Supplementary Information

Rhodium-catalyzed hydroarylation of alkynes via tetrazole-directed C–H activation

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1. General information:

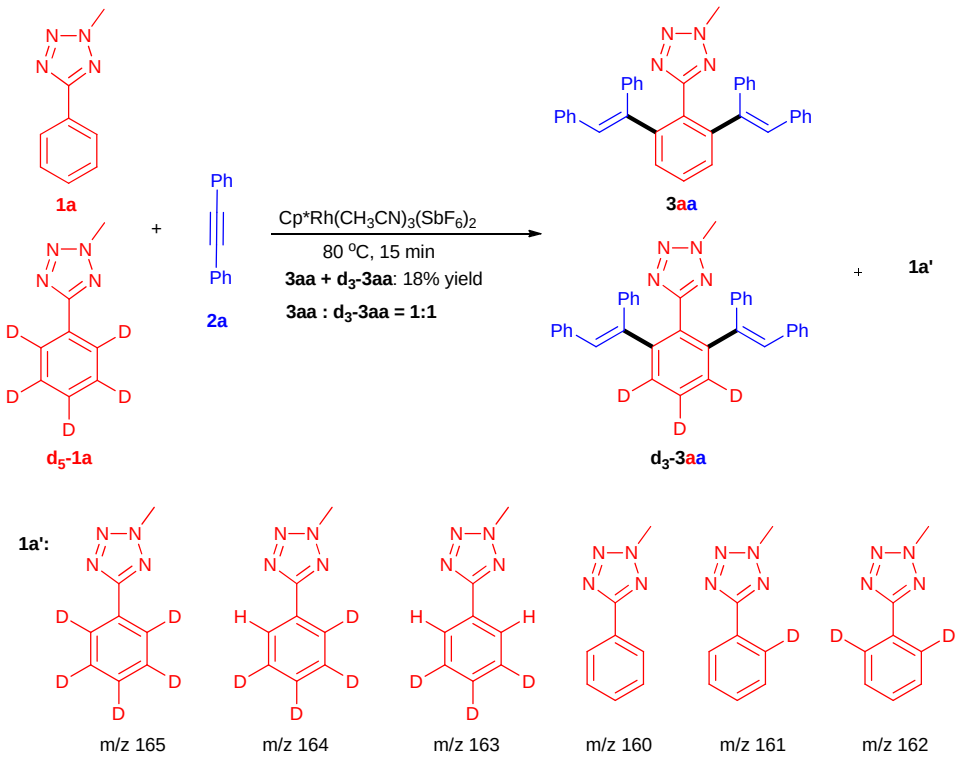
All chemicals were used as received without further purification unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 400 MHz NMR spectrometer (100 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm) and were referenced to $CDCl_3$ (7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 mesh).

Experimental procedure for the reaction: Under air, a 20 mL Schlenk tube equipped with a stir bar was charged with tetrazole **1** (0.1 mmol), alkyne **2** (0.3 mmol), benzoic acid (0.025 mmol), $Cp^*Rh(CH_3CN)_3(SbF_6)_2$ (2 mol%), acetic acid (2 mL) and sealed The reaction mixture was stirred at 80 °C for 14 h. After the completion of the reaction (monitored by TLC), the mixture was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-EtOAc as the eluent to give the desired product **3**.

Intermolecular competition experiment with 1a-d5: A 20 mL of Schlenk tube equipped with a stir bar was charged with 2-methyl-5-phenyl-2*H*-tetrazole **1a** and **d_5-1a** (1:1 0.2 mmol), 1,2-diphenylethyne **2a** (0.6 mmol), benzoic acid (0.05 mmol), $Cp^*Rh(CH_3CN)_3(SbF_6)_2$ (0.004 mmol) in 2 mL of AcOH. The tube was sealed with a Teflon lined cap. The reaction mixture was stirred at 80 °C for 15 min in oil bath. After that, the mixture was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-ethyl acetate as eluent to give product **3aa** and **d_3-3aa** in 18% yield. The mixture was analyzed using ^{1}H NMR spectrometer. As shown in Figure S1, the ratio of **3aa** and **d_3-3aa** is nearly 1:1.

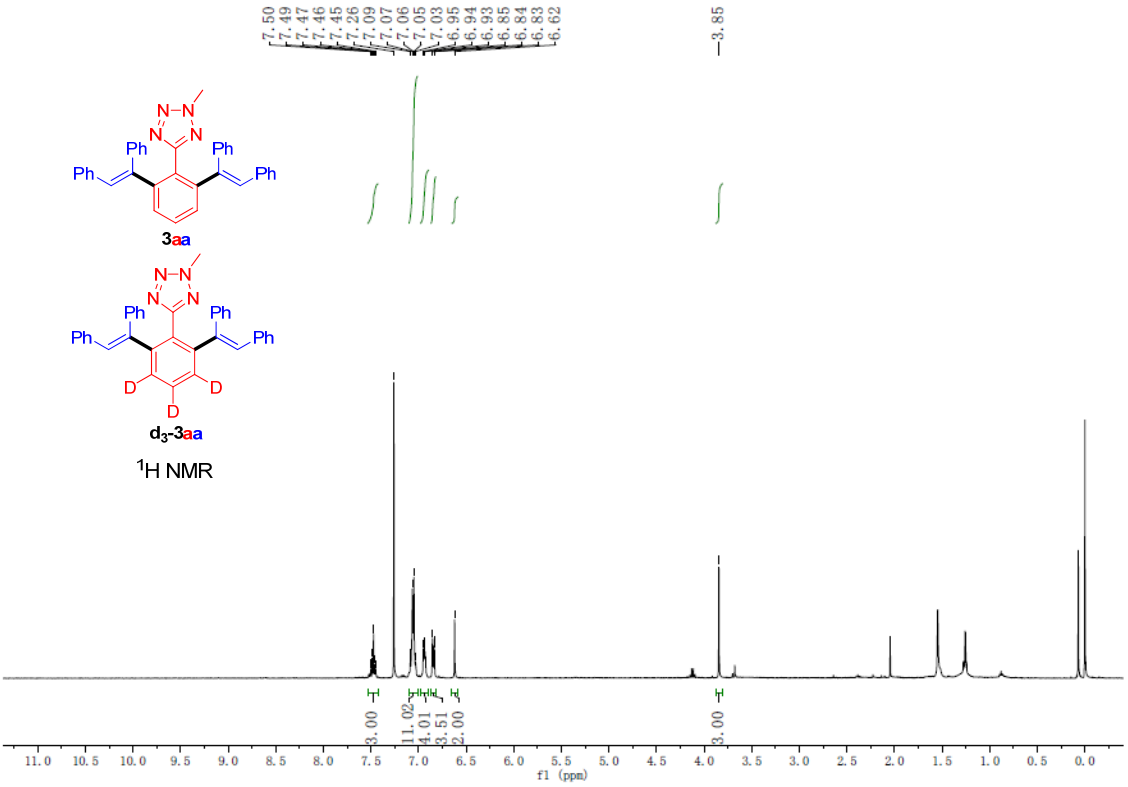
^{1}H NMR of **3aa** and **d_3-3aa** ($CDCl_3$, 400 MHz): δ 7.50-7.45 (m, 3H), 7.09-7.03 (m, 11H), 6.95-6.93 (m, 4H), 6.85-6.83 (m, 3.51H), 6.62 (s, 2H), 3.85 (s, 3H).

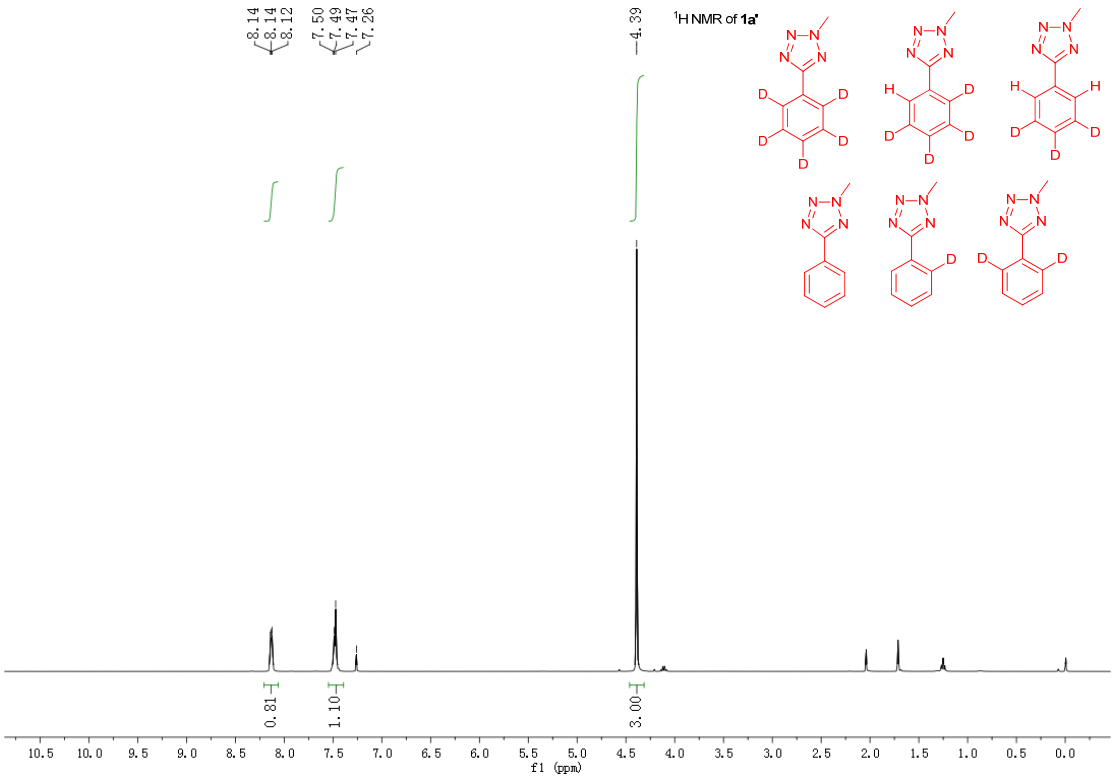
Recovered materials **1a'** of ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14-8.12(m, 0.81H), 7.50-7.47(m, 1.10H), 4.39 (s, 3H). m/z = 160, 161, 162, 163, 164, 165.



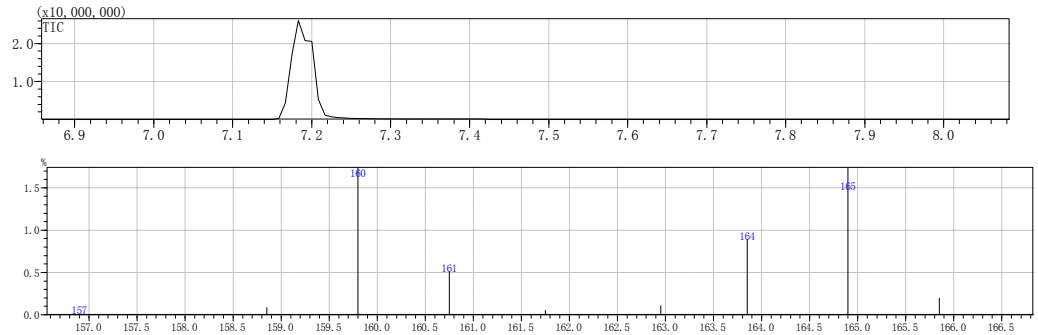
Scheme S1 Intermolecular competition experiment with **1a-d5:**

Figure S1 The ^{1}H NMR spectrum of the KIE results





The GC-MS spectra of 1a':



2. Experimental characterization data for compounds

5-(2,6-Bis((*E*)-1,2-diphenylvinyl)phenyl)-2-methyl-2*H*-tetrazole (3aa): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:25) give **3aa** (47.6 mg, 92% yield) as white solid. mp 182-184 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54-7.47 (m, 3H), 7.13-7.05 (m, 12H), 6.98-6.96 (m, 4H), 6.88 (d, J = 6.4 Hz, 4H), 6.65 (s, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.8, 146.2, 141.6, 139.9, 137.2, 131.5, 129.9, 129.8, 129.6, 129.4, 127.9, 126.8, 38.7. IR (KBr, cm^{-1}): 3074, 3051, 3018, 2955, 2922, 2851, 2360, 2341, 1519, 1489, 1443, 1406, 1357, 1186, 1078, 1029. HRMS (ESI) calcd for $C_{36}H_{29}N_4$ ([M + H]$^+$): 517.2387. Found: 517.2363.

5-(2,6-Bis((*E*)-1,2-diphenylvinyl)-4-methylphenyl)-2-methyl-2*H*-tetrazole (3ba): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ba** (50.6 mg, 94% yield) as white solid. mp 165-167 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.31 (s, 2H), 7.11-7.05 (m, 12H), 6.97-6.95 (m, 4H), 6.89 (d, J = 6.2 Hz, 4H), 6.63 (2, 2H), 3.85 (s, 3H), 2.46 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.9, 146.0, 141.8, 140.0, 139.4, 137.2, 131.2, 130.5, 129.9 129.4, 127.8, 126.8, 126.7, 123.9, 38.7, 21.4. IR (KBr, cm^{-1}): 3076, 3053, 3020, 2953, 2920, 2852, 2358, 2341, 1596, 1526, 1491, 1445, 1412, 1356, 1184, 1076, 1036, 1007. HRMS (ESI) calcd for $C_{37}H_{31}N_4$ ([M + H]$^+$): 531.2543. Found: 531.2530.

(*E*)-5-(2-(1,2-Diphenylvinyl)-5-methylphenyl)-2-methyl-2*H*-tetrazole (3ca): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ca** (33.1 mg, 94% yield) as white solid. mp 65-67 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.56 (s, 1H), 7.39-729 (m, 2H), 7.14-7.07 (m, 10H), 6.62 (s, 1H), 4.16 (s, 3H), 2.43 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 165.3, 141.9, 140.1, 137.6, 131.1, 130.9, 130.6, 130.4, 130.3, 129.4, 127.9, 127.6, 126.9, 126.7, 39.2, 21.0. IR (KBr, cm^{-1}): 3078, 3053, 3020, 2953, 2920, 2864, 2361, 2341, 1491, 1445, 1362, 1074, 1043, 1028. HRMS (ESI) calcd for $C_{23}H_{21}N_4$ ([M + H]$^+$): 353.1761. Found: 353.1754.

5-(2,6-Bis((*E*)-1,2-diphenylvinyl)-4-methoxyphenyl)-2-methyl-2*H*-tetrazole (3da): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3da** (51.1 mg, 93% yield) as white solid. mp 174-176 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.10-7.04 (m, 14H), 6.99-6.95 (m, 4H), 6.87 (d, J = 6.4Hz, 4H), 3.89 (s, 3H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.7, 160.1, 147.6, 141.7, 139.8, 137.1, 131.3, 129.9, 129.4, 127.9, 127.8, 126.8, 119.3, 115.3, 55.5, 38.6. IR (KBr, cm^{-1}): 3076, 3049, 3018, 2962, 2928, 2862, 2358, 2341, 1589, 1566, 1445, 1409, 1356, 1329, 1204, 1032. HRMS (ESI) calcd for $C_{37}H_{31}N_4O$ ([M + H]$^+$): 547.2492. Found: 547.2482.

5-(4,6-bis((*E*)-1,2-Diphenylvinyl)benzo[d][1,3]dioxol-5-yl)-2-methyl-2*H*-tetrazole (3ea): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ea** (48.7 mg, 87% yield) as white solid. mp 65-66 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.12-7.05 (m, 12H), 6.97-6.92 (m, 9H), 6.71 (s, 1H), 6.56 (s, 1H), 6.02 (s, 2H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.5, 148.4, 141.3, 140.7, 140.0, 137.1, 136.6, 134.6, 133.3, 131.2, 129.9, 129.7, 129.4, 129.3, 127.8, 126.9, 109.8, 101.6, 38.7. IR (KBr, cm^{-1}): 3078, 3053, 3020, 2957, 2918, 2853,

2358, 2341, 1716, 1599, 1491, 1456, 1393, 1263, 1220, 1080, 1065, 1032, 1007. HRMS (ESI) calcd for $C_{37}H_{29}N_4O_2$ ([M + H]$^+$): 561.2285. Found: 561.2259.

5-(4-Bromo-2,6-bis((*E*)-1,2-diphenylvinyl)phenyl)-2-methyl-2*H*-tetrazole (3fa): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3fa** (52.5 mg, 88% yield) as white solid. mp 80-82 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.65 (s, 2H), 7.12-7.05 (m, 12H), 6.95-6.93 (m, 4H), 6.84 (d, J = 6.4Hz, 4H), 6.64 (s, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.0, 147.9, 140.3, 139.3, 136.7, 132.4, 132.2, 129.8, 129.4, 128.0, 127.9, 127.1, 127.0, 125.8, 123.8, 38.7. IR (KBr, cm^{-1}): 3078, 3055, 3022, 2956, 2927, 2852, 2356, 2329, 1598, 1574, 1504, 1404, 1355, 1223, 1157, 1095, 1038, 1012. HRMS (ESI) calcd for $C_{36}H_{28}BrN_4$ ([M + H]$^+$): 595.1492. Found: 595.1487.

5-(2,6-Bis((*E*)-1,2-diphenylvinyl)-4-fluorophenyl)-2-methyl-2*H*-tetrazole (3ga): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ga** (47.2 mg, 88% yield) as white solid. mp 143-145 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.12-7.06 (m, 12H), 6.96 (s, 4H), 6.86 (d, J = 6.4 Hz, 4H), 6.64 (S, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.1, 148.5 (d, $J_{C\text{-}F}$ = 8.2 Hz), 140.6, 139.4, 136.7, 132.1, 129.8, 129.4, 127.9 (d, $J_{C\text{-}F}$ = 7.1 Hz), 127.0, 116.7 (d, $J_{C\text{-}F}$ = 21.6 Hz), 38.7. IR (KBr, cm^{-1}): 3055, 3022, 2955, 2926, 2869,2854, 2358, 2329, 1587, 1491, 1445, 1409, 1356, 1182, 1136, 1117, 1076, 1029. HRMS (ESI) calcd for $C_{36}H_{28}FN_4$ ([M + H]$^+$): 535.2293. Found: 535.2285.

5-(2,6-Bis((*E*)-1,2-diphenylvinyl)-4-(trifluoromethyl)phenyl)-2-methyl-2*H*-tetrazole (3ha): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ha** (50.6 mg, 86% yield) as white solid. mp 156-158 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.75 (s, 2H), 7.11-7.04 (m, 12H), 6.97-6.95 (m, 4H), 6.82 (d, J = 6.8Hz, 4H), 6.88 (s, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.7, 147.1, 140.4, 139.1, 136.6, 132.6, 131.6 (q, J = 137.9 Hz), 129.8, 129.4, 128.0, 127.9, 127.2, 127.1, 126.2 (q, J = 3.5 Hz), 38.7. IR (KBr, cm^{-1}): 3078, 3055, 3022, 2957, 2928, 2359, 2332, 1526, 1491, 1445, 1423, 1342, 1315, 1249, 1186, 1163, 1132, 1089, 1078. HRMS (ESI) calcd for $C_{37}H_{28}F_3N_4$ ([M + H]$^+$): 585.2261. Found: 585.2233.

3,5-bis((*E*)-1,2-diphenylvinyl)-4-(2-methyl-2*H*-tetrazol-5-yl)benzoic acid (3ia): Flash column chromatography on a silica gel (dichloromethane: ethyl acetate: petroleum ether, 1:1:3) give **3ia** (30.8 mg, 57% yield) as white solid. mp 213-215 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.93

(s, 2H), 7.11-7.02 (m, 12H), 6.95-6.93 (m, 4H), 6.83-6.81 (m, 4H), 6.68 (s, 2H), 3.84 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 168.8, 162.9, 146.9, 140.7, 139.3, 136.8, 134.3, 132.3, 130.2, 129.9, 129.4, 128.5, 128.0, 127.9, 127.1, 127.0, 38.7. IR (KBr, cm^{-1}): 3456, 3294, 3178, 2957, 2923, 2853, 2358, 2341, 1732, 1682, 1655, 1612, 1558, 1445, 1389, 1275. HRMS (ESI) calcd for $C_{37}H_{29}N_4O_2$ ($[M + H]^+$): 561.2285. Found: 561.2277.

(*E*)-5-(2-(1,2-Diphenylvinyl)-6-methylphenyl)-2-methyl-2*H*-tetrazole (3ja): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ja** (32.6 mg, 92% yield) as white solid. mp 89-91 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.42-7.35 (m, 2H), 7.29-7.26 (m, 1H), 7.11-7.05 (m, 6H), 7.01-6.98 (m, 2H), 6.87 (d, J = 6.8 Hz, 2H), 6.65 (s, 1H), 4.13 (s, 3H), 2.15 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.1, 145.9, 142.1, 140.1, 138.6, 137.3, 129.9, 129.6, 129.5, 129.4, 128.1, 127.9, 127.8, 126.8, 39.1, 20.2. IR (KBr, cm^{-1}): 3051, 3024, 2955, 2922, 2868, 2358, 2331, 1574, 1522, 1493, 1456, 1441, 1416, 1404, 1356, 1188, 1074, 1038. HRMS (ESI) calcd for $C_{23}H_{21}N_4$ ($[M + H]^+$): 353.1761. Found: 353.1754.

(*E*)-5-(2-Chloro-6-(1,2-diphenylvinyl)phenyl)-2-methyl-2*H*-tetrazole (3ka): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:20) give **3ka** (32.9 mg, 88% yield) as white solid. mp 122-124 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49-7.42 (m, 3H), 7.14-7.06 (m, 6H), 6.99-6.97 (m, 2H), 6.86 (d, J = 6.8Hz, 2H), 6.66 (s, 1H), 4.13 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 162.2, 147.9, 140.7, 139.4, 136.7, 135.3, 132.1, 130.9, 129.9, 129.4, 128.9, 128.8, 128.0, 127.9, 127.1, 127.0, 126.8, 39.2. IR (KBr, cm^{-1}): 3076, 3053, 3024, 2953, 2920, 2853, 2359, 2341, 1591, 1558, 1491, 1445, 1406, 1359, 1192, 1074. HRMS (ESI) calcd for $C_{22}H_{18}ClN_4$ ($[M + H]^+$): 373.1215. Found: 373.1209.

5-(2,6-Bis((*E*)-1,2-Dip-tolylvinyl)phenyl)-2-methyl-2*H*-tetrazole (3ab): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:25) give **3ab** (49.6 mg, 87% yield) as white solid. mp 79-81 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.51-7.43 (m, 3H), 6.92-6.84 (m, 12H), 6.78 (d, J = 8.0Hz, 4H), 6.56 (s, 2H), 3.88 (s, 3H), 2.26 (s, 6H), 2.25 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.9, 146.4, 140.7, 137.3, 136.3, 134.5, 130.9, 129.7, 129.6, 129.4, 129.2, 128.5, 126.6, 38.6, 21.3, 21.2. IR (KBr, cm^{-1}): 3076, 3045, 3020, 2953, 2918, 2864, 2358, 2341, 1508, 1456, 1406, 1354, 1182, 1034. HRMS (ESI) calcd for $C_{40}H_{37}N_4$ ($[M + H]^+$): 573.3013. Found: 573.2997.

5-(2,6-Bis((*E*)-1,2-bis(4-methoxyphenyl)vinyl)phenyl)-2-methyl-2*H*-tetrazole (3ac): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:5) give **3ac** (47.1 mg, 74% yield) as white solid. mp 80-82 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.46-7.40 (m, 3H), 6.89 (d, J = 8.8Hz, 4H), 6.78 (d, J = 8.8Hz, 4H), 6.63-6.59 (m, 8H), 6.49 (s, 2H), 3.87 (s, 3H), 3.74 (s, 6H) , 3.72 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 164.0, 158.3, 158.2, 146.5, 139.4, 132.7, 131.1, 130.5, 130.3, 130.1, 129.6, 129.4, 126.5, 113.3, 55.1, 38.6. IR (KBr, cm^{-1}): 3029, 3001, 2953, 2934, 2907, 2835, 2359, 2322, 1605, 1574, 1508, 1458, 1441, 1418, 1354, 1290, 1248, 1177, 1109, 1034. HRMS (ESI) calcd for $C_{40}H_{37}N_4O_4$ ($[M + H]^+$): 637.2809. Found: 637.2782.

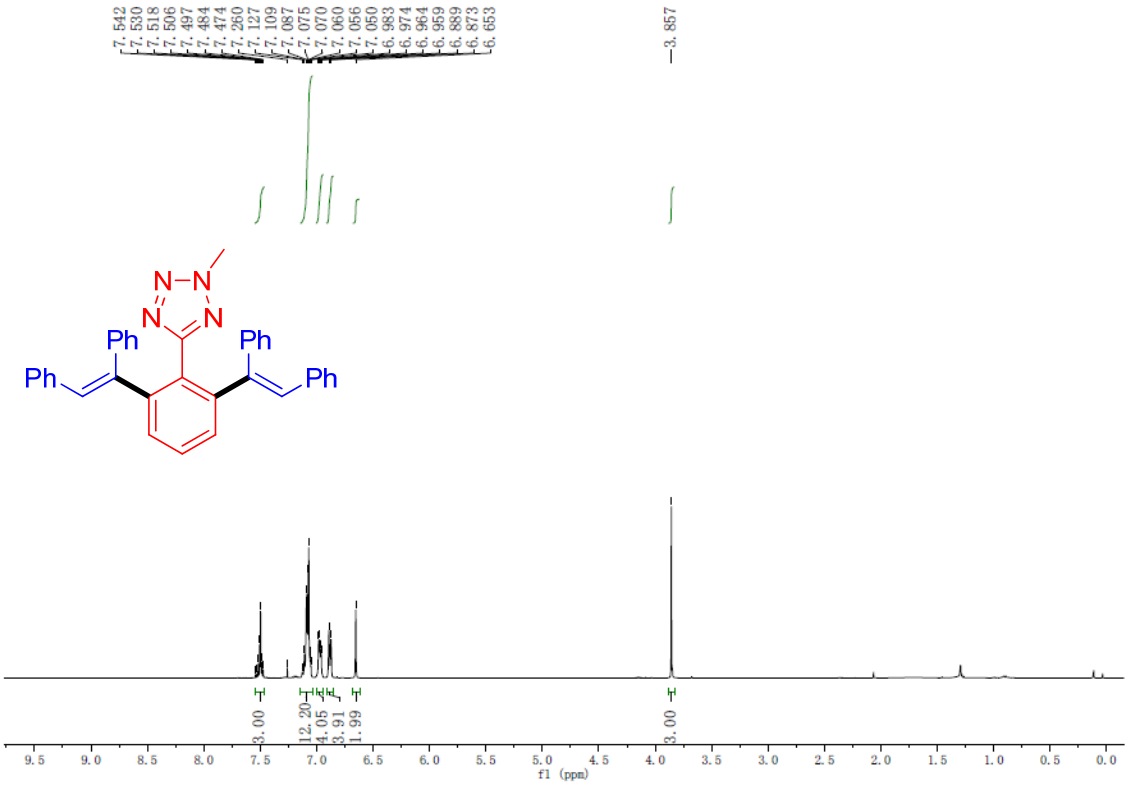
5-(2,6-Bis((*E*)-1,2-bis(4-chlorophenyl)vinyl)phenyl)-2-methyl-2*H*-tetrazole (3ad): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:25) give **3ad** (46.4 mg, 71% yield) as white solid. mp 87-89 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54-7.45 (m, 3H), 7.05 (t, J = 8.4Hz, 8H), 6.87 (d, J = 8.4Hz, 4H), 6.75 (d, J = 8.4Hz, 4H), 6.58 (s, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.5, 145.5, 140.9, 137.9, 135.1, 133.0, 132.9, 131.2, 130.6, 130.1, 129.9, 128.3, 126.5, 38.8. IR (KBr, cm^{-1}): 3051, 3028, 2955, 2924, 2853, 2357, 2329, 1591, 1489, 1456, 1398, 1354, 1180, 1092, 1034, 1013. HRMS (ESI) calcd for $C_{36}H_{25}Cl_4N_4$ ($[M + H]^+$): 653.0828. Found: 653.0826.

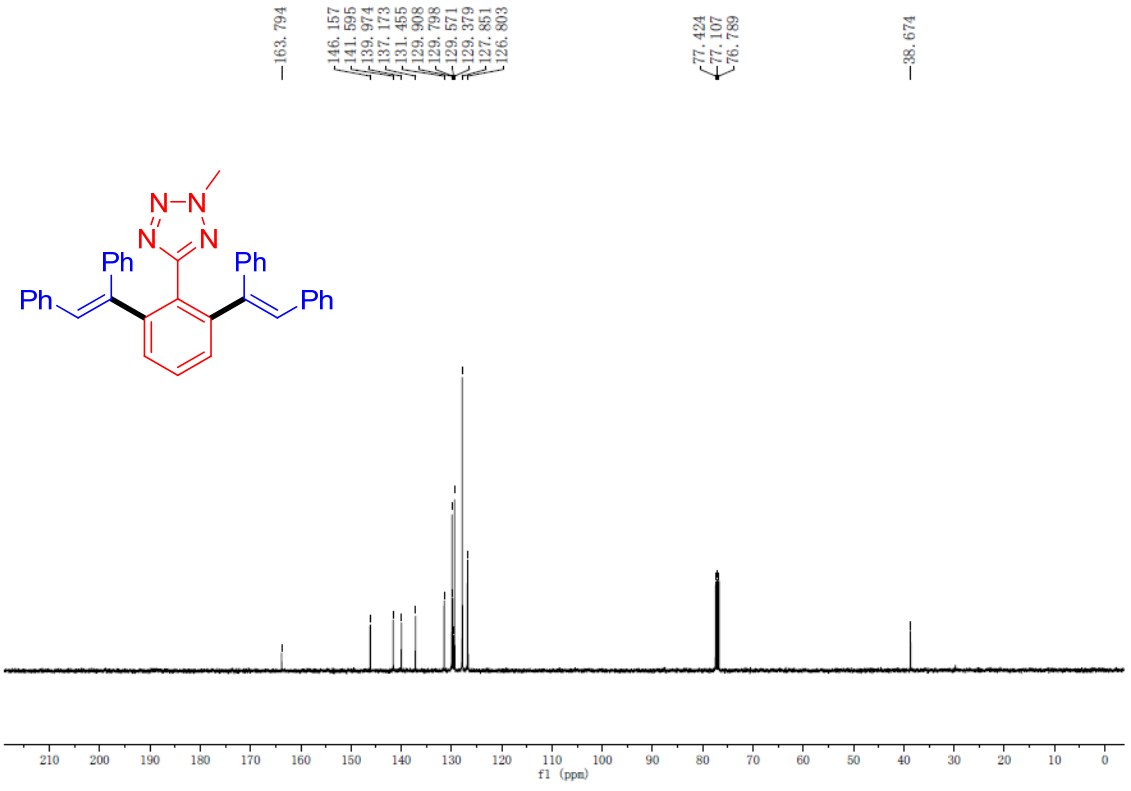
5-(2,6-Bis((*E*)-1,2-bis(4-bromophenyl)vinyl)phenyl)-2-methyl-2*H*-tetrazole (3ae): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:25) give **3ae** (59.9 mg, 72% yield) as white solid. mp 85-87 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58-7.48 (m, 3H), 7.28-7.22 (m, 4H), 7.15 (s, 2H), 7.01-6.80 (m, 11H), 6.61 (s, 2H), 4.01 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.3, 145.2, 141.4, 141.3, 138.5, 132.4, 132.3, 130.8, 130.2, 130.1, 129.8, 129.6, 128.4, 127.8, 126.7, 122.1, 121.9, 39.0. IR (KBr, cm^{-1}): 3057, 3011, 2953, 2926, 2852, 2359, 2332, 1589, 1558, 1472, 1418, 1404, 1356, 1157, 1070, 1036. HRMS (ESI) calcd for $C_{36}H_{25}Br_4N_4$ ($[M + H]^+$): 828.8807. Found: 832.8794.

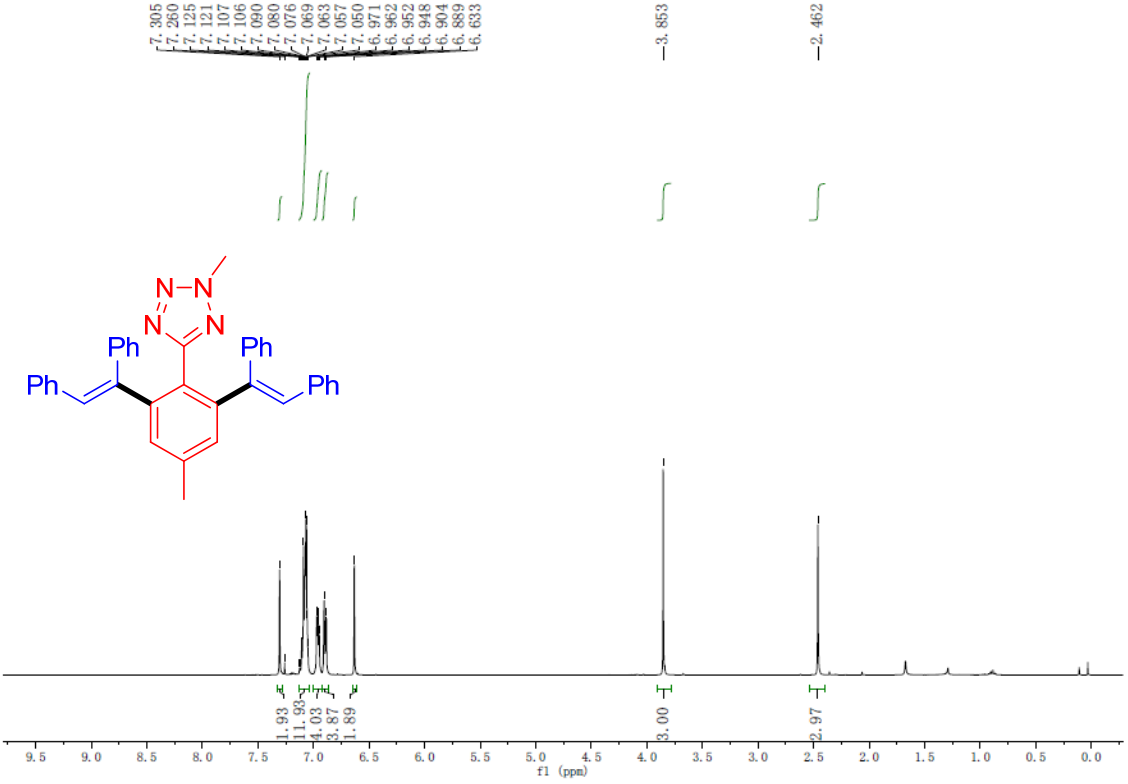
5-(2,6-Bis((*E*)-1,2-bis(4-fluorophenyl)vinyl)phenyl)-2-methyl-2*H*-tetrazole (3af): Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1:25) give **3af** (42.2 mg, 72% yield) as white solid. mp 176-178 °C. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.54-7.44 (m, 3H), 6.92-6.88 (m, 4H), 6.82-6.74 (m, 4H), 6.57 (s, 2H), 3.91 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.7, 162.9 (d, $J_{C\text{-}F}$ = 13.1 Hz), 160.5 (d, $J_{C\text{-}F}$ = 13.2 Hz), 145.8, 140.3, 135.6 (d, $J_{C\text{-}F}$ = 3.4 Hz),

132.9 (d, $J_{C\text{-}F}$ = 3.5 Hz), 131.5 (d, $J_{C\text{-}F}$ = 7.9 Hz), 130.9 (d, $J_{C\text{-}F}$ = 7.8 Hz), 130.5, 129.8 (d, $J_{C\text{-}F}$ = 10.0 Hz), 115.1 (d, $J_{C\text{-}F}$ = 2.0 Hz), 114.9(d, $J_{C\text{-}F}$ = 2.0 Hz), 38.8. IR (KBr, cm^{-1}): 3078, 3055, 3022, 2956, 2927, 2852, 2356, 2329, 1599, 1573, 1504, 1404, 1356, 1223, 1157, 1095, 1037, 1012. HRMS (ESI) calcd for $C_{36}H_{25}F_4N_4$ ($[M + H]^+$): 589.2010. Found: 589.2005.

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



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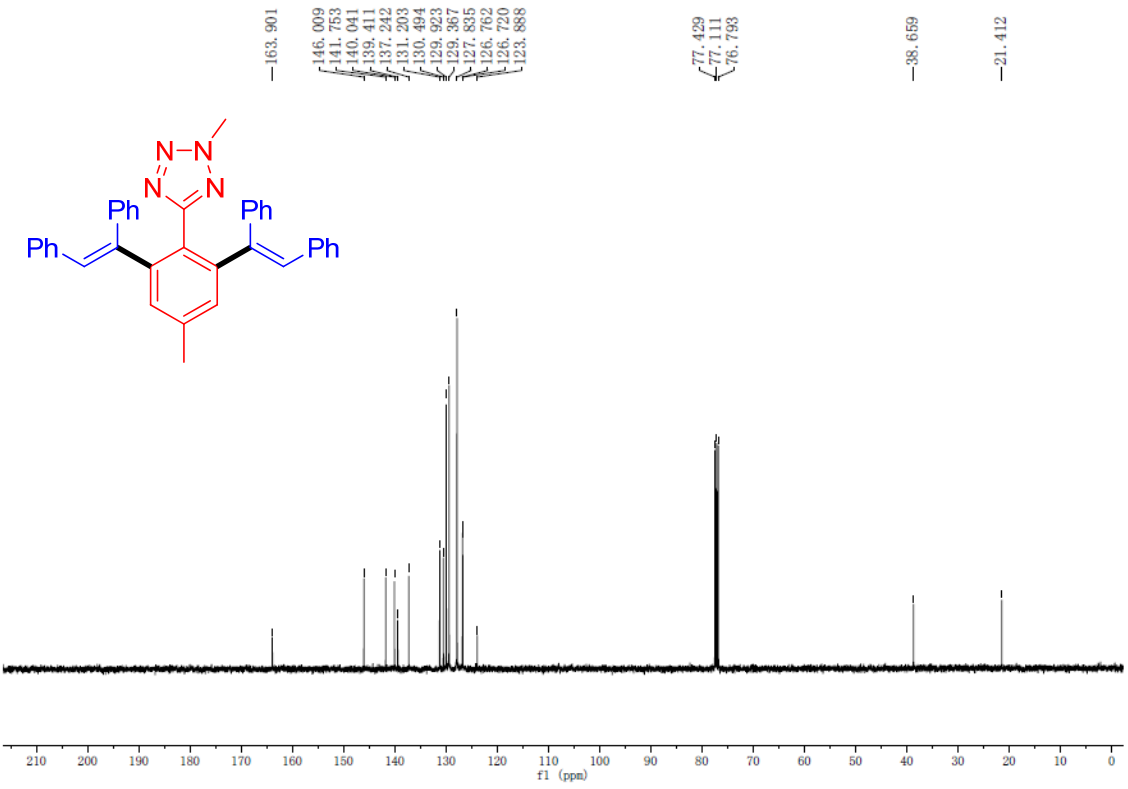
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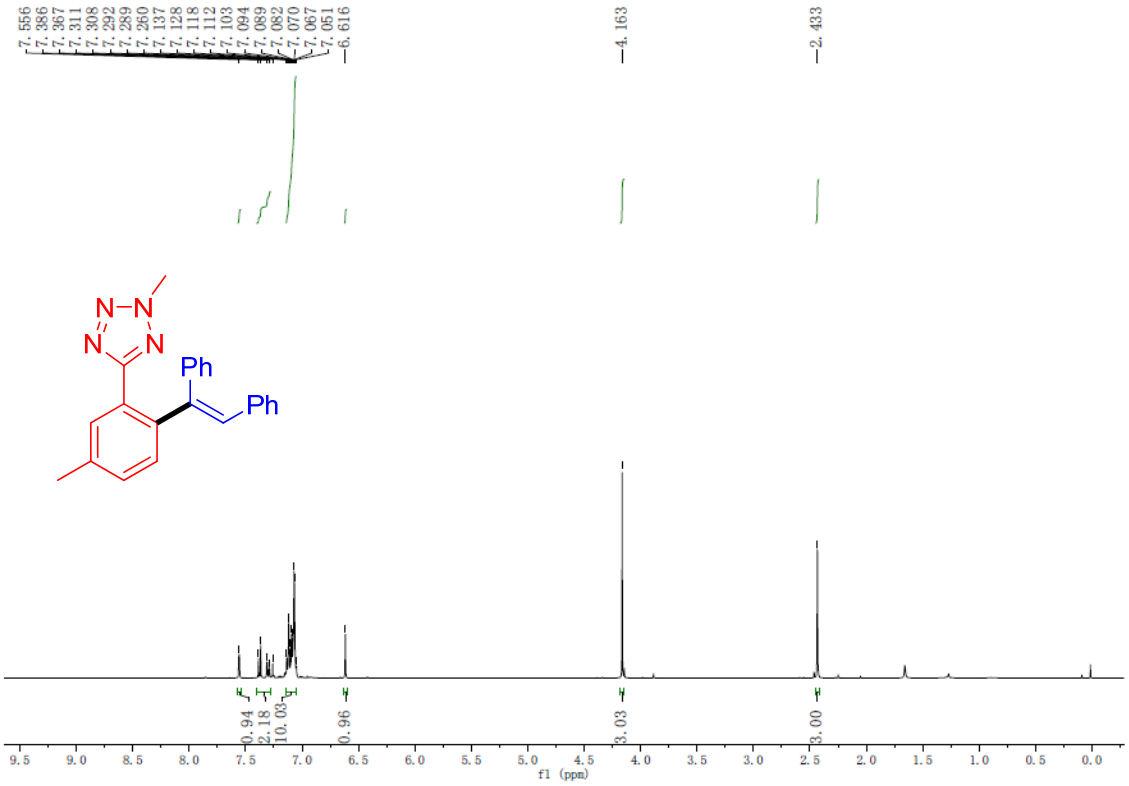
N–N
N
N
Ph
Ph
Ph
Ph
f1 (ppm)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7.386
7.367
7.311
7.308
7.292
7.289
7.260
7.137
7.128
7.118
7.112
7.103
7.094
7.089
7.082
7.070
7.067
7.051
6.616
4.163
2.433
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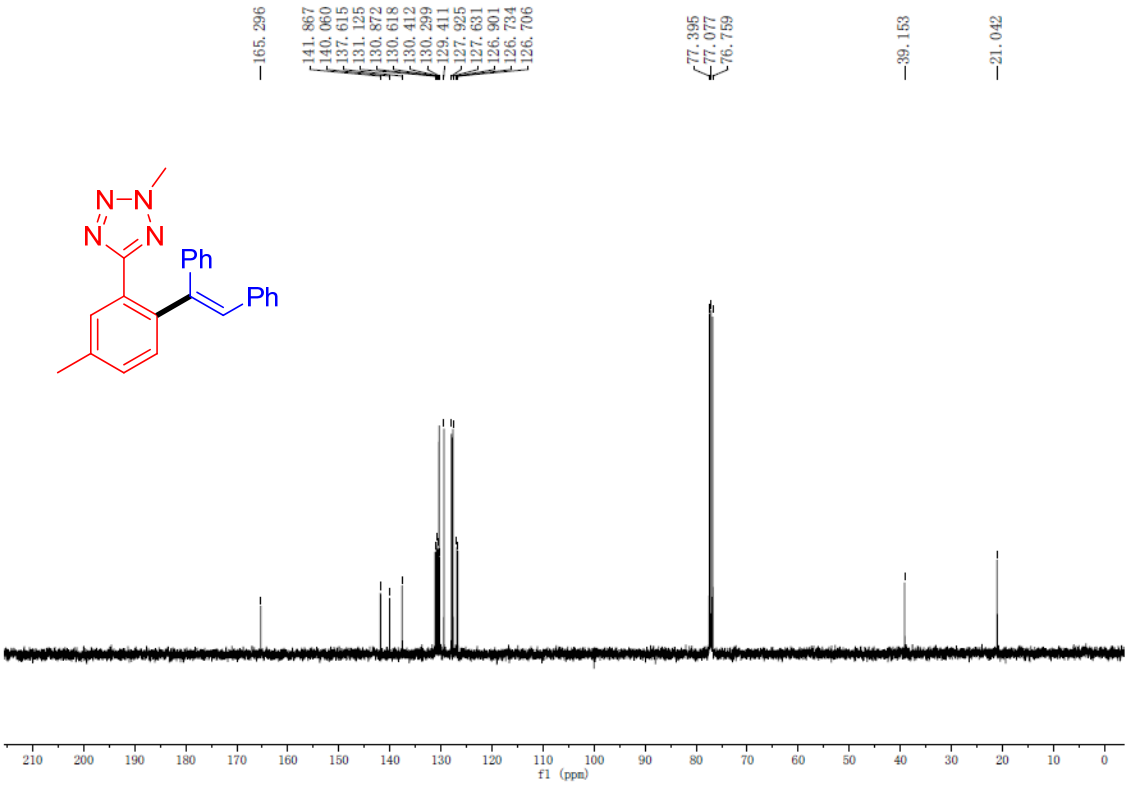
N
N
N
Ph
Ph
0.94
2.18
10.03
0.96
3.03
3.00
f1 (ppm)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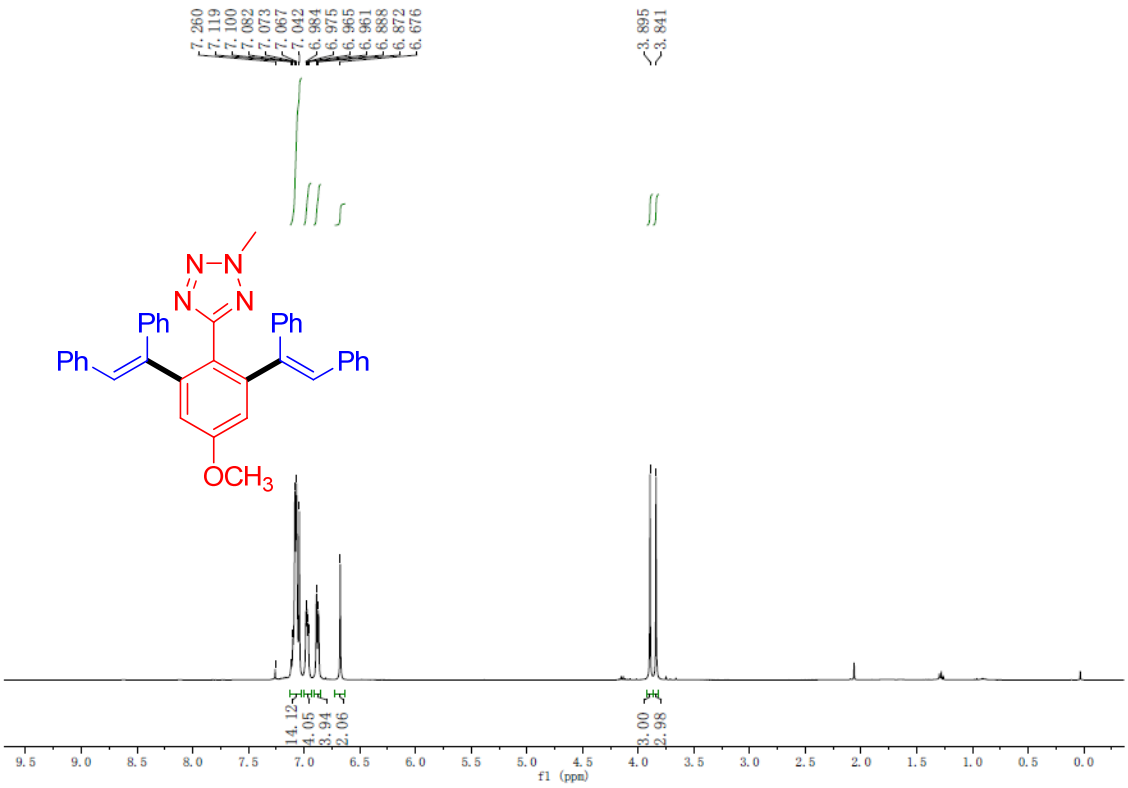
141.867
140.060
137.615
131.125
130.872
130.618
130.412
130.299
129.411
127.925
127.631
126.901
126.734
126.706
77.395
77.077
76.759
39.153
21.042
N
N
N
N
Ph
Ph
f1 (ppm)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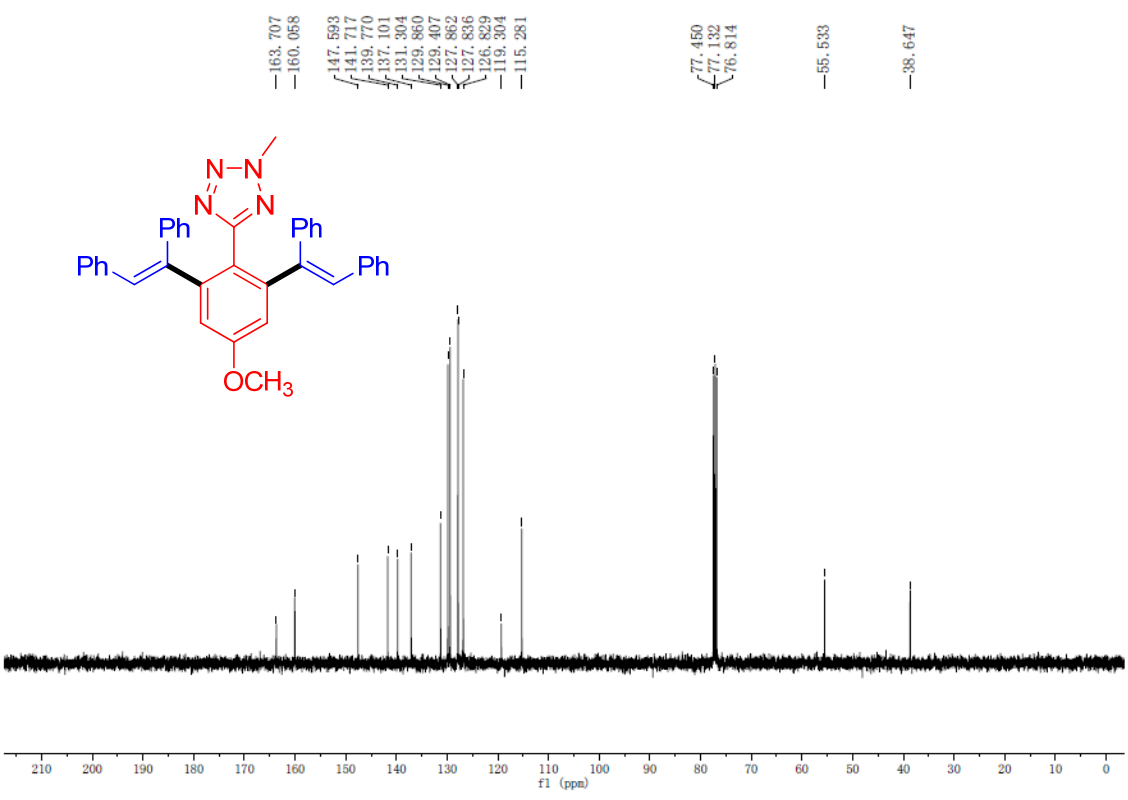
7.119
7.100
7.082
7.073
7.067
7.042
6.984
6.975
6.965
6.961
6.888
6.872
6.676
3.895
3.841
N–N
N
N
Ph
Ph
Ph
Ph
OCH3
14.12
4.05
3.94
2.06
3.00
2.98
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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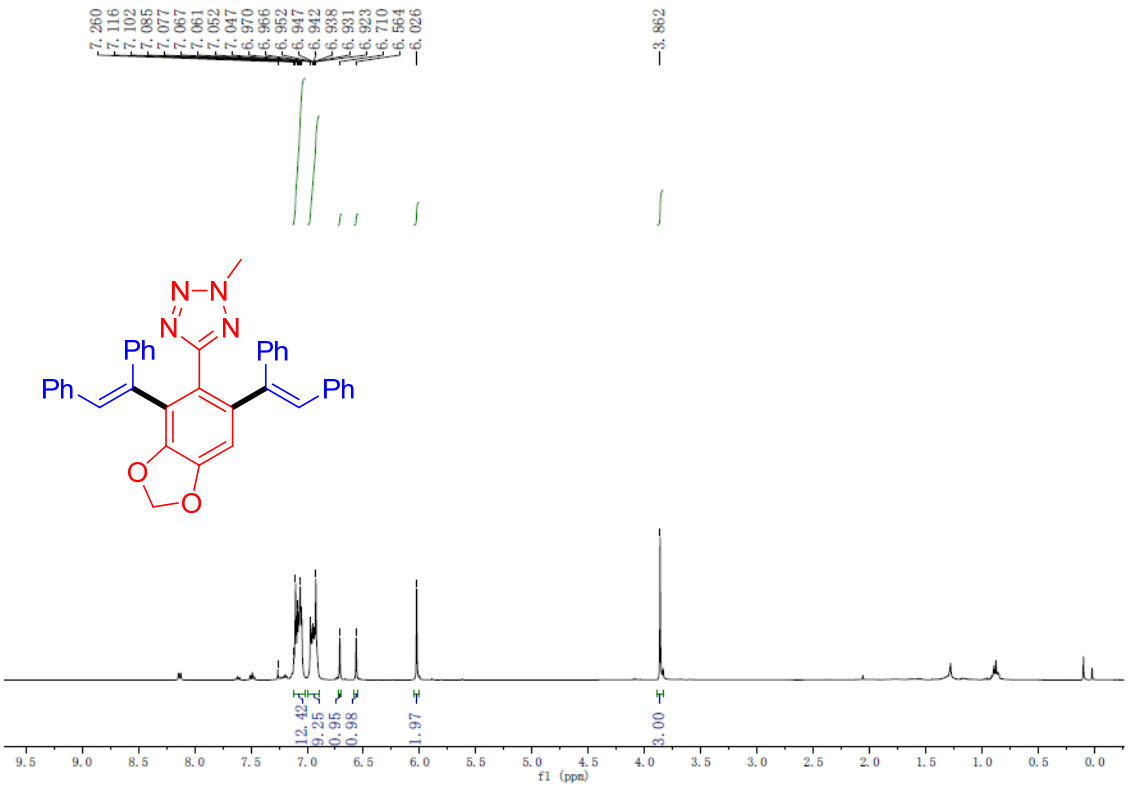
147.593
141.717
139.770
137.101
131.304
129.860
129.407
127.862
127.836
126.829
119.304
115.281
77.450
77.132
76.814
55.533
38.647
N–N
N
N
Ph
Ph
Ph
Ph
OCH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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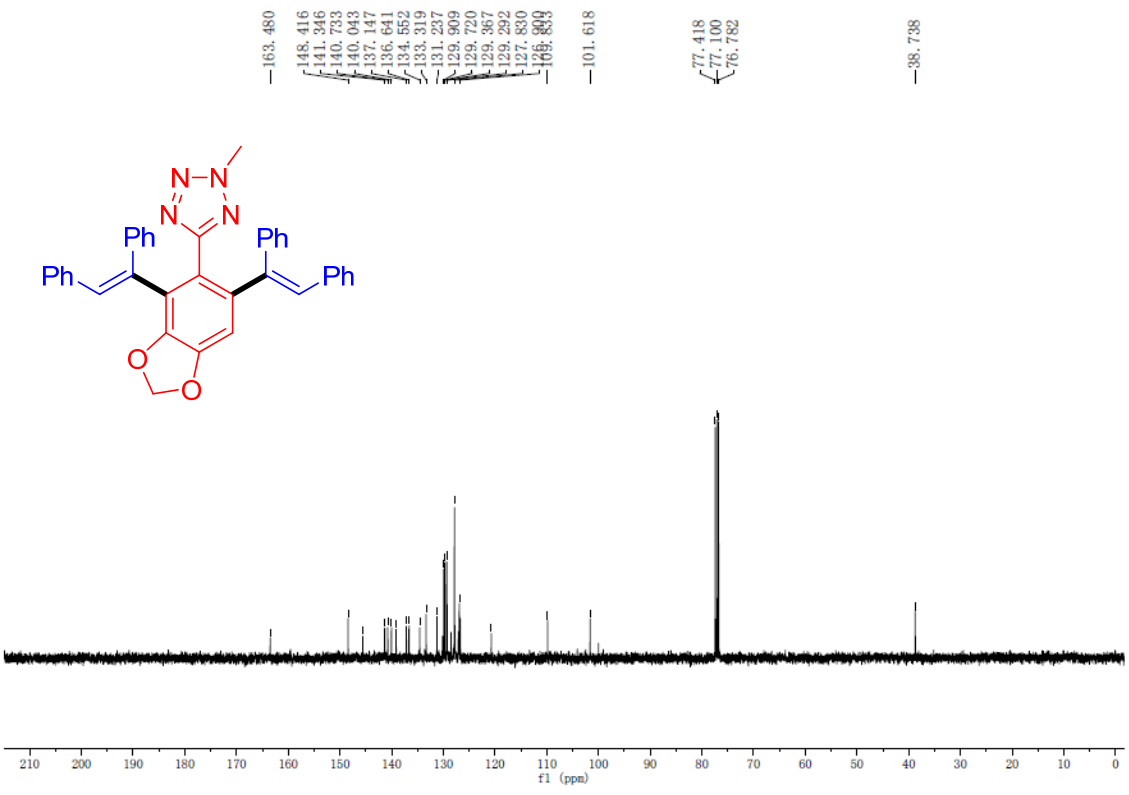
7.116
7.102
7.085
7.077
7.067
7.061
7.052
7.047
6.970
6.966
6.952
6.947
6.942
6.938
6.931
6.923
6.710
6.564
6.026
3.862
N
N
N
N
Ph
Ph
Ph
Ph
O
O
12.42
9.25
0.95
0.98
1.97
3.00
f1 (ppm)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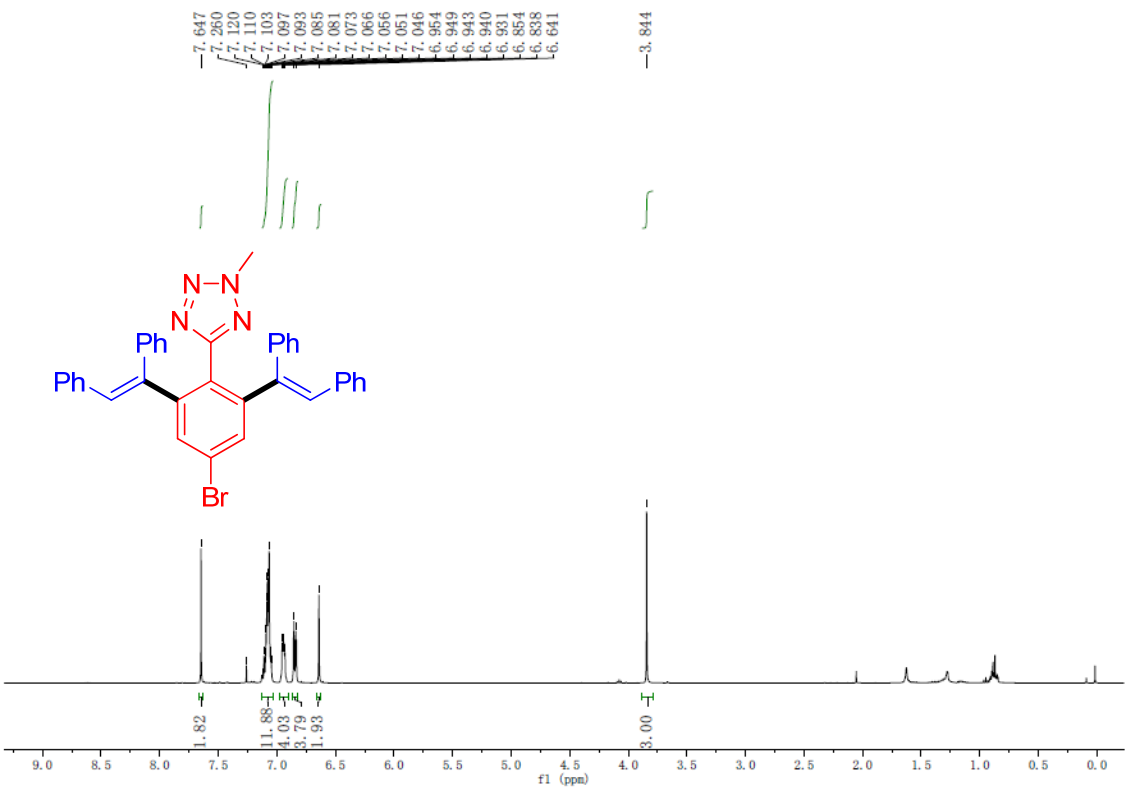
148.416
141.346
140.733
140.043
137.147
136.641
134.552
133.319
131.237
129.909
129.720
129.367
129.292
127.830
101.618
77.418
77.100
76.782
38.738
N
N
N
N
Ph
Ph
Ph
Ph
O
O
f1 (ppm)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7.260
7.120
7.110
7.103
7.097
7.093
7.085
7.081
7.073
7.066
7.056
7.051
7.046
6.964
6.949
6.943
6.940
6.931
6.854
6.838
6.641
3.844
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N
N
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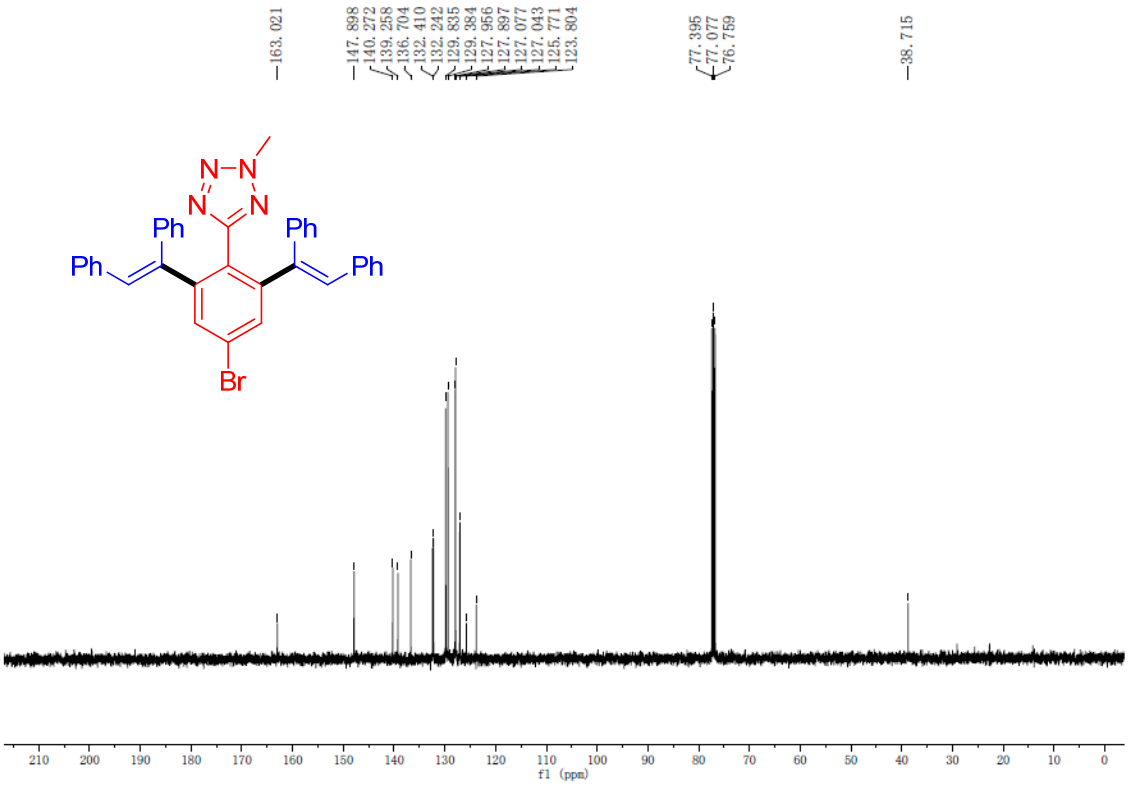
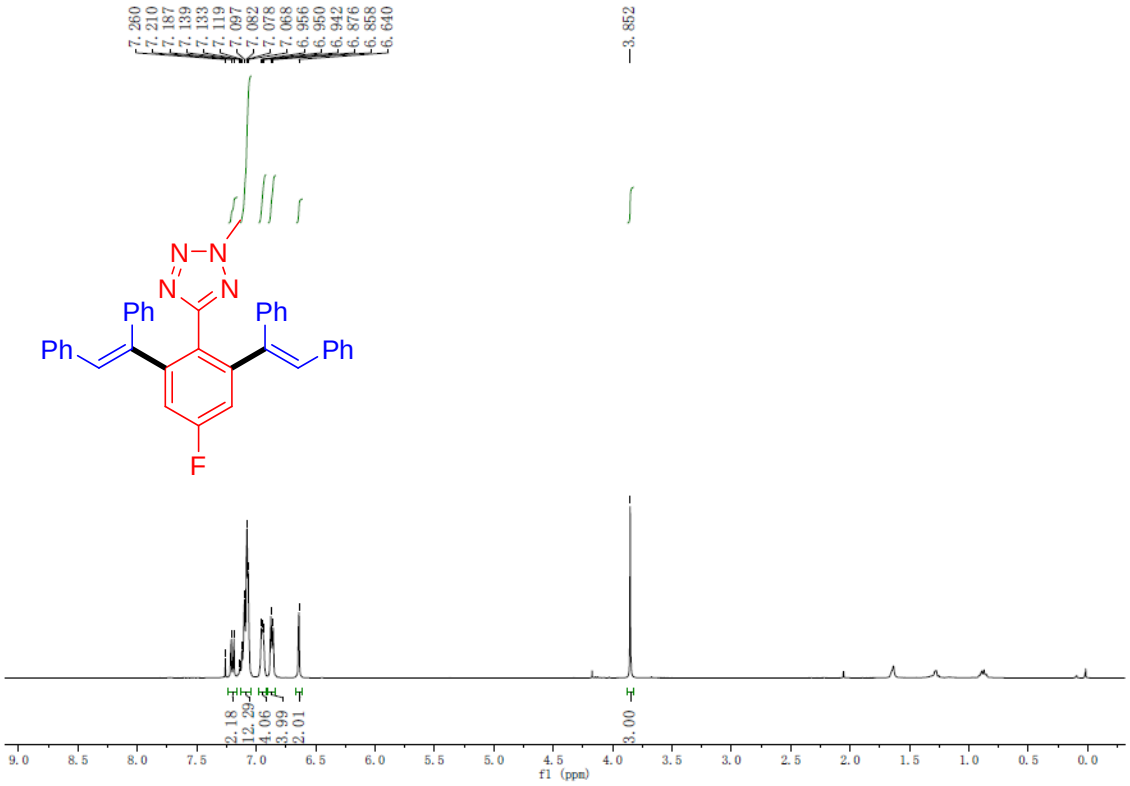
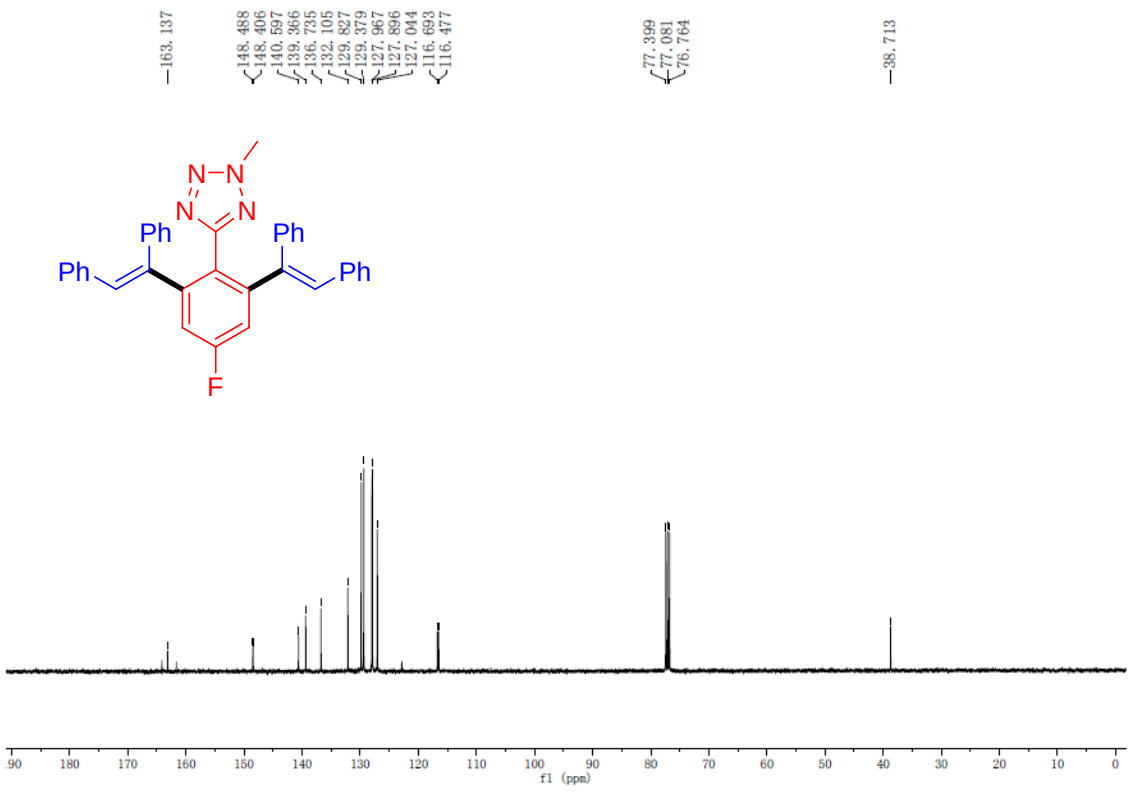
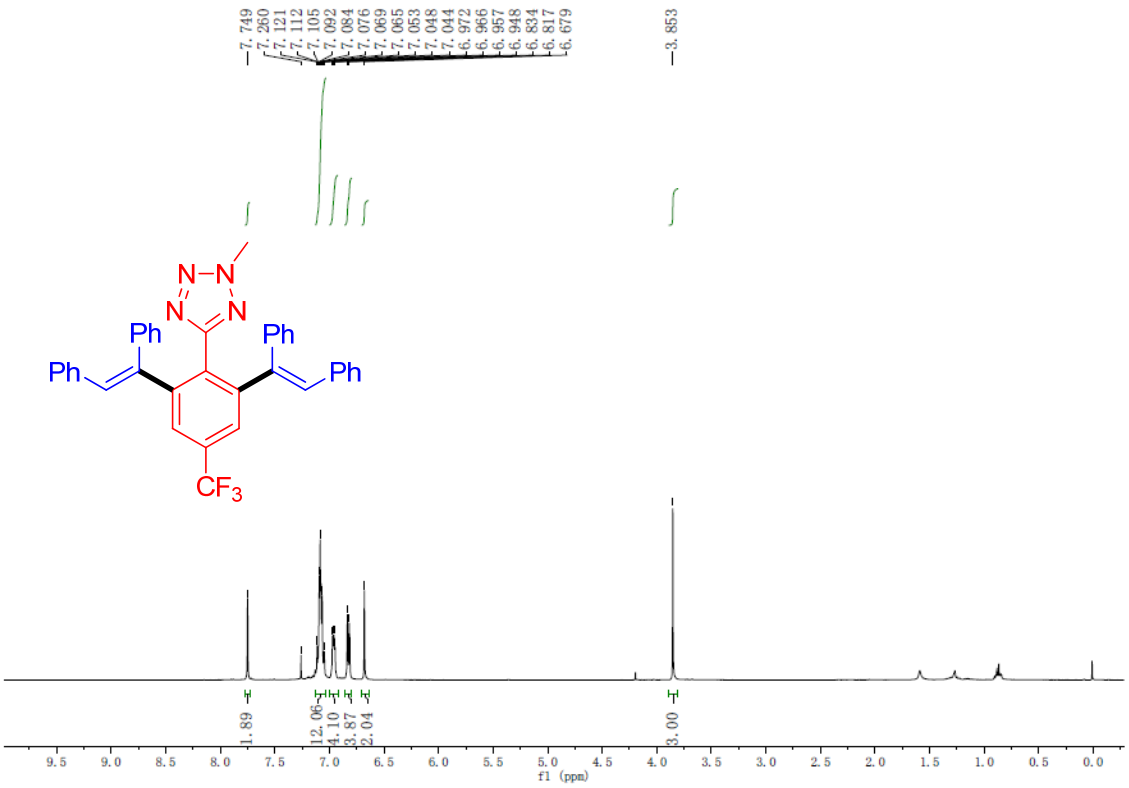
Ph
Ph
Ph
Br
1.82
11.88
4.03
3.79
1.93
3.00
f1 (ppm)


163.021
147.898
140.272
139.258
136.704
132.410
132.242
129.835
129.384
127.956
127.897
127.077
127.043
125.771
123.804
77.395
77.077
76.759
38.715
N
N
N
Ph
Ph
Ph
Ph
Br
f1 (ppm)


7.260
7.210
7.187
7.139
7.133
7.119
7.097
7.082
7.078
7.068
6.956
6.950
6.942
6.876
6.858
6.640
3.852
N
N
N
Ph
Ph
Ph
Ph
F
2.18
12.29
4.06
3.99
2.01
3.00
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)


163.137
148.488
148.406
140.597
139.366
136.735
132.105
129.827
129.379
127.967
127.896
127.044
116.693
116.477
77.399
77.081
76.764
38.713
N
N
N
Ph
Ph
Ph
Ph
F
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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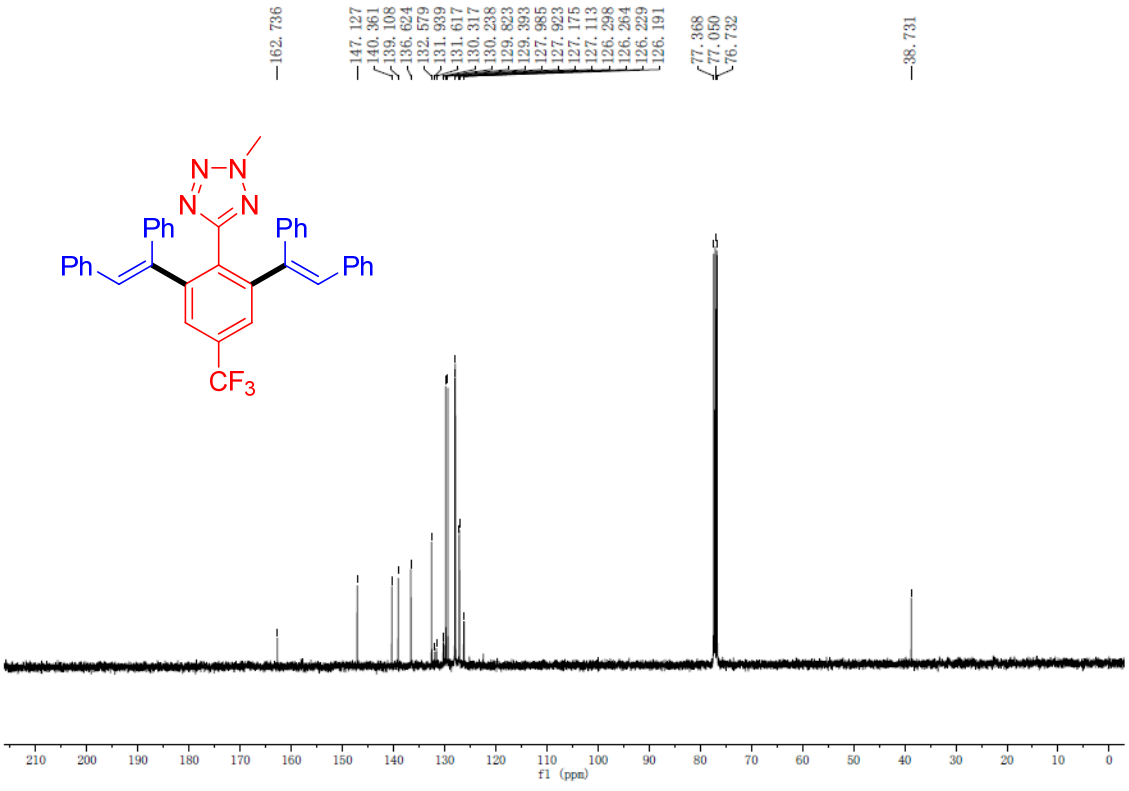
7.260
7.121
7.112
7.105
7.092
7.084
7.076
7.069
7.065
7.053
7.048
7.044
6.972
6.966
6.957
6.948
6.834
6.817
6.679
3.853
N–N
N
N
Ph
Ph
Ph
Ph
CF3
1.89
12.06
4.10
3.87
2.04
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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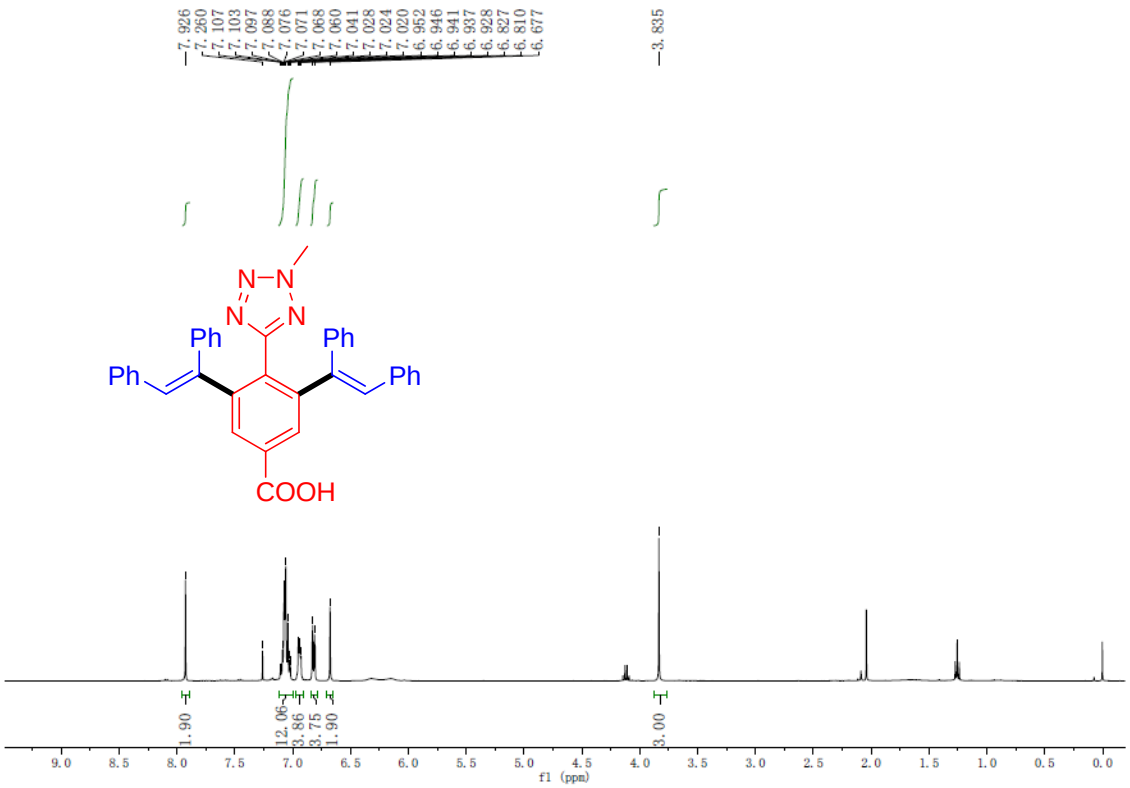
147.127
140.361
139.108
136.624
132.579
131.939
131.617
130.317
130.238
129.823
129.393
127.985
127.923
127.175
127.113
126.298
126.264
126.229
126.191
77.368
77.050
76.732
38.731
N–N
N
N
Ph
Ph
Ph
Ph
CF3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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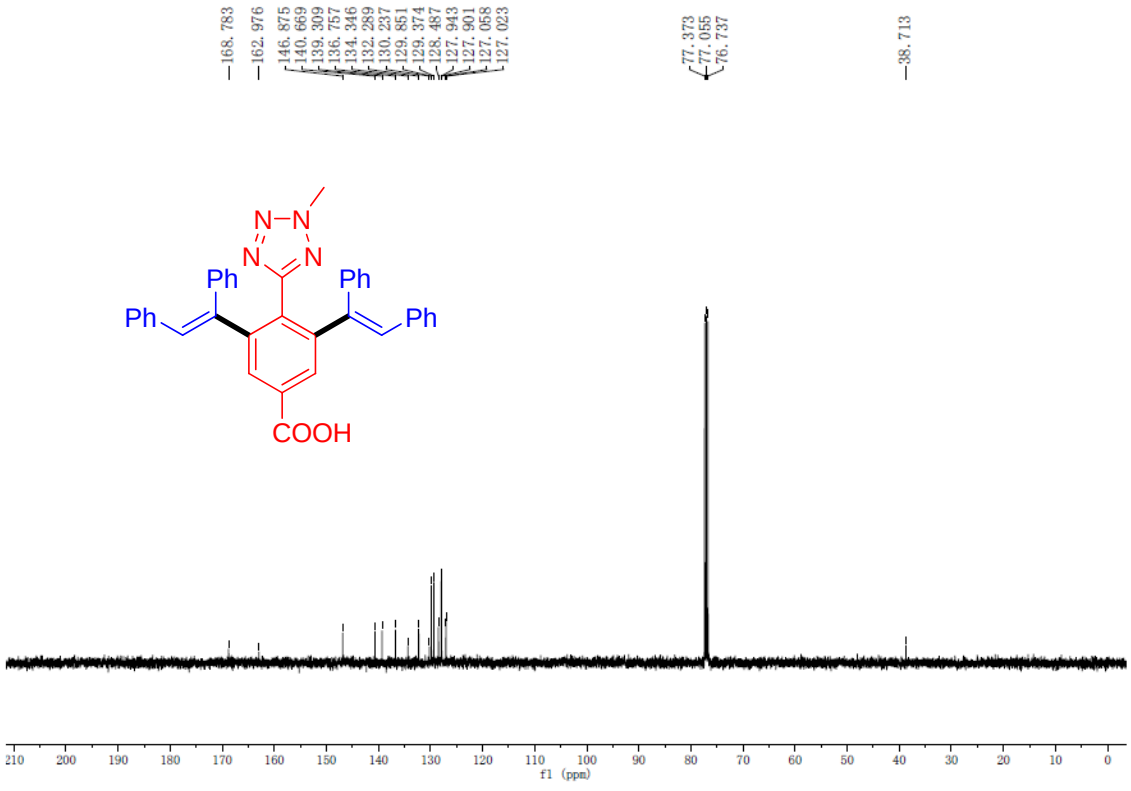
7.107
7.103
7.097
7.088
7.076
7.071
7.068
7.060
7.041
7.028
7.024
7.020
6.952
6.946
6.941
6.937
6.928
6.827
6.810
6.677
3.835
N–N
N
N
Ph
Ph
Ph
Ph
COOH
1.90
12.06
3.86
3.75
1.90
3.00
f1 (ppm)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162.976
146.875
140.669
139.309
136.757
134.946
132.289
130.237
129.851
129.374
128.487
127.943
127.901
127.058
127.023
77.373
77.055
76.737
38.713
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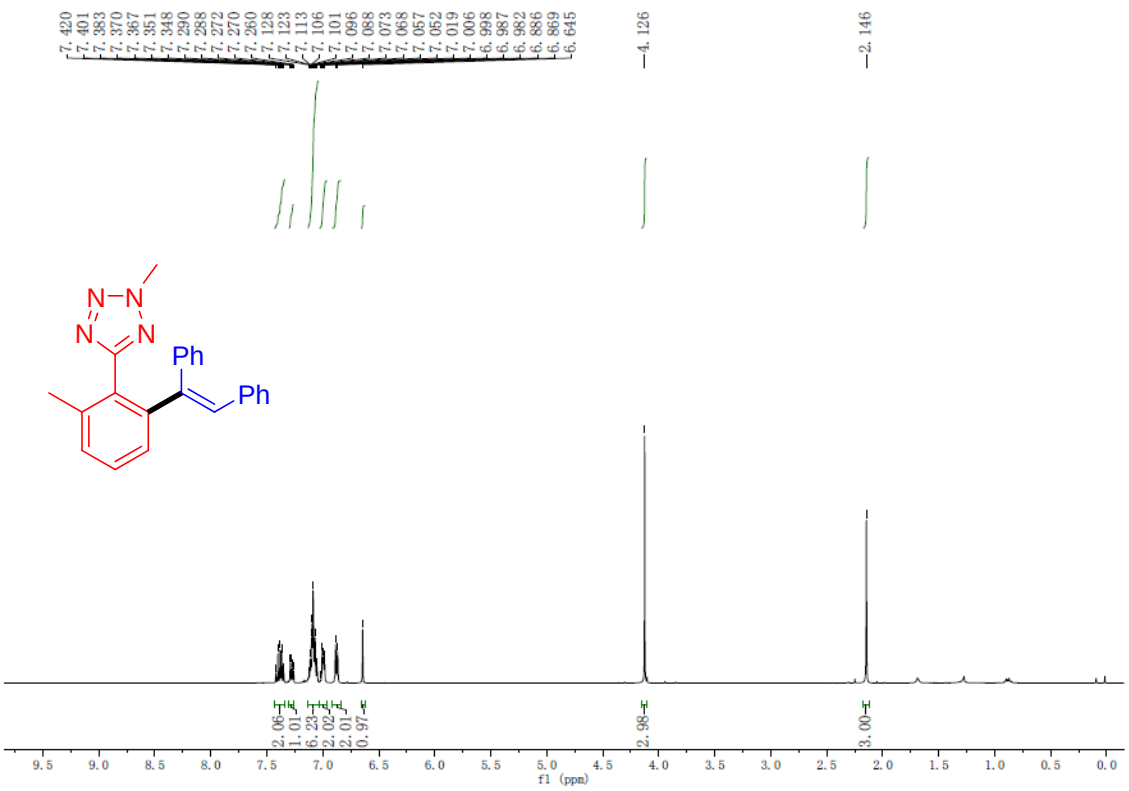
N
N
Ph
Ph
Ph
Ph
COOH
f1 (ppm)


7.420
7.401
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7.370
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7.351
7.348
7.290
7.288
7.272
7.270
7.260
7.128
7.123
7.113
7.106
7.101
7.096
7.088
7.073
7.068
7.057
7.052
7.019
7.006
6.998
6.987
6.982
6.886
6.869
6.645
4.126
2.146
N
N
N
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Ph
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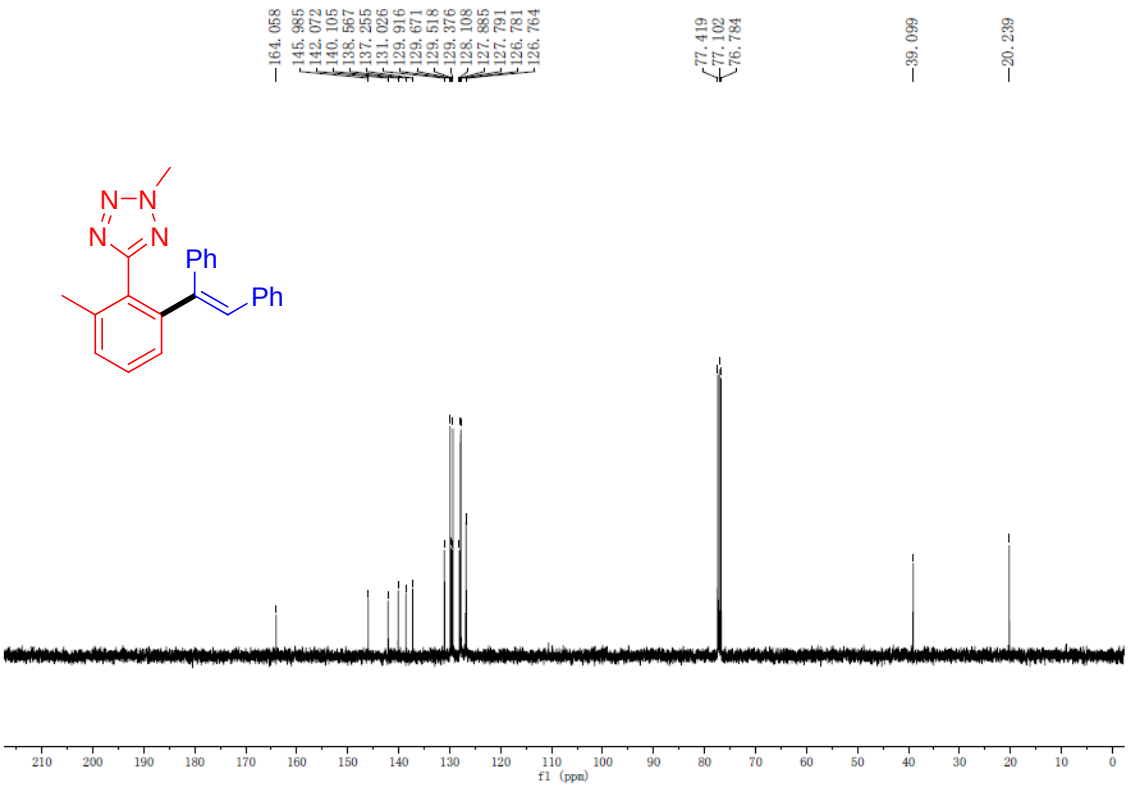
1.01
6.23
2.02
2.01
0.97
2.98
3.00
f1 (ppm)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137.255
131.026
129.916
129.671
129.518
129.376
128.108
127.885
127.791
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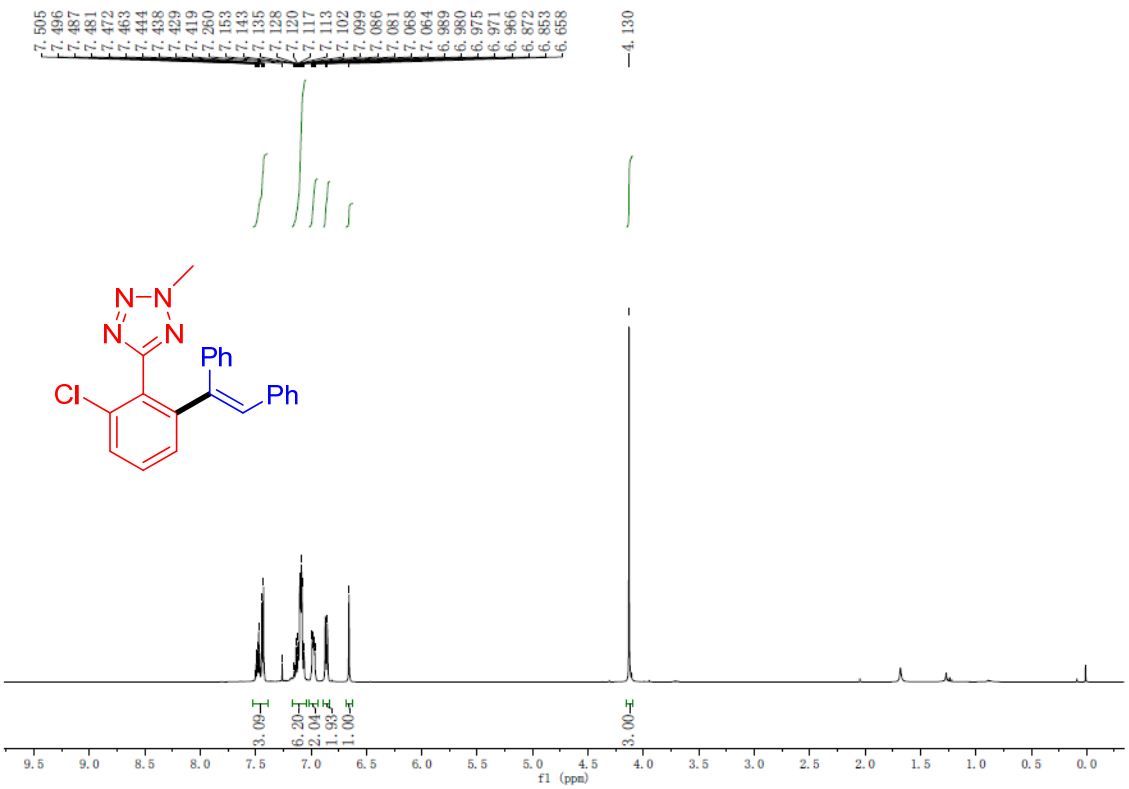
126.764
77.419
77.102
76.784
39.099
20.239
N
N
N
N
Ph
Ph
f1 (ppm)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7.487
7.481
7.472
7.463
7.444
7.438
7.429
7.419
7.260
7.153
7.143
7.135
7.128
7.120
7.117
7.113
7.102
7.099
7.086
7.081
7.068
7.064
6.989
6.980
6.975
6.971
6.966
6.872
6.853
6.658
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N
Ph
Cl
Ph
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2.04
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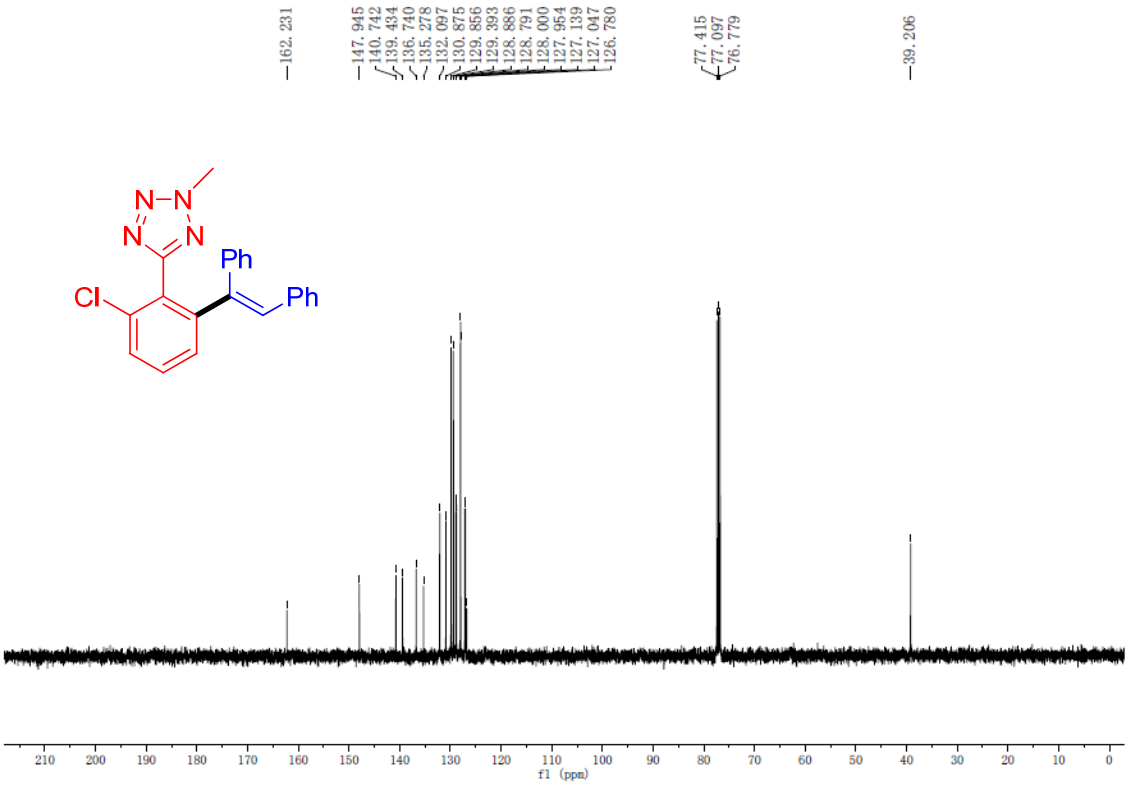
3.00
f1 (ppm)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130.875
129.856
129.393
128.886
128.791
128.000
127.954
127.139
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126.780
77.415
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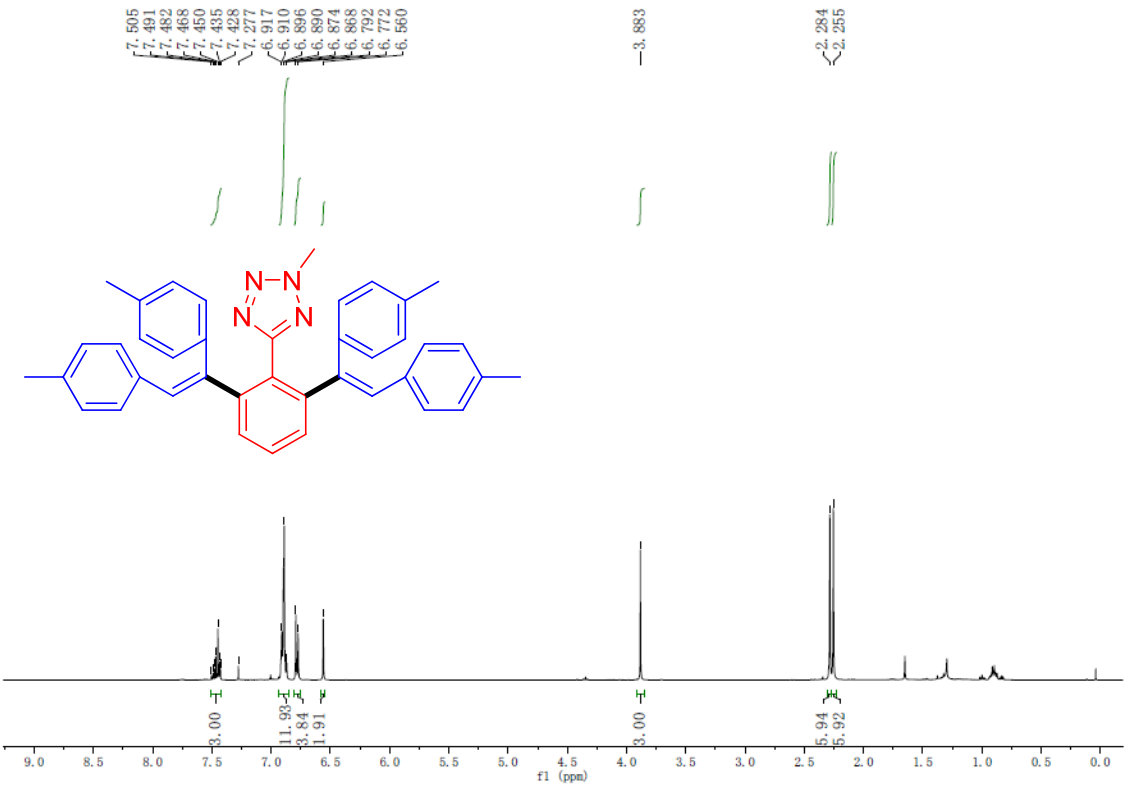
76.779
39.206
N
N
N
Ph
Cl
Ph
f1 (ppm)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7.491
7.482
7.468
7.450
7.435
7.428
7.277
6.917
6.910
6.896
6.890
6.874
6.868
6.792
6.772
6.560
3.883
2.284
2.255
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N
N
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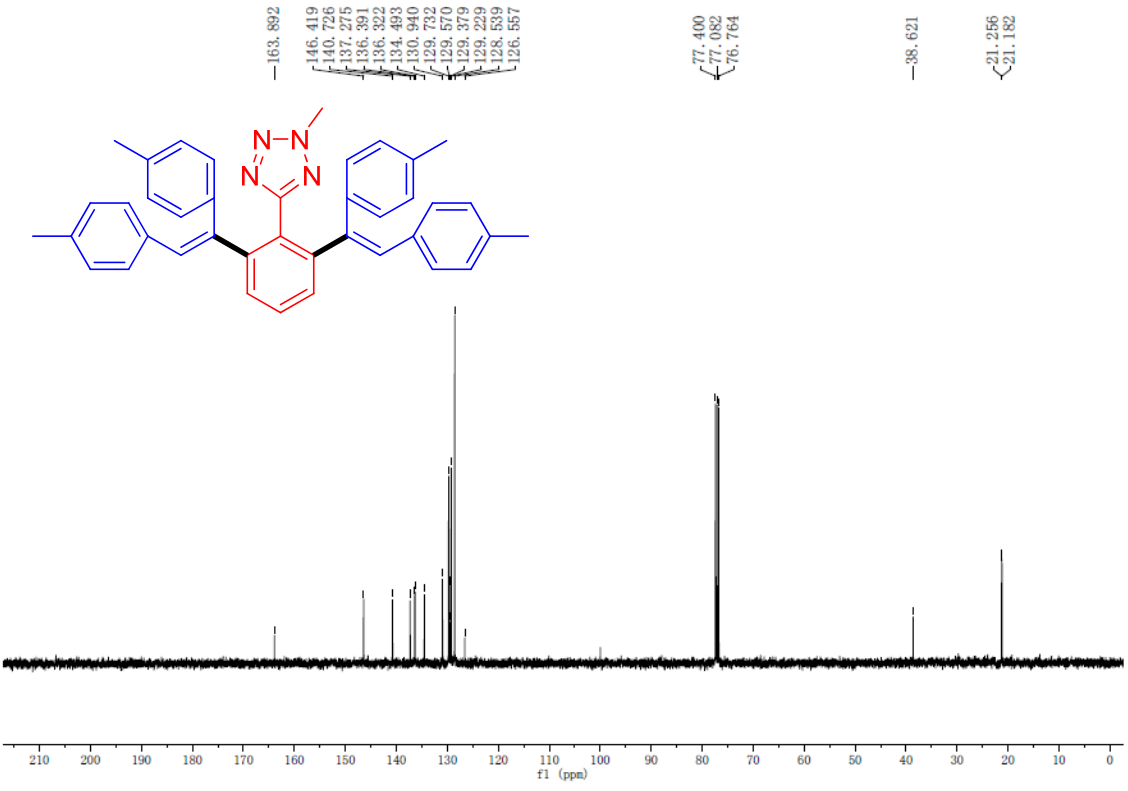
1.91
3.00
5.94
5.92
f1 (ppm)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136.322
134.493
130.940
129.732
129.570
129.379
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77.400
77.082
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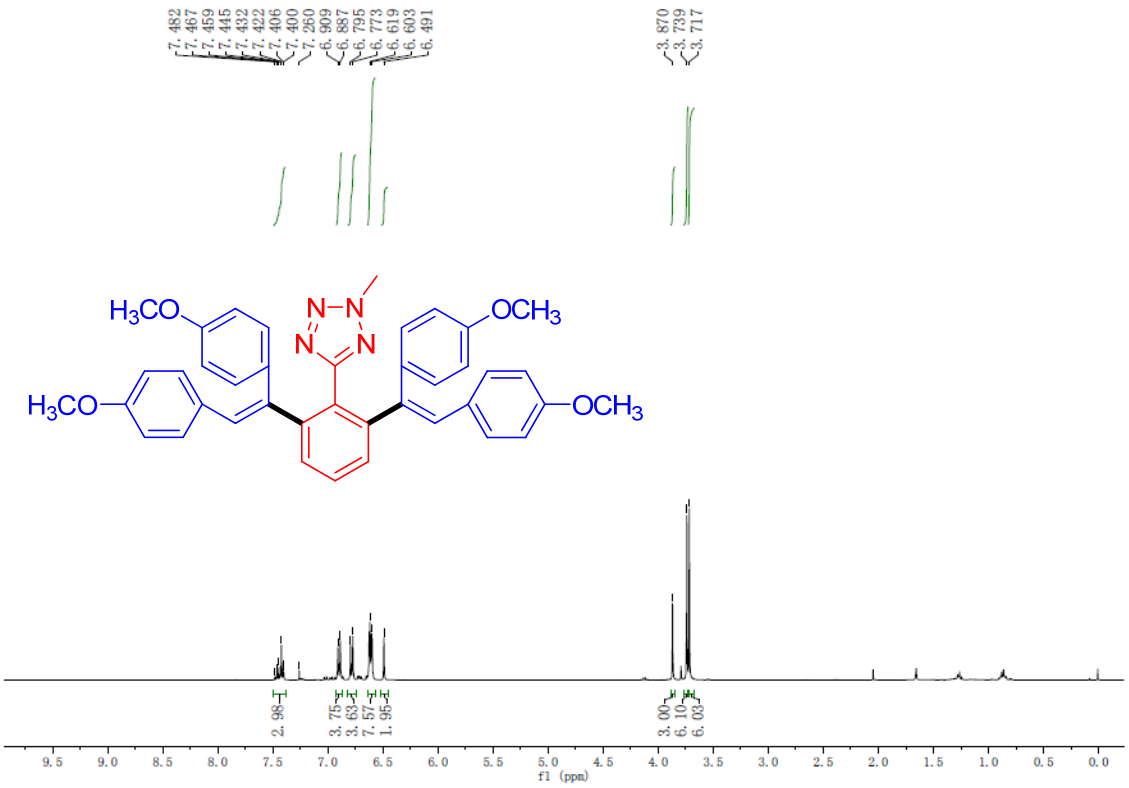
N
N
f1 (ppm)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7.422
7.406
7.400
7.260
6.909
6.887
6.795
6.773
6.619
6.603
6.491
3.870
3.739
3.717
H3CO
OCH3
H3CO
OCH3
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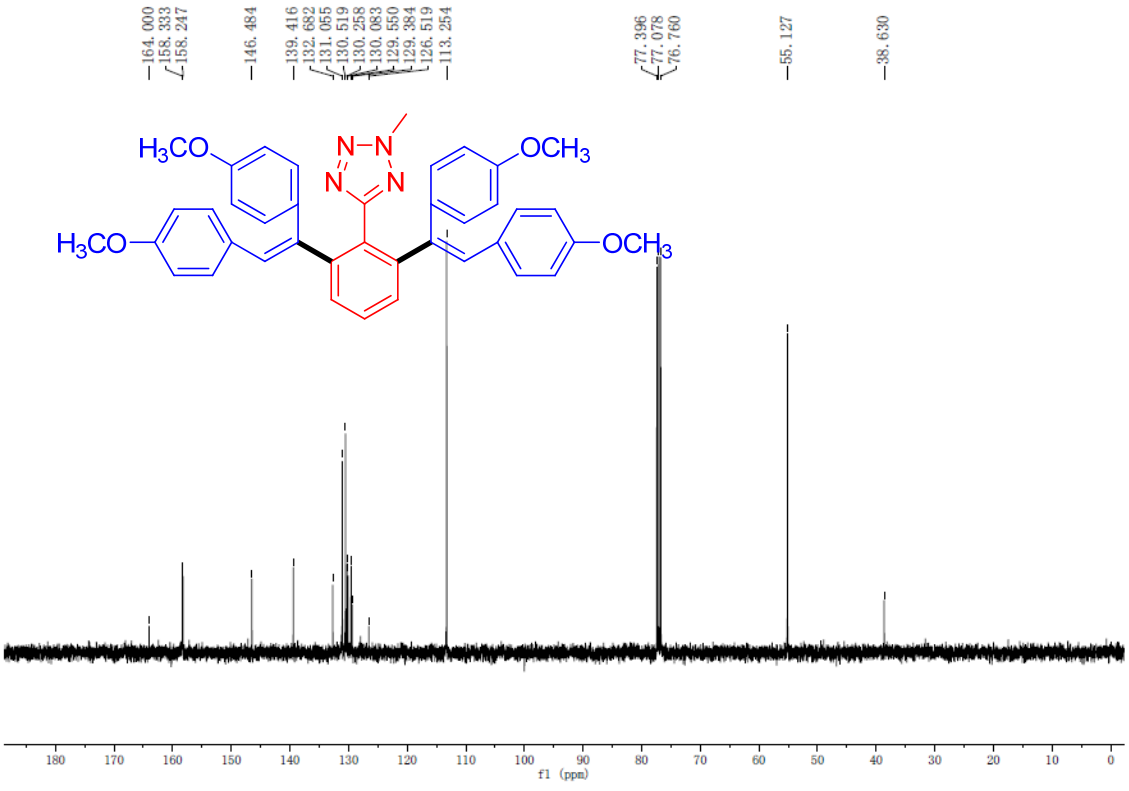
3.75
3.63
7.57
1.95
3.00
6.10
6.03
f1 (ppm)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131.055
130.519
130.258
130.083
129.550
129.384
126.519
113.254
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77.078
76.760
55.127
38.630
H3CO
OCH3
H3CO
OCH3
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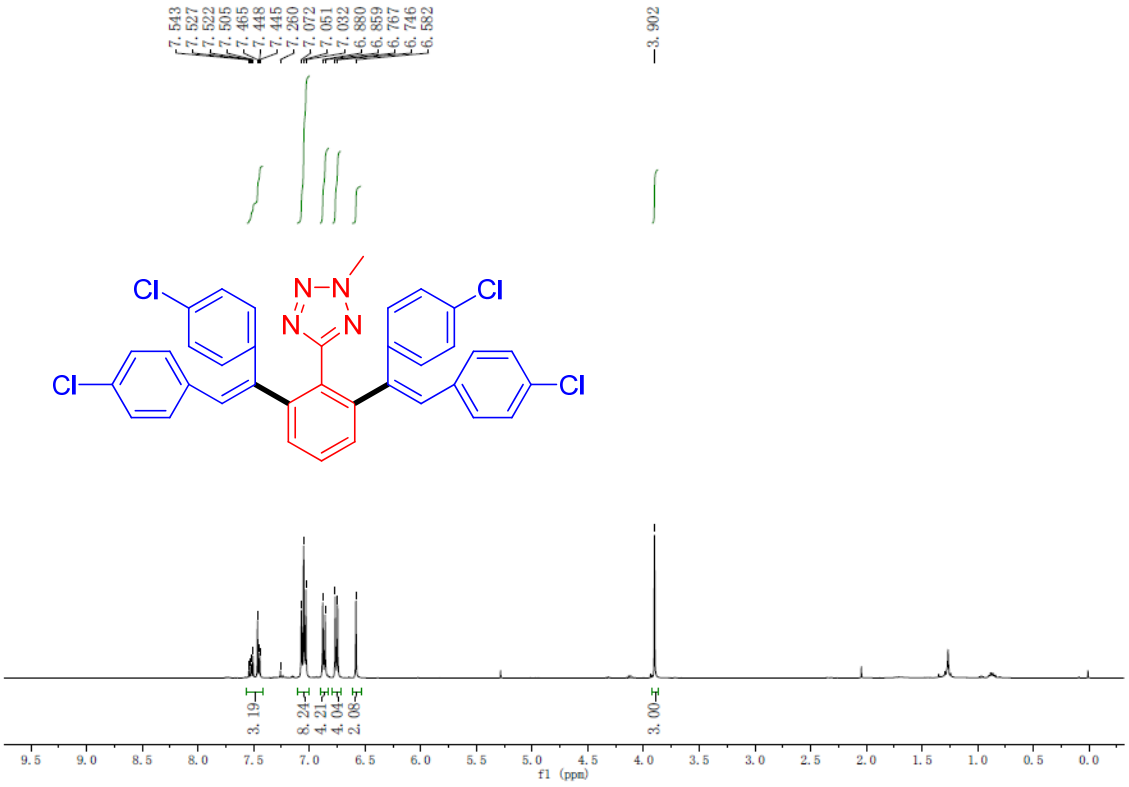
N
N
f1 (ppm)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7.448
7.445
7.260
7.072
7.051
7.032
6.880
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6.767
6.746
6.582
3.902
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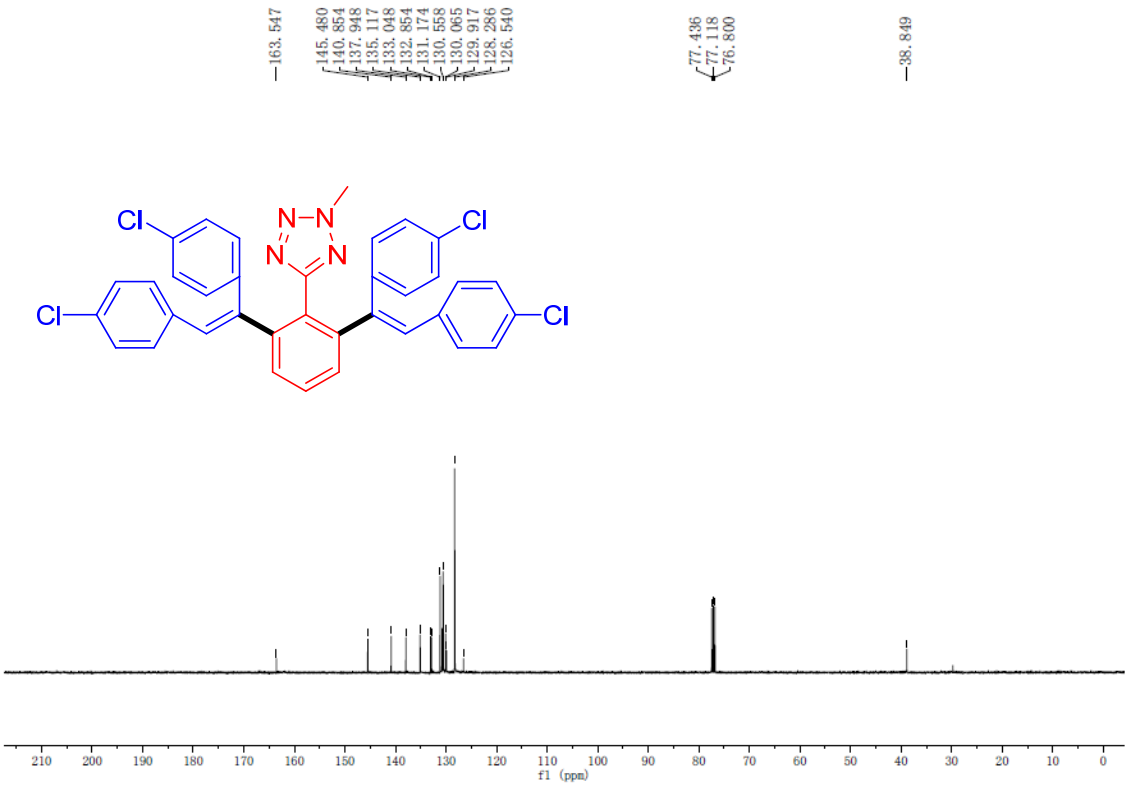
4.21
4.04
2.08
3.00
f1 (ppm)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133.048
132.854
131.174
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130.065
129.917
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77.118
76.800
38.849
Cl
Cl
Cl
Cl
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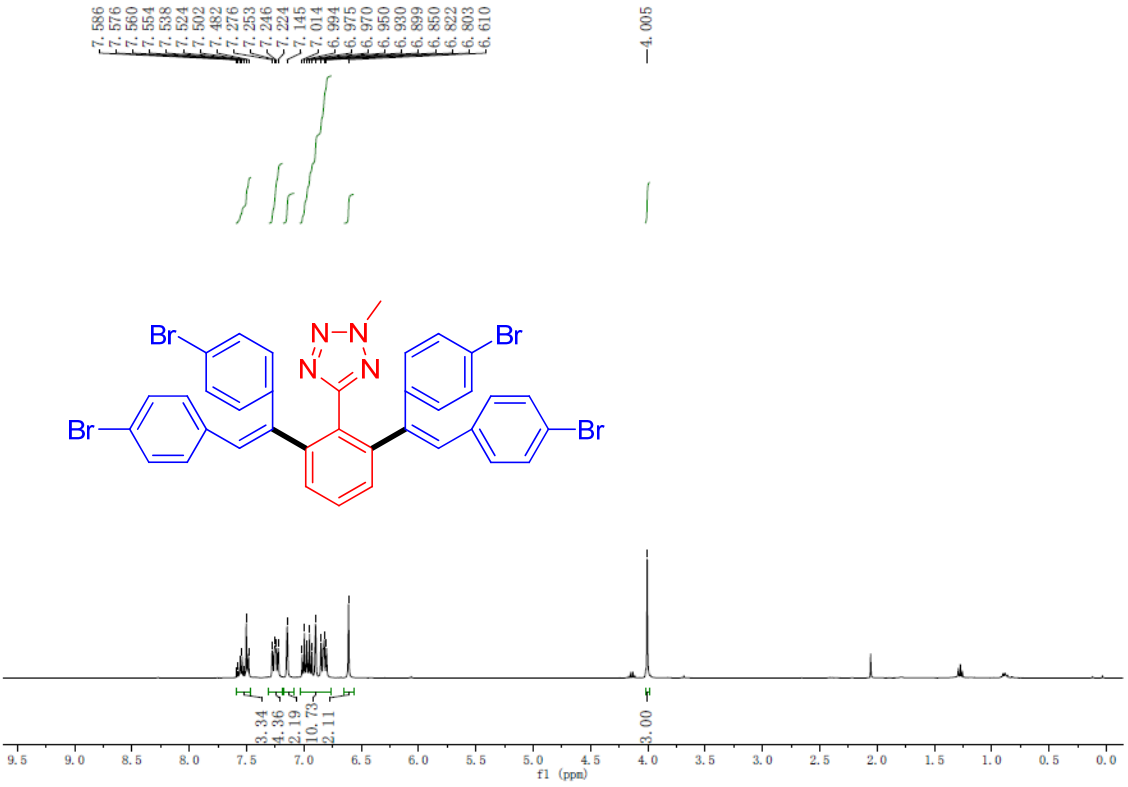
N
N
N
f1 (ppm)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7.014
6.994
6.975
6.970
6.950
6.930
6.899
6.850
6.822
6.803
6.610
4.005
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Br
Br
Br
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N
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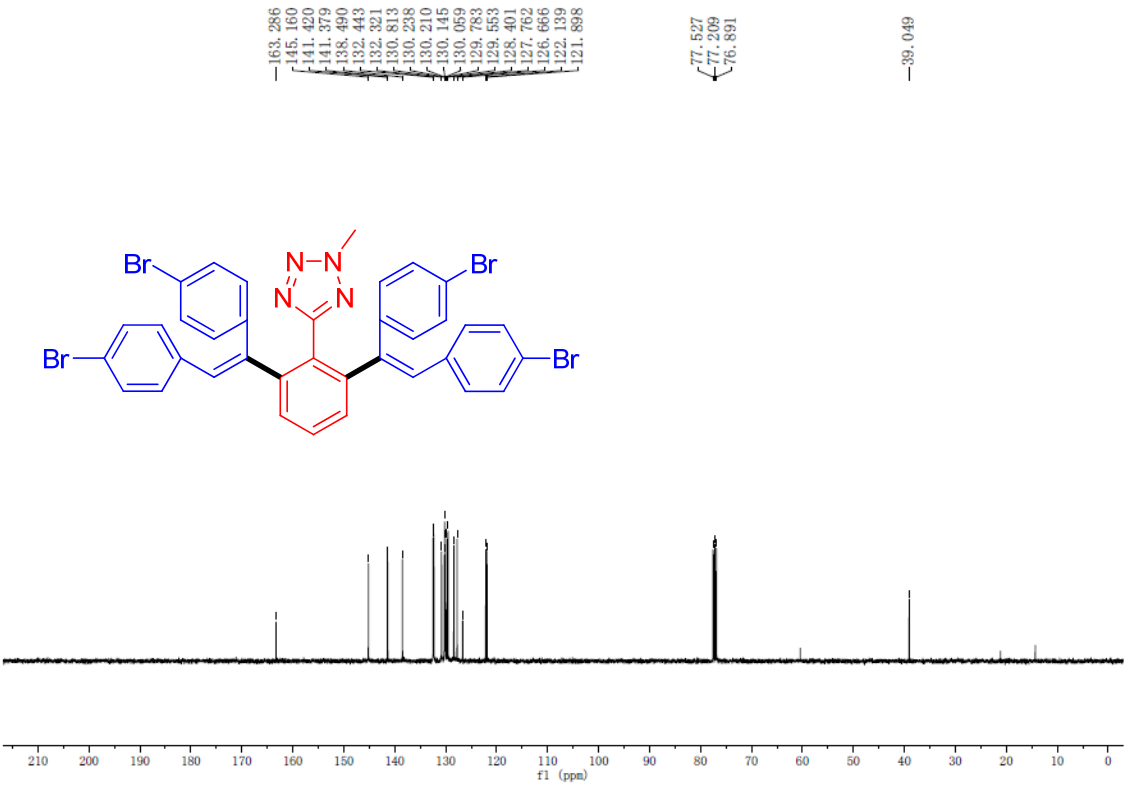
4.36
2.19
10.73
2.11
3.00
f1 (ppm)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145.160
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130.813
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130.210
130.145
130.059
129.783
129.553
128.401
127.762
126.666
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77.527
77.209
76.891
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Br
Br
Br
Br
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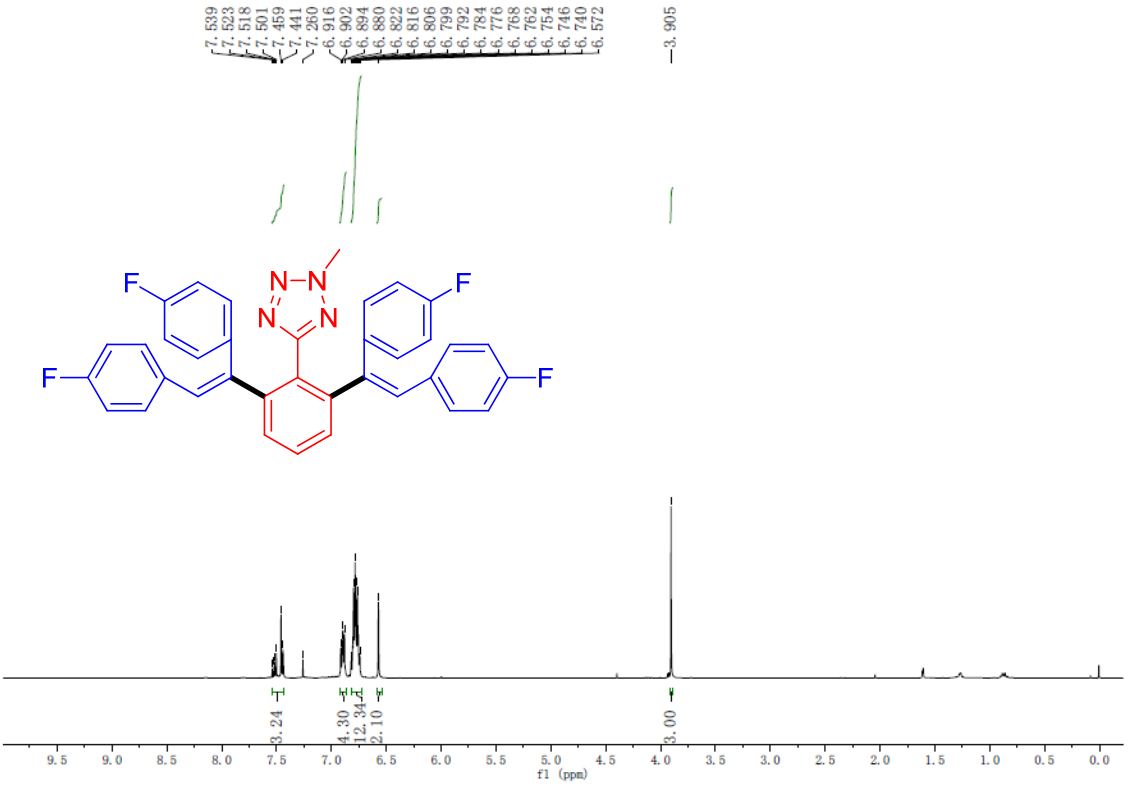
N
N
f1 (ppm)


7.539
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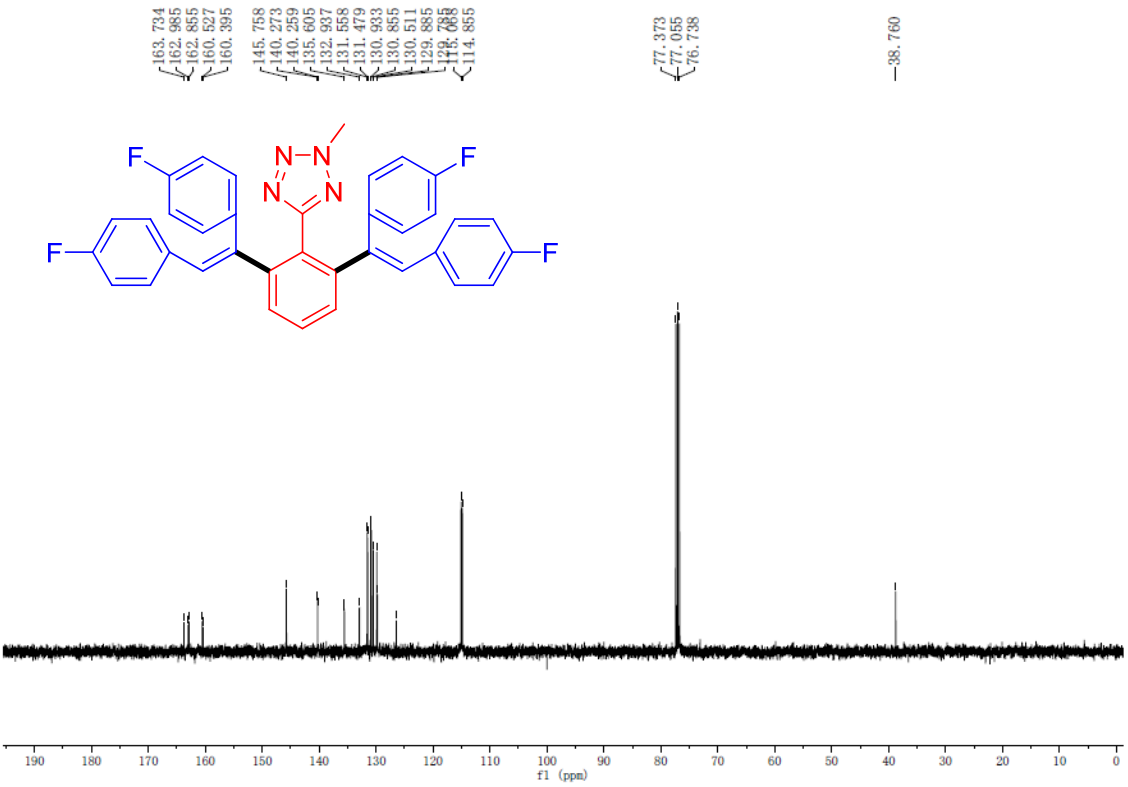
6.822
6.816
6.806
6.799
6.792
6.784
6.776
6.768
6.762
6.754
6.746
6.740
6.572
3.905
F
N–N
N
N
F
F
F
3.24
4.30
12.34
2.10
3.00
f1 (ppm)


163.734
162.985
162.855
160.527
160.395
145.758
140.273
140.259
135.605
132.937
131.558
131.479
130.933
130.855
130.511
129.885
129.785
114.855
77.373
77.055
76.738
38.760
F
N–N
N
N
F
F
F
f1 (ppm)