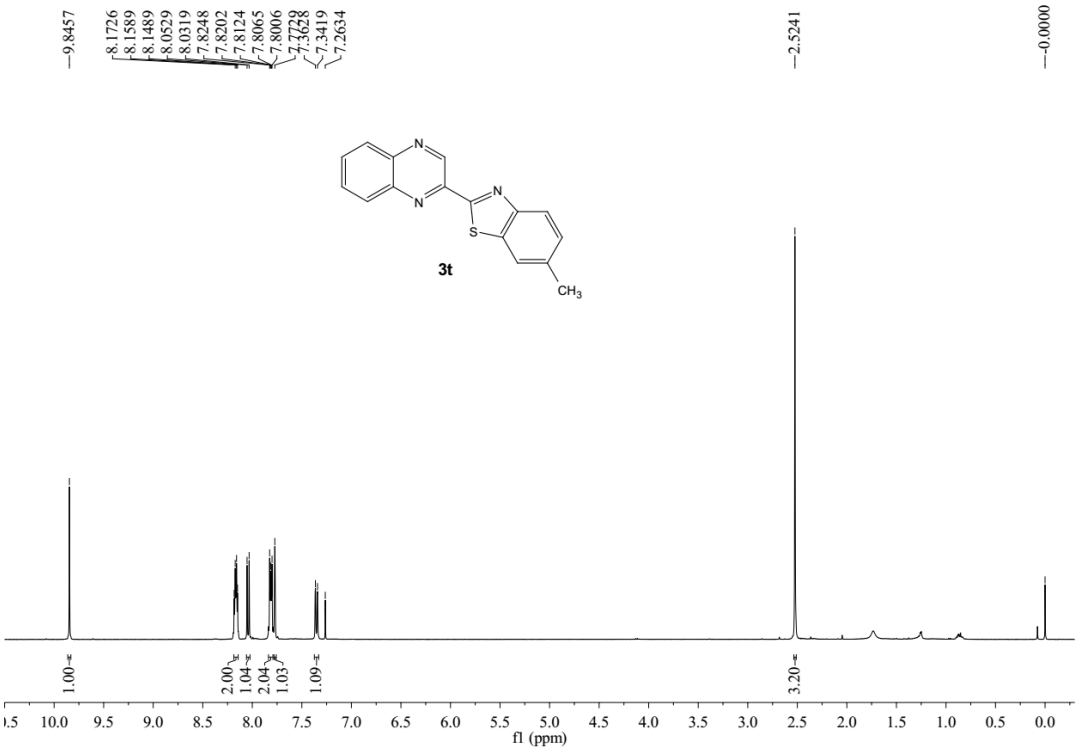
150.8667
147.9730
136.6047
136.0673
132.0445
131.6084
131.5179
129.4551
128.8098
128.0548
127.9804
127.7616
127.3419
126.3850
123.1676
123.0008
121.7463
118.3784
77.3175
77.0000
76.6825
21.6487
3s
CH3
f1 (ppm)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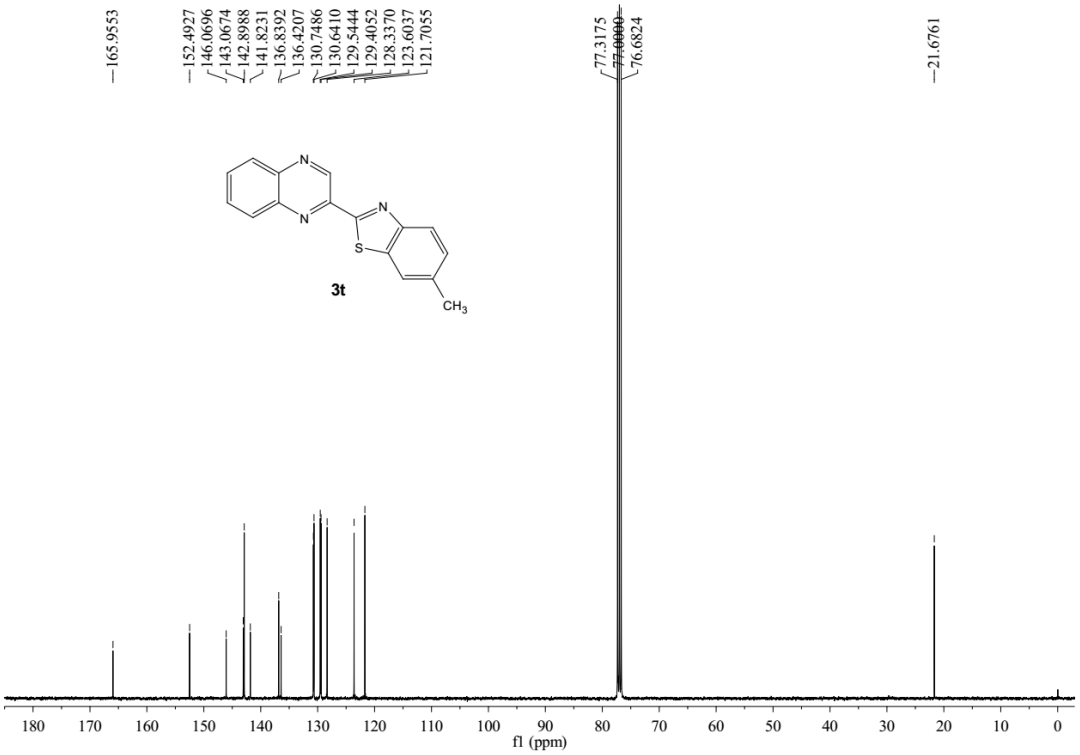
8.1589
8.1489
8.0529
8.0319
7.8248
7.8202
7.8124
7.8065
7.8006
7.3628
7.3419
7.2634
2.5241
0.0000
3t
1.00
2.00
1.04
2.04
1.03
1.09
3.20
fl (ppm)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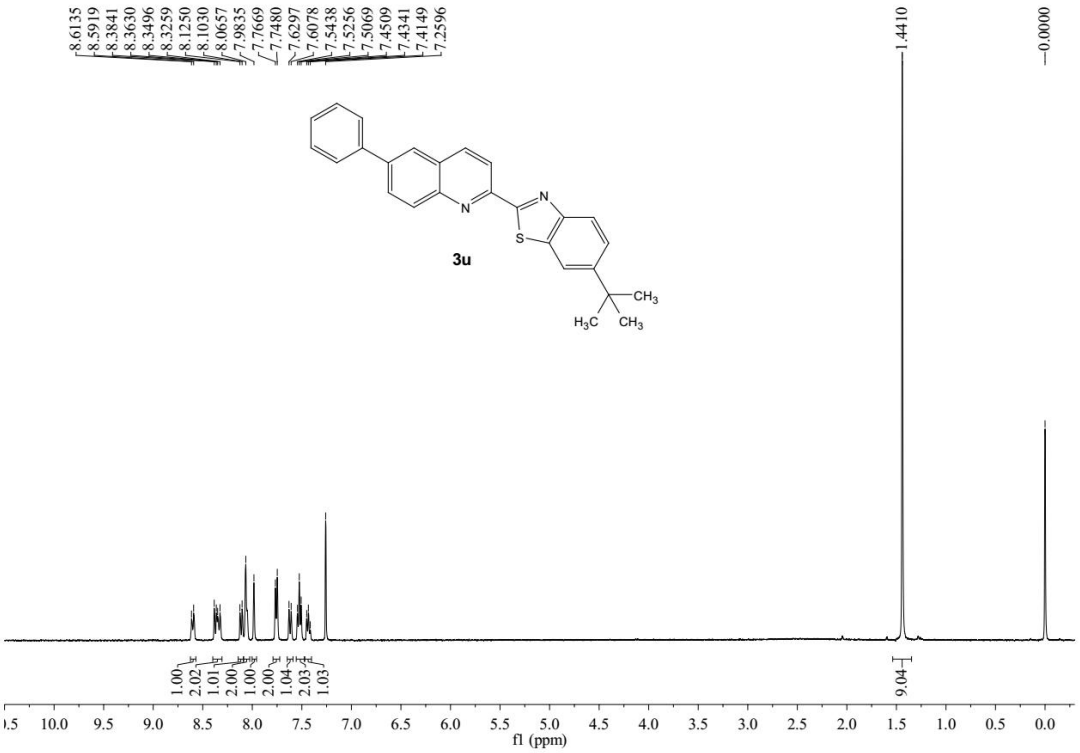
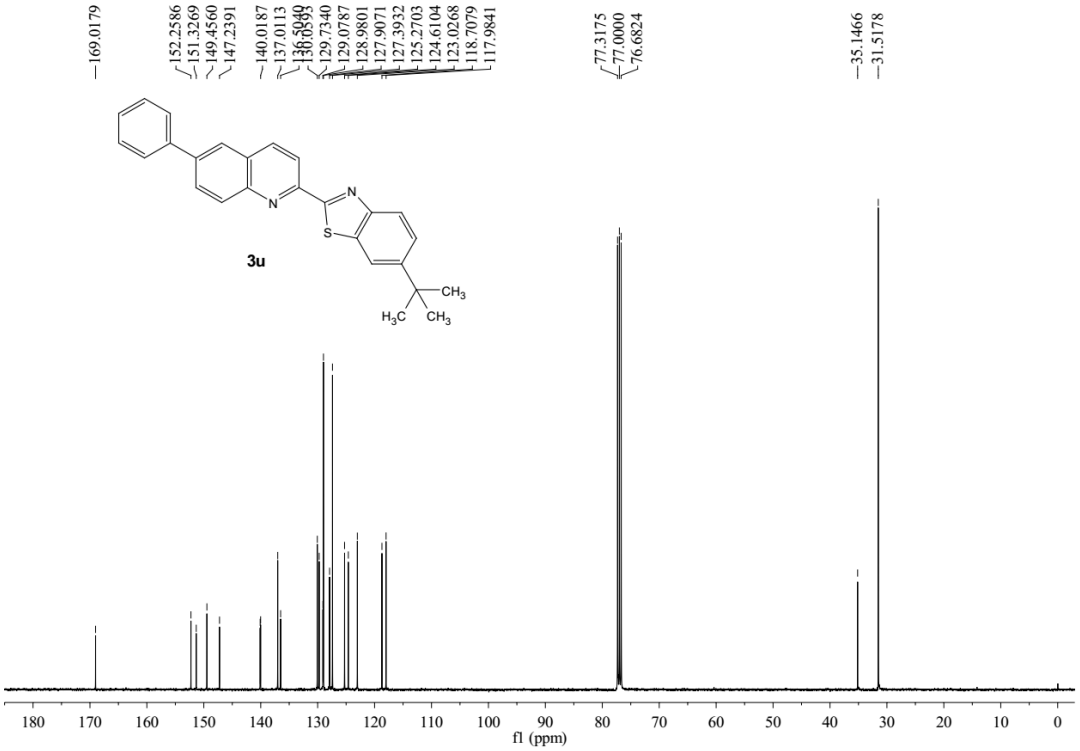
152.4927
146.0696
143.0674
142.8988
141.8231
136.8392
136.4207
130.7486
130.6410
129.5444
129.4052
128.3370
123.6037
121.7055
77.3175
77.0000
76.6824
21.6761
3t
fl (ppm)


8.6135
8.5919
8.3841
8.3630
8.3496
8.3259
8.1250
8.1030
8.0657
7.9835
7.7669
7.7480
7.6297
7.6078
7.5438
7.5256
7.5069
7.4509
7.4341
7.4149
7.2596
1.4410
0.0000
3u
CH3
H3C CH3
1.00
2.02
1.01
2.00
1.00
2.00
1.04
2.03
1.03
9.04
f1 (ppm)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151.3269
149.4560
147.2391
140.0187
137.0113
129.7340
129.0787
128.9801
127.9071
127.3932
125.2703
124.6104
123.0268
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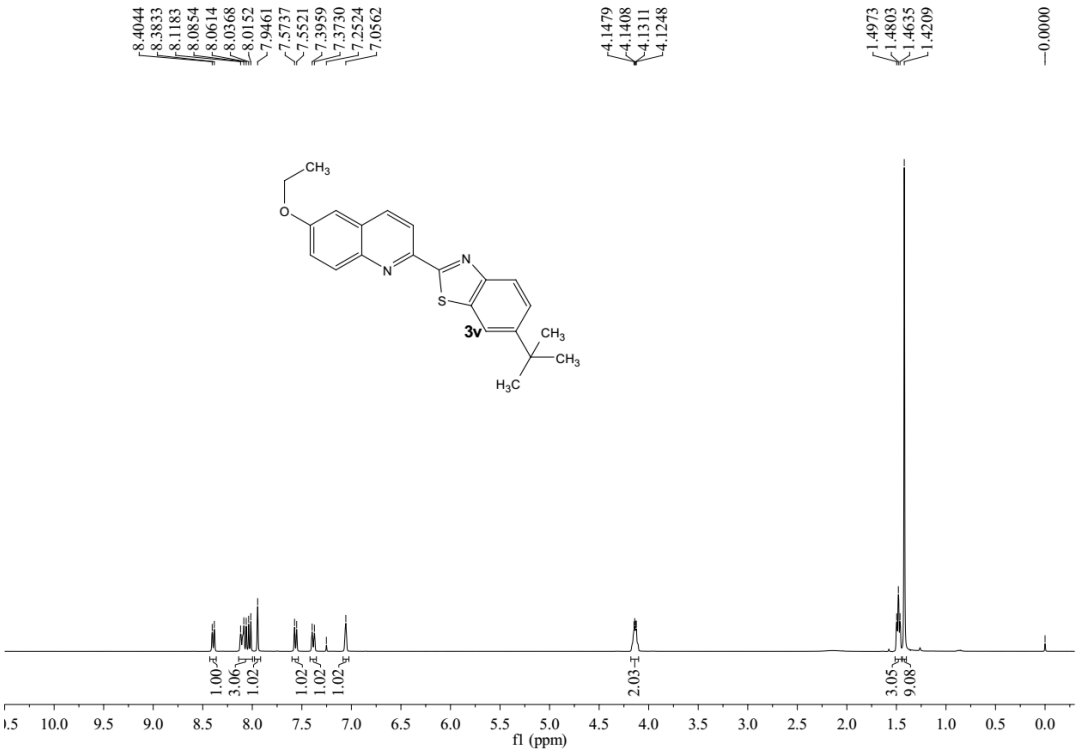
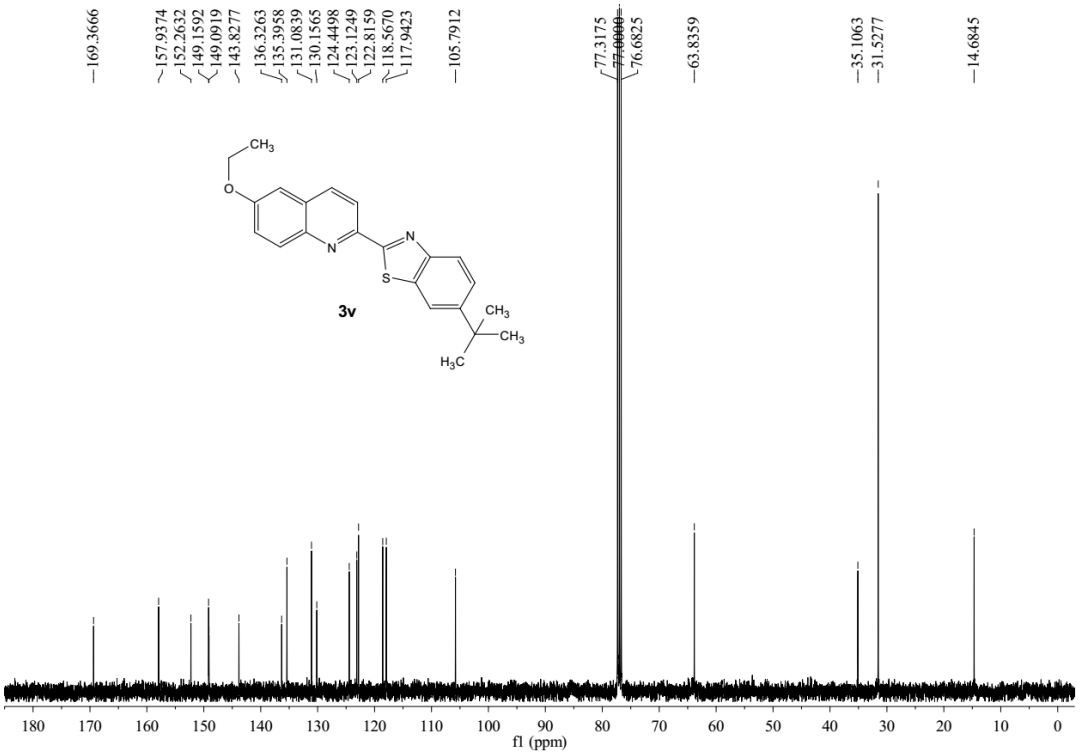
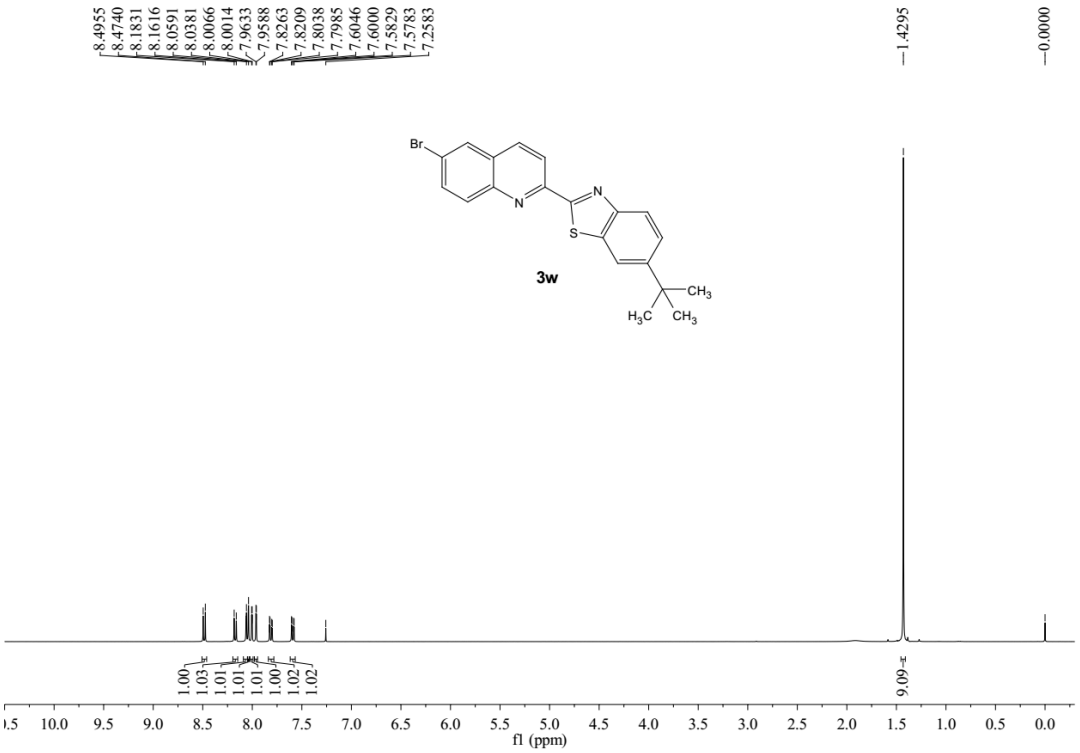
77.3175
77.0000
76.6824
35.1466
31.5178
3u
CH3
H3C CH3
f1 (ppm)


8.4044
8.3833
8.1183
8.0854
8.0614
8.0368
8.0152
7.9461
7.5737
7.5521
7.3959
7.3730
7.2524
7.0562
4.1479
4.1408
4.1311
4.1248
1.4973
1.4803
1.4635
1.4209
0.0000
3v
1.00
3.06
1.02
1.02
1.02
1.02
2.03
3.05
9.08
f1 (ppm)


169.3666
157.9374
152.2632
149.1592
149.0919
143.8277
136.3263
135.3958
131.0839
130.1565
124.4498
123.1249
122.8159
118.5670
117.9423
105.7912
77.3175
77.0000
76.6825
63.8359
35.1063
31.5277
14.6845
3v
f1 (ppm)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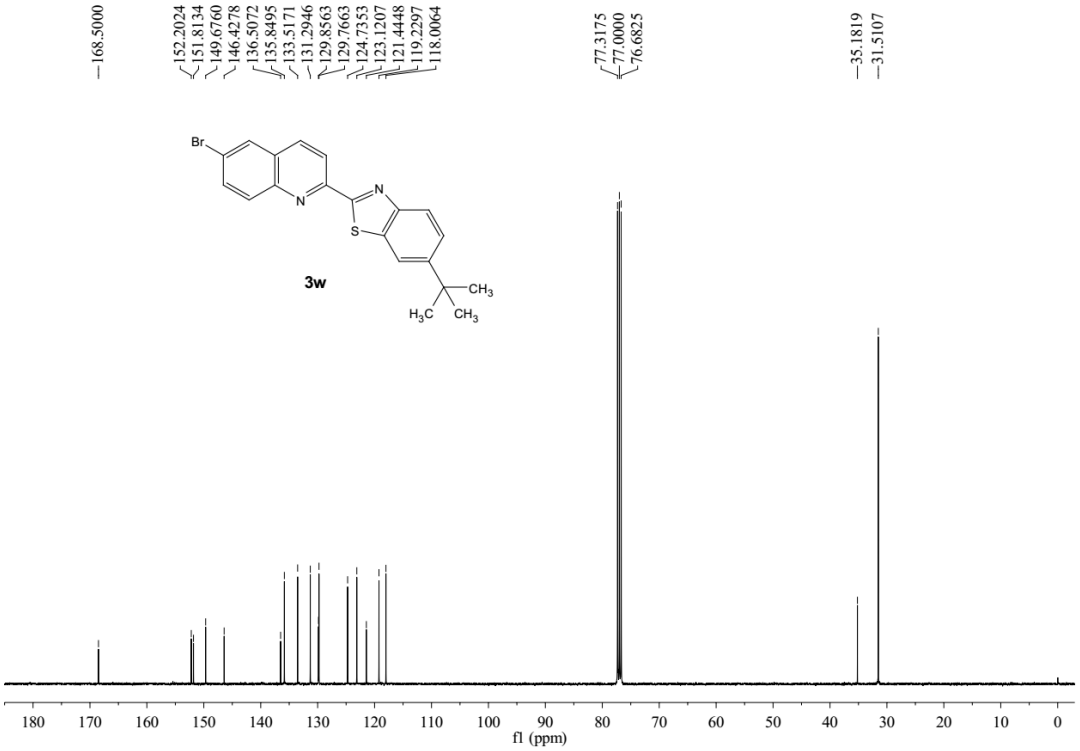
8.4740
8.1831
8.1616
8.0591
8.0381
8.0066
8.0014
7.9633
7.9588
7.8263
7.8209
7.8038
7.7985
7.6046
7.6000
7.5829
7.5783
7.2583
1.4295
0.0000
Br
N
N
S
CH3
H3C
CH3
3w
1.00
1.03
1.01
1.01
1.01
1.00
1.02
1.02
9.09
f1 (ppm)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149.6760
146.4278
136.5072
135.8495
133.5171
131.2946
129.8563
129.7663
124.7353
123.1207
121.4448
119.2297
118.0064
77.3175
77.0000
76.6825
35.1819
31.5107
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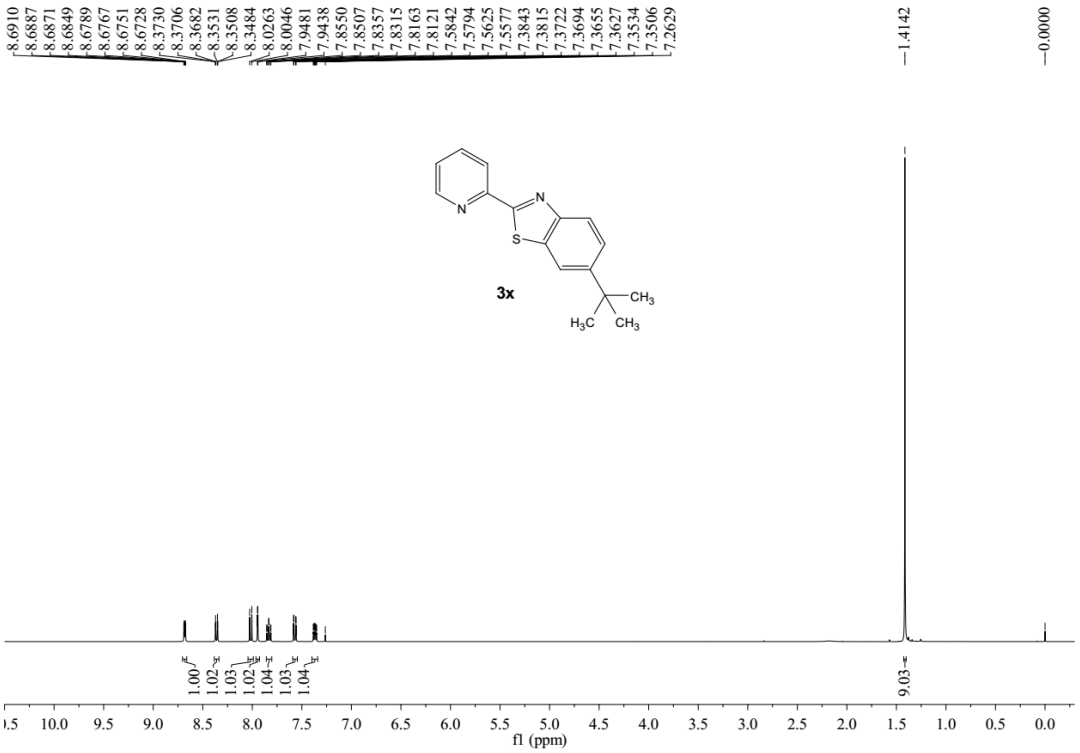
N
S
CH3
H3C
CH3
3w
f1 (ppm)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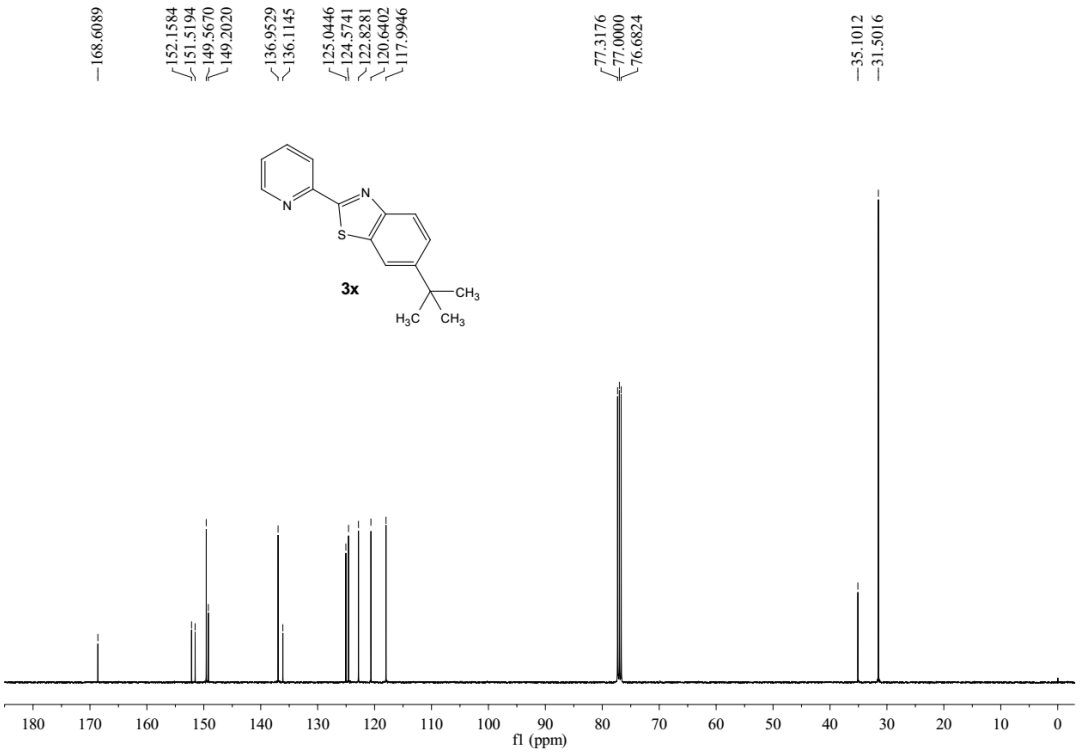
8.6871
8.6849
8.6789
8.6767
8.6751
8.6728
8.3730
8.3706
8.3682
8.3531
8.3508
8.3484
8.0263
8.0046
7.9481
7.9438
7.8550
7.8507
7.8357
7.8315
7.8163
7.8121
7.5842
7.5794
7.5625
7.5577
7.3843
7.3815
7.3722
7.3694
7.3655
7.3627
7.3534
7.3506
7.2629
1.4142
0.0000
3x
1.00
1.02
1.03
1.02
1.04
1.03
1.04
9.03
fl (ppm)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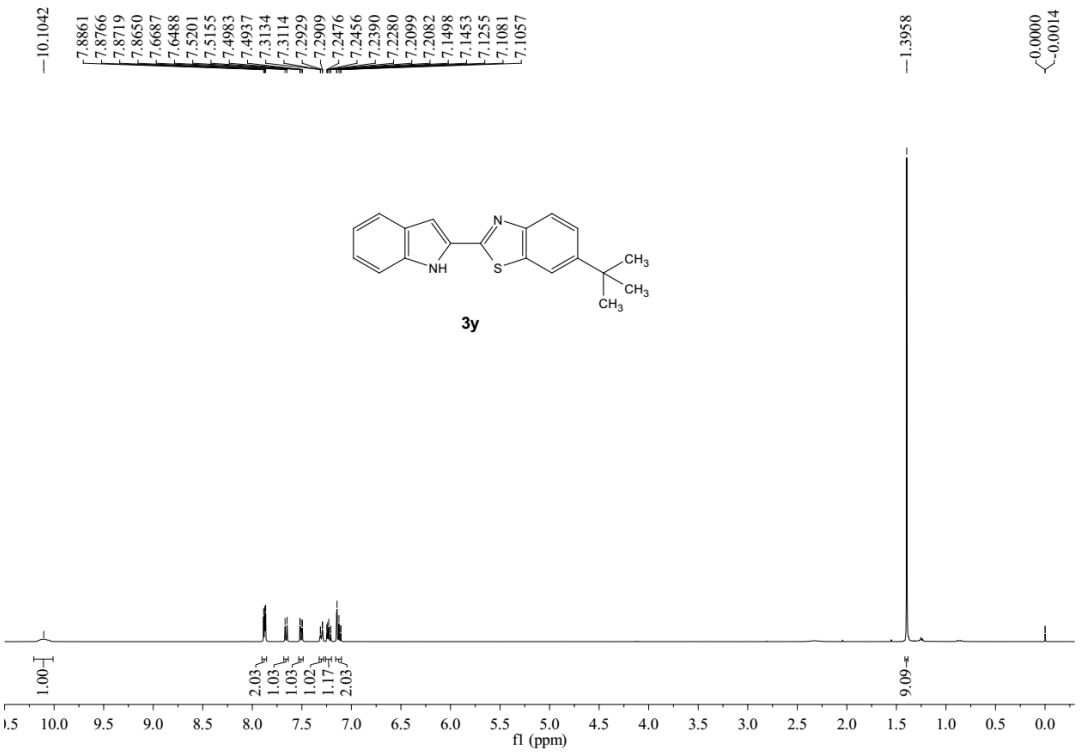
151.5194
149.5670
149.2020
136.9529
136.1145
125.0446
124.5741
122.8281
120.6402
117.9946
77.3176
77.0000
76.6824
35.1012
31.5016
3x
fl (ppm)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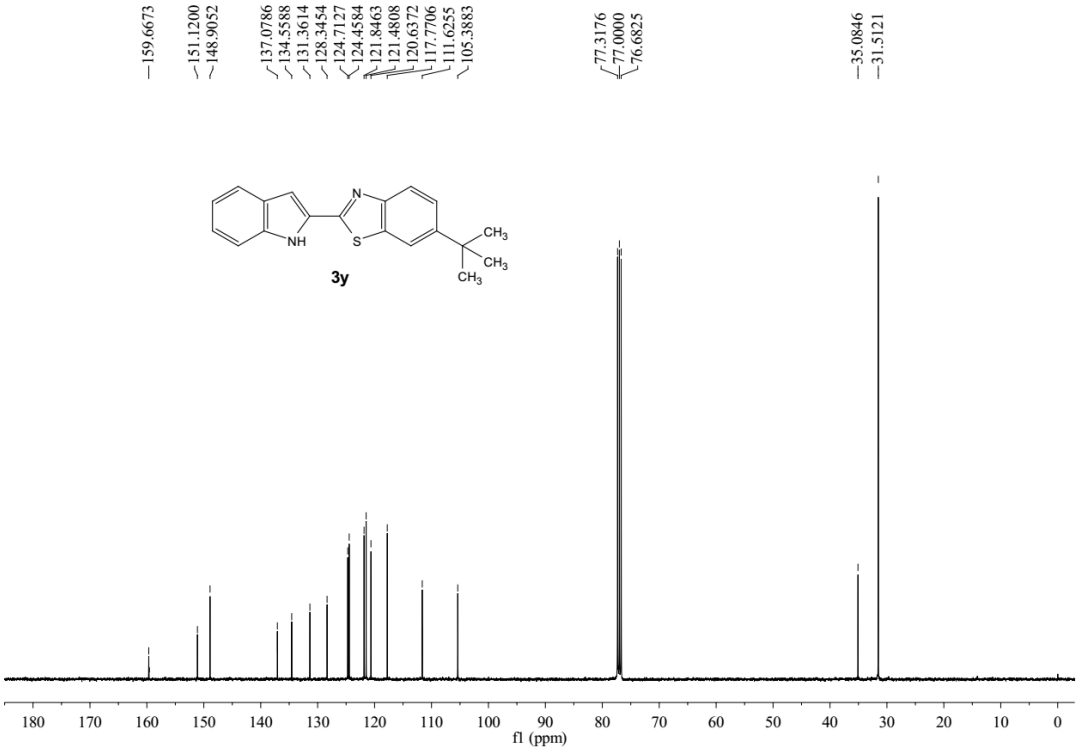
7.8719
7.8650
7.6687
7.6488
7.5201
7.5155
7.4983
7.4937
7.3134
7.3114
7.2929
7.2909
7.2476
7.2456
7.2390
7.2280
7.2099
7.2082
7.1498
7.1453
7.1255
7.1081
7.1057
1.3958
0.0000
-0.0014
N
NH
S
CH3
CH3
CH3
3y
1.00
2.03
1.03
1.03
1.02
1.17
2.03
9.09
f1 (ppm)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148.9052
137.0786
134.5588
131.3614
128.3454
124.7127
124.4584
121.8463
121.4808
120.6372
117.7706
111.6255
105.3883
77.3176
77.0000
76.6825
35.0846
31.5121
N
NH
S
CH3
CH3
CH3
3y
f1 (ppm)