Supporting Information

Rh(III)-catalyzed Cyclization Reaction of Azoles with Alkynes: Efficient Synthesis of Azole-fused-Pyridines

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1. General Information

Reagents and Solvents: $[RhCp^*Cl_2]_2$ and NaOAc were commercially available. PE refers to petroleum ether b.p. 60-90 °C and EA refers to ethyl acetate. All other starting materials and solvents were commercially available and were used without further purification unless otherwise stated. Room temperature reactions were carried out between 20-25 °C.

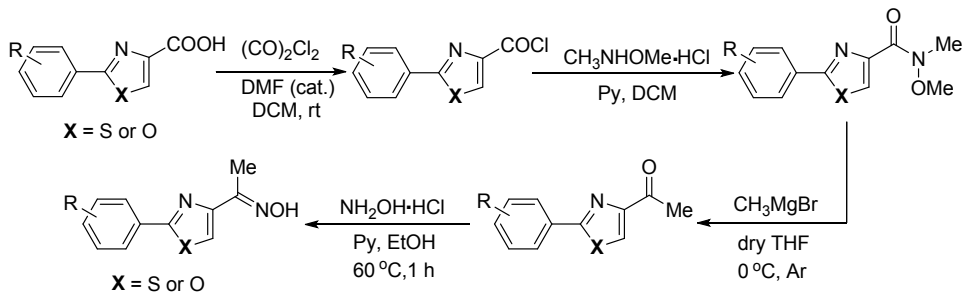
Chromatography: Flash column chromatography was carried out using commercially available 300-400 mesh under pressure unless otherwise indicated. Gradient flash chromatography was conducted eluting with PE/EA.

Data collection: ^1H and ^{13}C NMR spectra were collected on BRUKER AV-300 (300 MHz) spectrometer using $CDCl_3$ as solvent. Chemical shifts of ^1H NMR were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ = 0.00 ppm) with the solvent resonance as an internal standard ($CDCl_3$: δ = 7.26 ppm). Data are reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, brs = broad singlet, m = multiplet), coupling constant (Hz), and integration. Chemical shifts of ^{13}C NMR were reported in ppm with the solvent as the internal standard ($CDCl_3$: δ = 77.0 ppm). Infrared spectra (IR) were recorded on a Thermo Scientific iS10 FT/IR spectrometer; absorptions are reported in reciprocal centimeters. High Resolution Mass measurement was performed on Agilent QTOF 6520 mass spectrometer with electron spray ionization (ESI) as the ion source. Melting point (mp) was measured on a microscopic melting point apparatus.

2. General procedure for the preparation of substrates

2.1 Preparation of thiazole/oxazole substrates

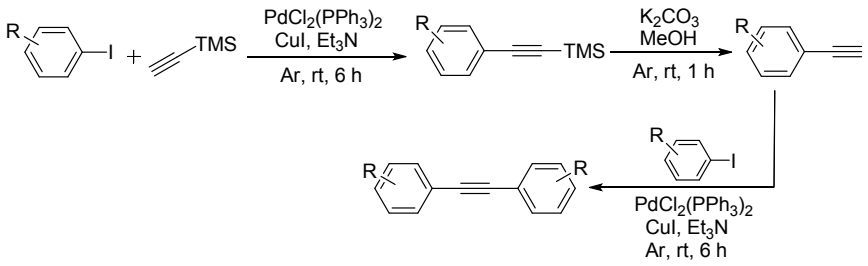
As shown in **Scheme S1**, starting materials thiazole/oxazole carboxylic acid were synthesized according to the literature.[1] Weinreb amidation followed by the reaction with methylmagnesium bromide to get the corresponding ketones.[2] The thiazole/oxazole substrates were formed by the condensition between the ketones and hydroxylamine hydrochloride.[3]



Scheme S1. Preparation of thiazole/oxazole substrates

2.2 Preparation of symmetrical alkynes

As shown in **Scheme S2**, the symmetrical alkynes were prepared from the corresponding phenyl iodide and ethynyltrimethylsilane as starting materials via sonogashira reaction, remove of trimethylsilane followed by another sonogashira reaction. For details see the reported literatures.[4]

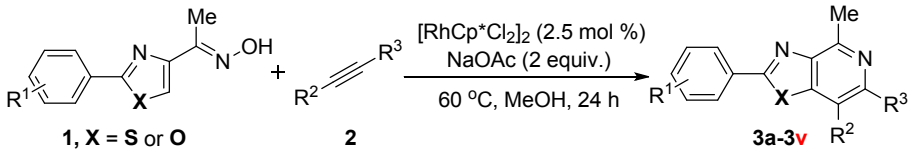


Scheme S2. Preparation of symmetrical alkynes

3. Rh(III)-catalyzed Cyclization Reaction of Azoles with Alkynes

3.1 General Procedure

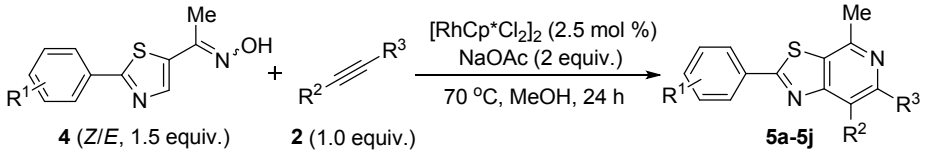
3.1.1 Typical Experimental Procedure for Synthesis of 3a-3v



1, X = S or **O** **2** **3a-3v**

A reaction tube was charged with catalyst $[RhCp^*Cl_2]_2$ (3.1 mg, 2.5 mol %), NaOAc (34 mg, 2.0 equiv.), **1** (0.2 mmol, 1.0 equiv.), **2** (0.24 mmol, 1.2 equiv.) in 2 mL methanol under air atmosphere. The reaction tube was sealed, and the mixture was vigorously stirred at 60 °C (oil temperature) for 24 h. After competition, the mixture was cooled to room temperature, diluted with dichloromethane and concentrated under reduced pressure then purified by flash chromatography on silica gel (PE/EA) to afford the corresponding products **3a-3v**.

3.1.2 Typical Experimental Procedure for Synthesis of 5a-5j



4 (*Z*/*E*, 1.5 equiv.) **2** (1.0 equiv.) **5a-5j**

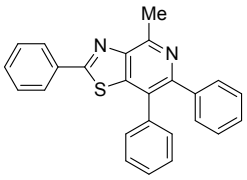
A reaction tube was charged with catalyst $[RhCp^*Cl_2]_2$ (3.1 mg, 2.5 mol %), NaOAc (34 mg, 2.0 equiv.), **4** (0.3 mmol, 1.5 equiv.), **2** (0.2 mmol, 1.0 equiv.) in 2 mL methanol under air atmosphere. The reaction tube was sealed, and the mixture was vigorously stirred at 70 °C (oil temperature) for 24 h. After competition, the mixture

was cooled to room temperature, diluted with dichloromethane and concentrated under reduced pressure then purified by flash chromatography on silica gel (petroleum ether/ethyl acetate) to afford the corresponding products **5a-5j**.

3.2 Characterization of the Cyclization Products

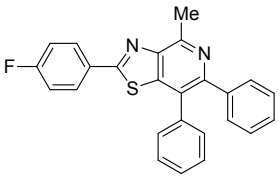
3.2.1 C_5-Cyclization Products

4-methyl-2,6,7-triphenylthiazolo[4,5-c]pyridine (3a)



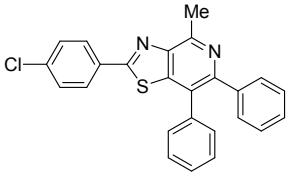
72 mg, 95% yield; white solid, mp: 210-212 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.47 (ddd, *J* = 6.0, 5.0, 2.2 Hz, 5H), 7.37 (s, 5H), 7.31-7.22 (m, 3H), 3.16 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.3, 152.8, 150.7, 148.6, 145.9, 139.9, 139.2, 133.3, 131.3, 130.4, 129.5, 129.1, 128.8, 128.0, 127.9, 127.6, 127.5, 127.2, 21.6; IR (KBr) 3050, 2920, 1599, 1549, 1477, 1419, 1307, 1252, 1172, 1027, 974, 762, 703 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{19}N_2S$ $[M+H]^+$ 379.1263, found 379.1265.

2-(4-fluorophenyl)-4-methyl-6,7-diphenylthiazolo[4,5-c]pyridine (3b)



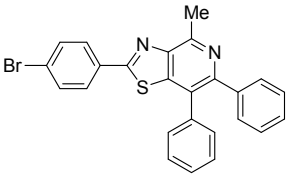
74 mg, 93% yield; white solid, mp: 214-216 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.5, 5.3 Hz, 2H), 7.46-7.26 (m, 7H), 7.22 (dd, *J* = 6.5, 3.3 Hz, 3H), 7.13 (t, *J* = 8.5 Hz, 2H), 3.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.0, 166.3, 162.9, 152.7, 150.8, 148.5, 145.9, 139.8, 139.1, 130.3, 129.7, 129.6, 129.4, 128.8, 128.0, 127.9, 127.6, 127.2, 116.4, 116.1, 21.6; IR (KBr) 3050, 2908, 1598, 1546, 1510, 1478, 1420, 1372, 1248, 1230, 1156, 974, 841, 764, 702 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{18}FN_2S$ $[M+H]^+$ 397.1169, found 397.1168.

2-(4-chlorophenyl)-4-methyl-6,7-diphenylthiazolo[4,5-c]pyridine (3c)



72 mg, 87% yield; white solid, mp: 193-195 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.4 Hz, 2H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.35 (dt, *J* = 12.8, 5.5 Hz, 7H), 7.25-7.17 (m, 3H), 3.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 152.9, 150.9, 148.5, 145.9, 139.7, 139.0, 132.3, 132.2, 130.3, 129.4, 128.9, 128.8, 128.0, 127.9, 127.6, 127.2, 125.8, 21.6; IR (KBr) 3050, 2920, 1584, 1546, 1469, 1413, 1375, 1248, 1174, 1074, 1007, 974, 810, 765, 703 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{18}ClN_2S$ $[M+H]^+$ 413.0874, found 413.0872.

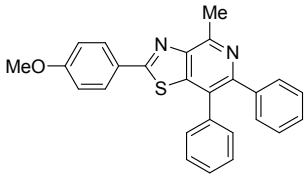
2-(4-bromophenyl)-4-methyl-6,7-diphenylthiazolo[4,5-c]pyridine (3d)



85 mg, 93% yield; pale yellow solid, mp: 215-217 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.47-7.27 (m, 9H), 7.26-7.18 (m, 3H), 3.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.9, 152.9, 150.9, 148.5, 145.9, 139.7, 139.0, 137.4, 131.7, 130.3, 129.4, 129.3, 128.8, 128.8, 128.0, 127.9, 127.6, 127.2, 21.6; IR (KBr) 3055, 2914, 1594, 1546, 1471, 1419, 1399, 1376,

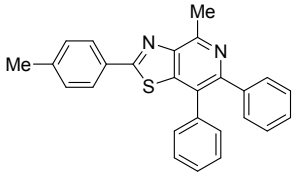
1249, 1087, 1014, 974, 877, 837, 765, 704 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{18}BrN_2S$ $[M+H]^+$ 457.0369, found 457.0371.

2-(4-methoxyphenyl)-4-methyl-6,7-diphenylthiazolo[4,5-c]pyridine (3e)



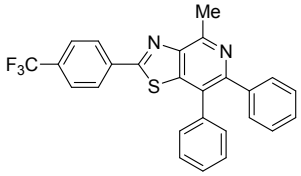
65 mg, 80% yield; White solid, mp: 198-200 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.6 Hz, 2H), 7.47-7.15 (m, 10H), 6.95 (d, *J* = 8.6 Hz, 2H), 3.84 (s, 3H), 3.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.1, 162.2, 152.2, 150.4, 148.7, 145.7, 140.0, 139.3, 130.3, 129.5, 129.2, 128.7, 127.8, 127.5, 127.1, 126.1, 114.4, 55.5, 21.6; IR (KBr) 3032, 2938, 1606, 1548, 1479, 1420, 1360, 1307, 1255, 1172, 1030, 877, 837, 762, 699 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2OS$ $[M+H]^+$ 409.1369, found 409.1371.

4-methyl-6,7-diphenyl-2-(p-tolyl)thiazolo[4,5-c]pyridine (3f)



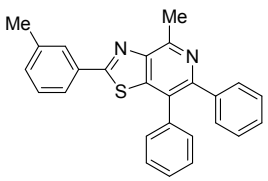
67 mg, 86% yield; white solid, mp: 196-198 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.9 Hz, 2H), 7.44-7.26 (m, 7H), 7.22 (d, *J* = 7.6 Hz, 5H), 3.09 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.5, 160.4, 152.5, 150.5, 148.7, 145.7, 141.8, 139.9, 139.2, 130.6, 130.4, 129.8, 129.5, 128.8, 127.9, 127.5, 127.2, 115.0, 21.6, 21.6; IR (KBr) 3056, 2920, 1599, 1547, 1480, 1420, 1375, 1254, 1177, 974, 877, 811, 768, 702 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2S$ $[M+H]^+$ 393.1420, found 393.1417.

4-methyl-6,7-diphenyl-2-(4-(trifluoromethyl)phenyl)thiazolo[4,5-c]pyridine (3g)



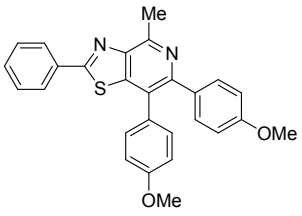
80 mg, 90% yield; white solid, mp: 205-207 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.1 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.50-7.31 (m, 7H), 7.30-7.22 (m, 3H), 3.15 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.3, 153.3, 151.2, 148.5, 146.1, 139.6, 138.9, 136.4, 132.8 (q, J_{C-F} = 32.5 Hz), 130.3, 129.4, 128.9, 128.1, 127.9, 127.9, 127.7, 127.3, 126.7 (q, J_{C-F} = 3.7 Hz), 123.8 (q, J_{C-F} = 270.7 Hz), 21.5; IR (KBr) 3061, 2932, 1616, 1546, 1419, 1338, 1322, 1251, 1170, 1118, 1066, 977, 844, 765, 698 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{18}F_3N_2S$ $[M+H]^+$ 447.1137, found 447.1136.

4-methyl-6,7-diphenyl-2-(m-tolyl)thiazolo[4,5-c]pyridine (3h)



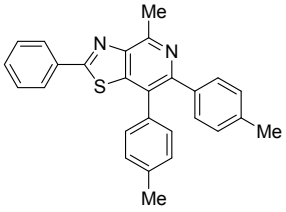
71 mg, 90% yield; white solid, mp: 184-186 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.41 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.36-7.26 (m, 6H), 7.23 (dd, *J* = 6.6, 2.9 Hz, 3H), 3.11 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.6, 152.7, 150.6, 148.6, 145.8, 139.9, 139.2, 138.9, 133.2, 132.1, 130.3, 130.0, 129.5, 129.0, 128.8, 128.1, 127.9, 127.5, 127.2, 124.9, 21.6, 21.4; IR (KBr) 3044, 2919, 1735, 1654, 1548, 1481, 1421, 1374, 1265, 1178, 1018, 921, 826, 790, 763, 699 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2S$ $[M+H]^+$ 393.1420, found 393.1419.

6,7-bis(4-methoxyphenyl)-4-methyl-2-phenylthiazolo[4,5-c]pyridine (3i)



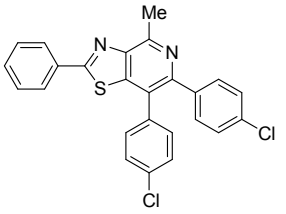
74 mg, 85% yield; pale yellow solid, mp: 154-156 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 3.5 Hz, 2H), 7.48 (d, *J* = 1.6 Hz, 3H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.25 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 6.78 (d, *J* = 8.5 Hz, 2H), 3.80 (d, *J* = 17.6 Hz, 6H), 3.08 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.0, 159.1, 152.3, 150.3, 148.3, 146.2, 133.4, 132.4, 131.6, 131.2, 130.6, 129.1, 128.8, 127.6, 126.4, 124.8, 114.2, 113.4, 55.3, 55.2, 21.5; IR (KBr) 2997, 2837, 1725, 1607, 1548, 1513, 1434, 1405, 1288, 1249, 1175, 1031, 927, 838, 817, 729, 685 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{27}H_{23}N_2O_2S$ $[M+H]^+$ 439.1475, found 439.1474.

4-methyl-2-phenyl-6,7-di-p-tolylthiazolo[4,5-c]pyridine (3j)



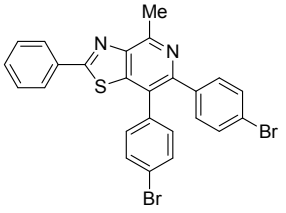
65 mg, 80% yield; white solid, mp: 201-203 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.11-7.99 (m, 2H), 7.51-7.39 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.25-7.10 (m, 4H), 7.03 (d, *J* = 8.0 Hz, 2H), 3.08 (s, 3H), 2.36 (s, 3H), 2.29 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.1, 152.5, 150.7, 148.4, 146.0, 137.6, 137.2, 137.1, 136.4, 133.4, 131.2, 130.2, 129.5, 129.3, 129.1, 128.6, 127.6, 126.9, 21.6, 21.4, 21.3; IR (KBr) 3025, 2916, 1611, 1547, 1477, 1431, 1376, 1253, 1182, 1030, 972, 829, 779, 765, 685 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{27}H_{23}N_2S$ $[M+H]^+$ 407.1576, found 407.1575.

6,7-bis(4-chlorophenyl)-4-methyl-2-phenylthiazolo[4,5-c]pyridine (3k)



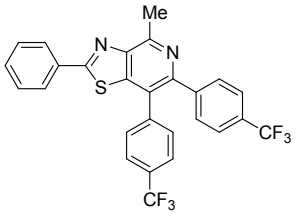
76 mg, 85% yield; pale yellow solid, mp: 206-208 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10–7.99 (m, 2H), 7.51–7.39 (m, 3H), 7.38–7.26 (m, 4H), 7.21 (dt, *J* = 4.1, 3.4 Hz, 4H), 3.06 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.5, 153.2, 149.3, 148.7, 145.6, 138.0, 137.2, 134.2, 133.9, 133.0, 131.6, 131.5, 130.8, 129.3, 129.1, 128.3, 127.6, 125.9, 21.6; IR (KBr) 3050, 2920, 1566, 1549, 1490, 1476, 1432, 1375, 1248, 1192, 1106, 1014, 839, 801, 765, 686 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{17}Cl_2N_2S$ $[M+H]^+$ 447.0484, found 447.0486.

6,7-bis(4-bromophenyl)-4-methyl-2-phenylthiazolo[4,5-c]pyridine (3l)



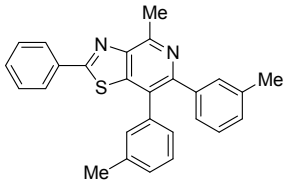
97 mg, 91% yield; pale yellow solid, mp: 238-240 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12-7.99 (m, 2H), 7.47 (qd, *J* = 8.7, 3.0 Hz, 5H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.30-7.22 (m, 2H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.07 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.6, 153.3, 149.3, 148.8, 145.6, 138.5, 137.7, 133.0, 132.3, 131.9, 131.5, 131.2, 131.0, 129.2, 127.6, 125.9, 122.4, 122.3, 21.6; IR (KBr) 3056, 2926, 1547, 1486, 1431, 1377, 1242, 1104, 1070, 1009, 971, 839, 801, 764, 686 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{17}Br_2N_2S$ $[M+H]^+$ 534.9474, found 534.9472.

4-methyl-2-phenyl-6,7-bis(4-(trifluoromethyl)phenyl)thiazolo[4,5-c]pyridine (3m)



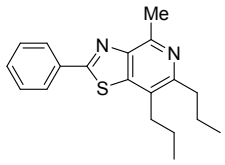
68 mg, 67% yield; white solid, mp: 227-230 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, J = 6.7 Hz, 2H), 7.66 (d, J = 7.8 Hz, 2H), 7.45-7.52 (m, 9H), 3.12 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.0, 153.8, 149.1, 149.0, 145.6, 143.0, 142.2, 132.9, 131.7, 130.6, 130.2, 130.1, 129.9, 129.6, 129.5, 129.2, 127.7, 126.1 (q, $J_{C\text{-}F}$ = 3.6 Hz), 125.9, 125.7, 125.0 (q, $J_{C\text{-}F}$ = 3.6 Hz), 122.3, 122.1, 118.7, 118.5, 21.6; IR (KBr) 3050, 2930, 1620, 1481, 1327, 1157, 1118, 1060, 1016, 845, 627 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{27}H_{16}F_6N_2S$ $[M+H]^+$ 515.1011, found 515.1009.

4-methyl-2-phenyl-6,7-di-m-tolylthiazolo[4,5-c]pyridine (3n)



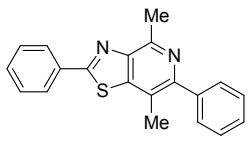
68 mg, 84% yield; pale yellow solid, mp: 139-141 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10-7.96 (m, 2H), 7.47-7.33 (m, 4H), 7.23-6.98 (m, 7H), 3.10 (s, 3H), 2.28 (d, J = 6.6 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 168.2, 152.5, 150.8, 148.5, 145.9, 139.8, 139.2, 138.4, 137.5, 133.3, 131.2, 131.0, 129.9, 129.5, 129.1, 128.6, 128.3, 127.9, 127.6, 127.5, 127.3, 126.6, 21.6, 21.5, 21.5; IR (KBr) 3020, 2914, 1596, 1584, 1550, 1476, 1445, 1373, 1252, 1089, 968, 906, 791, 761, 704, 685 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{27}H_{23}N_2S$ $[M+H]^+$ 407.1576, found 407.1574.

4-methyl-2-phenyl-6,7-dipropylthiazolo[4,5-c]pyridine (3o)



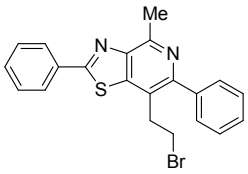
52 mg, 84% yield; white solid, mp: 66-68 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (ddd, J = 5.5, 3.0, 1.5 Hz, 2H), 7.53-7.37 (m, 3H), 2.96 (s, 3H), 2.90-2.74 (m, 4H), 1.86-1.62 (m, 4H), 1.04 (t, J = 7.3 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 166.5, 153.6, 151.0, 148.1, 144.4, 133.5, 131.0, 129.0, 127.5, 125.9, 36.8, 35.0, 23.9, 22.6, 21.2, 14.4, 14.3; IR (KBr) 2958, 2928, 2868, 1560, 1477, 1438, 1310, 1251, 1234, 1086, 1071, 974, 912, 839, 766, 689, 651 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{19}H_{23}N_2S$ $[M+H]^+$ 311.1576, found 311.1578.

4,7-dimethyl-2,6-diphenylthiazolo[4,5-c]pyridine (3p)



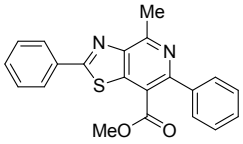
49 mg, 77% yield; white solid, mp: 136-138 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.17-8.03 (m, 2H), 7.63-7.52 (m, 2H), 7.53-7.34 (m, 6H), 3.02 (s, 3H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.5, 152.0, 151.2, 148.4, 145.3, 140.3, 133.4, 131.2, 129.6, 129.1, 128.2, 127.9, 127.6, 121.5, 21.4, 19.5; IR (KBr) 3056, 2908, 1560, 1478, 1451, 1421, 1250, 1121, 1021, 953, 886, 764, 685, 675 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{20}H_{17}N_2S$ $[M+H]^+$ 317.1107, found 317.1109.

7-(2-bromoethyl)-4-methyl-2,6-diphenylthiazolo[4,5-c]pyridine (3q)



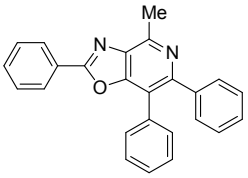
34 mg, 41% yield; white solid, mp: 128-130 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.64-7.36 (m, 8H), 3.58-3.35 (m, 4H), 3.04 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.7, 153.0, 152.5, 149.0, 144.8, 139.8, 133.1, 131.5, 129.2, 129.0, 128.6, 128.3, 127.8, 123.0, 36.7, 29.4, 21.5; IR (KBr) 3056, 2922, 1554, 1477, 1444, 1425, 1247, 1224, 1073, 1023, 980, 883, 800, 759, 705, 683 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{21}H_{18}BrN_2S$ $[M+H]^+$ 409.0369, found 409.0366.

methyl 4-methyl-2,6-diphenylthiazolo[4,5-c]pyridine-7-carboxylate (3r)



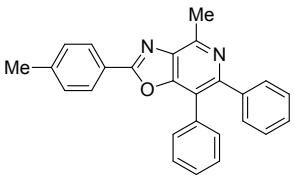
14 mg, 19% yield; white solid, mp: 158-160 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19-8.15 (m, 2H), 7.58-7.51 (m, 5H), 7.49-7.41 (m, 3H), 3.73 (s, 3H) , 3.11 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 167.6, 156.3, 155.1, 148.8, 144.9, 140.8, 133.1, 131.6, 129.2, 129.0, 128.4, 128.0, 127.7, 52.3, 21.9; IR (KBr) 3518, 3420, 3051, 2825, 1733, 1637, 1629, 1350, 1122, 1045, 720, 690 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{21}H_{16}N_2O_2S$ $[M+H]^+$ 361.1005, found 361.1009.

4-methyl-2,6,7-triphenyloxazolo[4,5-c]pyridine (3s)



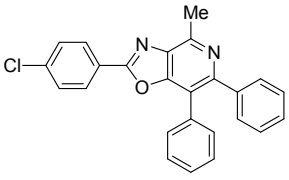
55 mg, 76% yield; white solid, mp: 196-198 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.22 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.50 (dt, *J* = 12.2, 4.5 Hz, 3H), 7.45-7.30 (m, 7H), 7.25 (t, *J* = 3.2 Hz, 3H), 2.97 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2, 154.8, 152.6, 150.2, 139.9, 137.4, 133.6, 132.0, 130.5, 130.4, 128.9, 128.5, 128.0, 127.9, 127.8, 127.7, 126.5, 117.9, 20.2; IR (KBr) 3059, 2908, 1627, 1593, 1550, 1492, 1425, 1380, 1207, 1121, 1018, 914, 769, 708, 690 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{19}N_2O$ $[M+H]^+$ 363.1492, found 363.1491.

4-methyl-6,7-diphenyl-2-(p-tolyl)oxazolo[4,5-c]pyridine (3t)



49 mg, 65% yield; white solid, mp: 206-208 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 2H), 7.46-7.38 (m, 2H), 7.38-7.29 (m, 5H), 7.24 (dd, *J* = 8.5, 5.3 Hz, 5H), 2.95 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.5, 154.7, 152.4, 149.9, 142.6, 140.0, 137.5, 133.6, 130.5, 130.4, 129.7, 128.4, 128.0, 127.9, 127.7, 127.6, 123.7, 117.8, 21.8, 20.2; IR (KBr) 3032, 2914, 1626, 1612, 1500, 1422, 1379, 1313, 1206, 1121, 1041, 1015, 915, 833, 766, 731, 698 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2O$ $[M+H]^+$ 377.1648, found 377.1645.

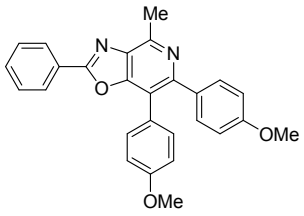
2-(4-chlorophenyl)-4-methyl-6,7-diphenyloxazolo[4,5-c]pyridine (3u)



66 mg, 83% yield; white solid, mp: 183-185 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.6 Hz, 2H), 7.51-7.28 (m, 9H), 7.28-7.16 (m, 3H), 2.94 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.2, 154.8, 152.8, 150.3, 139.8, 138.2, 137.3,

133.4, 130.5, 130.4, 129.3, 129.1, 128.5, 128.0, 127.8, 127.7, 125.0, 117.9, 20.2; IR (KBr) 3050, 2920, 1625, 1606, 1483, 1419, 1404, 1378, 1257, 1090, 1042, 1012, 909, 832, 732, 696 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{18}ClN_2O$ $[M+H]^+$ 397.1102, found 397.1100.

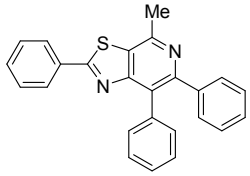
6,7-bis(4-methoxyphenyl)-4-methyl-2-phenyloxazolo[4,5-c]pyridine (3v)



79 mg, 94% yield; pale yellow solid, mp: 177-179 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.19 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.47 (q, *J* = 5.5 Hz, 3H), 7.37 (d, *J* = 8.7 Hz, 2H), 7.29 (d, *J* = 8.7 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 8.7 Hz, 2H), 3.80 (d, *J* = 15.9 Hz, 6H), 2.93 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.0, 159.2, 159.0, 154.9, 152.1, 149.6, 137.1, 132.6, 132.3, 131.8, 131.6, 128.9, 127.8, 126.6, 125.9, 117.1, 114.0, 113.5, 55.2, 55.2, 20.1; IR (KBr) 3055, 2926, 1605, 1513, 1437, 1372, 1289, 1248, 1173, 1118, 1031, 912, 821, 780, 706 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{27}H_{23}N_2O_3$ $[M+H]^+$ 423.1703, found 423.1707.

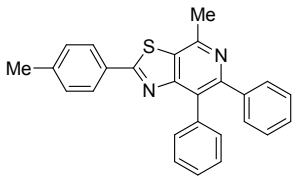
3.2.2 C_4-Cyclization Product

4-methyl-2,6,7-triphenylthiazolo[5,4-c]pyridine (5a)



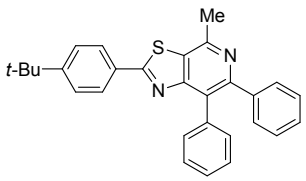
64 mg, 85% yield; white solid, mp: 174-176 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 7.8, 1.5 Hz, 2H), 7.50-7.35 (m, 7H), 7.35-7.25 (m, 3H), 7.26-7.17 (m, 3H), 2.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.7, 158.9, 153.9, 151.0, 140.5, 136.5, 133.1, 131.8, 131.6, 130.4, 130.2, 129.0, 128.4, 128.1, 127.9, 127.8, 127.4, 127.2, 25.0; IR (KBr) 3044, 2908, 1549, 1537, 1502, 1474, 1446, 1413, 1328, 1310, 1177, 1065, 962, 765, 698, 683 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{19}N_2S$ $[M+H]^+$ 379.1263, found 379.1267.

4-methyl-6,7-diphenyl-2-(p-tolyl)thiazolo[5,4-c]pyridine (5b)



73 mg, 93% yield; white solid, mp: 223-225 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 4.3 Hz, 4H), 7.29 (d, *J* = 5.3 Hz, 3H), 7.19 (d, *J* = 7.7 Hz, 5H), 2.87 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.9, 159.0, 153.8, 150.8, 142.5, 140.4, 136.5, 131.6, 130.4, 130.2, 129.7, 128.0, 127.9, 127.8, 127.4, 127.3, 127.2, 24.9, 21.7; IR (KBr) 3056, 2920, 1608, 1542, 1518, 1480, 1419, 1264, 1177, 1069, 961, 818, 767, 746, 702 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2S$ $[M+H]^+$ 393.1420, found 393.1422.

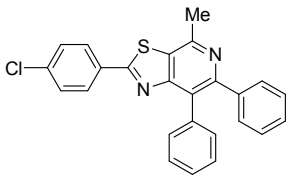
2-(4-(tert-butyl)phenyl)-4-methyl-6,7-diphenylthiazolo[5,4-c]pyridine (5c)



74 mg, 85% yield; white solid, mp: 144-146 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.42-7.34 (m, 4H), 7.34-7.25 (m, 3H), 7.21 (dd, *J* = 5.0, 1.7 Hz, 3H), 2.88 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.7, 159.0, 155.5, 153.9, 150.9, 140.6,

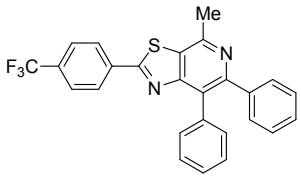
136.6, 131.7, 130.5, 130.4, 130.2, 128.0, 127.9, 127.7, 127.4, 127.3, 127.1, 126.0, 35.1, 31.2, 25.0; IR (KBr) 3038, 2955, 1631, 1619, 1540, 1479, 1416, 1263, 1065, 962, 838, 765, 751, 704 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{29}H_{27}N_2S$ $[M+H]^+$ 435.1889, found 435.1893.

2-(4-chlorophenyl)-4-methyl-6,7-diphenylthiazolo[5,4-c]pyridine (5d)



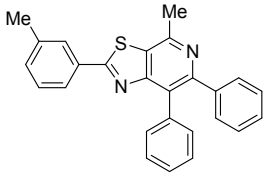
77mg, 94% yield; white solid, mp: 176-178 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.6 Hz, 2H), 7.43 (s, 1H), 7.42-7.29 (m, 8H), 7.24 (dd, *J* = 6.1, 1.8 Hz, 3H), 2.91 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.1, 158.8, 154.1, 151.0, 140.4, 137.9, 136.4, 131.6, 130.4, 130.2, 129.3, 129.2, 127.9, 127.8, 127.6, 127.5, 127.4, 127.3, 25.0; IR (KBr) 3061, 2896, 1590, 1538, 1474, 1419, 1399, 1350, 1089, 1068, 1013, 960, 831, 761, 704, 693 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{25}H_{18}ClN_2S$ $[M+H]^+$ 413.0874, found 413.0873.

4-methyl-6,7-diphenyl-2-(4-(trifluoromethyl)phenyl)thiazolo[5,4-c]pyridine (5e)



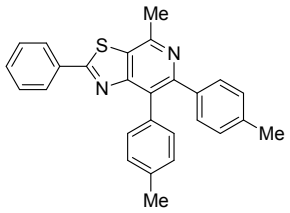
79 mg, 88% yield; white solid, mp: 171-173 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 8.2 Hz, 2H), 7.48-7.35 (m, 4H), 7.31 (dd, *J* = 4.9, 1.7 Hz, 3H), 7.26-7.16 (m, 3H), 2.89 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.6, 158.7, 154.2, 151.2, 140.2, 136.3, 136.2, 133.2 (q, $J_{C\text{-}F}$ = 32.6 Hz), 131.5, 130.4, 130.3, 128.3, 127.9, 127.8, 127.6, 127.5, 127.3, 126.0 (d, $J_{C\text{-}F}$ = 3.7 Hz), 123.7 (q, $J_{C\text{-}F}$ = 270.8 Hz), 24.9; IR (KBr) 3061, 3032, 1611, 1534, 1520, 1482, 1419, 1319, 1190, 1175, 1128, 1064, 1017, 965, 846, 761, 746, 706, 698 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{18}F_3N_2S$ $[M+H]^+$ 447.1137, found 447.1134.

4-methyl-6,7-diphenyl-2-(m-tolyl)thiazolo[5,4-c]pyridine (5f)



73 mg, 93% yield; white solid, mp: 180-182 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 3.4, 2.7 Hz, 2H), 7.46-7.35 (m, 4H), 7.35-7.26 (m, 5H), 7.25-7.19 (m, 3H), 2.89 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.9, 158.9, 153.9, 150.9, 140.5, 138.9, 136.5, 133.1, 132.6, 131.6, 130.4, 130.2, 128.9, 128.6, 127.9, 127.8, 127.4, 127.3, 127.2, 125.4, 25.0, 21.4; IR (KBr) 3050, 2914, 1731, 1541, 1492, 1461, 1420, 1267, 1166, 1071, 906, 776, 765, 749, 698 cm^{-1}; HRMS (ESI) *m/z* calcd for $C_{26}H_{21}N_2S$ $[M+H]^+$ 393.1420, found 393.1423.

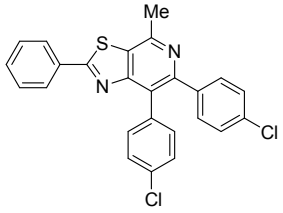
4-methyl-2-phenyl-6,7-di-p-tolylthiazolo[5,4-c]pyridine (5g)



67 mg, 82% yield; white solid, mp: 175-177 °C; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 7.6, 1.4 Hz, 2H), 7.41 (q, *J* = 6.2 Hz, 3H), 7.37-7.23 (m, 4H), 7.12 (d, *J* = 7.9 Hz, 2H), 7.04 (d, *J* = 7.9 Hz, 2H), 2.86 (s, 3H), 2.36 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3, 159.0, 153.9, 150.6, 137.8, 137.0, 136.7, 133.6, 133.2, 131.7, 131.4, 130.3, 129.9,

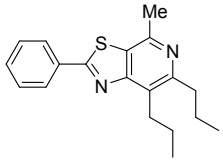
129.0, 128.6, 128.6, 128.1, 127.2, 25.0, 21.5, 21.3; IR (KBr) 3032, 2920, 1652, 1550, 1507, 1476, 1430, 1310, 1260, 1107, 1071, 961, 832, 786, 686 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{27}H_{23}N_2S$ $[M+H]^+$ 407.1576, found 407.1575.

6,7-bis(4-chlorophenyl)-4-methyl-2-phenylthiazolo[5,4-c]pyridine (5h)



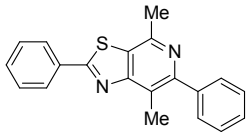
76 mg, 85% yield; white solid, mp: 185-187 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.04 (d, *J* = 6.5 Hz, 2H), 7.54-7.39 (m, 3H), 7.32 (d, *J* = 7.6 Hz, 6H), 7.23 (d, *J* = 8.4 Hz, 2H), 2.88 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.2, 158.7, 152.4, 151.5, 138.6, 134.7, 133.7, 133.4, 132.9, 132.8, 132.0, 131.7, 130.5, 129.1, 128.3, 128.2, 128.0, 126.1, 24.9; IR (KBr) 3061, 2908, 1740, 1549, 1491, 1476, 1432, 1237, 1091, 1014, 964, 831, 795, 767, 687 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{25}H_{17}Cl_2N_2S$ $[M+H]^+$ 447.0484, found 447.0483.

4-methyl-2-phenyl-6,7-dipropylthiazolo[5,4-c]pyridine (5i)



48 mg, 77% yield; white solid, mp: 50-52 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.20-8.05 (m, 2H), 7.58-7.38 (m, 3H), 3.13 (dd, *J* = 8.7, 6.9 Hz, 2H), 2.98-2.82 (m, 2H), 2.73 (s, 3H), 1.77 (dp, *J* = 15.1, 7.5 Hz, 4H), 1.06 (td, *J* = 7.3, 3.0 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.5, 159.3, 156.1, 148.8, 133.5, 131.4, 129.0, 128.5, 127.8, 126.9, 36.8, 30.3, 24.6, 24.2, 24.0, 14.5, 14.4; IR (KBr) 2959, 2928, 2868, 1559, 1508, 1477, 1439, 1261, 1123, 1065, 1033, 980, 801, 764, 685 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{19}H_{23}N_2S$ $[M+H]^+$ 311.1576, found 311.1577.

4,7-dimethyl-2,6-diphenylthiazolo[5,4-c]pyridine (5j)



51 mg, 81% yield; white solid, mp: 155-157 °C; ^1H NMR (300 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 7.3, 2.1 Hz, 2H), 7.58 (d, *J* = 7.0 Hz, 2H), 7.45 (ddd, *J* = 23.7, 10.1, 4.3 Hz, 6H), 2.81 (s, 3H), 2.73 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 171.3, 159.8, 154.8, 149.1, 140.6, 133.3, 131.7, 129.5, 129.1, 128.5, 128.2, 127.9, 127.7, 122.6, 24.7, 15.5; IR (KBr) 3044, 2914, 1554, 1475, 1450, 1422, 1321, 1252, 1177, 1067, 988, 909, 803, 760, 706, 686 cm^{-1}; HRMS (ESI) *m*/*z* calcd for $C_{20}H_{17}N_2S$ $[M+H]^+$ 317.1107, found 317.1108.

References

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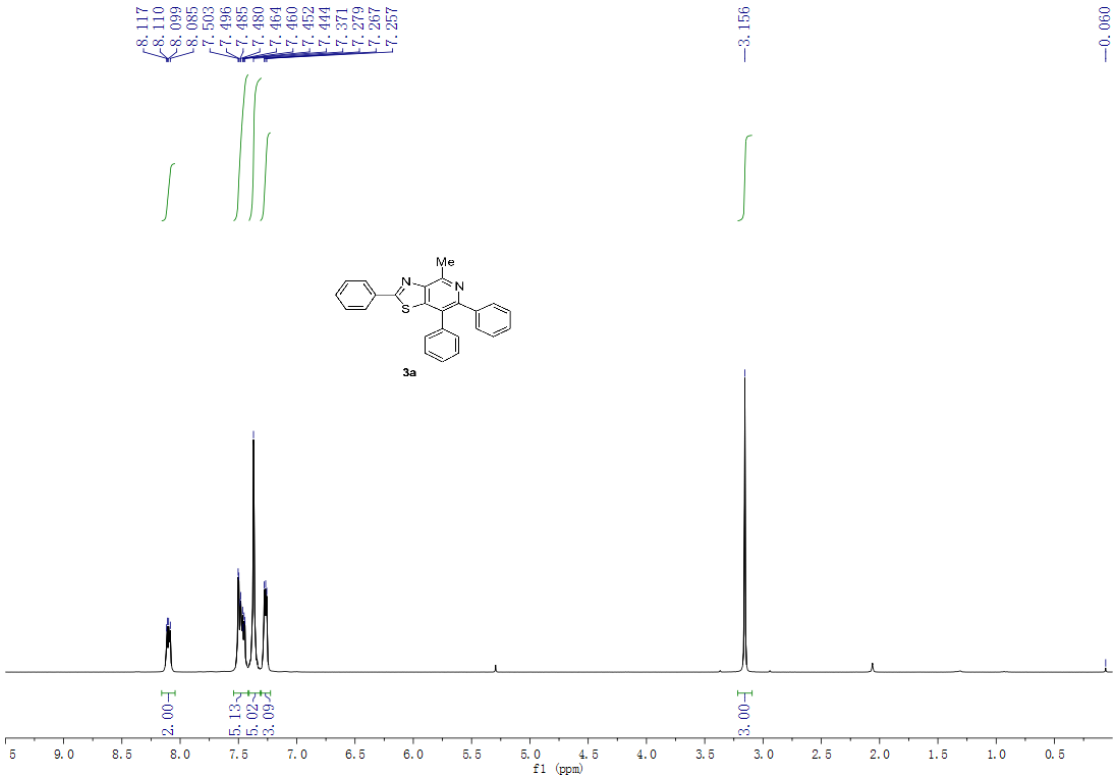
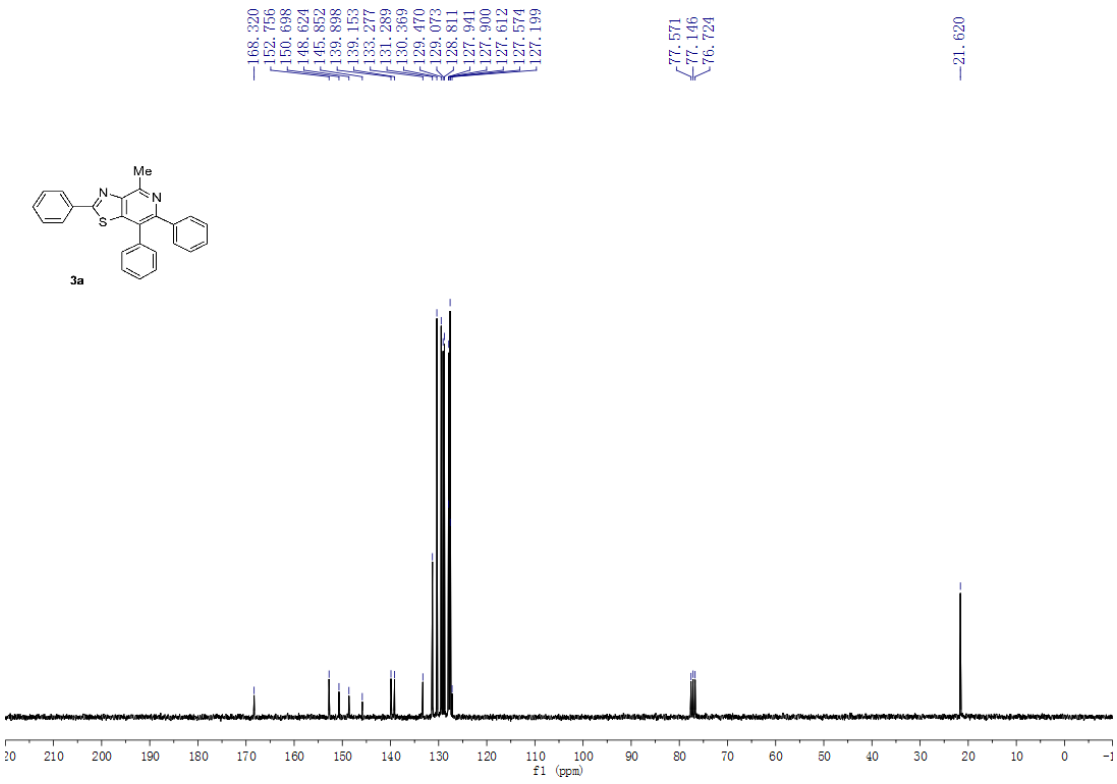
2. Labeeuw, O.; Phansavath, P.; Genêt, J.-P. *Tetrahedron Lett.* **2004**, *45*, 7107. Žinić, J. Kuftinec, H. Hofman, F. Kajfež, Z. Meić, *J. Org. Chem.* **1985**, *50*, 697-700.

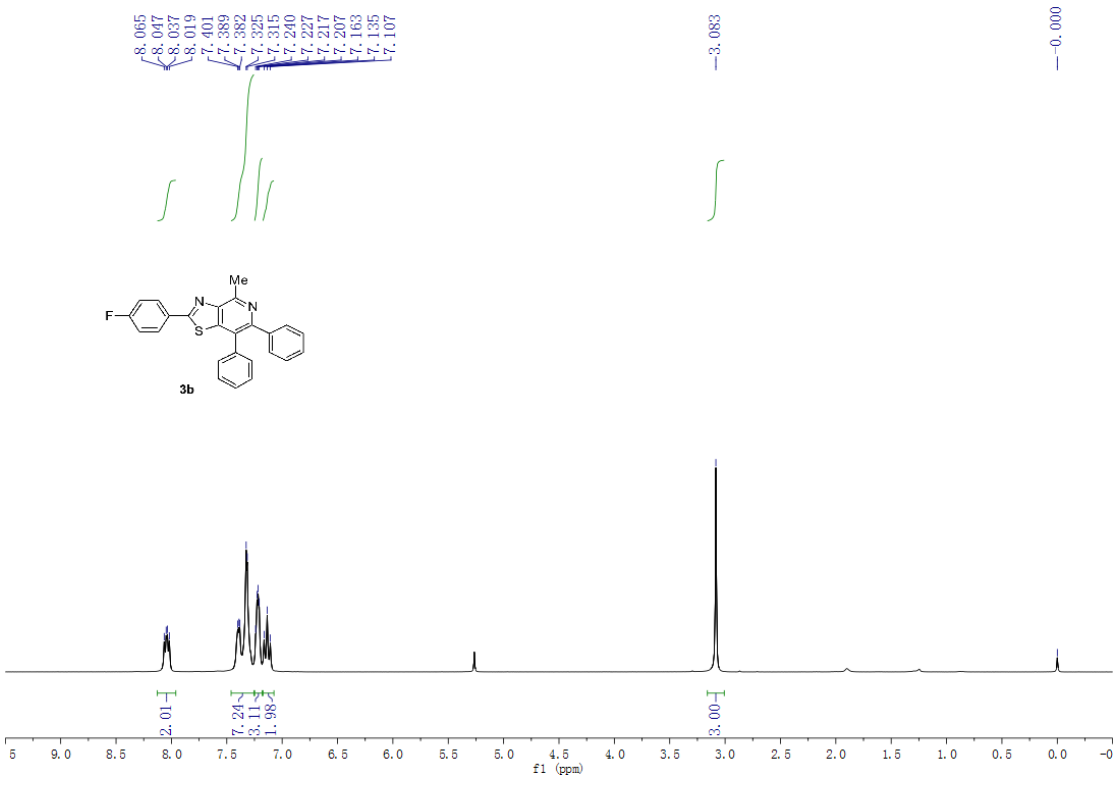
3. Parthasarathy, K.; Cheng, C. H. *J. Org. Chem.* **2009**, *74*, 9359.

4. (a) Mio, M. J.; Kopel, L. C.; Braun, J. B.; Gadzikwa, T. L.; Hull, K. L.; Brisbois, R. G.; Markworth, C. J.; Grieco, P. A. *Org. Lett.* **2002**, *4*, 3199. (b) Xu, Y. P.; Hu, R. H.; Cai, M. Z. *Chin. Chem. Lett.* **2008**, *19*, 783.

^{13}C and ^{1}H-NMR Spectra of Title Compounds



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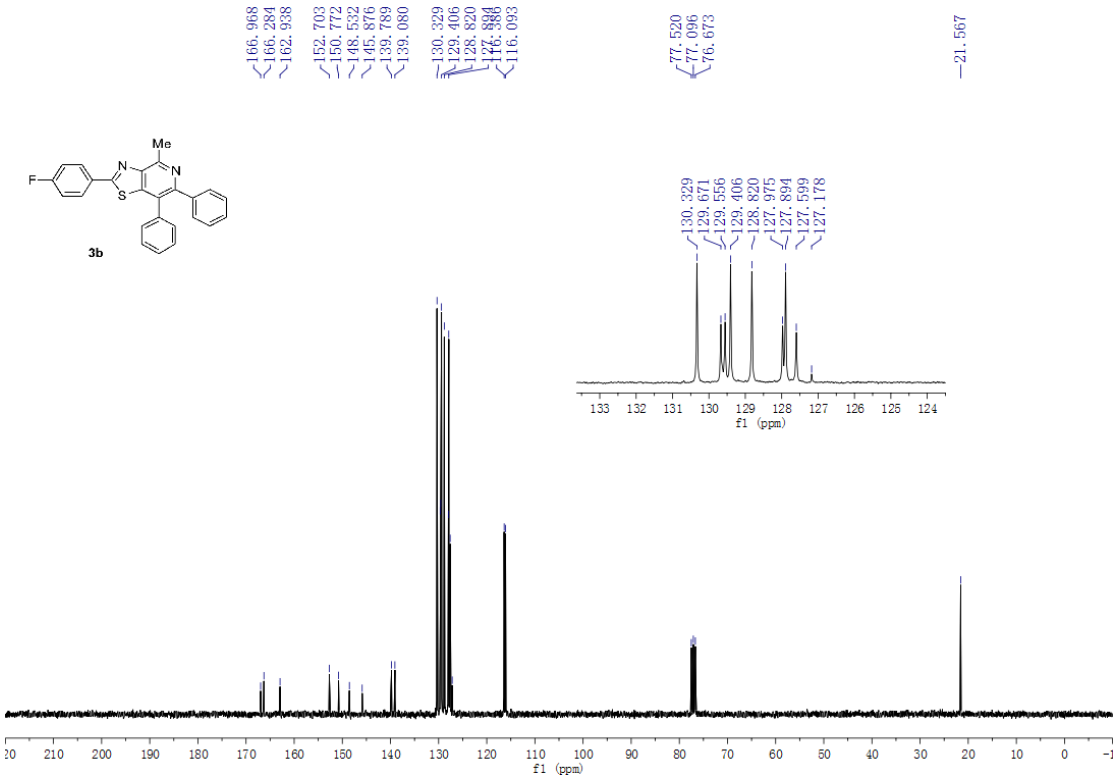
7.163
7.135
7.107
3.083
0.000
Me
F
N
S
N
3b
2.01
7.24
3.11
1.98
3.00
f1 (ppm)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139.789
139.080
130.329
129.406
128.820
127.894
116.093
77.520
77.096
76.673
21.567
Me
F
N
S
N
3b
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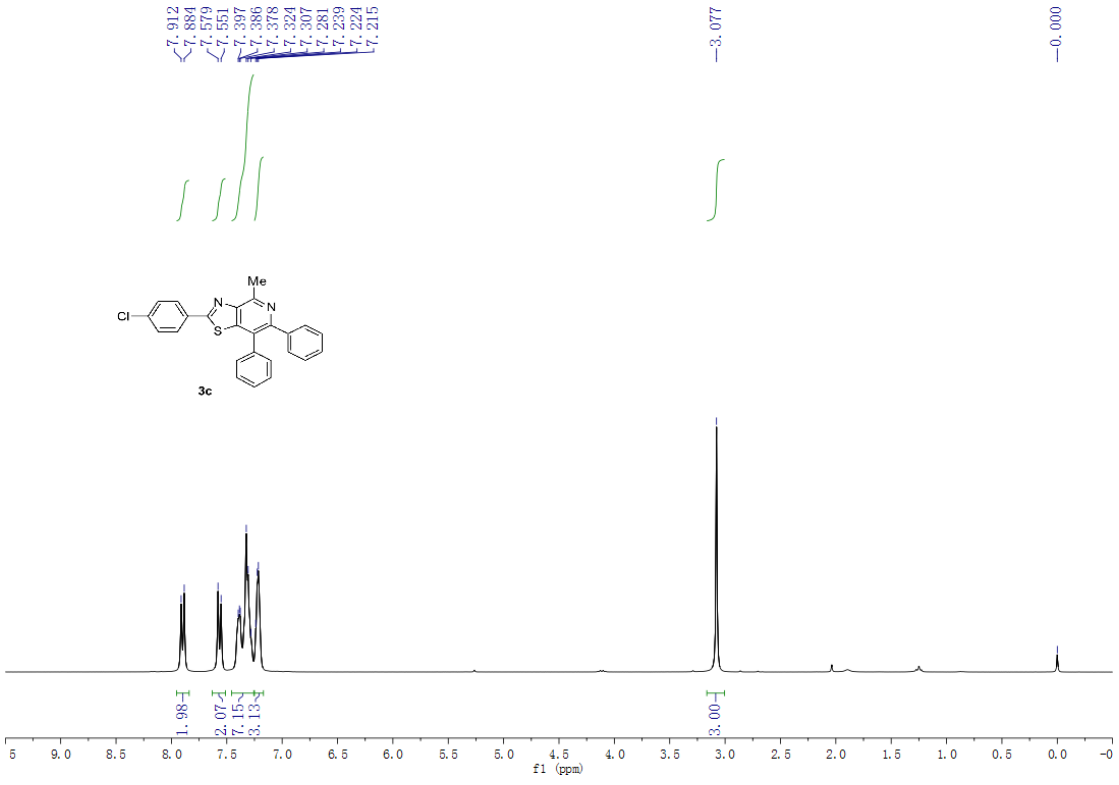
f1 (ppm)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S
Cl
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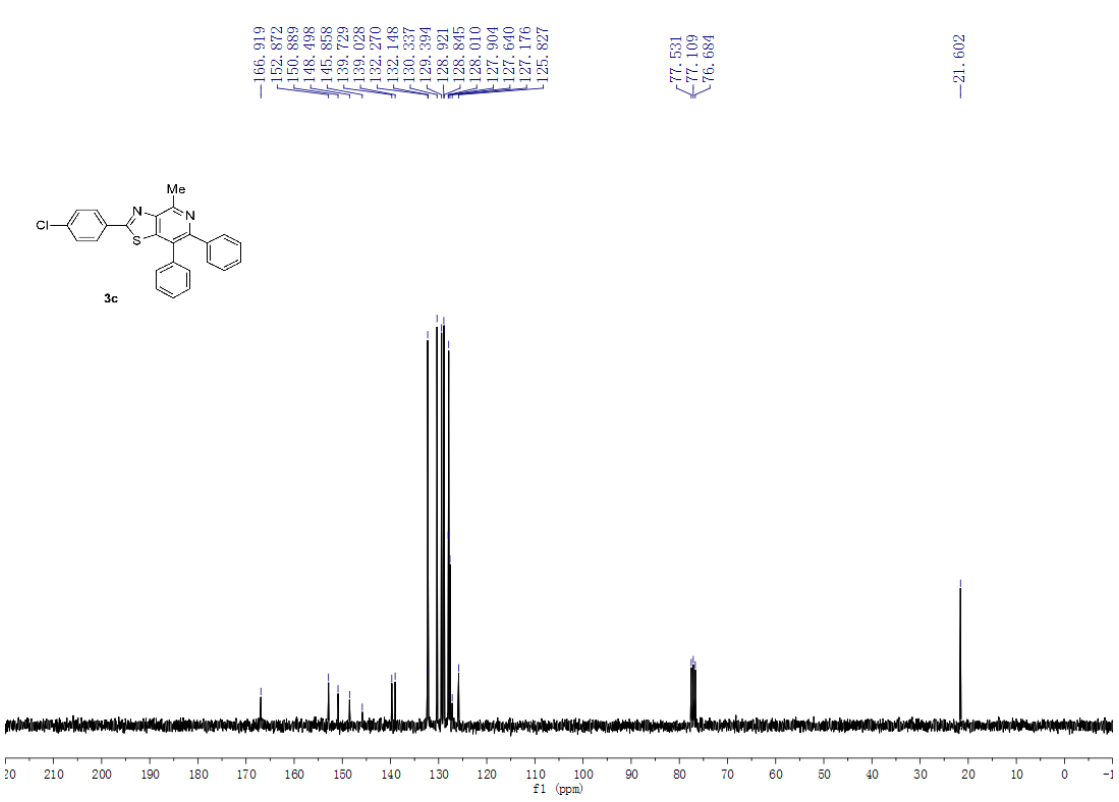
3.13
3.00
f1 (ppm)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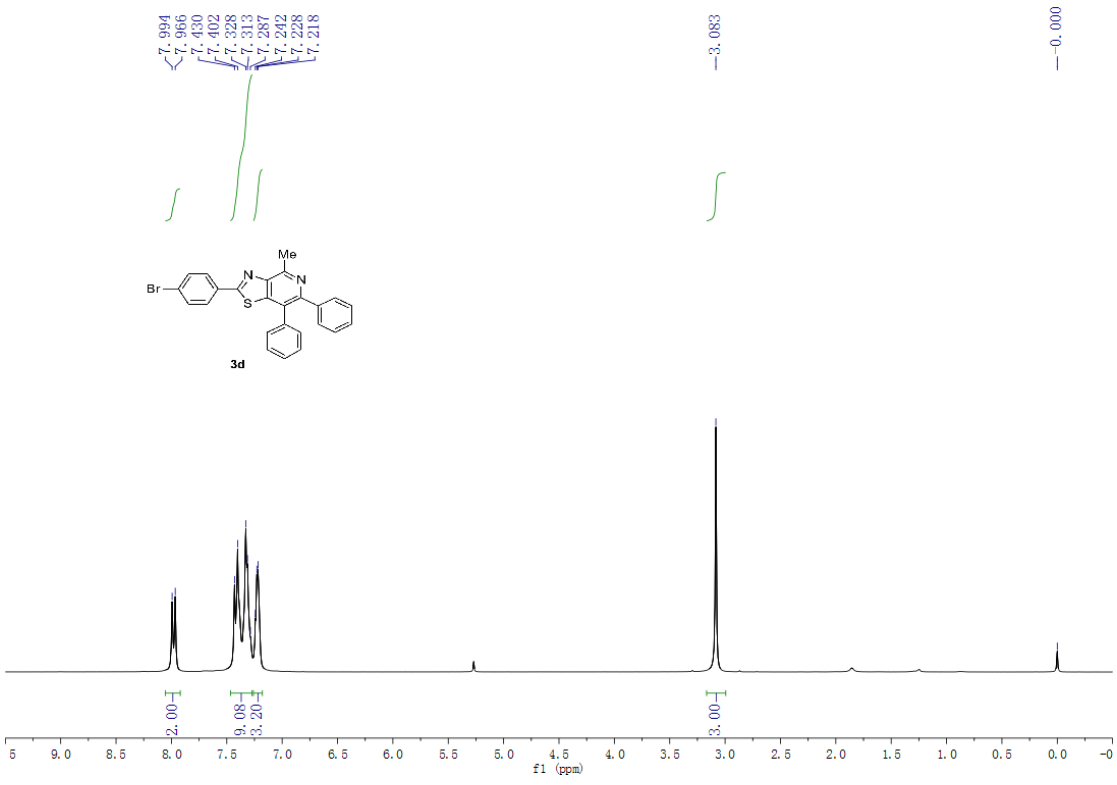
Cl
3c
f1 (ppm)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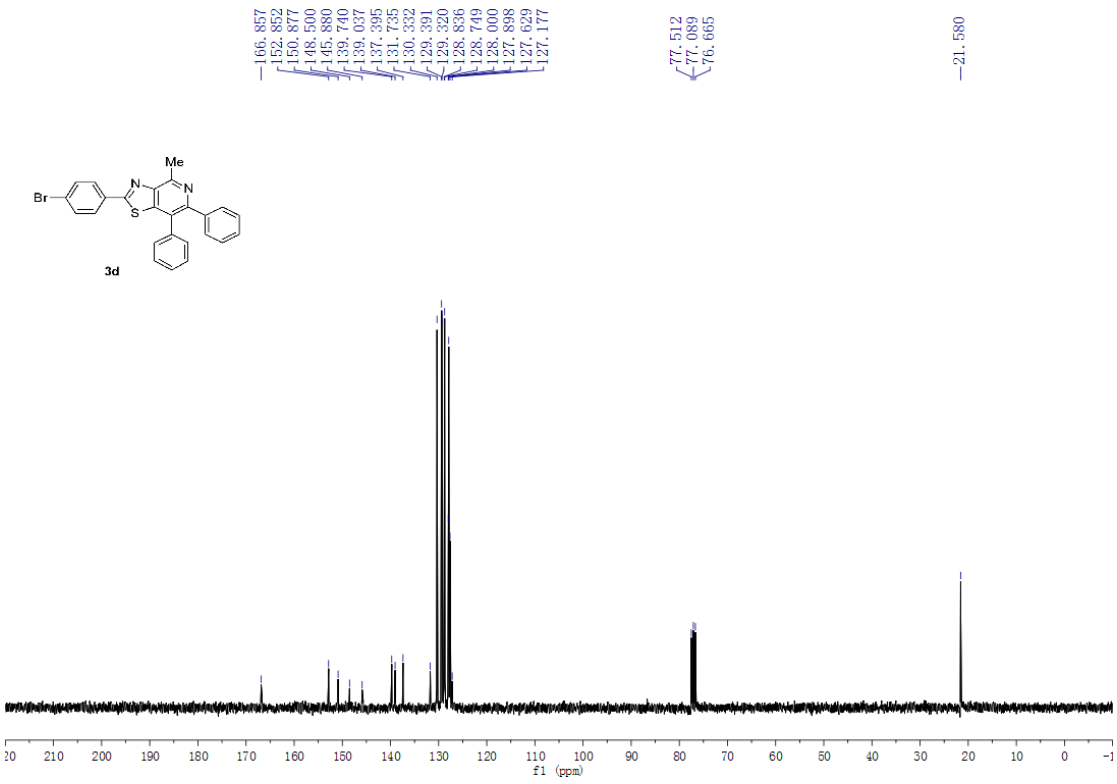
3.00
f1 (ppm)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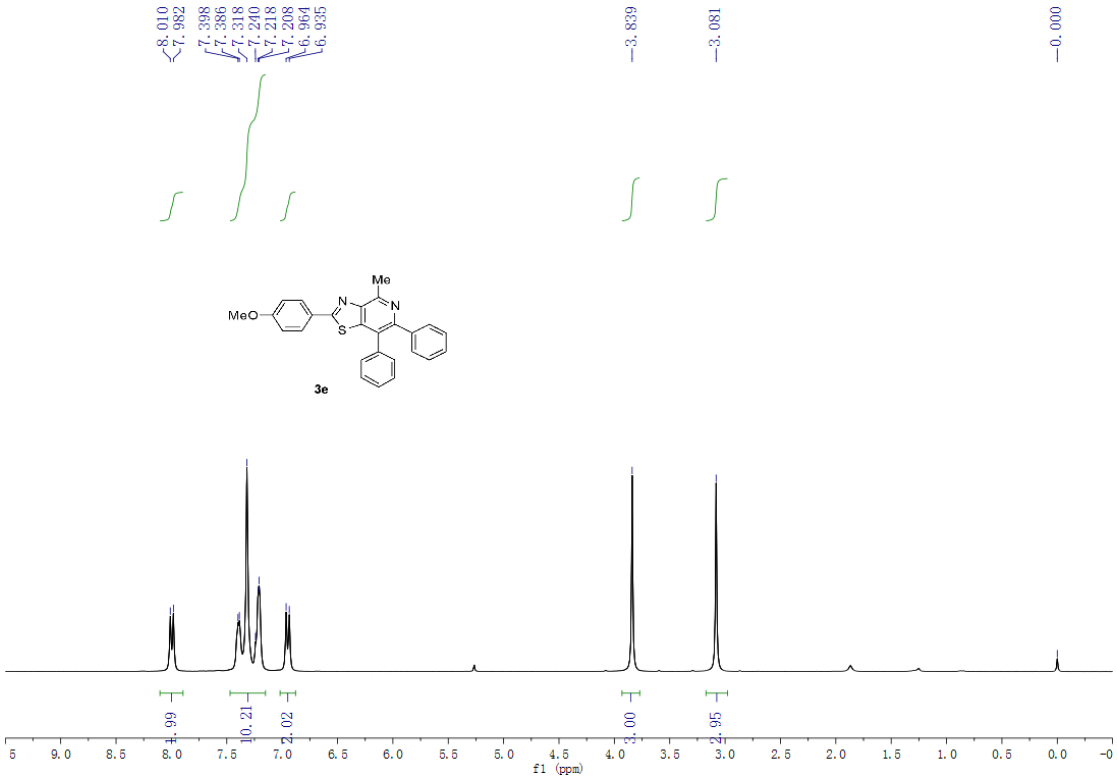
f1 (ppm)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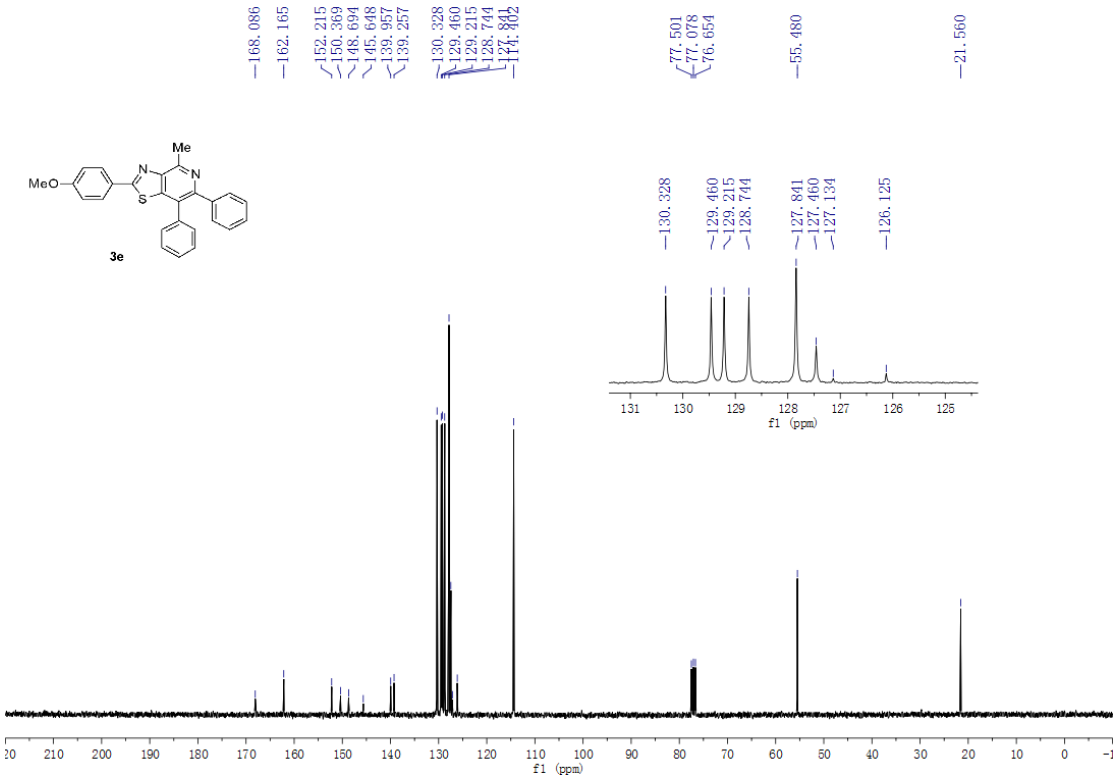
f1 (ppm)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126.125
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55.480
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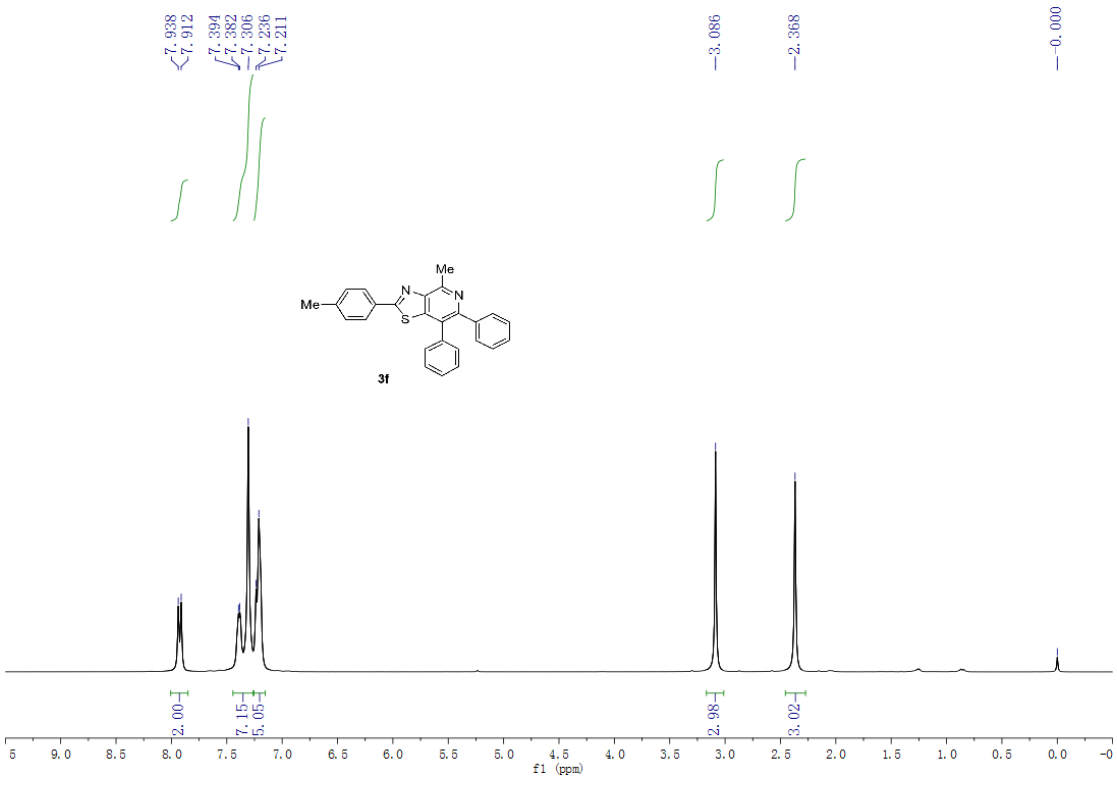
MeO
N
S
N
3e
f1 (ppm)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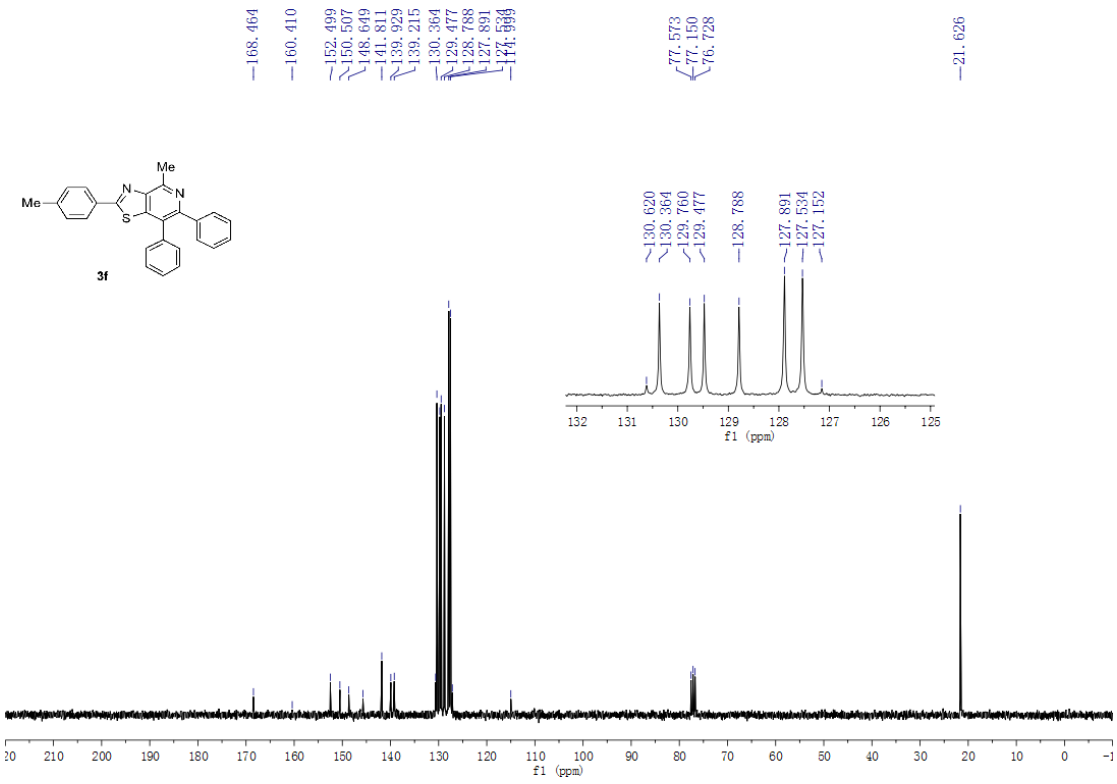
f1 (ppm)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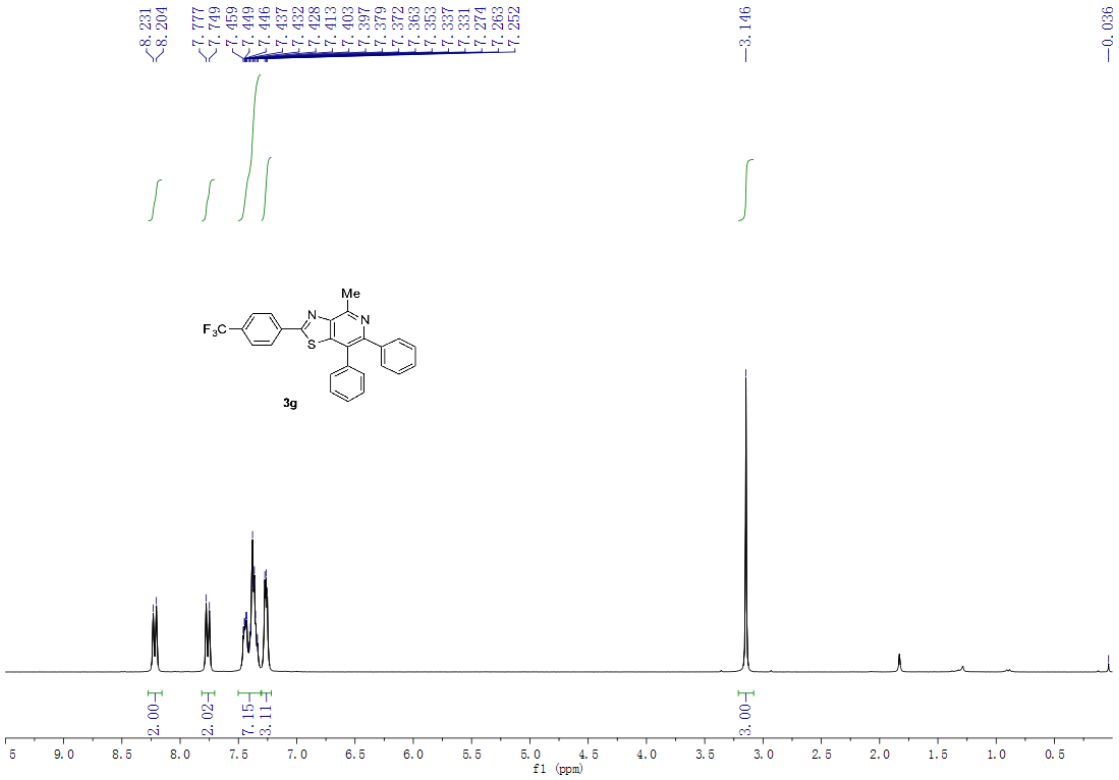
f1 (ppm)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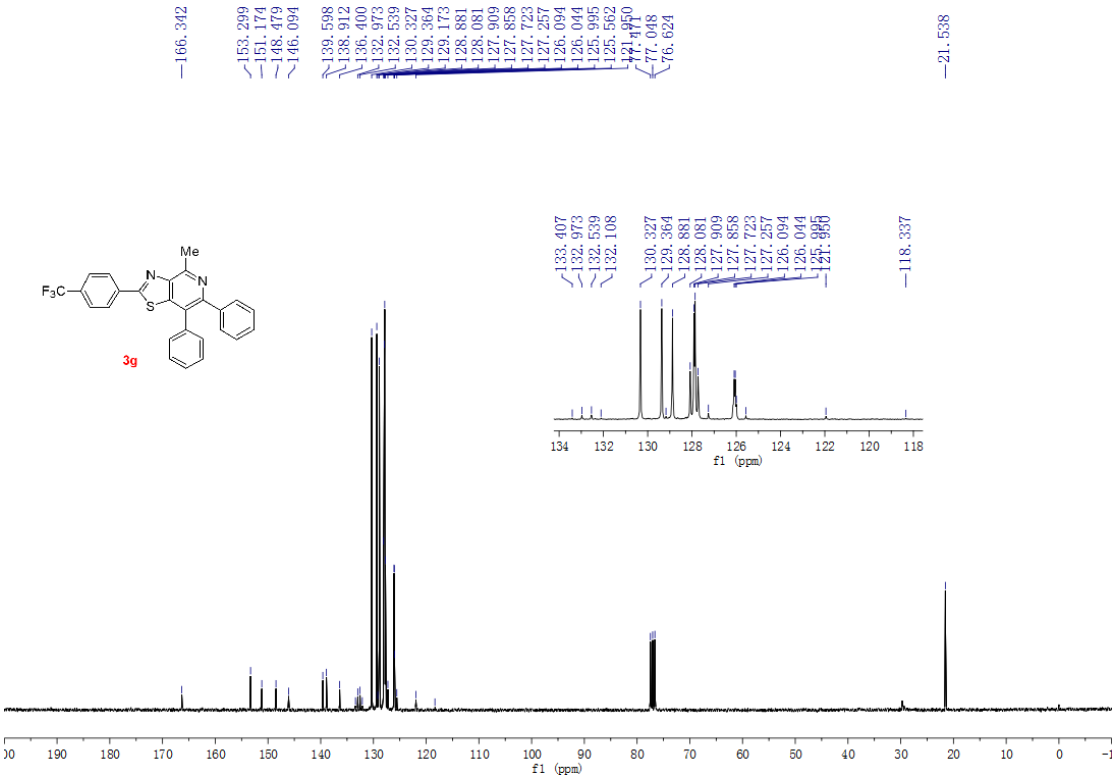
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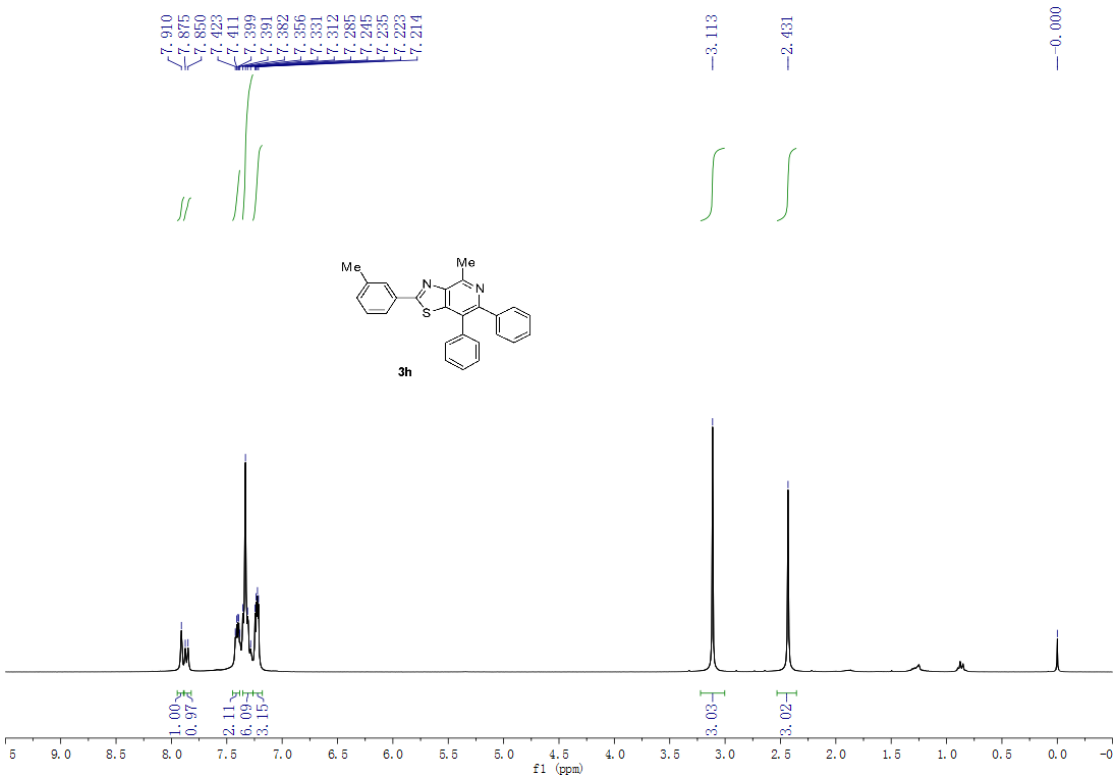
f1 (ppm)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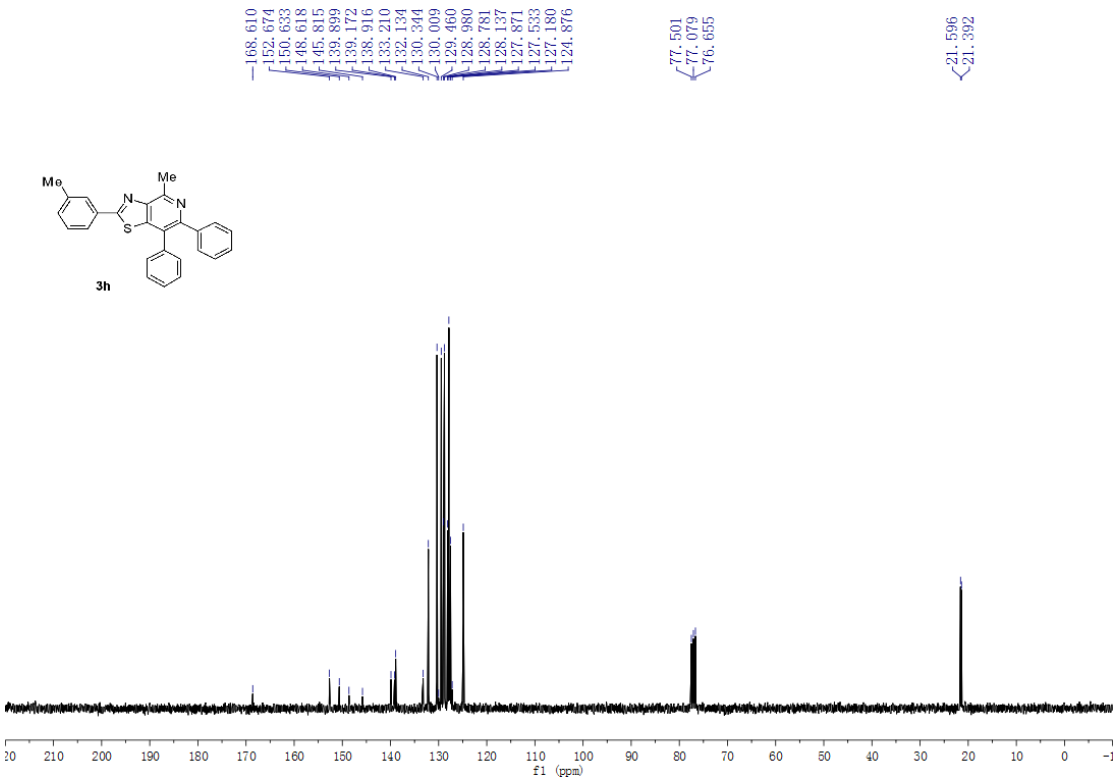
f1 (ppm)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3h
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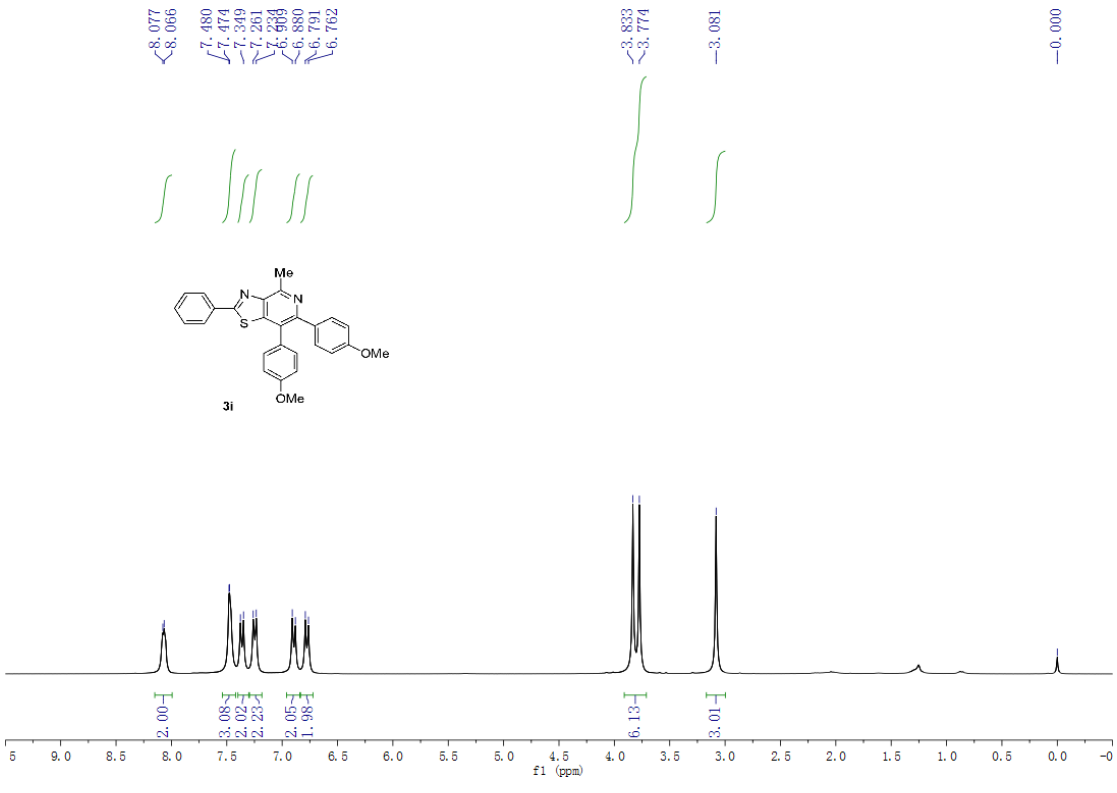
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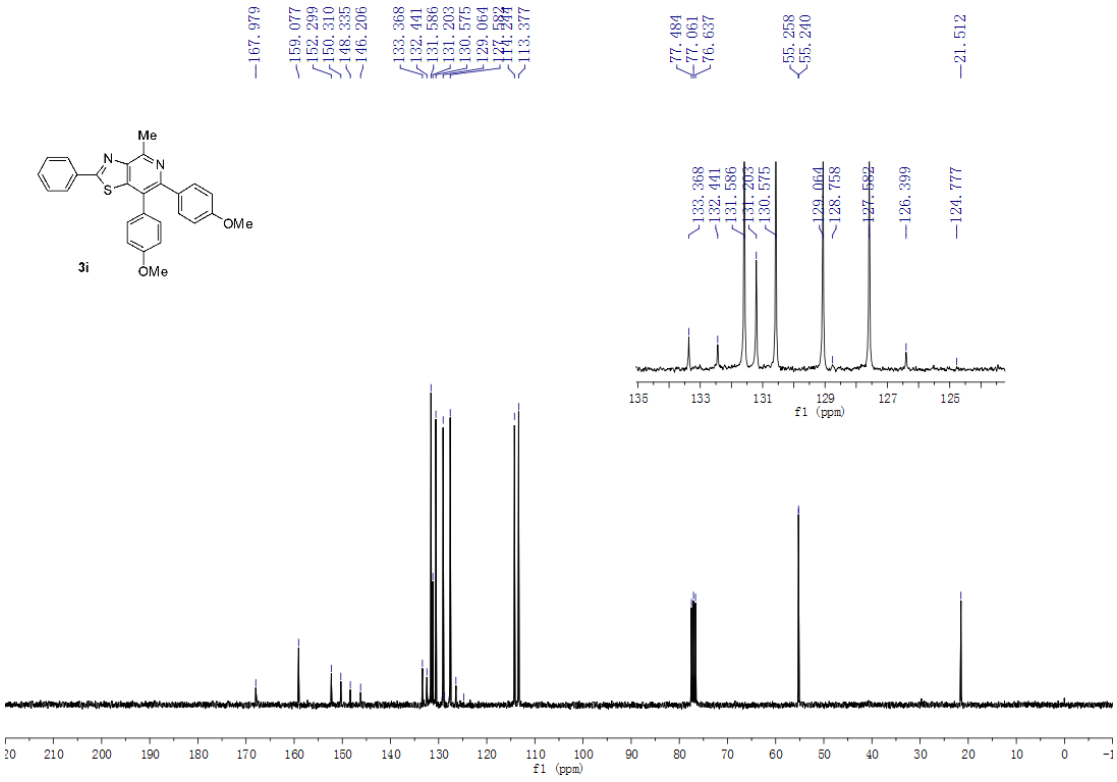
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OMe
3i
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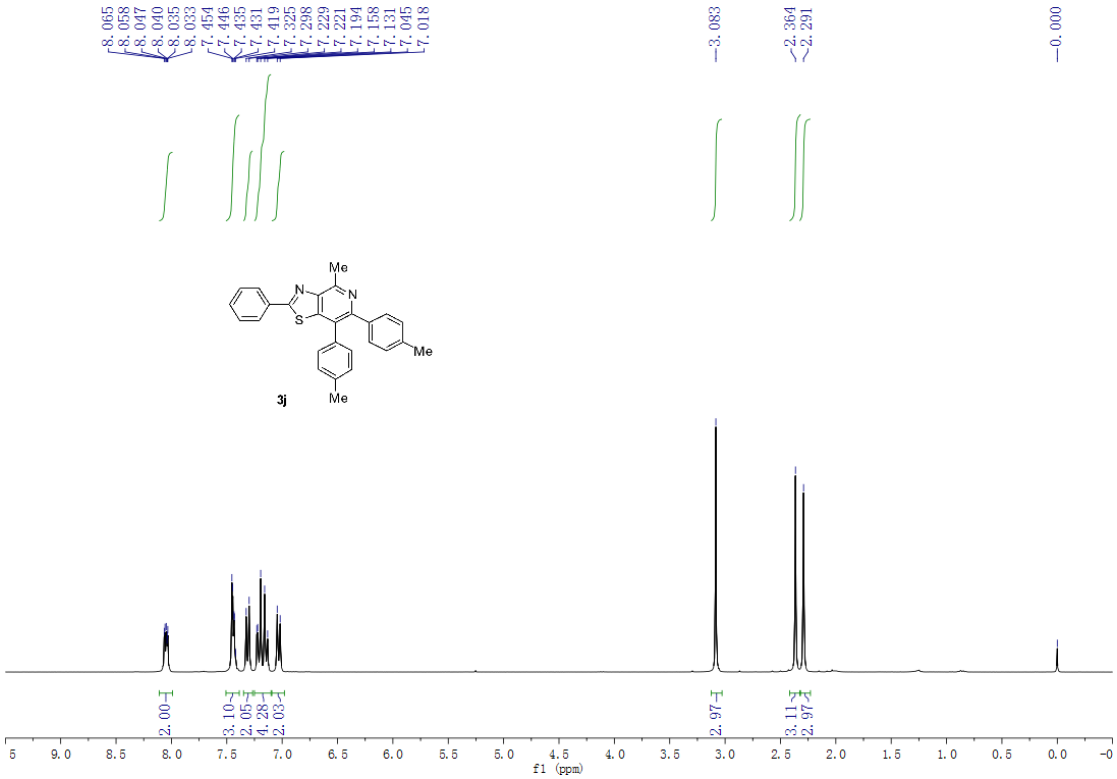
f1 (ppm)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7.131
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7.018
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2.364
2.291
0.000
Me
N
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Me
Me
3j
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2.05
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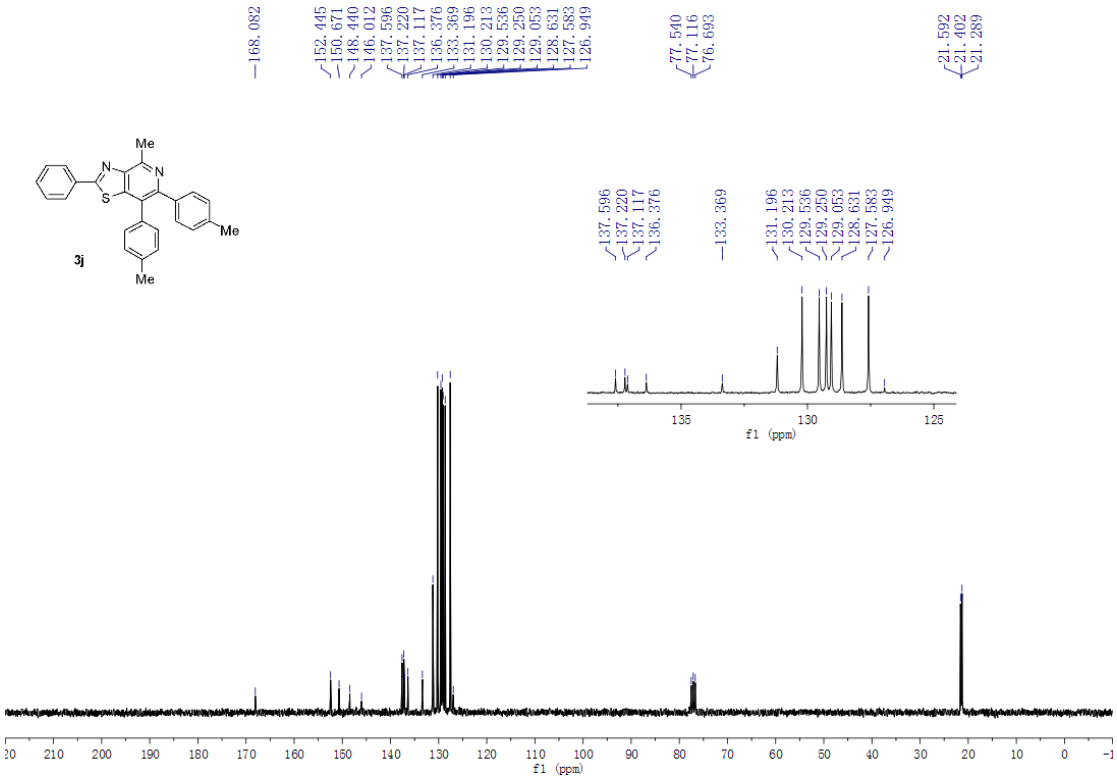
2.03
2.97
3.11
2.97
f1 (ppm)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21.592
21.402
21.289
Me
N
S
N
Me
Me
3j
137.596
137.220
137.117
136.376
133.369
131.196
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129.053
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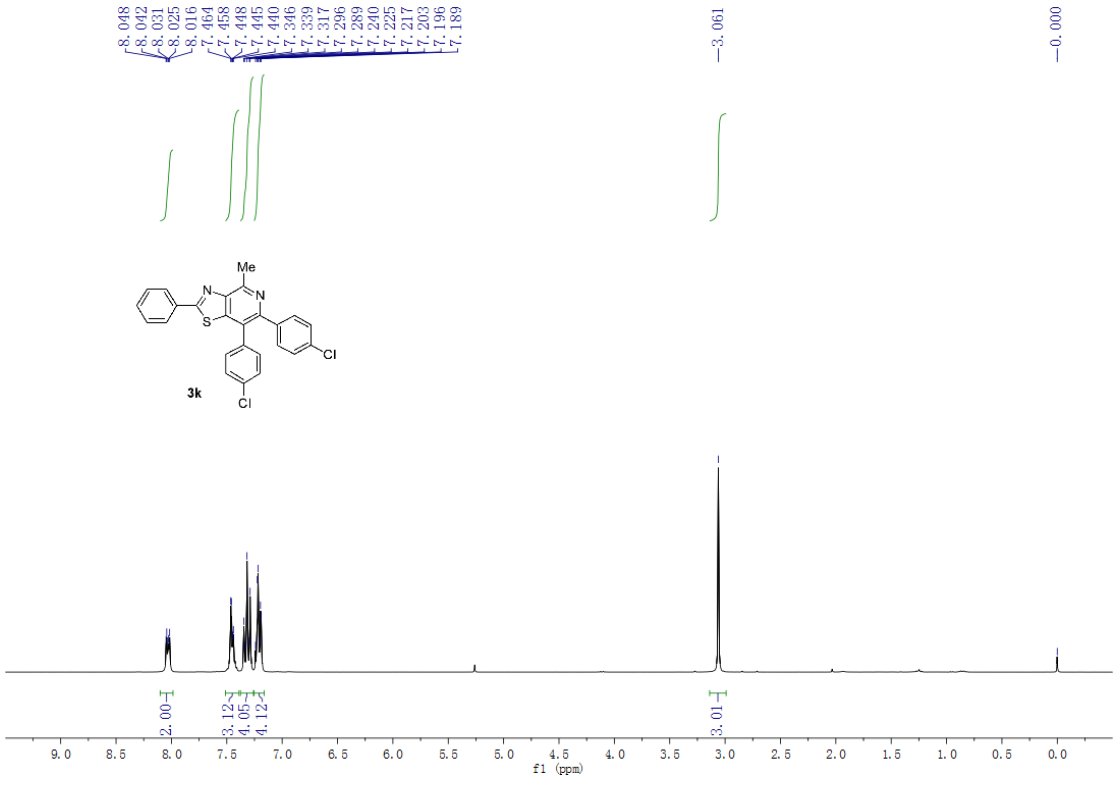
135
130
125
f1 (ppm)
f1 (ppm)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7.440
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7.217
7.203
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S
Cl
Cl
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3.12
4.05
4.12
3.01
9.0
8.5
8.0
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6.5
6.0
5.5
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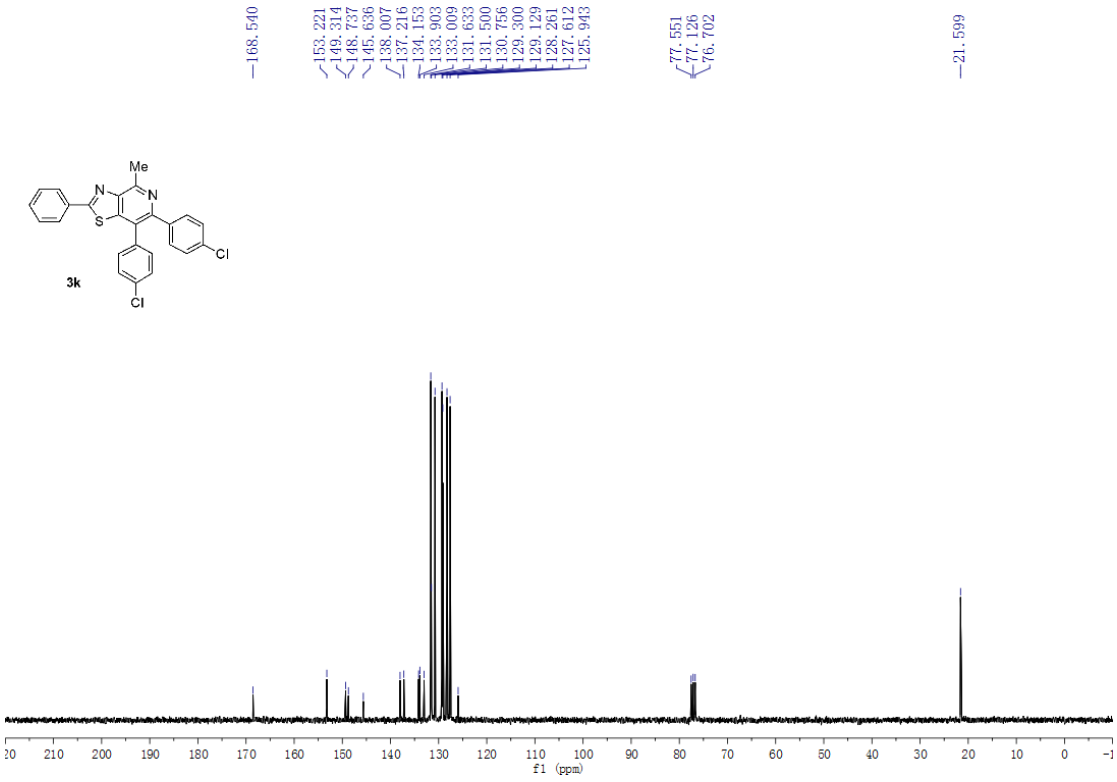
f1 (ppm)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Cl
Cl
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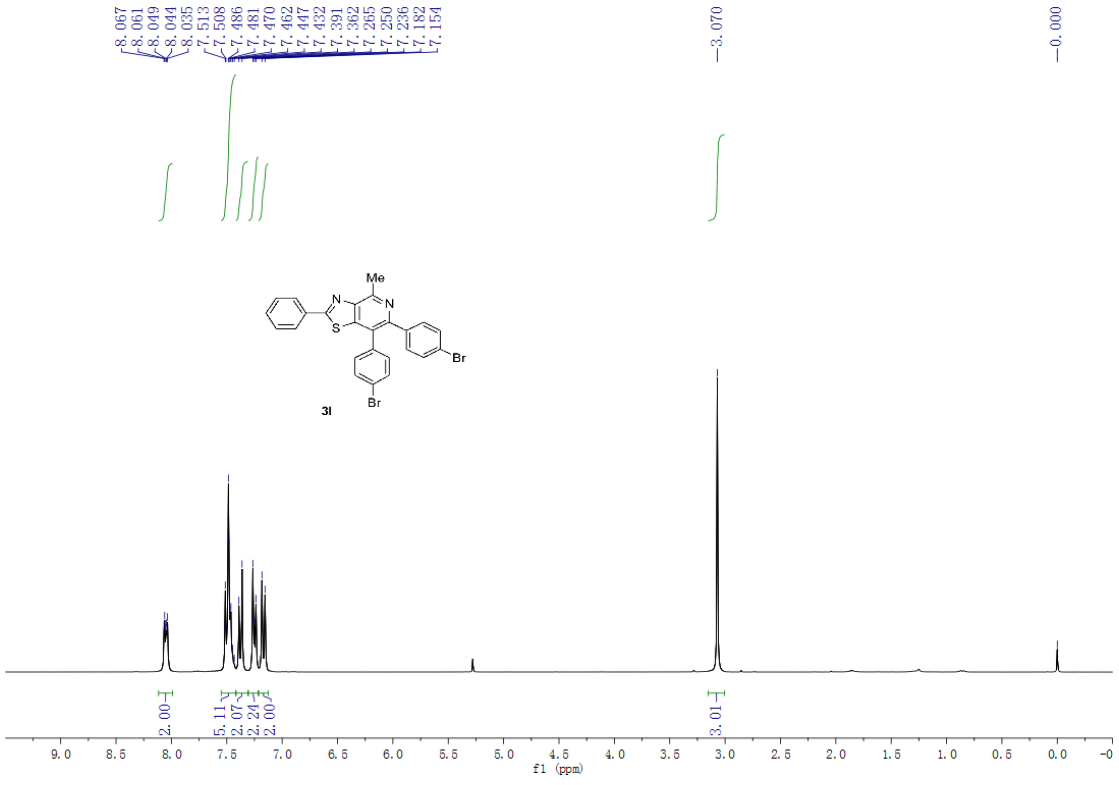
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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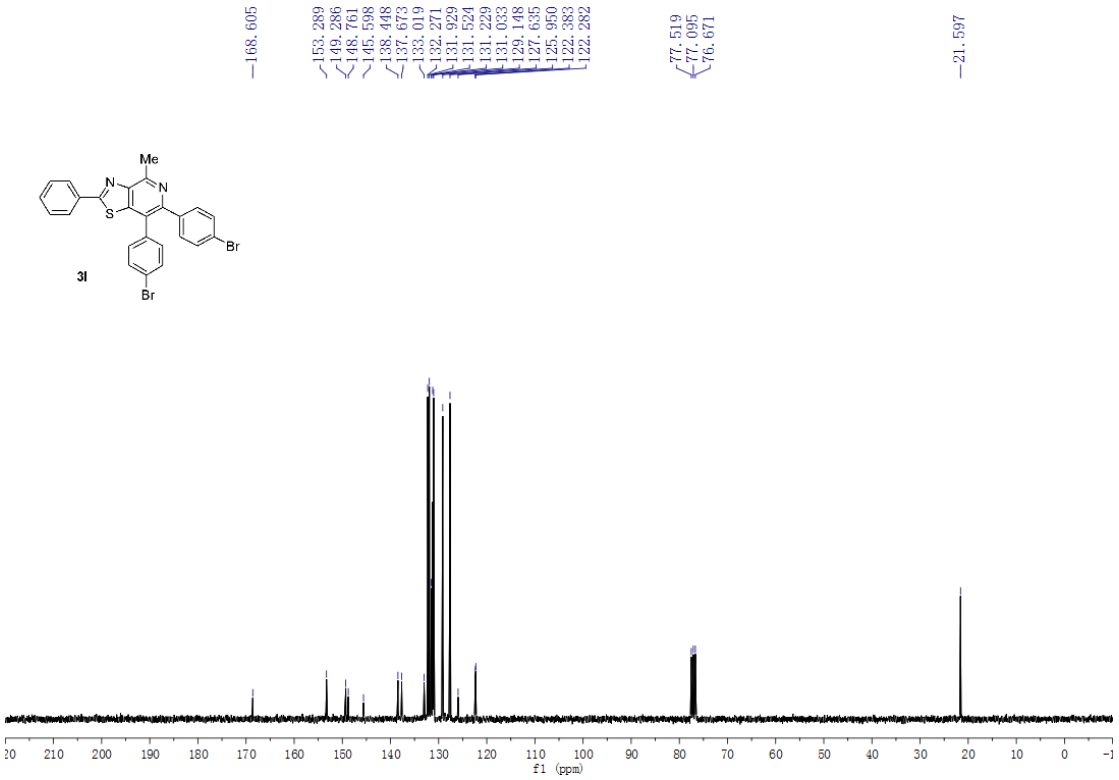
7.486
7.481
7.470
7.462
7.447
7.432
7.391
7.362
7.265
7.250
7.236
7.182
7.154
3.070
0.000
Me
N
S
N
Br
Br
3l
2.00
5.11
2.07
2.24
2.00
3.01
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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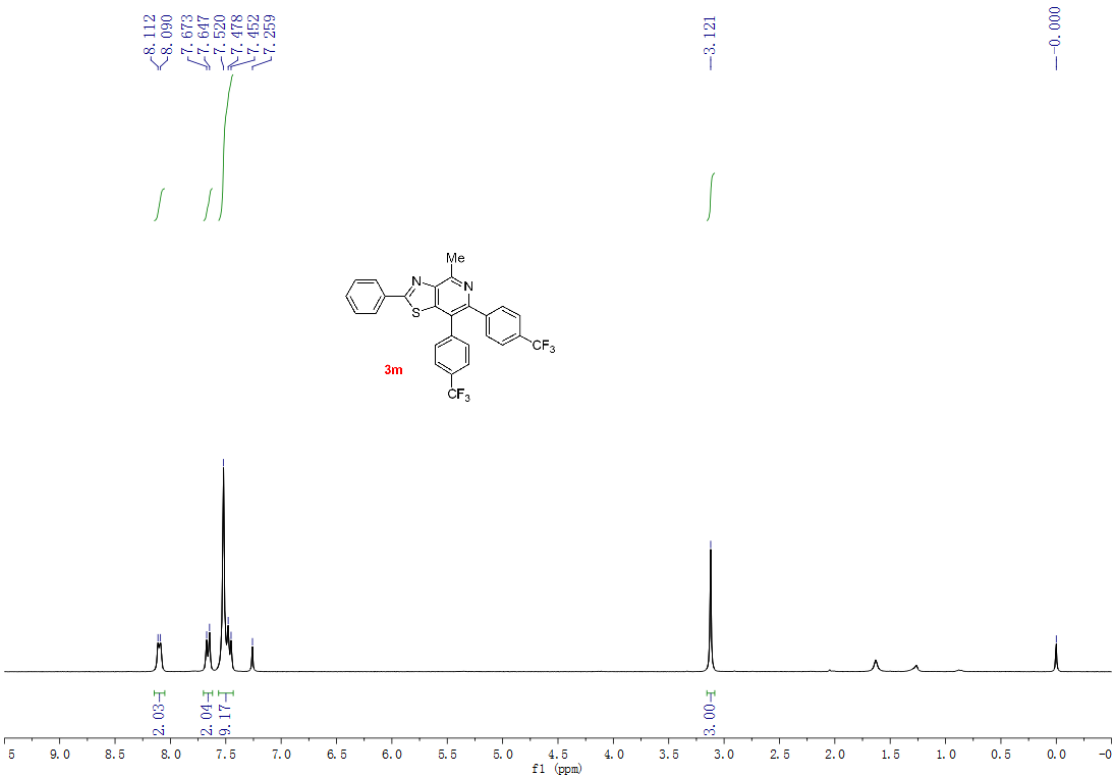
149.286
148.761
145.598
138.448
137.673
133.019
132.271
131.929
131.524
131.229
131.033
129.148
127.635
125.950
122.383
122.282
77.519
77.095
76.671
21.597
Me
N
S
N
Br
Br
3l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.520
7.478
7.452
7.259
3.121
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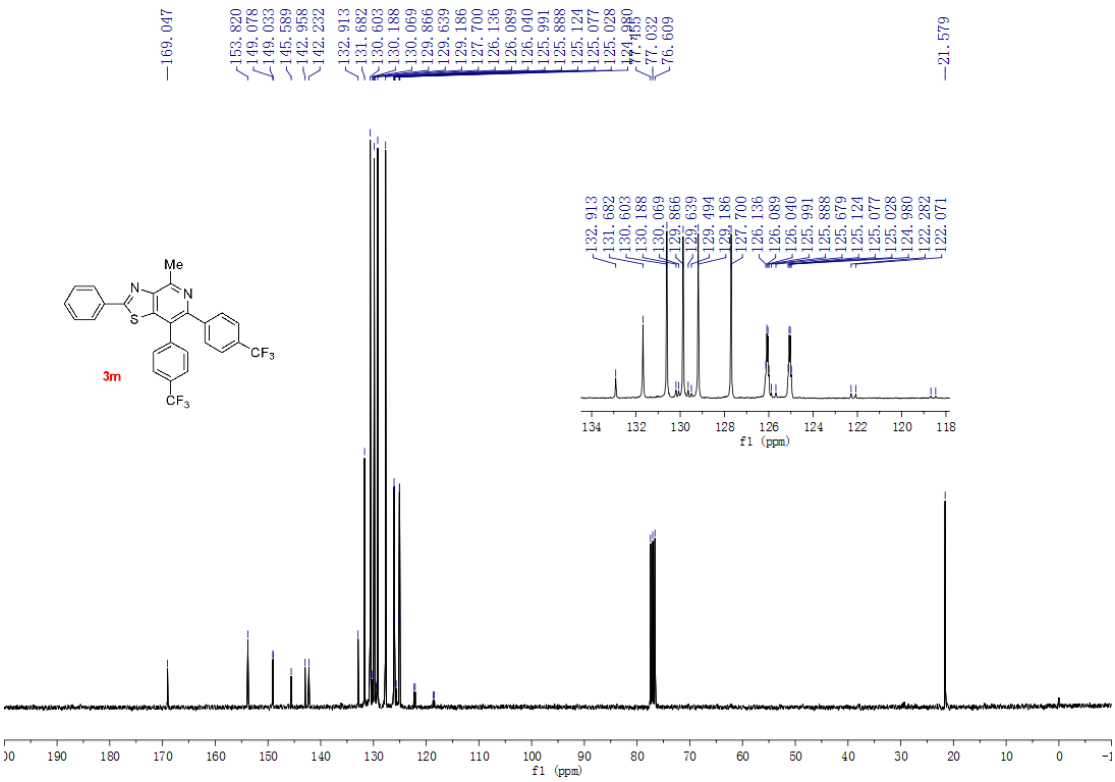
S
N
CF3
CF3
3m
2.03
2.04
9.17
3.00
f1 (ppm)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142.232
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130.069
129.866
129.639
129.186
127.700
126.136
126.089
126.040
125.991
125.888
125.124
125.077
125.028
124.980
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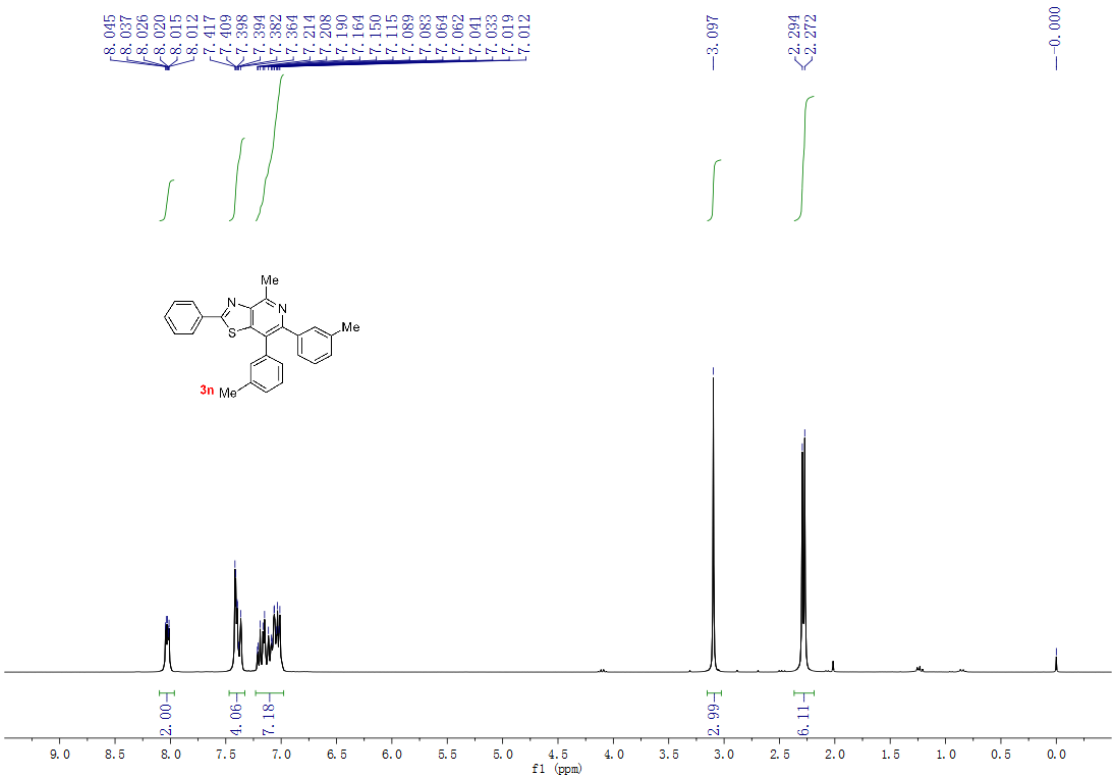
76.609
21.579
Me
N
S
N
CF3
CF3
3m
f1 (ppm)
f1 (ppm)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8.026
8.020
8.015
8.012
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7.409
7.398
7.394
7.382
7.364
7.214
7.208
7.190
7.164
7.150
7.115
7.089
7.083
7.064
7.062
7.041
7.033
7.019
7.012
3.097
2.294
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N
S
Me
3n Me
2.00
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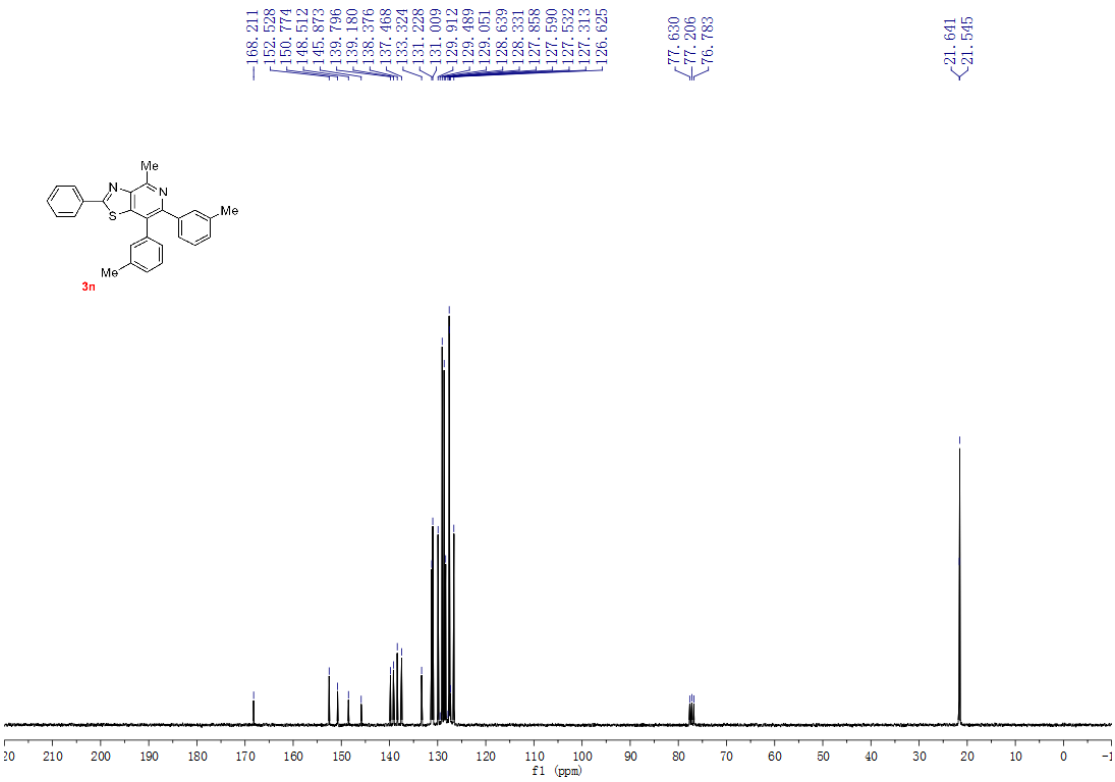
7.18
2.99
6.11
f1 (ppm)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139.180
138.376
137.468
133.324
131.228
131.009
129.912
129.489
129.051
128.639
128.331
127.858
127.590
127.532
127.313
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77.206
76.783
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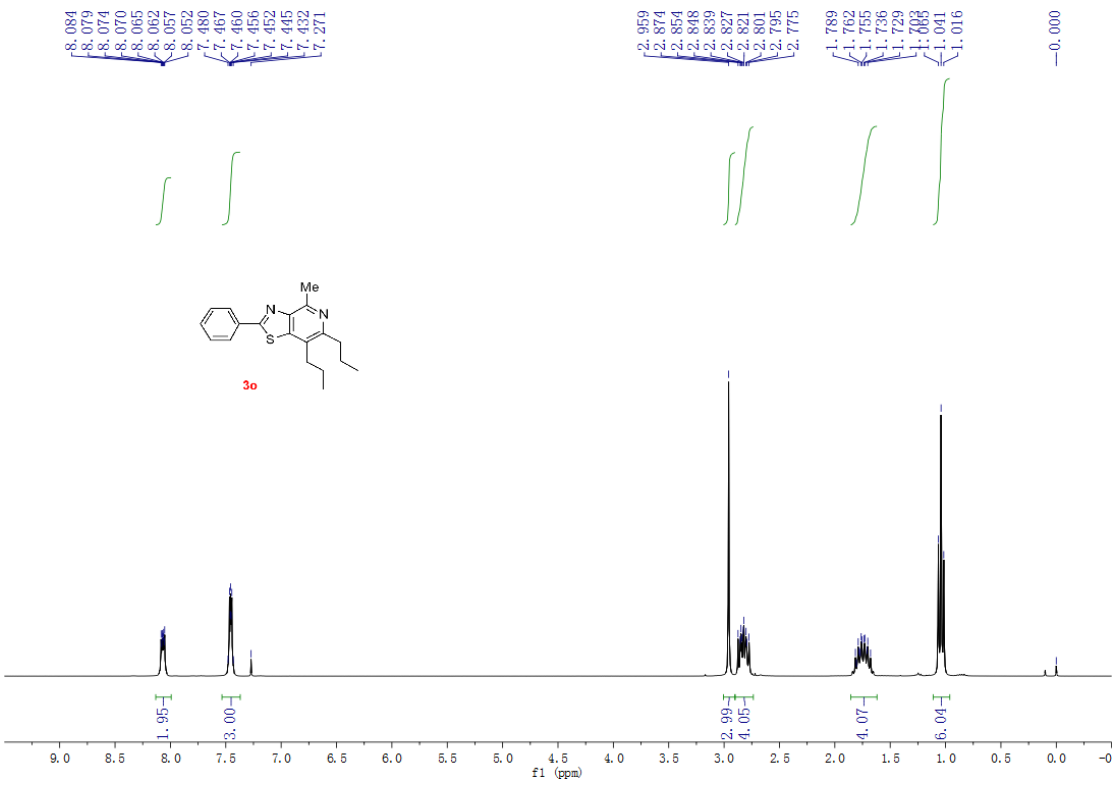
Me
N
N
S
Me
Me
3n
f1 (ppm)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8.070
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8.062
8.057
8.052
7.480
7.467
7.460
7.456
7.452
7.445
7.432
7.271
2.959
2.874
2.854
2.848
2.839
2.827
2.821
2.801
2.795
2.775
1.789
1.762
1.755
1.736
1.729
1.041
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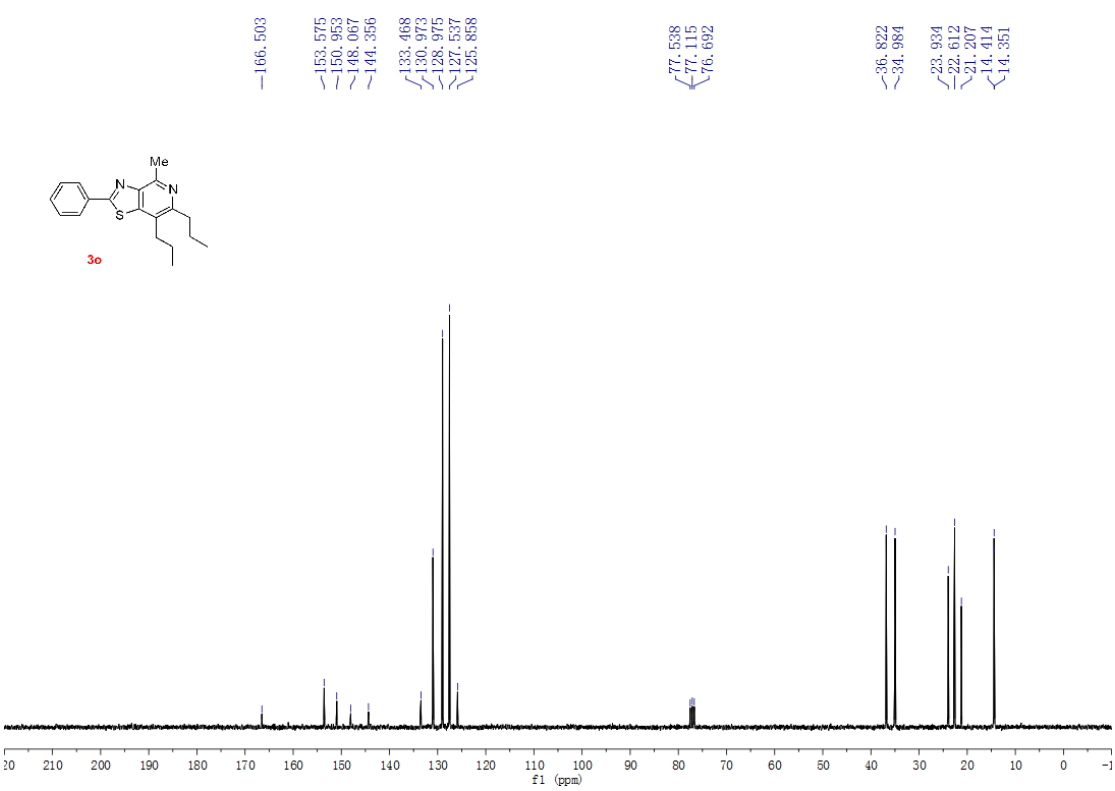
N
S
3o
1.95
3.00
2.99
4.05
4.07
6.04
f1 (ppm)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133.468
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128.975
127.537
125.858
77.538
77.115
76.692
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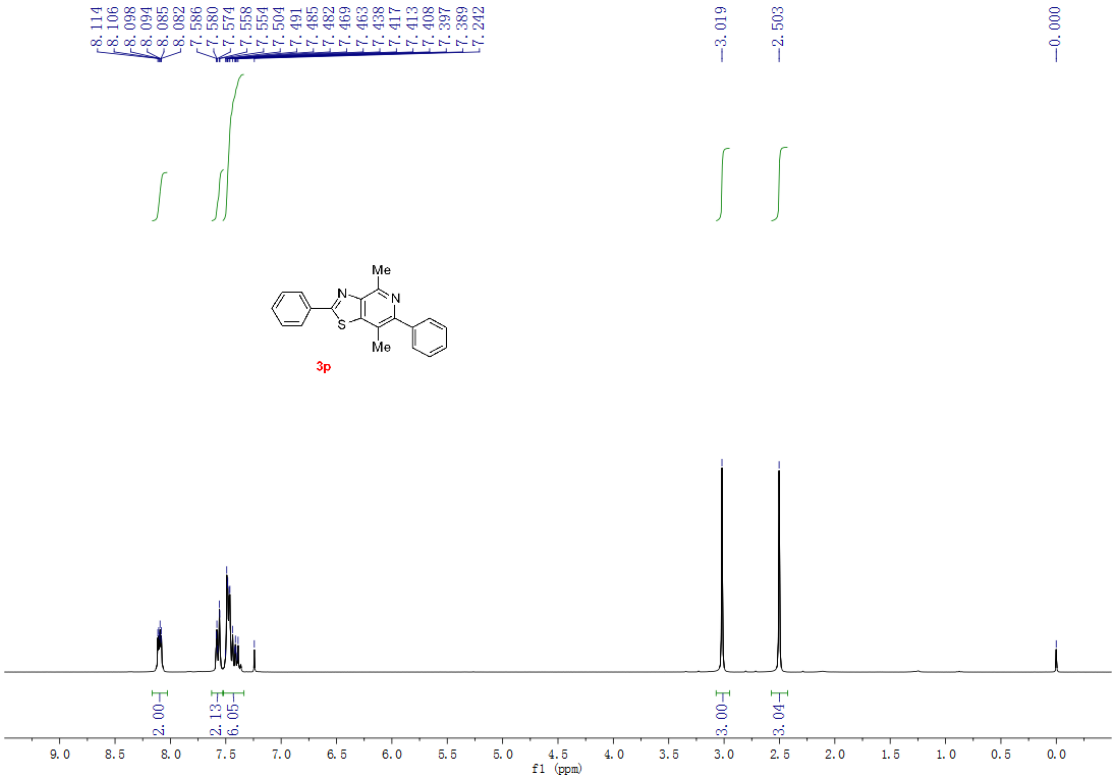
34.984
23.934
22.612
21.207
14.414
14.351
Me
N
N
S
3o
f1 (ppm)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8.106
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8.082
7.586
7.580
7.574
7.558
7.554
7.504
7.491
7.485
7.482
7.469
7.463
7.438
7.417
7.413
7.408
7.397
7.389
7.242
3.019
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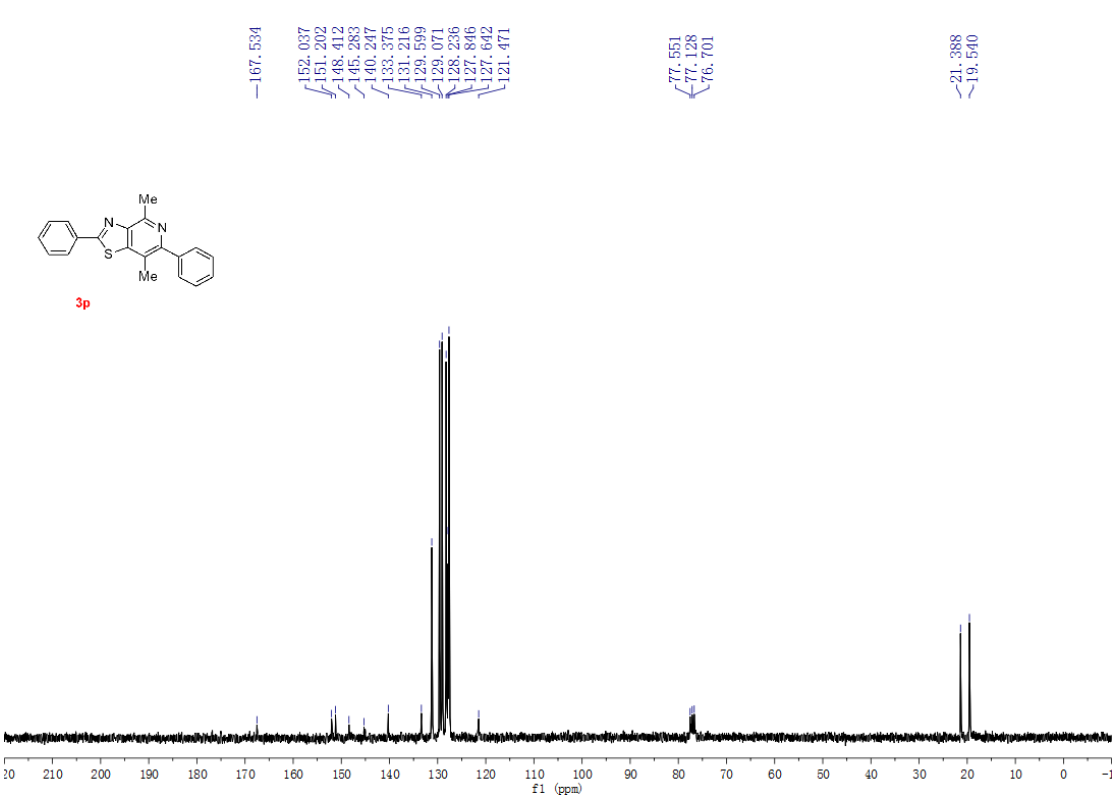
Me
N
S
N
Me
3p
2.00
2.13
6.05
3.00
3.04
f1 (ppm)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131.216
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128.236
127.846
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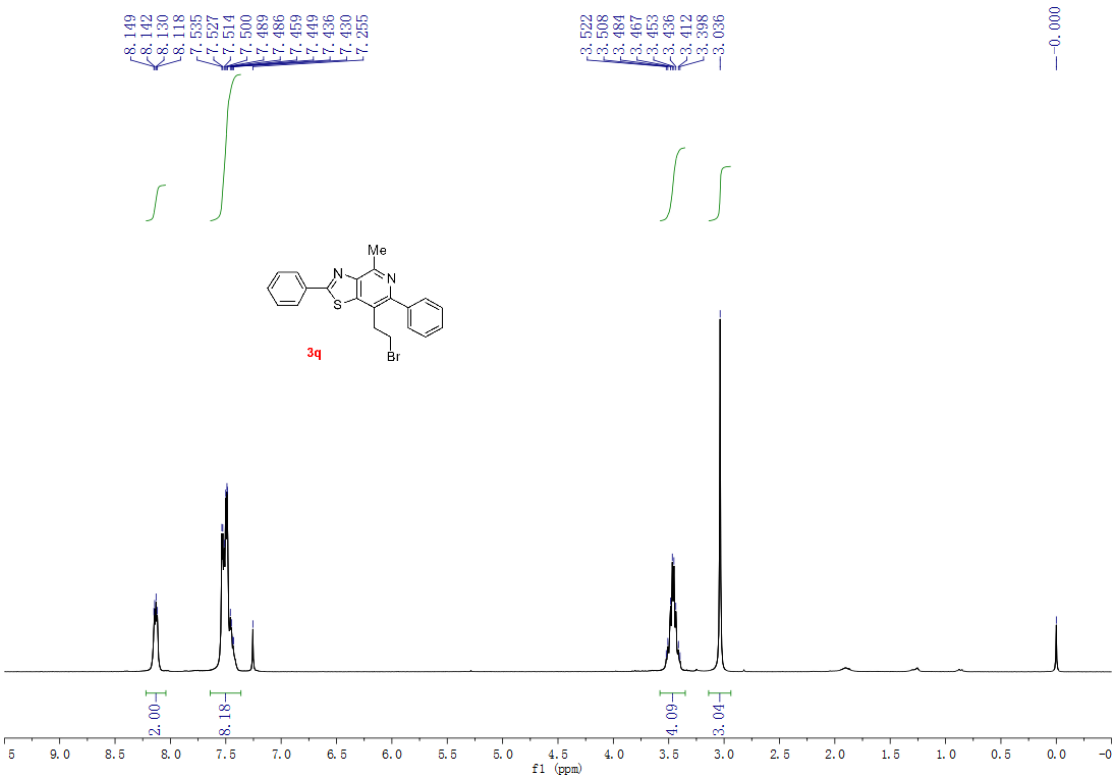
121.471
77.551
77.128
76.701
21.388
19.540
Me
N
S
N
Me
3p
f1 (ppm)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8.142
8.130
8.118
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7.527
7.514
7.500
7.489
7.486
7.459
7.449
7.436
7.430
7.255
3.522
3.508
3.484
3.467
3.453
3.436
3.412
3.398
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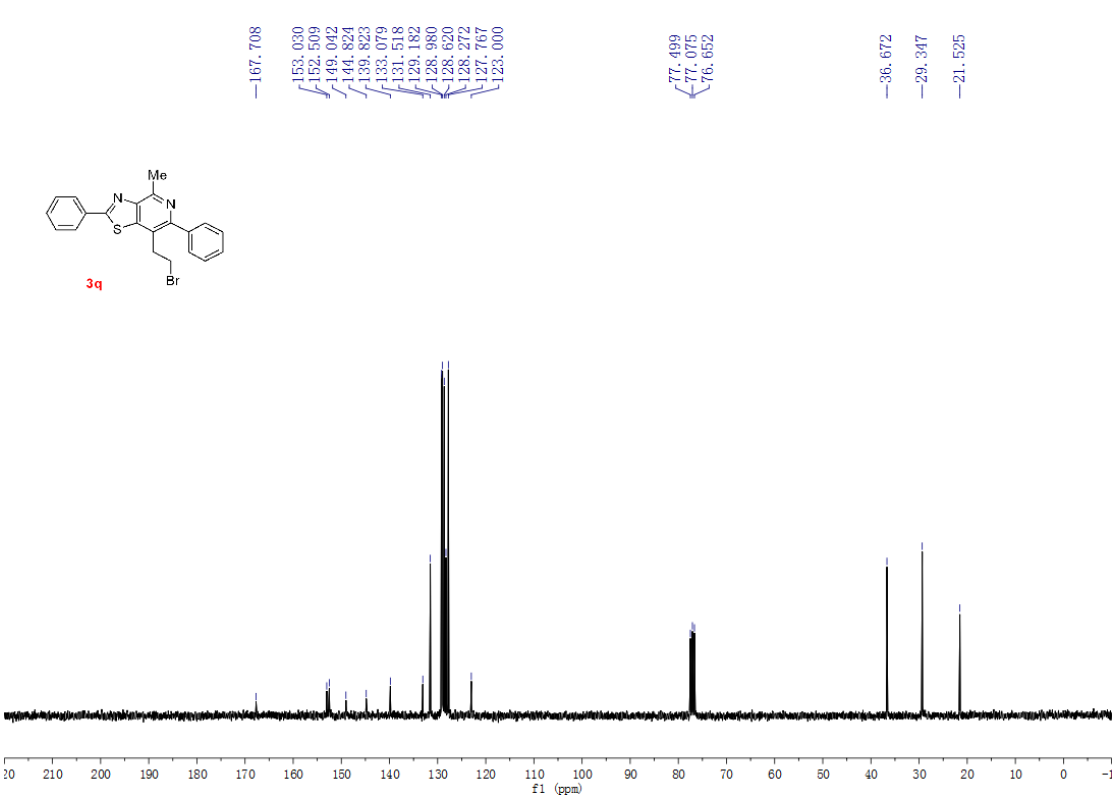
Me
N
N
S
Br
3q
2.00
8.18
4.09
3.04
f1 (ppm)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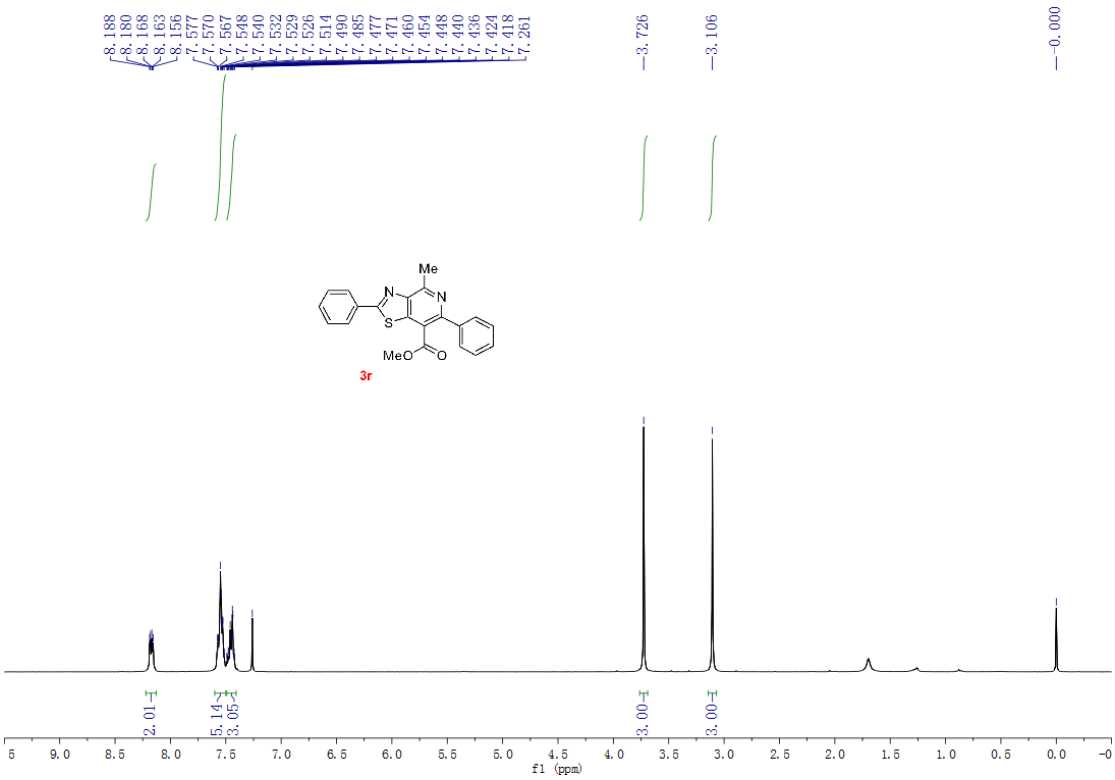
149.042
144.824
139.823
133.079
131.518
129.182
128.980
128.620
128.272
127.767
123.000
77.499
77.075
76.652
36.672
29.347
21.525
Me
N
N
S
Br
3q
f1 (ppm)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8.168
8.163
8.156
7.577
7.570
7.567
7.548
7.540
7.532
7.529
7.526
7.514
7.490
7.485
7.477
7.471
7.460
7.454
7.448
7.440
7.436
7.424
7.418
7.261
3.726
3.106
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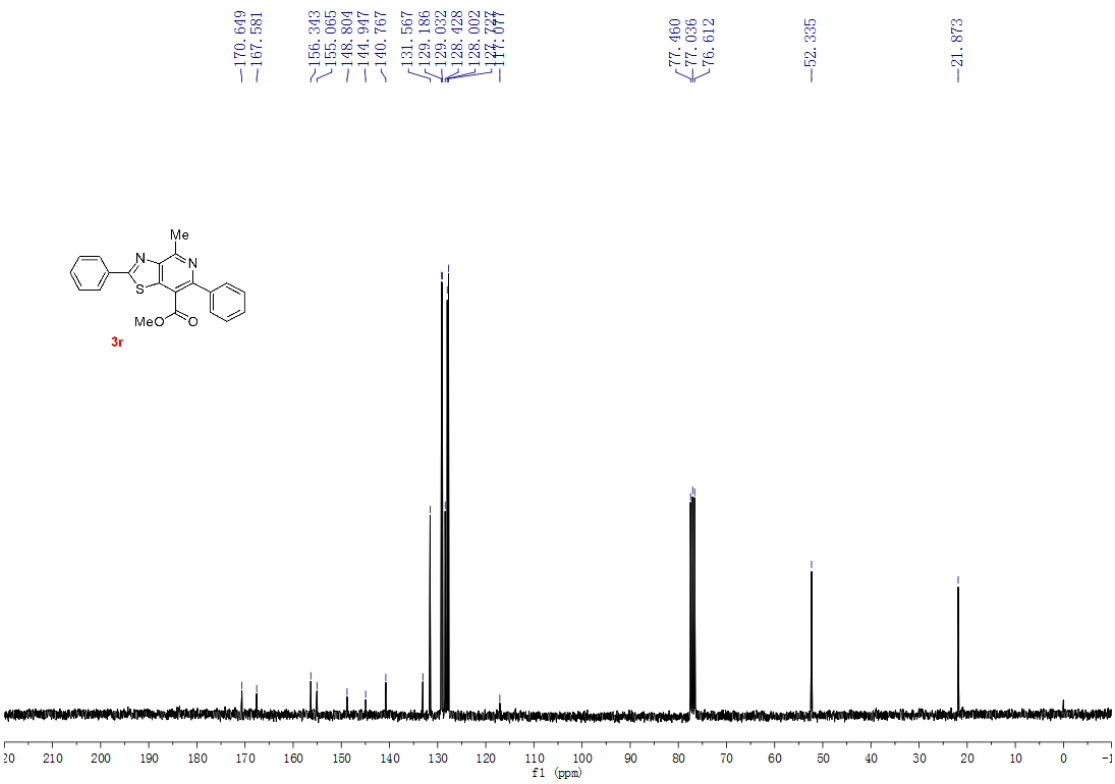
Me
N
N
S
MeO
O
3r
2.01
5.14
3.05
3.00
3.00
f1 (ppm)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156.343
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144.947
140.767
131.567
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128.428
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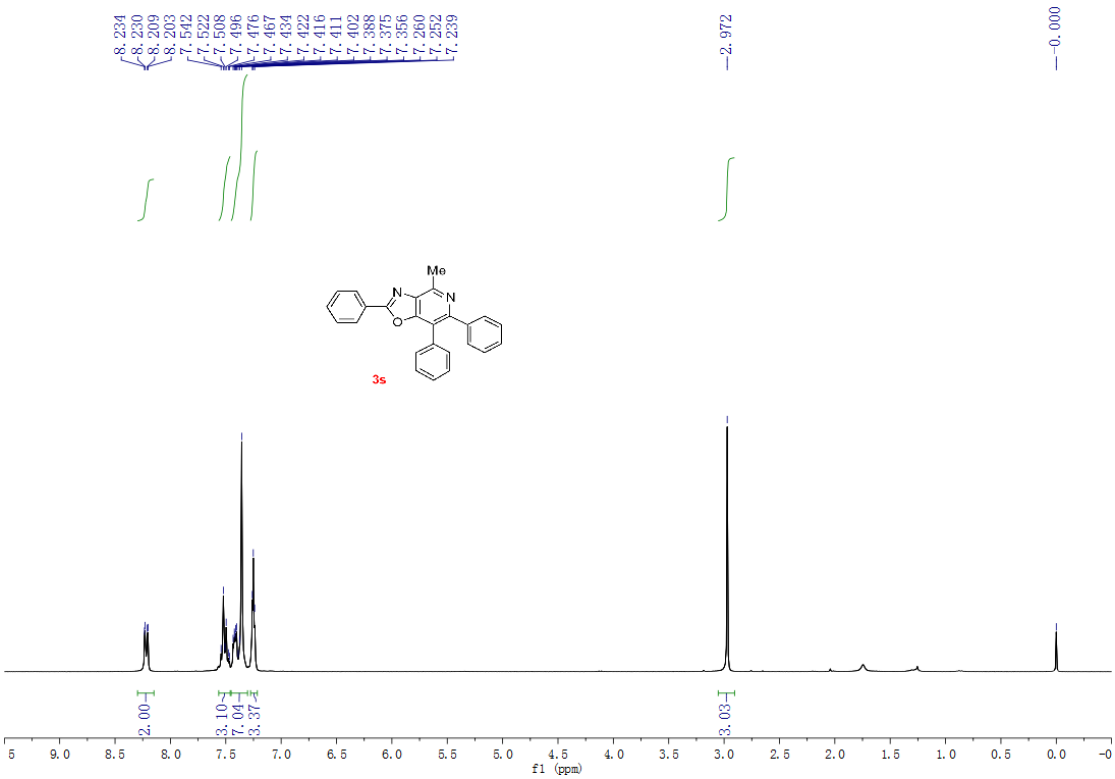
N
N
S
MeO
O
3r
f1 (ppm)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8.203
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7.522
7.508
7.496
7.476
7.467
7.434
7.422
7.416
7.411
7.402
7.388
7.375
7.356
7.260
7.252
7.239
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Me
N
N
O
3s
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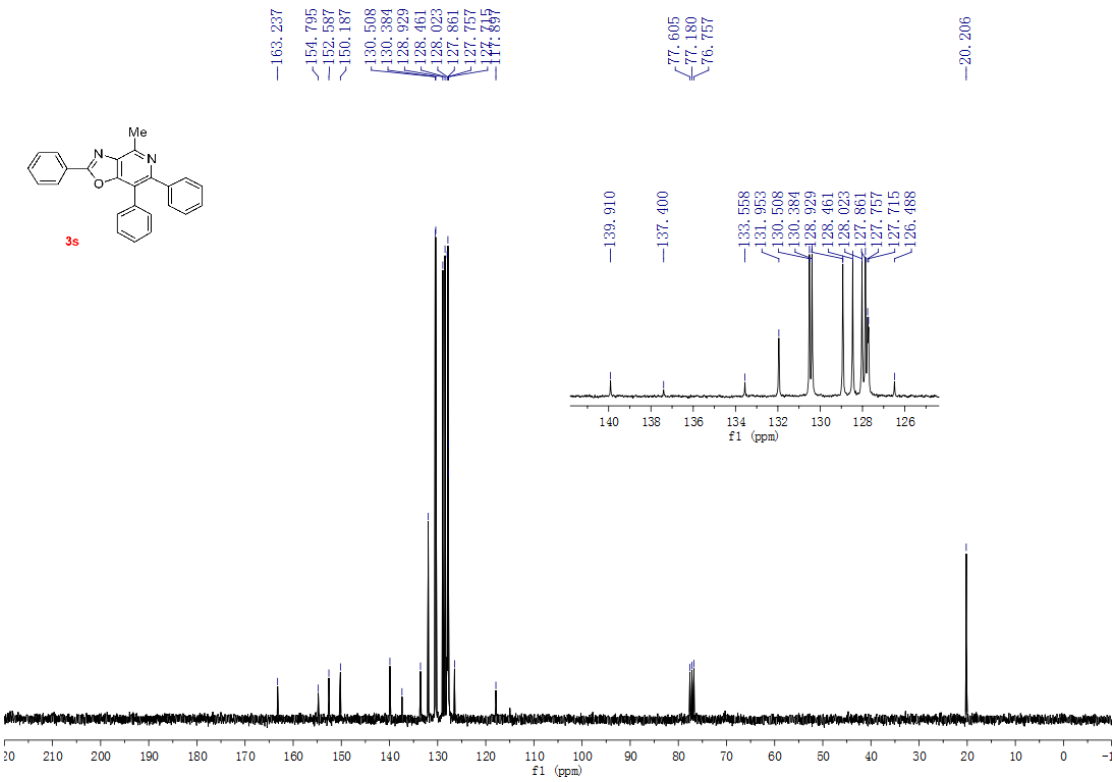
7.04
3.37
3.03
f1 (ppm)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127.715
117.897
77.605
77.180
76.757
20.206
Me
N
N
O
3s
139.910
137.400
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128.929
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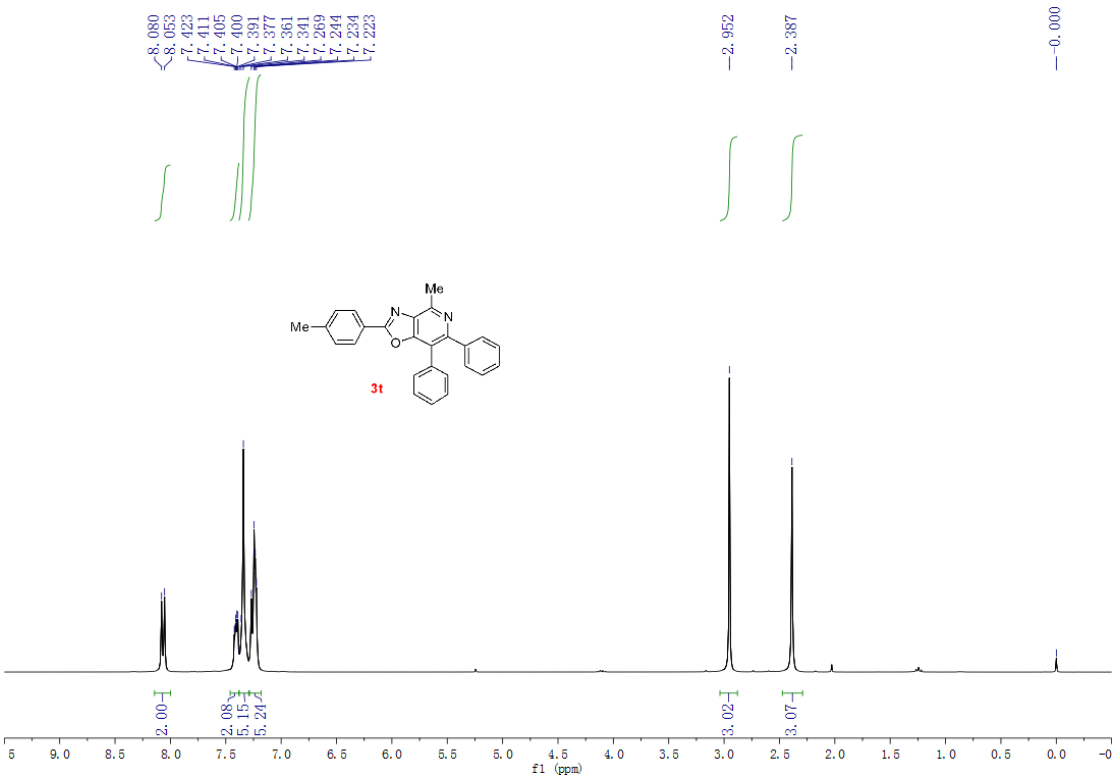
127.757
127.715
126.488
f1 (ppm)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7.400
7.391
7.377
7.361
7.341
7.269
7.244
7.234
7.223
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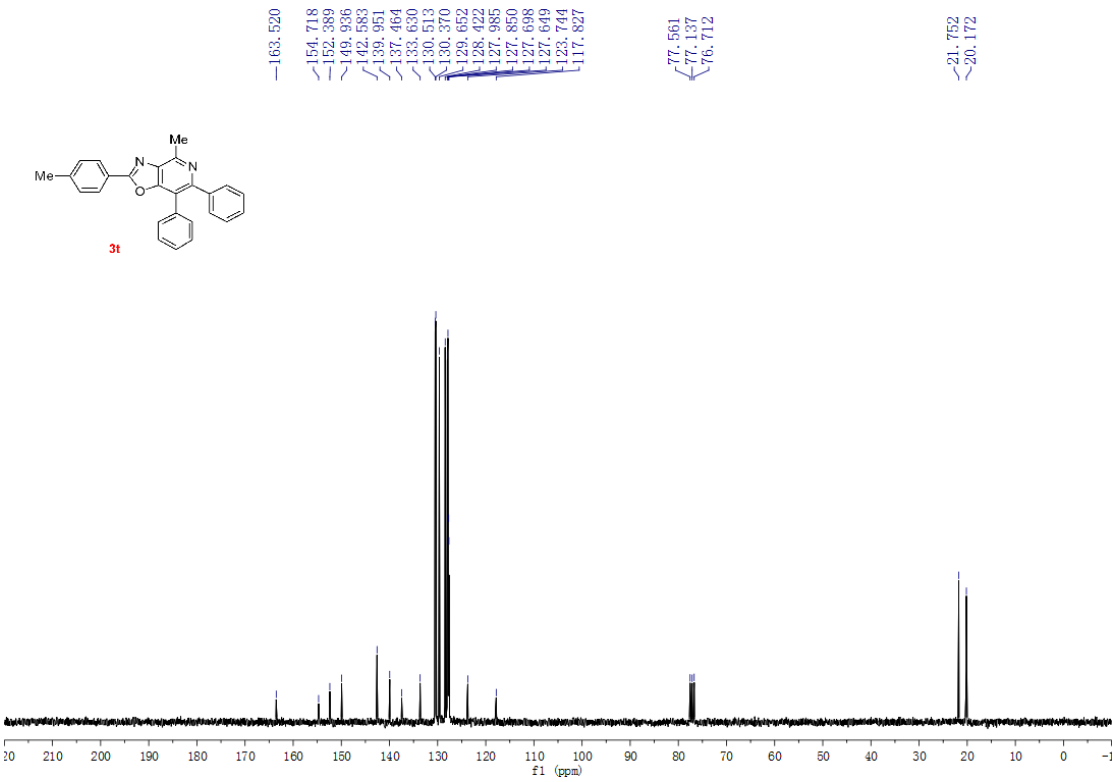
Me
Me
3t
2.00
2.08
5.15
5.24
3.02
3.07
f1 (ppm)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128.422
127.985
127.850
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77.561
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76.712
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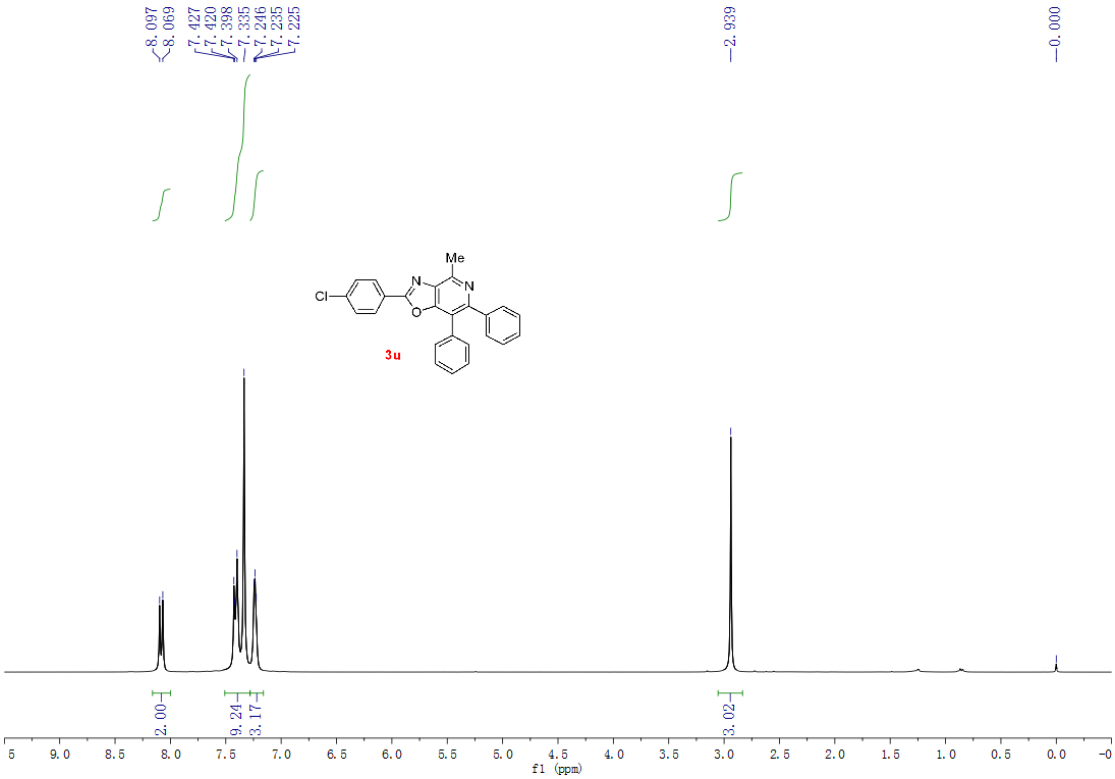
20.172
Me
Me
3t
f1 (ppm)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7.246
7.235
7.225
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Me
Cl
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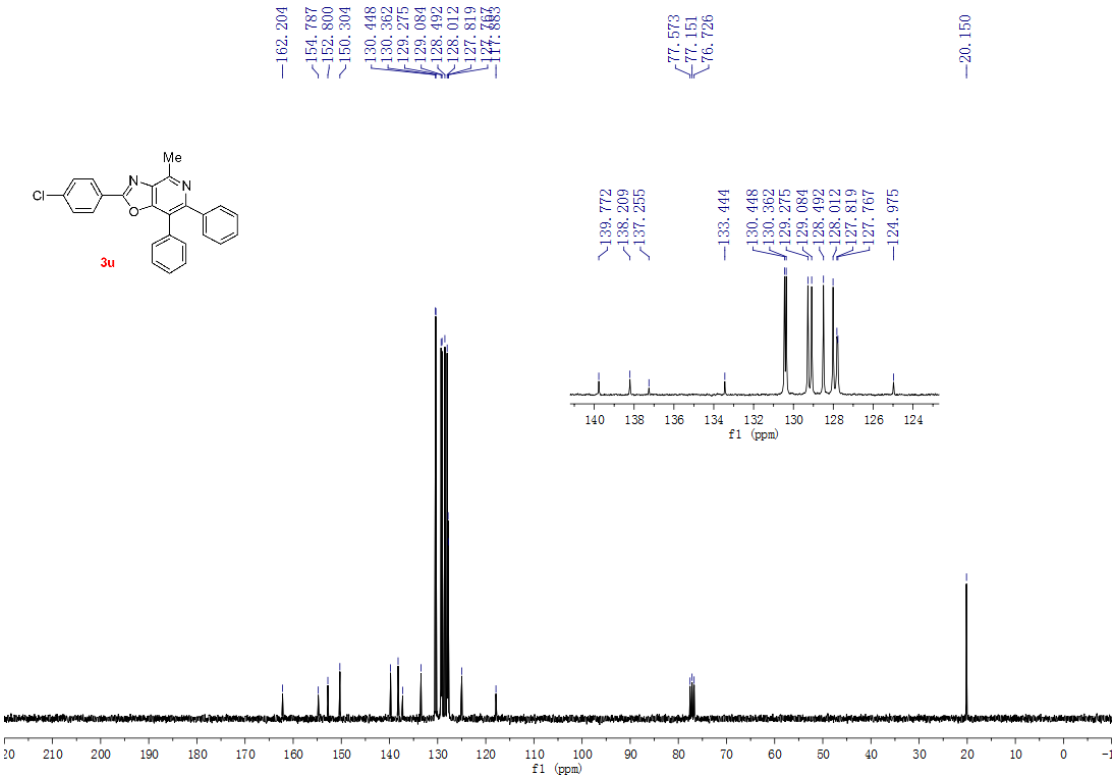
N
O
3u
2.00
9.24
3.17
3.02
f1 (ppm)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127.819
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77.151
76.726
20.150
Me
Cl
N
N
O
3u
139.772
138.209
137.255
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129.275
129.084
128.492
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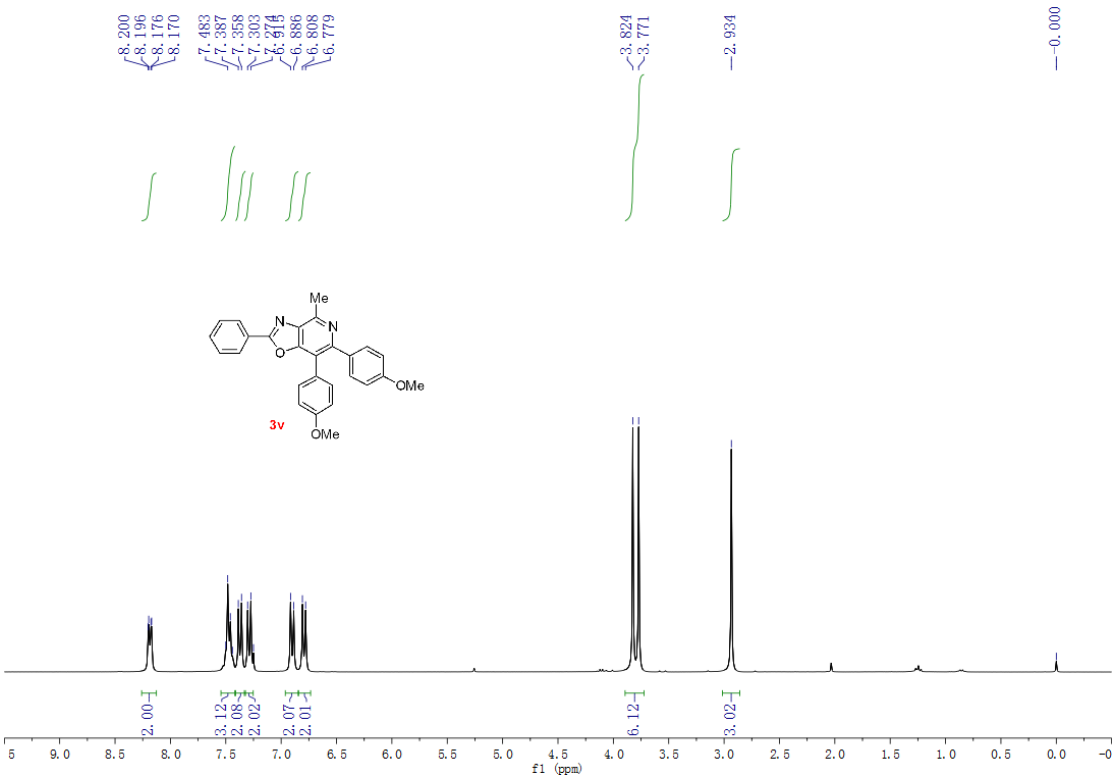
127.819
127.767
124.975
f1 (ppm)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7.303
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6.808
6.779
3.824
3.771
2.934
0.000
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OMe
OMe
3v
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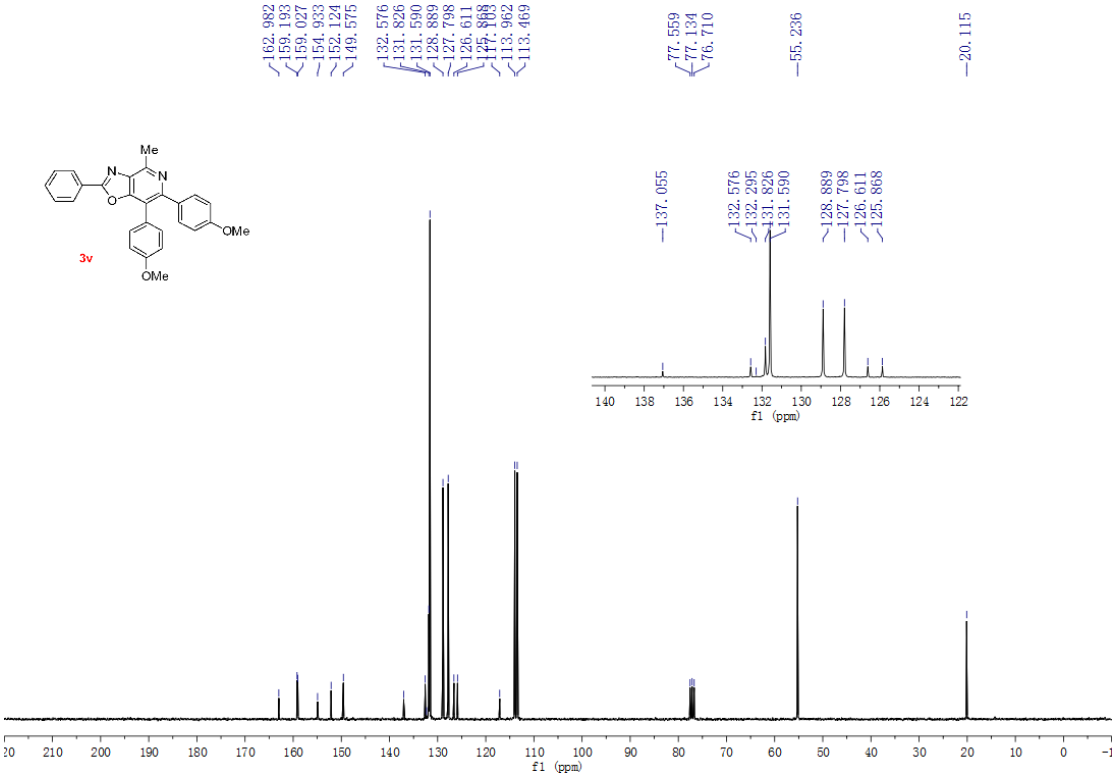
2.08
2.02
2.07
2.01
6.12
3.02
f1 (ppm)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113.962
113.469
77.559
77.134
76.710
55.236
20.115
Me
OMe
OMe
3v
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128.889
127.798
126.611
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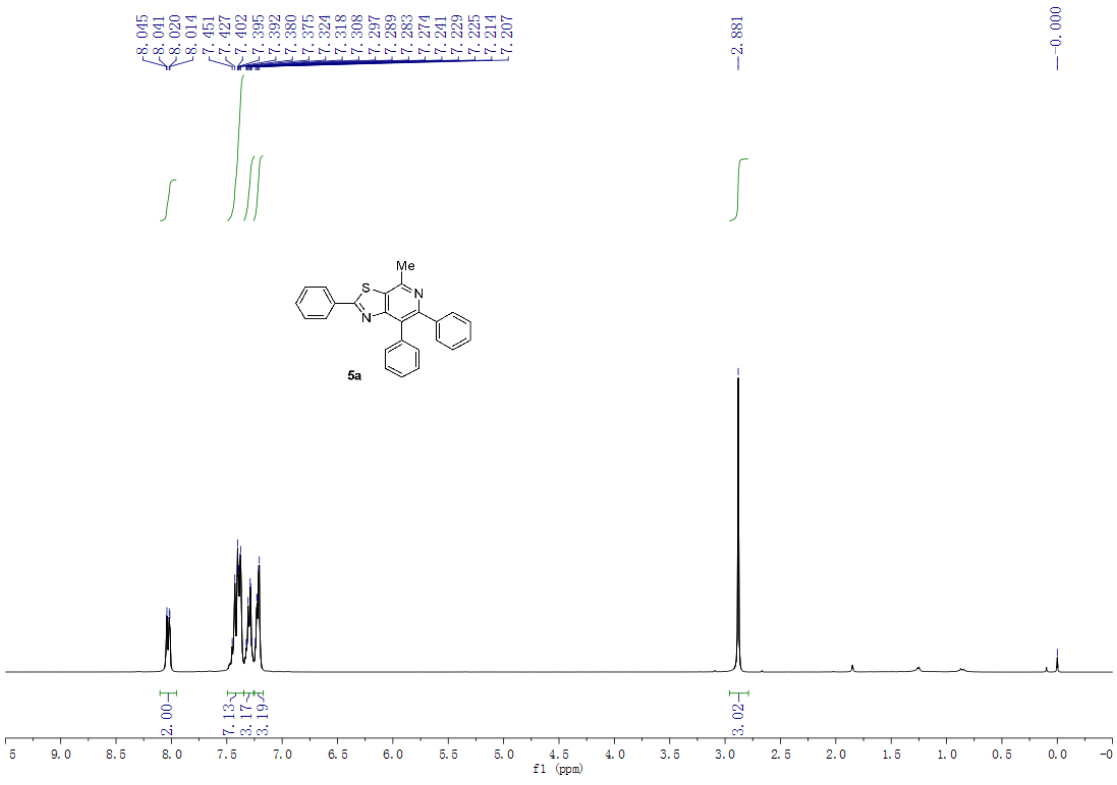
f1 (ppm)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8.014
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7.318
7.308
7.297
7.289
7.283
7.274
7.241
7.229
7.225
7.214
7.207
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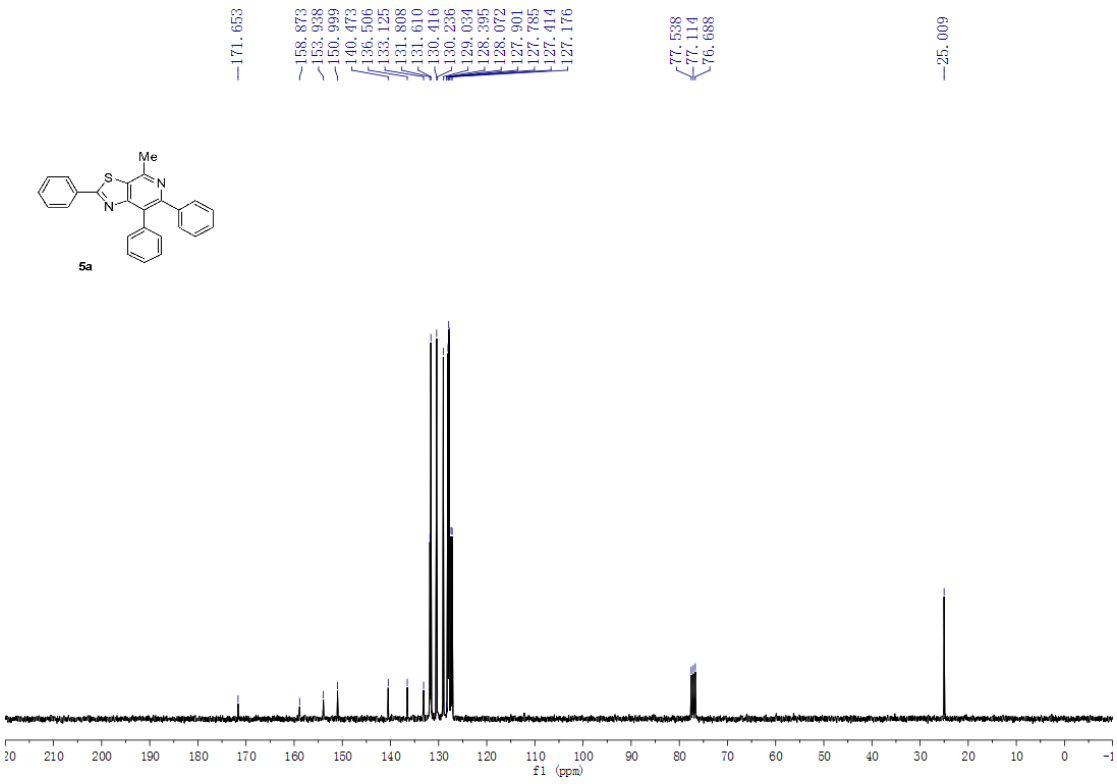
3.17
3.19
3.02
f1 (ppm)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130.236
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128.395
128.072
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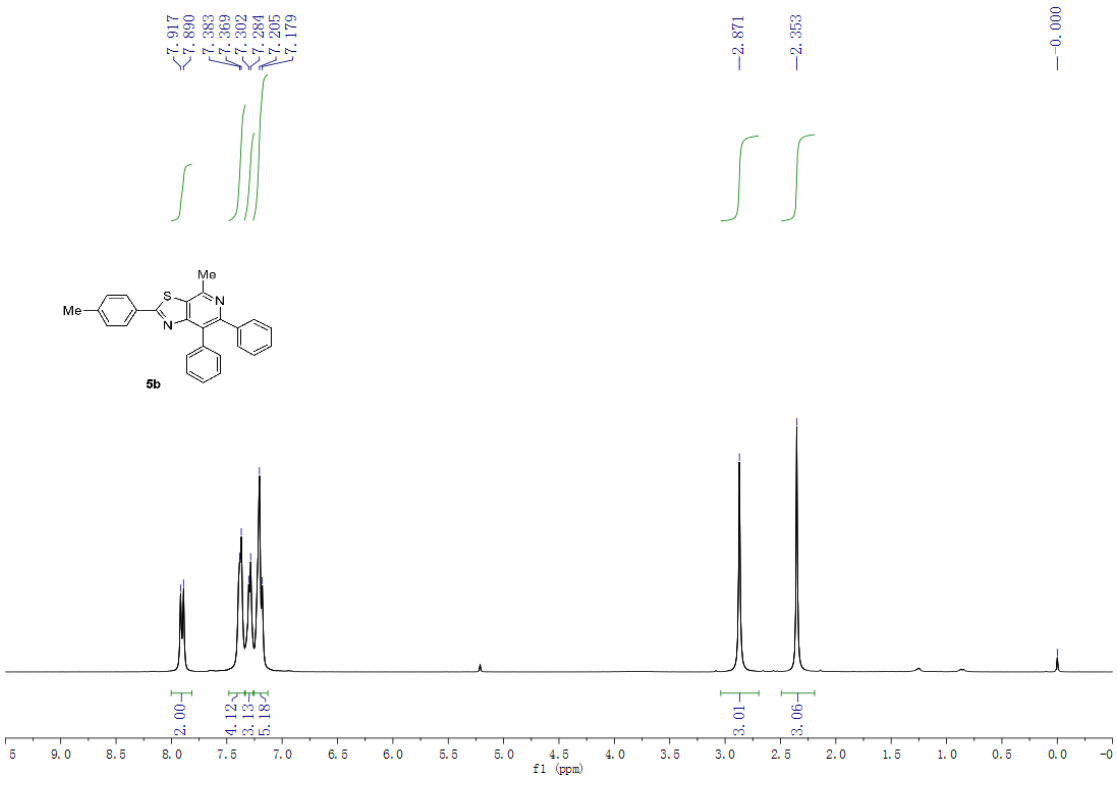
127.176
77.538
77.114
76.688
25.009
Me
S
N
N
5a
f1 (ppm)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7.284
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7.179
2.871
2.353
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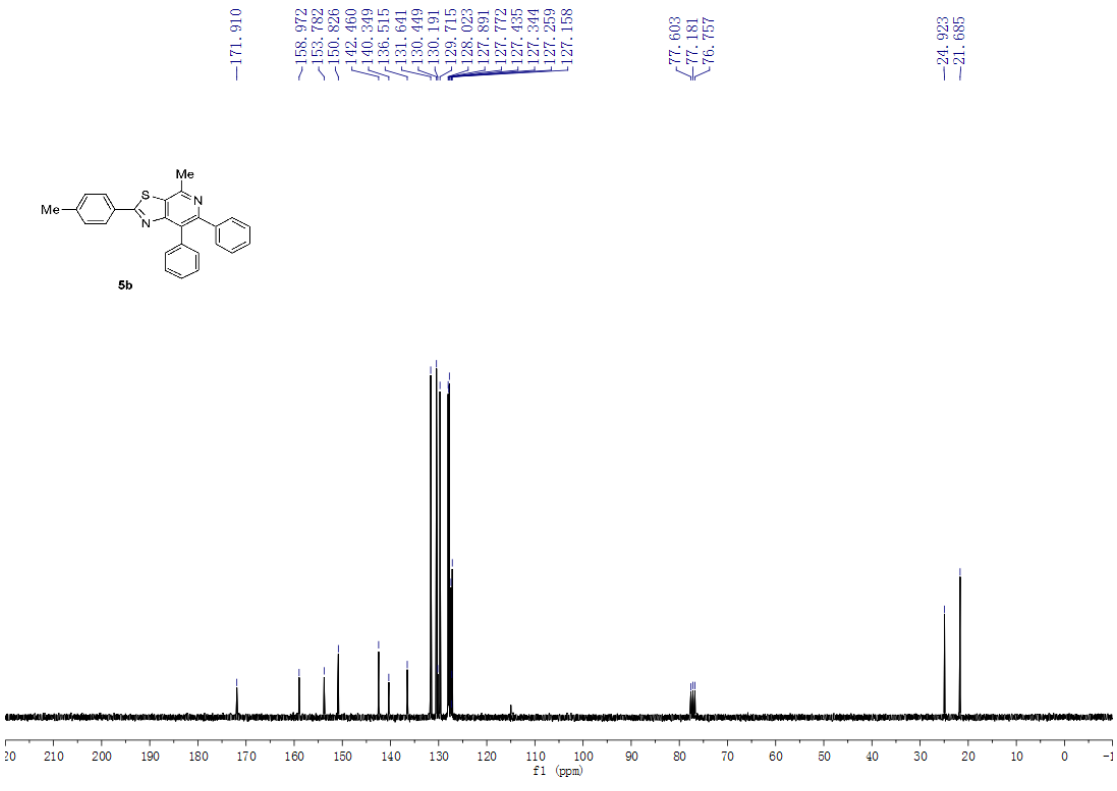
Me
S
N
N
5b
2.00
4.12
3.13
5.18
3.01
3.06
f1 (ppm)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129.715
128.023
127.891
127.772
127.435
127.344
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77.181
76.757
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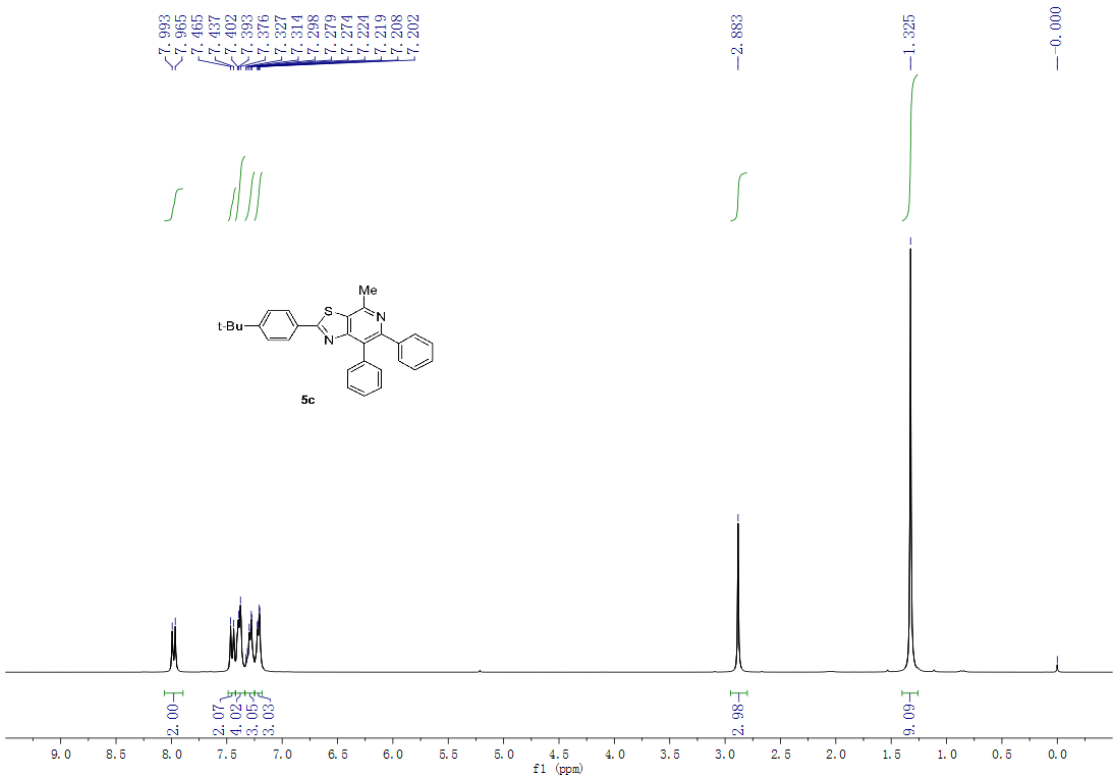
21.685
Me
Me
S
N
N
5b
f1 (ppm)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7.274
7.224
7.219
7.208
7.202
2.883
1.325
0.000
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N
5c
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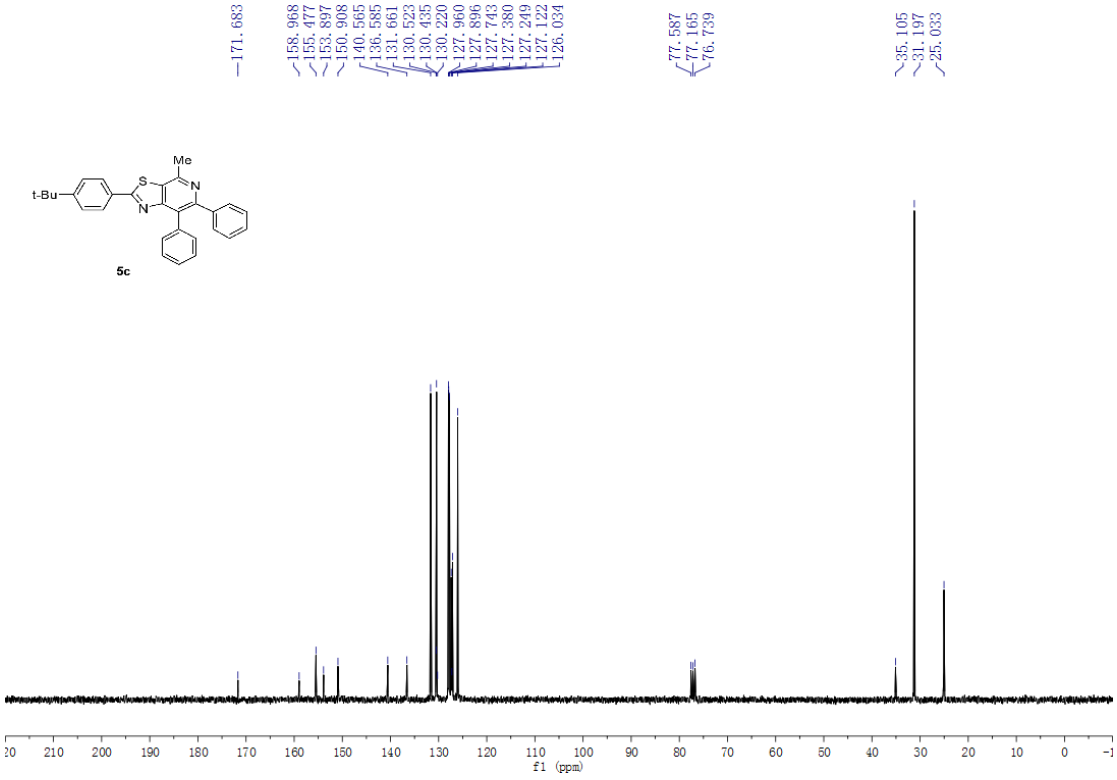
2.07
4.02
3.05
3.03
2.98
9.09
f1 (ppm)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131.661
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130.435
130.220
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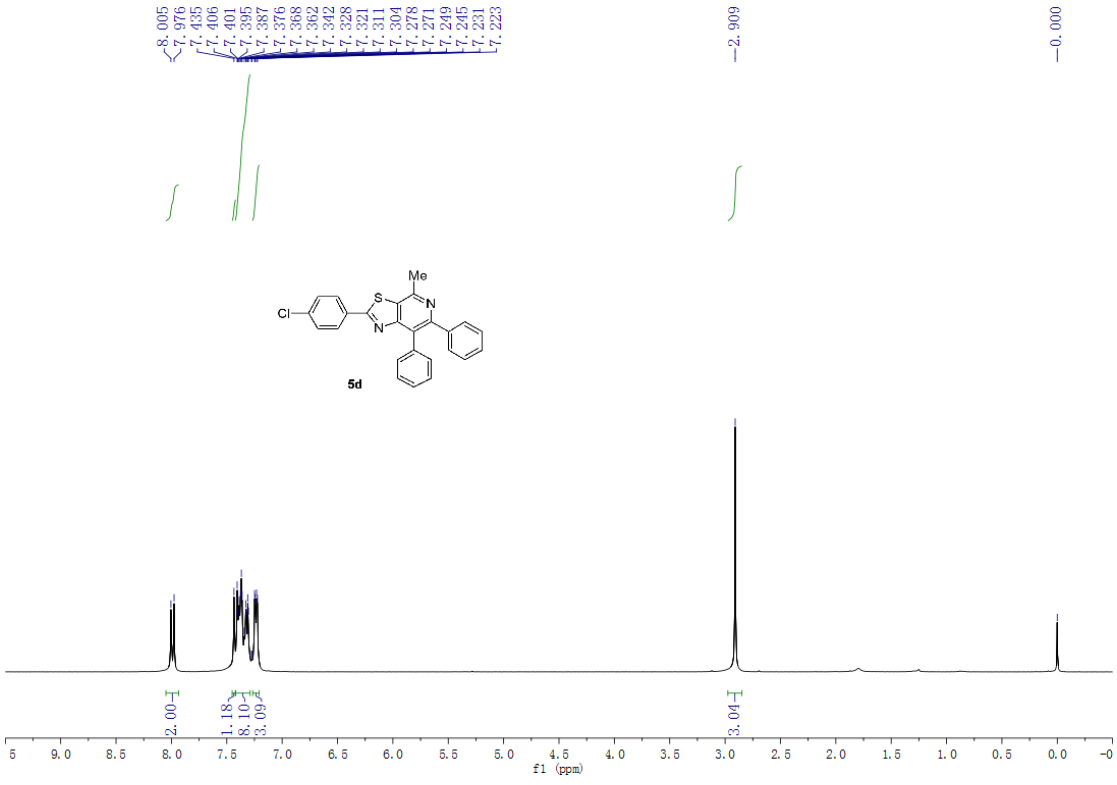
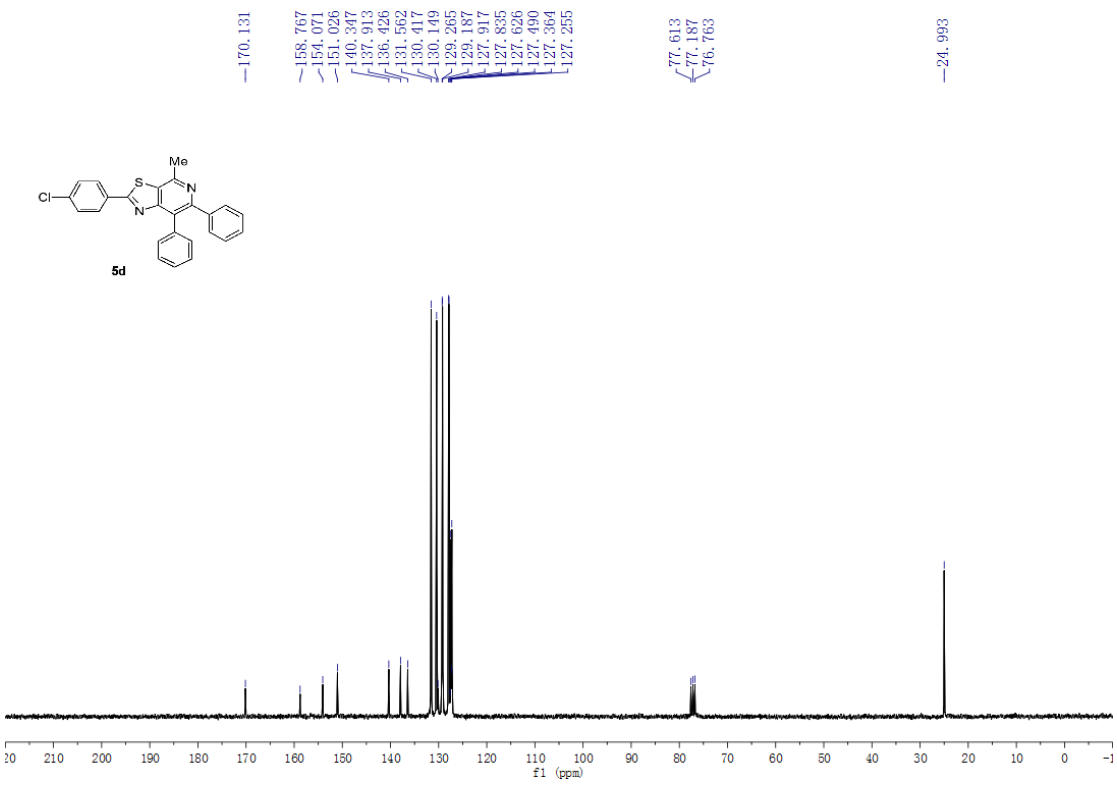
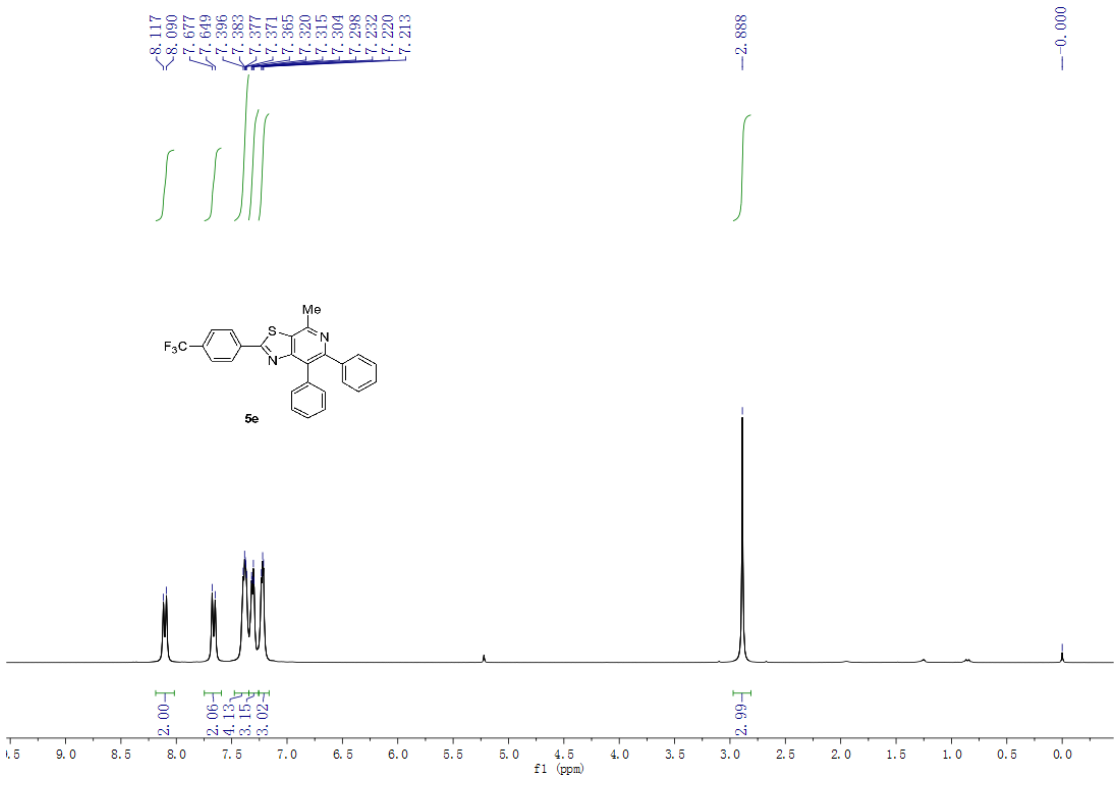
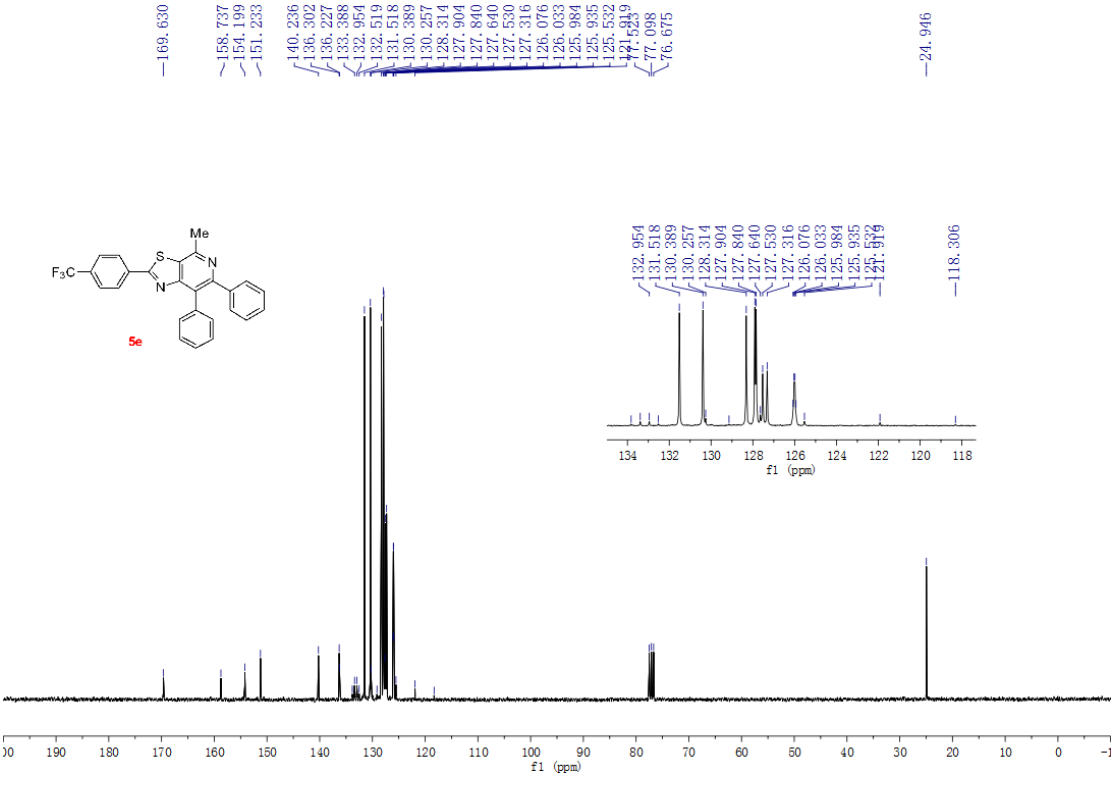
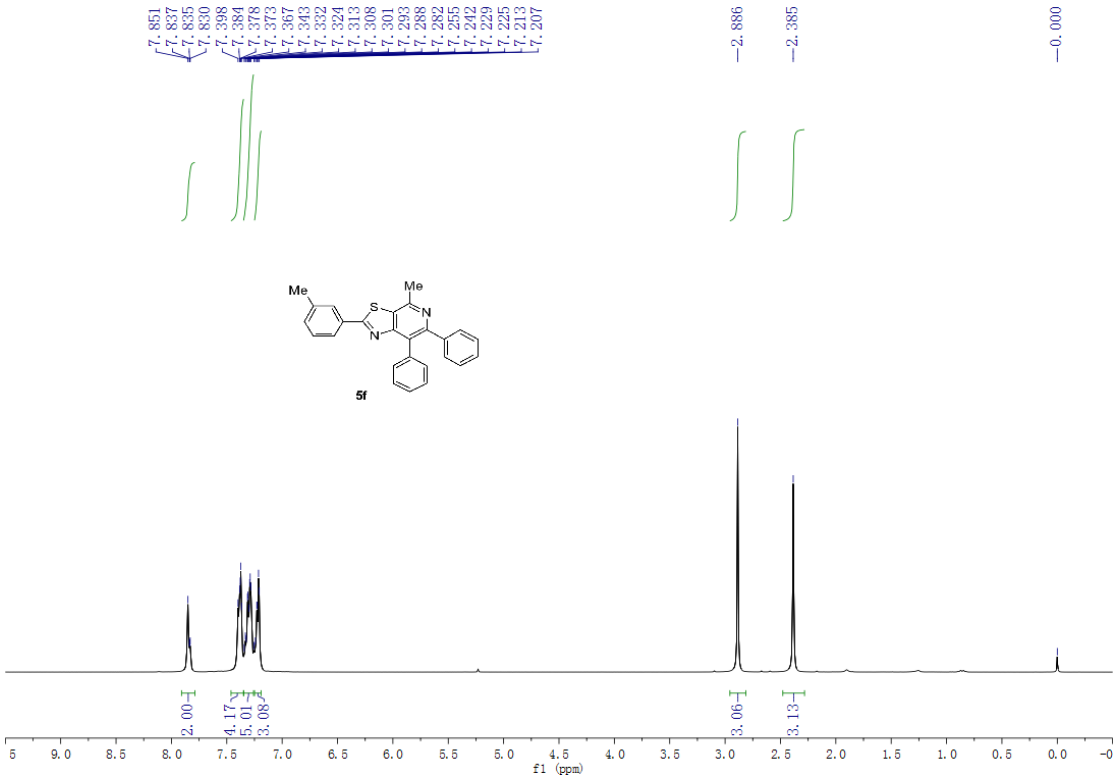
127.896
127.743
127.380
127.249
127.122
126.034
77.587
77.165
76.739
35.105
31.197
25.033
Me
t-Bu
S
N
N
5c
f1 (ppm)

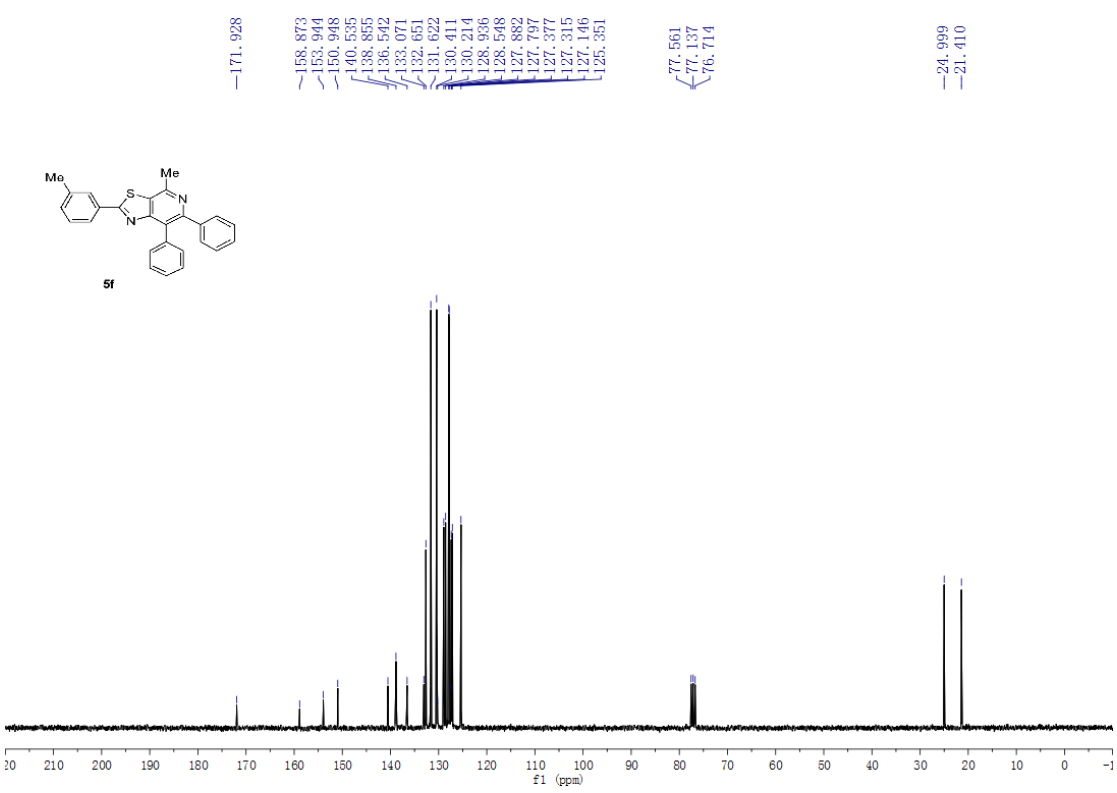

8.005
7.976
7.435
7.406
7.401
7.395
7.387
7.376
7.368
7.362
7.342
7.328
7.321
7.311
7.304
7.278
7.271
7.249
7.245
7.231
7.223
2.909
0.000
Me
Cl
S
N
N
5d
2.00
1.18
8.10
3.09
3.04
f1 (ppm)

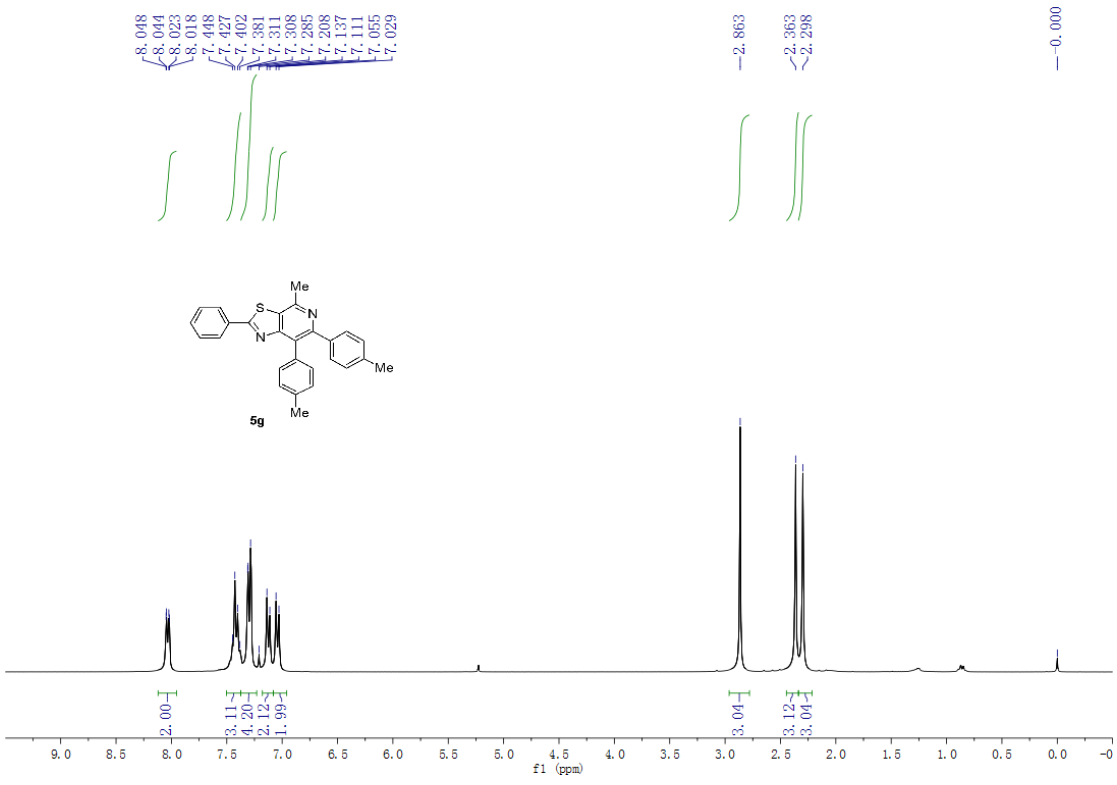

170.131
158.767
154.071
151.026
140.347
137.913
136.426
131.562
130.417
130.149
129.265
129.187
127.917
127.835
127.626
127.490
127.364
127.255
77.613
77.187
76.763
24.993
Me
Cl
S
N
N
5d
f1 (ppm)

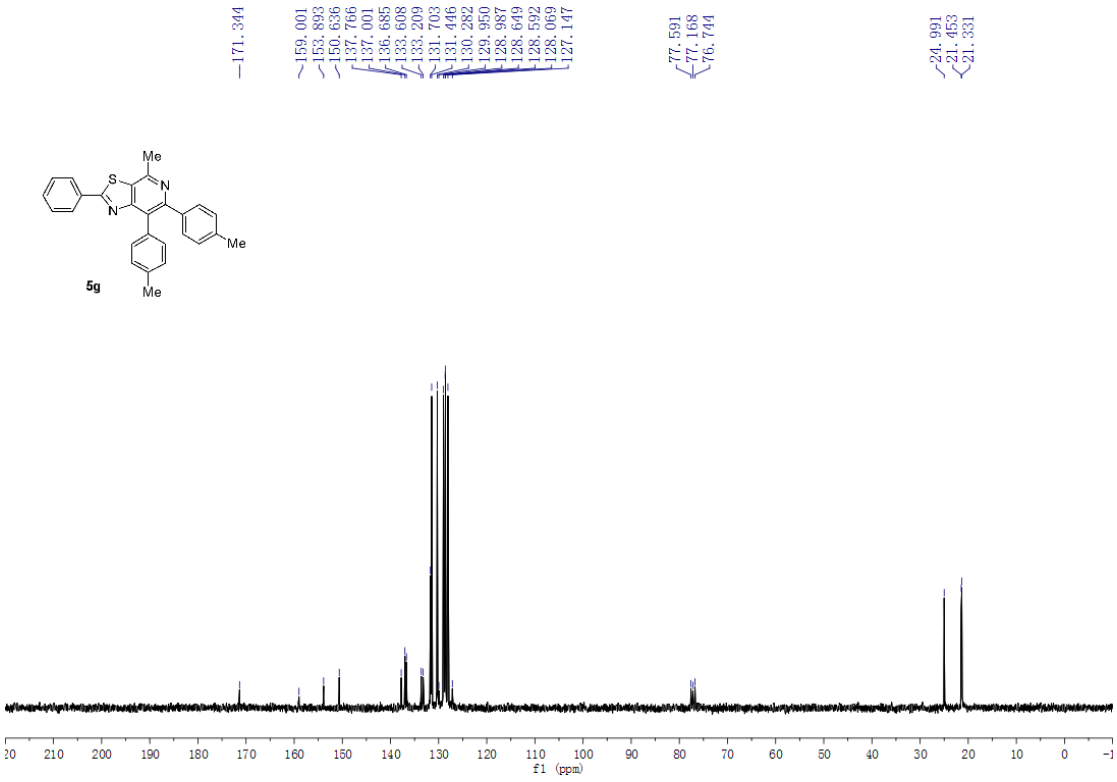

8.117
8.090
7.677
7.649
7.396
7.383
7.377
7.371
7.365
7.320
7.315
7.304
7.298
7.232
7.220
7.213
2.888
-0.000
Me
F3C
S
N
N
5e
2.00
2.06
4.13
3.15
3.02
2.99
f1 (ppm)

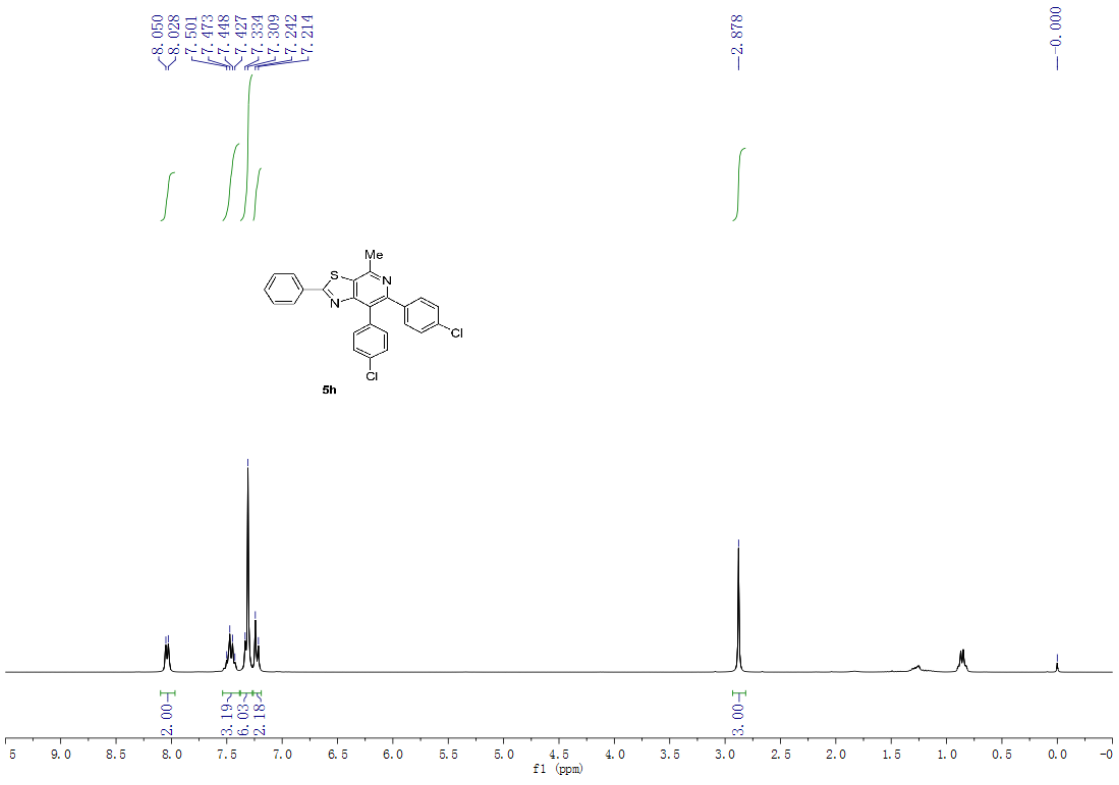

169.630
158.737
154.199
151.233
140.236
136.302
136.227
133.388
132.954
132.519
131.518
130.389
130.257
128.314
127.904
127.840
127.640
127.530
127.316
126.076
126.033
125.984
125.935
125.532
121.919
77.523
77.098
76.675
24.946
118.306
Me
F3C
S
N
N
5e
f1 (ppm)

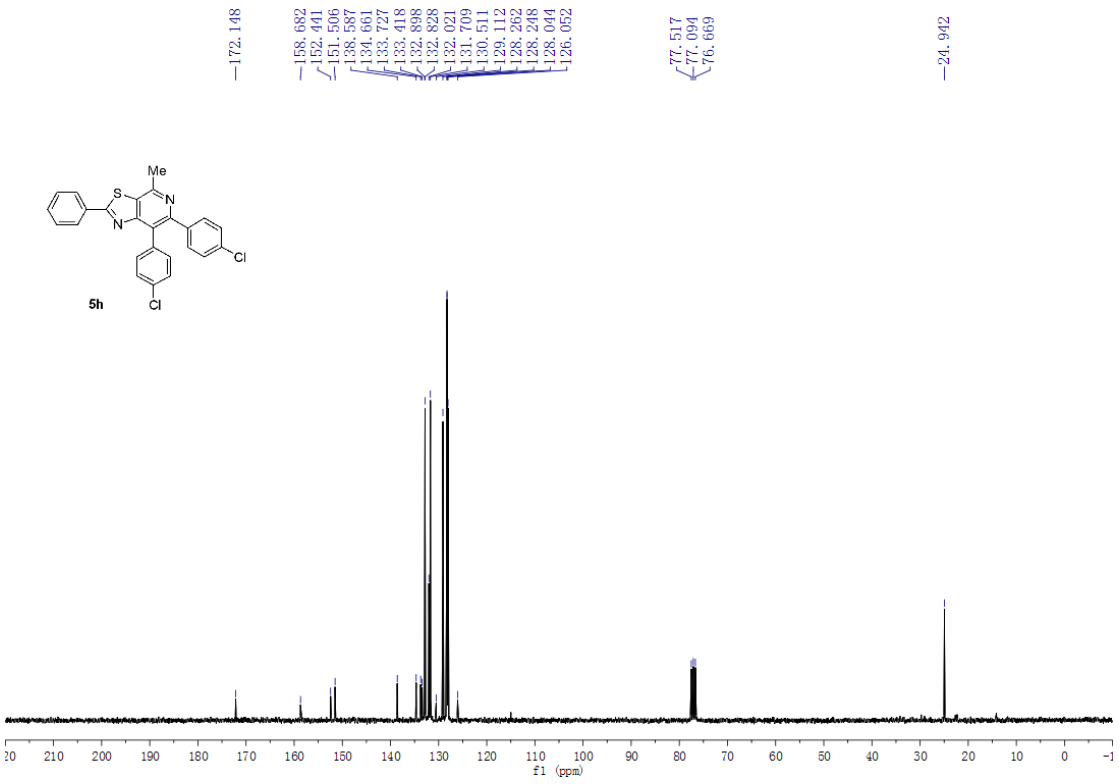

7.851
7.837
7.835
7.830
7.398
7.384
7.378
7.373
7.367
7.343
7.332
7.324
7.313
7.308
7.301
7.293
7.288
7.282
7.255
7.242
7.229
7.225
7.213
7.207
2.886
2.385
0.000
Me
Me
S
N
N
5f
2.00
4.17
5.01
3.08
3.06
3.13
f1 (ppm)

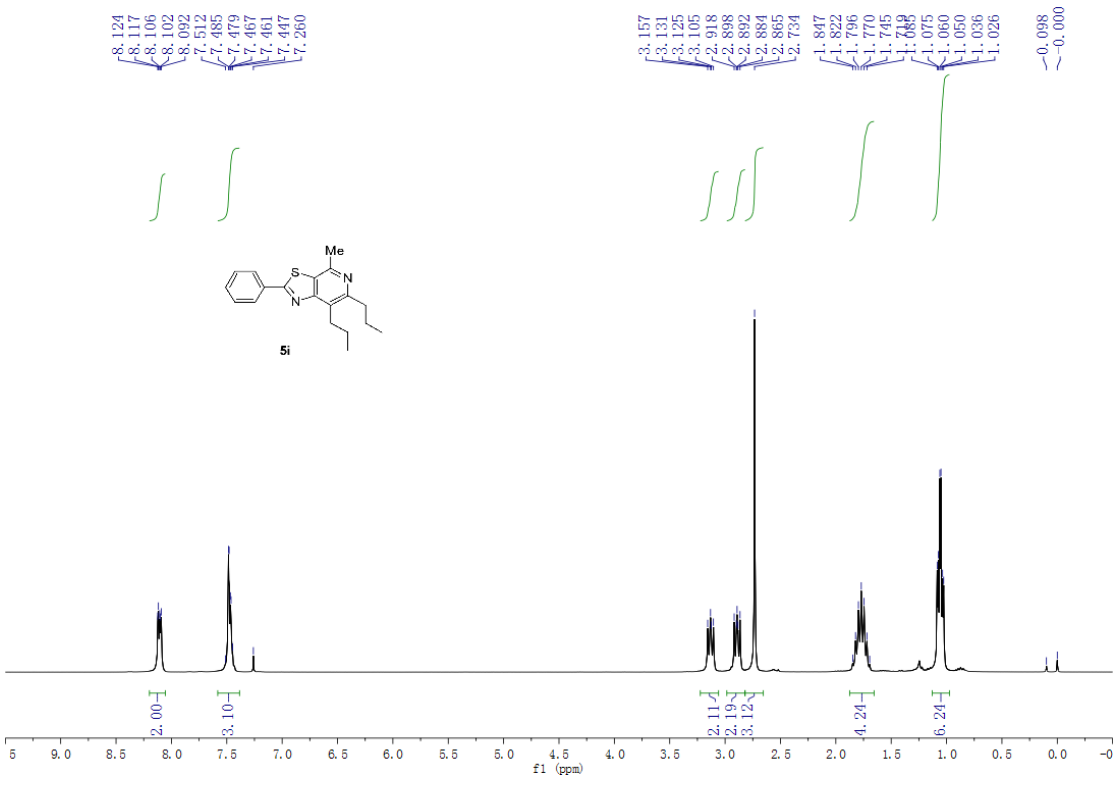

171.928
158.873
153.944
150.948
140.535
138.855
136.542
133.071
132.651
131.622
130.411
130.214
128.936
128.548
127.882
127.797
127.377
127.315
127.146
125.351
77.561
77.137
76.714
24.999
21.410
Me
Me
S
N
N
5f
f1 (ppm)

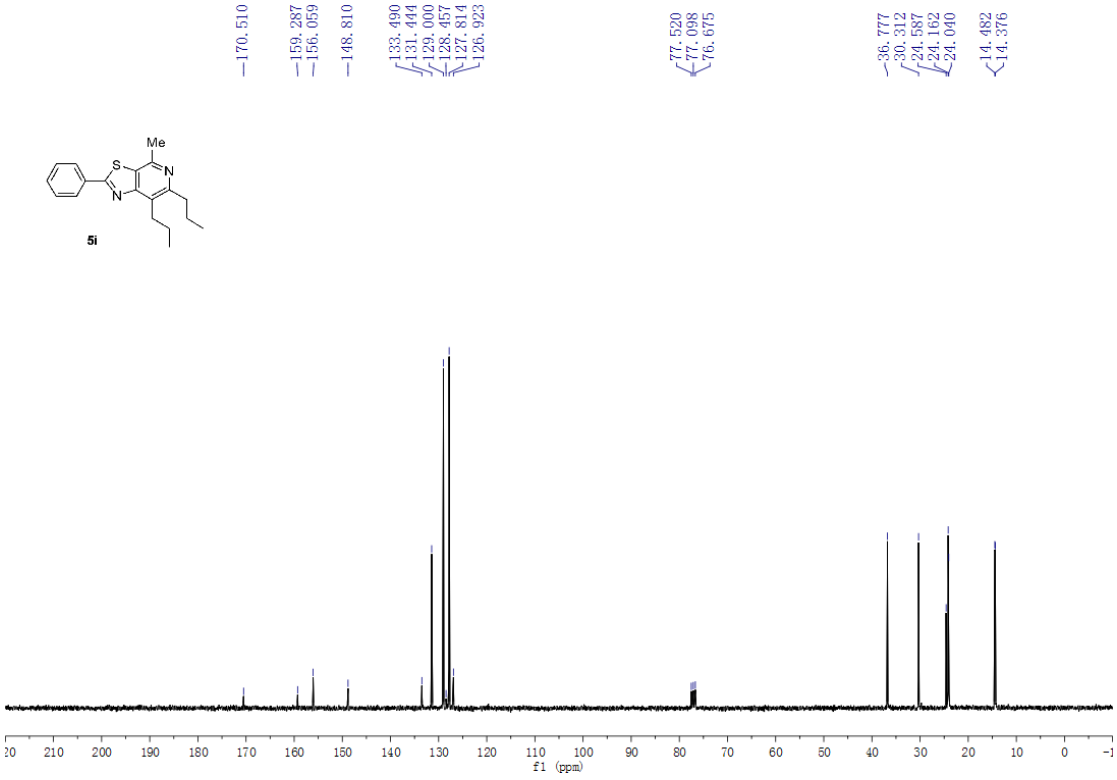

8.048
8.044
8.023
8.018
7.448
7.427
7.402
7.381
7.311
7.308
7.285
7.208
7.137
7.111
7.055
7.029
2.863
2.363
2.298
0.000
Me
Me
Me
5g
2.00
3.11
4.20
2.12
1.99
3.04
3.12
3.04
f1 (ppm)

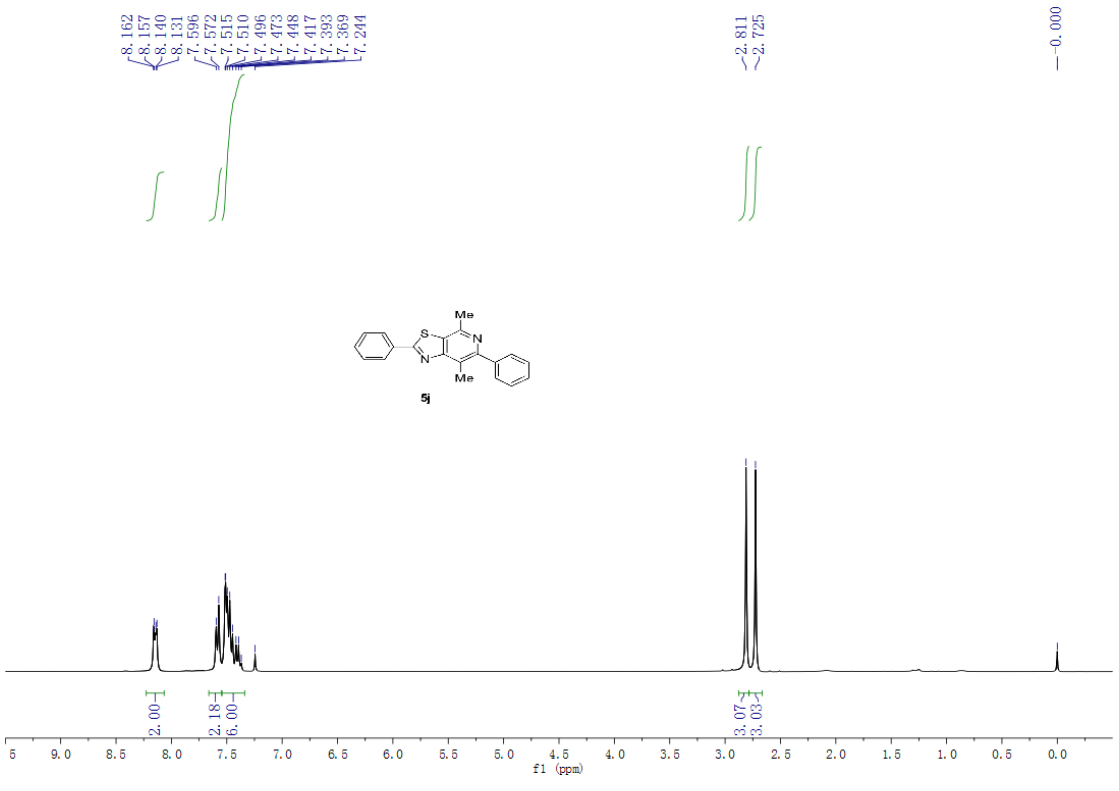

171.344
159.001
153.893
150.636
137.766
137.001
136.685
133.608
133.209
131.703
131.446
130.282
129.950
128.987
128.649
128.592
128.069
127.147
77.591
77.168
76.744
24.991
21.453
21.331
Me
Me
Me
5g
f1 (ppm)

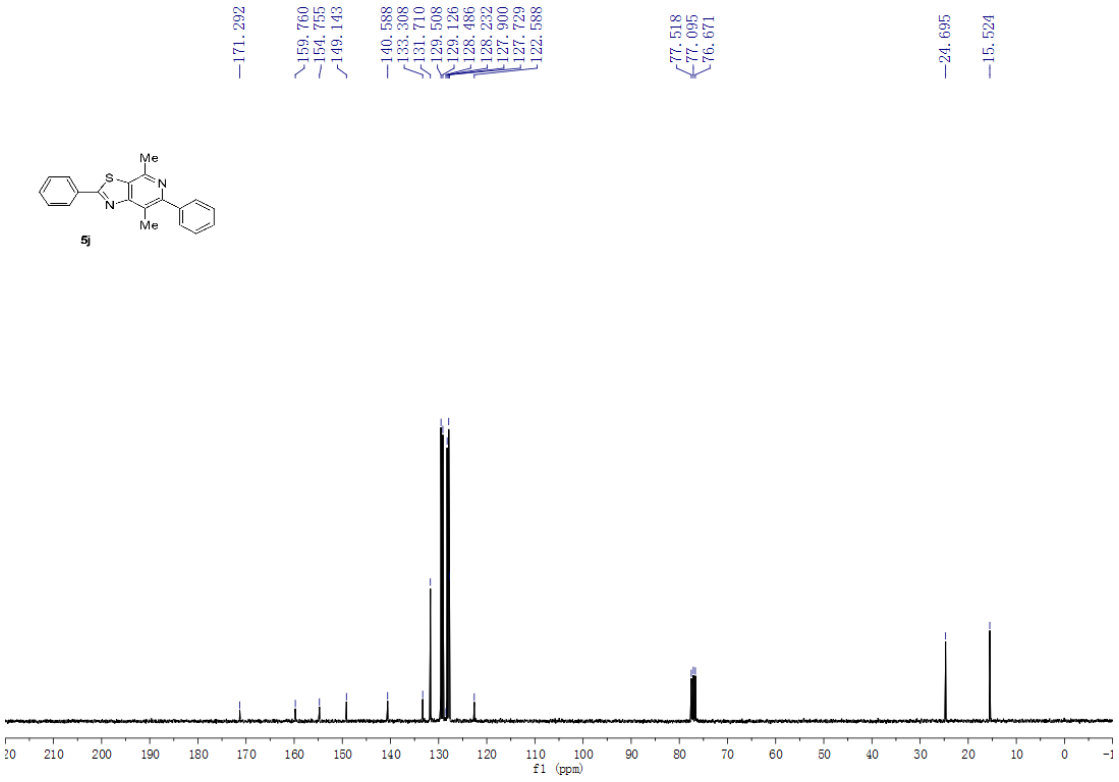

8.050
8.028
7.501
7.473
7.448
7.427
7.334
7.309
7.242
7.214
2.878
0.000
Me
S
N
N
Cl
Cl
5h
2.00
3.19
6.03
2.18
3.00
f1 (ppm)


172.148
158.682
152.441
151.506
138.587
134.661
133.727
133.418
132.898
132.828
132.021
131.709
130.511
129.112
128.262
128.248
128.044
126.052
77.517
77.094
76.669
24.942
Me
S
N
N
Cl
Cl
5h
f1 (ppm)


8.124
8.117
8.106
8.102
8.092
7.512
7.485
7.479
7.467
7.461
7.447
7.260
3.157
3.131
3.125
3.105
2.918
2.898
2.892
2.884
2.865
2.734
1.847
1.822
1.796
1.770
1.745
1.075
1.060
1.050
1.036
1.026
0.098
-0.000
Me
5i
2.00
3.10
2.11
2.19
3.12
4.24
6.24
f1 (ppm)


170.510
159.287
156.059
148.810
133.490
131.444
129.000
128.457
127.814
126.923
77.520
77.098
76.675
36.777
30.312
24.587
24.162
24.040
14.482
14.376
Me
5i
f1 (ppm)


8.162
8.157
8.140
8.131
7.596
7.572
7.515
7.510
7.496
7.473
7.448
7.417
7.393
7.369
7.244
2.811
2.725
0.000
Me
S
N
N
Me
5j
2.00
2.18
6.00
3.07
3.03
f1 (ppm)


171.292
159.760
154.755
149.143
140.588
133.308
131.710
129.508
129.126
128.486
128.232
127.900
127.729
122.588
77.518
77.095
76.671
24.695
15.524
Me
S
N
N
Me
5j
f1 (ppm)