Electronic Supplementary Material (ESI) for Chemical Communications


# Accessing *N*-Heteroarylated Indoles and Benzimidazoles from 2-Alkynyl Cyclohexadienimines and Cyclohexadienones through Metal-Catalyzed Tandem Reactions

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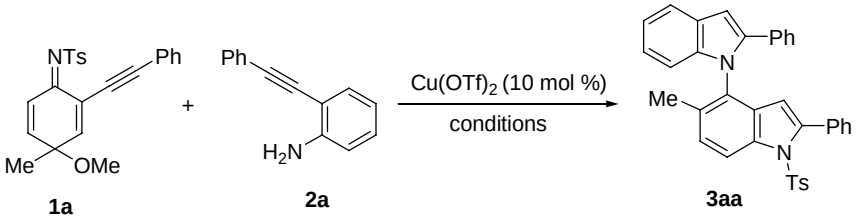
## Supporting Information

## General experimental methods:

All reactions were performed in Schlenk tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 25–35 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

## General procedure

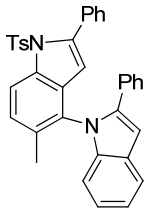
### 1. Synthesis of *N,C4*-coupled biheteroaryl alkaloids from 2-alkynyl cyclohexadienimines via tandem reaction



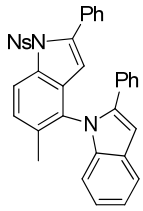

**1a** **2a** **3aa**

| Entry | Conditions | **3aa** (%) |
|---|---|---|
| 1 | $ClCH_2CH_2Cl$, rt | 95 |
| 2 | $CH_3CN$, rt | 0 |
| 3 | THF, rt | 25 |
| 4 | toluene, rt | 0 |
| 5 | DMF, rt | 0 |
| 6 | 1,4-dioxane, rt | 11 |
| 7 | $ClCH_2CH_2Cl$, reflux | 90 |
| 8 | $ClCH_2CH_2Cl$, rt | 77 |

$Cu(OTf)_2$ (4 mg, 0.01 mmol) was added into the solution of compound **1a** (39 mg, 0.1 mmol) and compound **2a** (23 mg, 0.12 mmol) in DCE (2 mL) at room temperature. Upon completion determined by TLC, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 20:1) to afford the pure product **3aa** (52 mg, 95% yield).

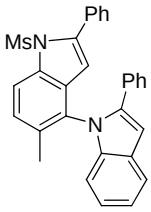



**1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3aa:** colorless solid; m.p. 183-185 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.25 (d, $J$ = 8.2 Hz, 1 H), 7.66 (d, $J$ = 7.4 Hz, 1 H), 7.34-7.38 (m, 2 H), 7.33-7.34 (m, 3 H), 7.22 (m, 3 H), 7.01-7.12 (m, 9 H), 6.82 (s, 1 H), 6.56 (d, $J$ = 7.8 Hz, 1 H), 6.07 (s, 1 H), 2.37 (s, 3 H), 1.88 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.4, 143.6, 141.2, 138.5, 137.6, 133.9, 132.9, 132.4, 131.8, 130.5, 130.1, 129.1, 128.8, 128.3, 128.0, 127.6, 127.4, 127.1, 126.8, 122.1, 120.5, 117.0, 111.6, 110.6, 102.6, 21.6, 17.1; IR (KBr) 3055, 3024, 2963, 2916, 2850, 1597, 1478, 1458, 1443, 1371 cm$^{-1}$; HRMS m/z calcd for $C_{36}H_{29}N_2O_2S$ ($[M+H]^+$): 553.1944, found 553.1939.



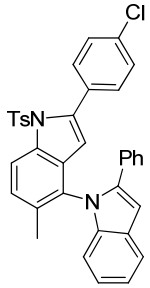

**1-(5-methyl-1-(4-nitrophenylsulfonyl)-2-phenyl-1H-indol-4-yl)-2-phenyl-1 H-indole 3ba:** yellow solid; m.p. 217-219 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.21 (d, $J$ = 8.2 Hz, 1 H), 8.07 (d, $J$ = 7.8 Hz, 2 H), 7.66 (d, $J$ = 7.3 Hz, 1 H), 7.30-7.42 (m, 8 H), 7.01-7.12 (m, 7 H), 6.81 (s, 1 H), 6.59 (d, $J$ = 7.8 Hz, 1 H), 6.00 (s, 1 H), 2.08 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 150.3, 143.2, 141.7, 141.3, 138.5, 137.2, 133.8, 132.4, 131.1, 130.6, 129.9, 129.7, 129.2, 128.4, 128.1, 128.0, 127.9, 127.7, 127.6, 127.2, 123.7, 122.4, 120.7, 120.6, 116.9, 112.4, 110.5, 103.1, 17.3; IR (KBr) 3101, 3060, 3029, 2957, 2916, 2845, 1607, 1535, 1473, 1448, 1386 cm$^{-1}$; HRMS m/z calcd for $C_{35}H_{26}N_3O_4S$ ($[M+H]^+$): 584.1639, found 584.1634.

**1-(5-methyl-1-(methylsulfonyl)-2-phenyl-1H-indol-4-yl)-2-phenyl-1H-indol e 3ca:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.06 (d, $J$ = 8.3 Hz, 1 H), 7.71 (d, $J$ = 7.4 Hz, 1 H), 7.28-7.39 (m, 6 H), 7.21-7.23 (m, 2 H), 7.13-7.17 (m,



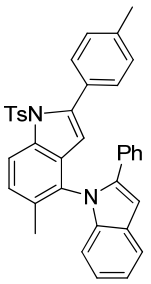

5 H), 6.87-6.89 (m, 2 H), 6.15 (s, 1 H), 2.59 (s, 3 H), 2.07 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 143.0, 141.4, 138.5, 137.2, 133.0, 132.7, 131.3, 129.9, 129.5, 129.0, 128.4, 128.1, 127.8, 127.6, 127.3, 122.4, 120.6, 116.0, 110.8, 110.7, 102.9, 38.8, 17.2; IR (KBr) 3060, 3035, 2957, 2927, 2865, 1602, 1576, 1484, 1463, 1437, 1365 cm$^{-1}$; HRMS m/z calcd for $C_{30}H_{25}N_2O_2S$ ($[M+H]^+$): 477.1631, found 477.1646.

**1-(2-(4-chlorophenyl)-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole**



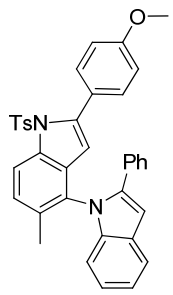

**3fa:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.24 (d, $J$ = 8.2 Hz, 1 H), 7.66 (d, $J$ = 7.8 Hz, 1 H), 7.31-7.32 (m, 4 H), 7.19-7.26 (m, 3 H), 7.02-7.14 (m, 9 H), 6.83 (s, 1 H), 6.55 (d, $J$ = 8.2 Hz, 1 H), 6.06 (s, 1 H), 2.38 (s, 3 H), 1.89 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.7, 142.3, 141.2, 138.5, 137.6, 134.9, 133.8, 133.1, 132.4, 131.2, 130.4, 129.1, 128.3, 128.0, 127.9, 127.8, 127.6, 127.2, 126.7, 122.2, 120.5, 117.0, 111.9, 110.6, 102.7, 21.6, 17.1; IR (KBr) 3055, 3029, 2952, 2921, 2850, 1591, 1494, 1473, 1458, 1365 cm$^{-1}$; HRMS m/z calcd for $C_{36}H_{28}ClN_2O_2S$ ($[M+H]^+$): 587.1555, found 587.1542.

**1-(5-methyl-2-p-tolyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ga:**

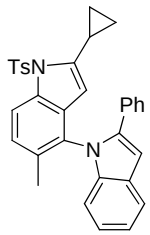



colorless solid; m.p. 154-156 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.23 (d, $J$ = 8.7 Hz, 1 H), 7.66 (d, $J$ = 7.8 Hz, 1 H), 7.30 (d, $J$ = 7.3 Hz, 2 H), 7.23 (m, 3 H), 7.15 (d, $J$ = 7.8 Hz, 2 H), 7.06-7.12 (m, 6 H), 7.00-7.03 (m, 3 H), 6.82 (s, 1 H), 6.54 (d, $J$ = 7.8Hz, 1 H), 6.05 (s, 1 H), 2.37 (s, 6 H), 1.86 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.4, 143.9, 141.2, 138.8, 138.5, 137.6, 133.9, 132.9, 132.4, 130.7, 129.9, 129.0, 128.2, 128.0, 127.6, 127.4, 127.1, 126.8, 122.1, 120.4, 117.1, 111.2, 110.7, 102.6, 21.6, 21.4, 17.0; IR (KBr) 3060, 3024, 2957, 2916, 2850, 1597, 1478, 1448, 1365 cm$^{-1}$; HRMS m/z calcd for $C_{37}H_{31}N_2O_2S$ ($[M+H]^+$): 567.2101, found 567.2119.

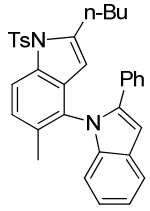
**1-(2-(4-methoxyphenyl)-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ha:** colorless solid; m.p. 181-183 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.23 (d, $J$ = 8.2 Hz, 1 H), 7.66 (d, $J$ = 7.8 Hz, 1 H), 7.32 (d, $J$ = 8.2 Hz, 2 H), 7.21 (d, $J$ = 7.3 Hz, 3 H), 7.06-7.12 (m, 6 H), 7.02-7.04 (m, 3 H), 6.87 (d, $J$ = 8.2 Hz, 2



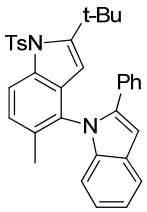

H), 6.82 (s, 1 H), 6.55 (d, $J$ = 8.2 Hz, 1 H), 6.01 (s, 1 H), 3.83 (s, 3 H), 2.37 (s, 3 H), 1.87 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.1, 144.4, 143.6, 141.2, 138.8, 138.5, 137.5, 134.0, 132.8, 132.5, 131.4, 130.7, 129.0, 128.9, 128.3, 128.0, 127.6, 127.2, 127.1, 126.8, 124.2, 122.1, 120.4, 117.1, 112.9, 110.7, 102.6, 52.2, 21.6, 17.0; IR (KBr) 3055, 3029, 2952, 2927, 2850, 1612, 1576, 1504, 1478, 1448, 1371 cm$^{-1}$; HRMS m/z calcd for $C_{37}H_{31}N_2O_3S$ ([M+H]$^+$): 583.2050, found 583.2048.



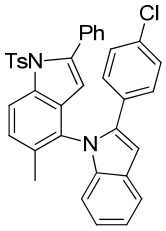

**1-(2-cyclopropyl-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ia:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.14 (d, $J$ = 8.2 Hz, 1 H), 7.69 (d, $J$ = 7.3 Hz, 1 H), 7.63 (d, $J$ = 7.8 Hz, 2 H), 7.22 (d, $J$ = 8.2 Hz, 2 H), 7.05-7.15 (m, 8 H), 6.85 (s, 1 H), 6.75 (d, $J$ = 7.8 Hz, 1 H), 5.65 (s, 1 H), 2.40 (s, 3 H), 2.30-2.34 (m, 1 H), 1.88 (s, 3 H), 0.82-0.84 (m, 2 H), 0.31-0.42 (m, 2 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 145.3, 144.6, 141.4, 138.5, 136.4, 136.3, 132.5, 131.7, 129.6, 129.0, 128.5, 128.3, 128.0, 127.6, 127.2, 126.5, 122.1, 120.4, 114.6, 110.8, 103.5, 102.5, 21.6, 17.0, 9.3, 8.7, 8.4; IR (KBr) 3050, 3027, 2957, 2916, 2850, 1597, 1575, 1489, 1455, 1372 cm$^{-1}$; HRMS m/z calcd for $C_{33}H_{29}N_2O_2S$ ([M+H]$^+$): 517.1944, found 517.1943.



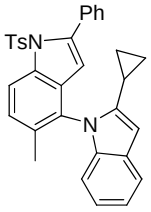

**1-(2-butyl-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ja:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.11 (d, $J$ = 8.7 Hz, 1 H), 7.70 (d, $J$ = 7.3 Hz, 1 H), 7.54 (d, $J$ = 7.8 Hz, 2 H), 7.20 (d, $J$ = 7.8 Hz, 2 H), 7.10-7.15 (m, 5 H), 7.03-7.08 (m, 3 H), 6.85 (s, 1 H), 6.73 (d, $J$ = 7.8 Hz, 1 H), 5.88 (s, 1 H), 2.80-2.87 (m, 2 H), 2.38 (s, 3 H), 1.87 (s, 3 H), 1.50-1.56 (m, 2 H), 1.23-1.28 (m, 2 H), 0.84 (t, $J$ = 7.1 Hz, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.6, 143.7, 141.4, 138.5, 136.3, 136.0, 132.5, 131.8, 129.7, 129.4, 128.4, 128.3, 128.0, 127.6, 127.2, 126.5, 126.1, 122.1, 120.4, 114.9, 110.8, 106.4, 102.5, 30.7, 28.7, 22.3, 21.6, 17.0, 13.8; IR (KBr) 3060, 3024, 2963, 2927, 2865, 1597, 1561, 1494, 1458, 1437, 1371 cm$^{-1}$; HRMS m/z calcd for $C_{34}H_{33}N_2O_2S$ ([M+H]$^+$): 533.2257, found 533.2269.



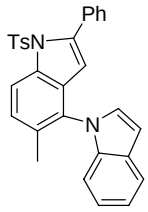

**1-(2-tert-butyl-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ka:** colorless solid; m.p. 268-270 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.62 (d, $J$ = 7.4 Hz, 4 H), 7.22 (d, $J$ = 7.3 Hz, 3 H), 7.08-7.16 (m, 6 H), 7.03 (t, $J$ = 7.3 Hz, 2 H), 6.74 (s, 1 H), 6.44 (d, $J$ = 7.8 Hz, 1 H), 2.44 (s, 3 H), 1.71 (s, 3 H), 0.75 (s, 9H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 143.9, 140.2, 139.2, 137.8, 135.8, 135.5, 134.6, 132.6, 130.5, 129.5, 128.2, 127.6, 127.3, 121.7, 121.5, 120.2, 117.7, 110.6, 110.5, 102.4, 30.0, 27.9, 21.6, 17.4; IR (KBr) 3055, 3029, 2962, 2922, 2870, 1596, 1576, 1482, 1457, 1391 cm$^{-1}$; HRMS m/z calcd for $C_{34}H_{33}N_2O_2S$ ($[M+H]^+$): 533.2257, found 533.2254.



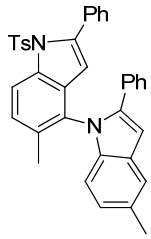

**2-(4-chlorophenyl)-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-indole 3ab:** colorless solid; m.p. 159-161 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.26 (d, $J$ = 8.3 Hz, 1 H), 7.65 (d, $J$ = 7.3 Hz, 1 H), 7.33-7.39 (m, 5 H), 7.22-7.25 (m, 3 H), 7.09-7.12 (m, 3 H), 7.04 (t, $J$ = 7.6 Hz, 1 H), 6.94-6.99 (m, 4 H), 6.81 (s, 1 H), 6.60 (d, $J$ = 8.2 Hz, 1 H), 6.06 (s, 1 H), 2.39 (s, 3 H), 1.86 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.7, 143.9, 139.8, 138.6, 137.5, 133.9, 133.1, 132.8, 131.7, 130.9, 130.4, 130.1, 129.1, 128.8, 128.7, 128.3, 128.1, 127.6, 127.5, 126.8, 122.5, 120.7, 120.6, 117.1, 111.2, 110.7, 103.0, 21.6, 17.0; IR (KBr) 3049, 3024, 2952, 2922, 2845, 1597, 1473, 1452, 1375 cm$^{-1}$; HRMS m/z calcd for $C_{36}H_{28}ClN_2O_2S$ ($[M+H]^+$): 587.1555, found 587.1553.



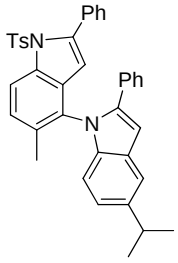

**2-cyclopropyl-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-indole 3ac:** colorless solid; m.p. 202-204 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.31 (d, $J$ = 8.2 Hz, 1 H), 7.53 (d, $J$ = 7.8 Hz, 1 H), 7.40-7.43 (m, 2 H), 7.33-7.38 (m, 4 H), 7.24-7.26 (m, 2 H), 7.03-7.06 (m, 3 H), 6.96 (t, $J$ = 7.3 Hz, 1 H), 6.53 (d, $J$ = 7.8 Hz, 1 H), 6.16 (s, 1 H), 5.99 (s, 1 H), 2.31 (s, 3 H), 2.05 (s, 3 H), 1.22-1.26 (m, 1 H), 0.60-0.64 (m, 2 H), 0.56-0.58 (m, 1 H), 0.42-0.48 (m, 1 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.6, 144.1, 143.6, 137.8, 137.5, 133.8, 133.6, 131.9, 131.0, 130.0, 128.9, 128.8, 128.3, 128.0, 127.5, 127.3, 126.8, 120.9, 119.8, 117.4, 111.7, 109.6, 96.7, 21.5, 17.0, 7.6, 7.6; IR (KBr) 3065, 3038, 2957, 2922, 2850, 1591, 1545, 1480, 1456, 1375 cm$^{-1}$; HRMS m/z calcd for $C_{33}H_{29}N_2O_2S$ ($[M+H]^+$): 517.1944, found 517.1953.



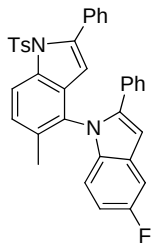

**1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-1H-indole 3ad:** yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.30 (d, $J$ = 8.7 Hz, 1 H), 7.67 (dd, $J$ = 6.8 Hz, 1 H), 7.31-7.39 (m, 6 H), 7.27-7.29 (m, 2 H), 7.11-7.13 (m, 2 H), 7.06-7.09 (m, 3 H), 6.71 (d, $J$ = 7.8 Hz, 1 H), 6.66 (d, $J$ = 2.8 Hz, 1 H), 6.02 (s, 1 H), 2.31 (s, 3 H), 2.10 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.7, 143.0, 137.4, 136.7, 134.4, 131.8, 131.7, 130.2, 129.5, 129.2, 128.8, 128.6, 128.2, 127.4, 126.8, 122.0, 120.9, 119.9, 116.6, 111.0, 110.5, 102.8, 21.5, 17.2; IR (KBr) 3050, 3029, 2947, 2916, 2855, 1730, 1597, 1509, 1478, 1453, 1371 cm$^{-1}$; HRMS m/z calcd for $C_{30}H_{25}N_2O_2S$ ($[M+H]^+$): 477.1630, found 477.1647.



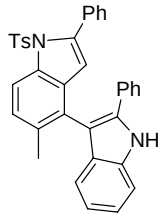

**5-methyl-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ae:** colorless solid; m.p. 226-228 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.23 (d, $J$ = 8.2 Hz, 1 H), 7.45 (s, 1H), 7.33-7.40 (m, 5 H), 7.21-7.23 (m, 3 H), 7.01-7.10 (m, 7 H), 6.86 (dd, $J$ = 8.3 Hz, 1 H), 6.75 (s, 1 H), 6.46 (d, $J$ = 8.2 Hz, 1 H), 6.08 (s, 1 H), 2.43 (s, 3 H), 2.38 (s, 3 H), 1.88 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.4, 143.5, 141.2, 137.6, 136.9, 133.9, 132.9, 131.9, 130.5, 130.1, 129.8, 129.2, 129.1, 128.8, 128.5, 128.0, 127.5, 127.4, 127.0, 126.8, 123.7, 120.2, 116.9, 111.7, 110.3, 102.2, 21.6, 21.4, 17.1; IR (KBr) 3055, 3028, 2957, 2911, 2855, 1607, 1494, 1478, 1437, 1376 cm$^{-1}$; HRMS m/z calcd for $C_{37}H_{31}N_2O_2S$ ($[M+H]^+$): 567.2101, found 567.2109.



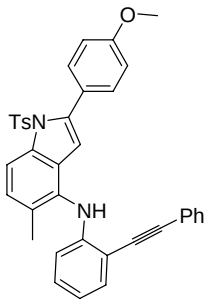

**5-isopropyl-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3af:** colorless solid; m.p. 153-155 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.23 (d, $J$ = 8.2 Hz, 1 H), 7.50 (s, 1H), 7.38-7.40 (m, 2 H), 7.33-7.36 (m, 3 H), 7.21-7.23 (m, 3 H), 7.05-7.10 (m, 4 H), 7.00-7.02 (m, 2 H), 6.92 (dd, $J$ = 8.5 Hz, 1 H), 6.77 (s, 1 H), 6.51 (d, $J$ = 8.2 Hz, 1 H), 6.10 (s, 1 H), 2.95-3.02 (m, 1H), 2.37 (s, 3 H), 1.89 (s, 3 H), 1.30 (s, 3 H), 1.29 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.4, 143.5, 141.3, 141.1, 137.6, 137.2, 133.9, 132.9, 132.6, 131.9, 130.5, 130.1, 129.3, 129.1, 128.7, 128.4, 128.0, 127.5, 127.4, 127.0, 126.8, 121.5, 117.3, 116.9, 111.7, 110.4, 102.4, 34.1, 24.5, 21.6, 21.4, 17.1; IR (KBr) 3050, 3024, 2958, 2924, 2870, 1735, 1598, 1479, 1444, 1375 cm$^{-1}$; HRMS m/z calcd for $C_{39}H_{35}N_2O_2S$ ($[M+H]^+$): 595.2414, found 595.2434.




**5-fluoro-1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-indole 3ag:** colorless solid; m.p. 200-202 °C; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.25 (d, $J$ = 8.7 Hz, 1 H), 7.35-7.41 (m, 5 H), 7.30 (d, $J$ = 7.6 Hz, 1 H), 7.22-7.24 (m, 3 H), 7.03-7.13 (m, 7 H), 6.73-6.78 (m, 2 H), 6.46-6.48 (m, 1 H), 6.06 (s, 1 H), 2.38 (s, 3 H), 1.86 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.5, 143.8, 142.8, 137.6, 135.0, 133.9, 132.8, 132.2, 131.7, 130.4, 130.1, 129.1, 128.9, 128.8, 128.5, 128.1, 127.6, 127.5, 127.4, 126.8, 117.2, 111.2, 110.5, 110.3, 105.4, 105.1, 102.5, 34.1, 24.5, 21.6, 21.4, 17.0; IR (KBr) 3045, 3024, 2963, 2922, 2845, 1591, 1484, 1466, 1443, 1375 cm$^{-1}$; HRMS m/z calcd for $C_{36}H_{28}FN_2O_2S$ ($[M+H]^+$): 571.1850, found 571.1858.



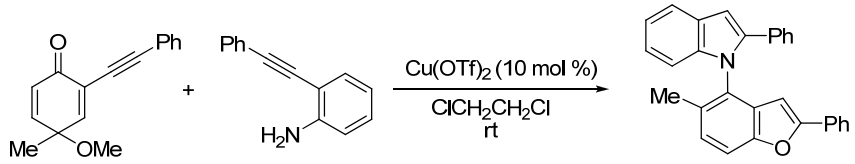

**5-methyl-2-phenyl-4-(2-phenyl-1H-indol-3-yl)-1-tosyl-1H-indole 5aa:** yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.38 (s, 1 H), 8.20 (d, $J$ = 8.7 Hz, 1 H), 7.42 (d, $J$ = 7.8 Hz, 1 H), 7.36-7.39 (m, 2 H), 7.25-7.31 (m, 6 H), 7.11-7.21 (m, 6 H), 7.07 (d, $J$ = 8.2 Hz, 2 H), 6.99 (t, $J$ = 6.8 Hz, 1 H), 6.91 (d, $J$ = 7.8 Hz, 1 H), 6.11 (s, 1 H), 2.35 (s, 3 H), 2.03 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 144.1, 142.4, 137.1, 135.9, 134.3, 133.9, 132.6, 132.4, 129.9, 129.2, 128.9, 128.6, 128.3, 127.4, 127.3, 127.2, 126.9, 126.5, 126.3, 122.6, 120.0, 119.9, 116.0, 114.9, 111.3, 110.8, 21.6, 19.6; IR (KBr) 3399, 3060, 2922, 2844, 1602, 1489, 1448, 1371 cm$^{-1}$; HRMS m/z calcd for $C_{36}H_{29}N_2O_2S$ ($[M+H]^+$): 553.1944, found 553.1953.




**2-(4-methoxyphenyl)-5-methyl-N-(2-(2-phenylethynyl)phenyl)-1-tosyl-1H-indol-4-amine 8ha:** yellow oil; $^{1}$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.09 (d, $J$ = 8.7 Hz, 1 H), 7.50-7.52 (m, 2 H), 7.37-7.40 (m, 3 H), 7.32-7.34 (m, 3 H), 7.24-7.27 (m, 3 H), 7.05 (d, $J$ = 8.2 Hz, 2 H), 6.96 (t, $J$ = 7.8 Hz, 1 H), 6.90 (d, $J$ = 8.7 Hz, 2 H), 6.68 (t, $J$ = 7.4 Hz, 1 H), 6.32 (s, 1 H), 6.25 (s, 1 H), 6.07 (d, $J$ = 8.2 Hz, 1 H), 3.85 (s, 3 H), 2.32 (s, 3 H), 2.30 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.0, 146.7, 144.4, 142.1, 137.8, 134.3, 132.1, 131.5, 131.4, 130.6, 130.0, 129.5, 129.1, 128.6, 128.4, 127.4, 126.8, 124.6, 123.0, 117.8, 114.5, 112.9, 111.7, 111.4, 107.9, 95.5, 85.7, 52.3, 21.5, 17.5; IR (KBr) 3378, 3050, 2957,

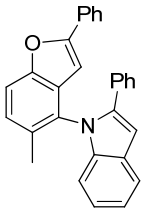
2916, 2850, 1607, 1576, 1499, 1448, 1371 $cm^{-1}$; HRMS m/z calcd for $C_{37}H_{31}N_2O_3S$ ($[M+H]^+$): 583.2050, found 583.2043.

## 2. Synthesis of *N,C4*-coupled biheteroaryl alkaloids from 2-alkynyl cyclohexadienones via tandem reaction

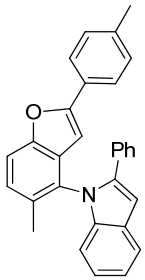



**6a** **2a** **7aa**

$Cu(OTf)_2$ (4 mg, 0.01 mmol) was added into the solution of compound **6a** (24 mg, 0.1 mmol) and compound **2a** (23 mg, 0.12 mmol) in DCE (2 mL) at room temperature. Upon completion determined by TLC, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 50:1) **7aa** (37 mg, 92% yield).

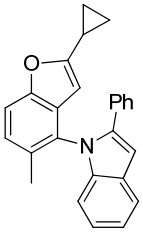



**1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-indole 7aa:** colorless solid; m.p. 244-246 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 77.74 (d, $J$ = 7.8 Hz, 3 H), 7.47 (d, $J$ = 8.3 Hz, 1 H), 7.37 (t, $J$ = 7.1 Hz, 2 H), 7.27-7.31 (m, 3 H), 7.12-7.20 (m, 6 H), 6.91 (s, 1 H), 6.88 (d, $J$ = 8.1 Hz, 1 H), 6.63 (s, 1 H), 1.88 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.0, 153.9, 141.6, 138.8, 132.7, 131.4, 130.1, 129.4, 129.2, 128.9, 128.5, 128.4, 127.9, 126.9, 125.1, 122.4, 120.7, 120.6, 111.3, 111.1, 102.8, 99.5, 17.2; IR (KBr) 3049, 3025, 2957, 2922, 2845, 1591, 1582, 1478, 1453 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{22}NO$ ($[M+H]^+$):400.1696, found 400.1682.

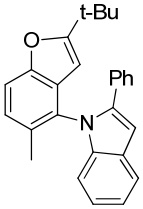



**1-(5-methyl-2-p-tolylbenzofuran-4-yl)-2-phenyl-1H-indole 7fa:** colorless solid; m.p. 224-226 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.74 (d, $J$ = 7.3 Hz, 1 H), 7.64 (d, $J$ = 6.9 Hz, 2 H), 7.46 (d, $J$ = 8.2 Hz, 1 H), 7.27-7.28 (m, 2 H), 7.10-7.20 (m, 8 H), 6.87-6.90 (m, 2 H), 6.57 (s, 1 H), 2.35 (s, 3 H), 1.87 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.1, 153.6, 141.4, 138.9, 138.6, 132.5,

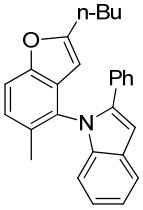
131.1, 129.4, 129.1, 128.4, 128.2, 127.7, 127.4, 127.2, 126.5, 124.9, 122.3, 120.5, 120.4, 111.0, 110.9, 102.6, 98.7, 21.4, 17.1; IR (KBr) 2963, 2922, 2850, 1602, 1489, 1448 $cm^{-1}$; HRMS m/z calcd for $C_{30}H_{24}NO$ ($[M+H]^+$): 414.1852, found 414.1852.




**1-(2-cyclopropyl-5-methylbenzofuran-4-yl)-2-phenyl-1H-indole 7ha:** colorless solid; m.p. 153-155 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.71 (d, $J$ = 7.8 Hz, 1 H), 7.31 (d, $J$ = 8.3 Hz, 1 H), 7.22-7.26 (m, 2 H), 7.15-7.18 (m, 4 H), 7.09-7.12 (m, 1 H), 7.02 (d, $J$ = 8.2 Hz, 1 H), 6.87 (s, 1 H), 6.83 (d, $J$ = 7.8 Hz, 1 H), 5.94 (s, 1 H), 1.89-1.93 (m, 1 H), 1.84 (s, 3 H), 0.88-0.94 (m, 4 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.6, 153.1, 141.4, 138.6, 132.7, 130.6, 128.9, 128.4, 128.3, 128.2, 127.7, 127.3, 125.2, 122.1, 120.4, 110.9, 110.5, 102.5, 98.5, 17.0, 9.4, 7.6; IR (KBr) 3055, 3019, 2947, 2932, 2855, 1586, 1489, 1453, 1437, 1371 $cm^{-1}$; HRMS m/z calcd for $C_{26}H_{22}NO$ ($[M+H]^+$): 364.1696, found 364.1676.

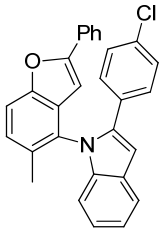



**1-(2-tert-butyl-5-methylbenzofuran-4-yl)-2-phenyl-1H-indole 7ia:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.72 (d, $J$ = 7.3 Hz, 1 H), 7.37 (d, $J$ = 8.3 Hz, 1 H), 7.23-7.25 (m, 2 H), 7.12-7.15 (m, 5 H), 7.06 (d, $J$ = 8.2 Hz, 1 H), 6.85-6.88 (m, 2 H), 5.92 (s, 1 H), 1.87 (s, 3 H), 1.28 (s, 9 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 168.4, 153.5, 141.5, 138.6, 132.7, 130.4, 128.9, 128.6, 128.3, 128.1, 127.8, 127.3, 125.4, 122.1, 120.4, 111.0, 110.7, 102.5, 97.2, 33.0, 28.8, 17.1; IR (KBr) 3055, 3029, 2968, 2922, 2855, 1597, 1581, 1494, 1458, 1437, 1371 $cm^{-1}$; HRMS m/z calcd for $C_{27}H_{26}NO$ ($[M+H]^+$): 380.2009, found 380.2019.

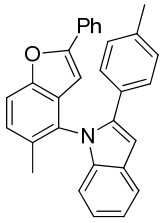



**1-(2-butyl-5-methylbenzofuran-4-yl)-2-phenyl-1H-indole 7ja:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.71 (d, $J$ = 7.8 Hz, 1 H), 7.36 (d, $J$ = 7.8 Hz, 1 H), 7.23-7.25 (m, 2H), 7.11-7.16 (m, 5H), 7.06 (d, $J$ = 8.2 Hz, 1 H), 6.87 (s, 1 H), 6.85 (d, $J$ = 8.1 Hz, 1 H), 5.95 (s, 1 H), 2.66 (t, $J$ = 6.9 Hz, 2 H), 1.88 (s, 3 H), 1.60-1.64 (m, 2H), 1.29-1.34 (m, 2H), 0.89 (t, $J$ = 6.7 Hz, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 160.8, 153.5, 141.4, 138.6, 132.7, 130.5, 128.8, 128.7, 128.3,

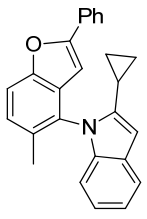
128.1, 127.7, 127.3, 125.4, 122.1, 120.4, 110.9, 110.6, 102.5, 100.0, 29.5, 28.1, 22.2, 17.1, 13.7; IR (KBr) 3055, 3024, 2957, 2922, 2855, 1586, 1489, 1458, 1437, 1376 $cm^{-1}$; HRMS m/z calcd for $C_{27}H_{26}NO$ ($[M+H]^+$): 380.2009, found 380.2013.




**2-(4-chlorophenyl)-1-(5-methyl-2-phenylbenzofuran-4-yl)-1H-indole 7ab:** colorless solid; m.p. 202-204 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.73-7.77 (m, 3 H), 7.50 (d, $J$ = 8.2 Hz, 1 H), 7.39 (t, $J$ = 7.1 Hz, 2 H), 7.33 (d, $J$ = 6.4 Hz, 1 H), 7.12-7.21 (m, 7 H), 6.90 (s, 1 H), 6.88 (d, $J$ = 8.2 Hz, 1 H), 6.60 (s, 1 H), 1.87 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.0, 153.8, 140.1, 138.8, 133.4, 131.2, 130.1, 129.9, 129.0, 128.9, 128.8, 128.5, 128.3, 126.8, 125.0, 122.6, 120.7, 120.6, 111.3, 111.0, 103.0, 99.2, 17.1; IR (KBr) 3050, 3024, 2957, 2922, 2854, 1596, 1581, 1484, 1453 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{21}ClNO$ ($[M+H]^+$): 434.1306, found 434.1311.

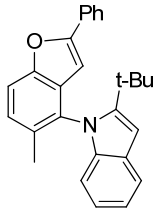



**1-(5-methyl-2-phenylbenzofuran-4-yl)-2-p-tolyl-1H-indole 7ah:** colorless solid; m.p. 203-205 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.72-7.77 (m, 3 H), 7.49 (d, $J$ = 8.2 Hz, 1 H), 7.39 (t, $J$ = 7.3 Hz, 2 H), 7.32 (d, $J$ = 6.9 Hz, 1 H), 7.11-7.17 (m, 5 H), 6.96 (d, $J$ = 7.4 Hz, 2 H), 6.86-6.87 (m, 2 H), 6.63 (s, 1 H), 2.24 (s, 3 H), 1.89 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 156.7, 153.7, 141.5, 138.5, 137.2, 131.2, 130.0, 129.7, 129.4, 129.1, 129.0, 128.7, 128.4, 127.6, 126.7, 124.9, 122.1, 120.5, 120.3, 111.1, 110.9, 102.2, 99.5, 21.1, 17.1; IR (KBr) 3050, 3024, 2947, 2922, 2855, 1597, 1581, 1494, 1473, 1448 $cm^{-1}$; HRMS m/z calcd for $C_{30}H_{24}NO$ ($[M+H]^+$): 414.1852, found 414.1865.

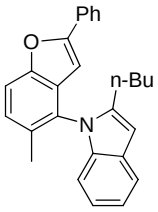



**2-cyclopropyl-1-(5-methyl-2-phenylbenzofuran-4-yl)-1H-indole 7ac:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.79-7.82 (m, 2 H), 7.68 (t, $J$ = 7.7 Hz, 1 H), 7.60 (t, $J$ = 7.0 Hz, 1 H), 7.61 (d, $J$ = 7.8 Hz, 1 H), 7.41-7.43 (m, 2 H), 7.32-7.36 (m, 2 H), 7.14-7.20 (m, 1 H), 7.07-7.13 (m, 1 H), 6.86 (t, $J$ = 8.2 Hz, 1 H), 6.61 (d, $J$ = 8.1 Hz, 1 H), 6.32 (d, $J$ = 8.1 Hz, 1 H), 2.14 (d, $J$ = 7.3 Hz, 3 H), 1.53-1.60 (m, 1 H), 0.79-0.82 (m, 4 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 156.8, 153.9, 144.4, 137.6, 131.9, 130.0, 129.4, 128.7, 128.1, 128.5, 124.9,

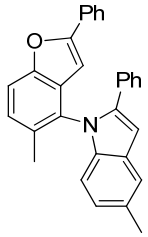
121.0, 119.9, 119.7, 111.3, 109.9, 99.4, 96.4, 17.0, 8.0, 7.7; IR (KBr) 3081, 3055, 3009, 2952, 2921, 2855, 1607, 1556, 1499, 1484, 1458, 1396 $cm^{-1}$; HRMS m/z calcd for $C_{26}H_{22}NO$ ($[M+H]^+$): 364.1696, found 364.1716.




**2-tert-butyl-1-(5-methyl-2-phenylbenzofuran-4-yl)-1H-indole 7ai:** colorless solid; m.p. 234-236 °C; $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ 7.74 (d, $J$ = 7.8 Hz, 2 H), 7.62 (d, $J$ = 7.4 Hz, 1 H), 7.56 (d, $J$ = 8.3 Hz, 1 H), 7.37 (t, $J$ = 7.1 Hz, 2 H), 7.23-7.31 (m, 2 H), 7.09 (t, $J$ = 7.1 Hz, 1 H), 6.98 (t, $J$ = 7.3 Hz, 1 H), 6.57 (s, 1 H), 6.53 (s, 1 H), 6.51 (d, $J$ = 8.2 Hz, 1 H), 1.95 (s, 3 H), 1.23 (s, 9 H); $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ 156.5, 153.3, 150.1, 139.2, 132.9, 130.9, 130.1, 128.7, 127.1, 126.5, 125.0, 121.4, 119.9, 119.7, 111.6, 109.8, 100.1, 99.7, 33.2, 30.4, 17.1; IR (KBr) 3060, 3026, 2968, 2927, 2865, 1602, 1576, 1504, 1484, 1453 $cm^{-1}$; HRMS m/z calcd for $C_{27}H_{26}NO$ ($[M+H]^+$): 380.2009, found 380.2026.

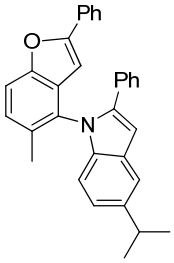



**2-butyl-1-(5-methyl-2-phenylbenzofuran-4-yl)-1H-indole 7aj:** yellow oil; $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ 7.74 (d, $J$ = 7.4 Hz, 2 H), 7.64 (d, $J$ = 7.8 Hz, 1 H), 7.54 (d, $J$ = 8.4 Hz, 1 H), 7.37 (t, $J$ = 7.5 Hz, 2 H), 7.26-7.31 (m, 2 H), 7.11 (t, $J$ = 7.3 Hz, 1 H), 7.03 (t, $J$ = 7.5 Hz, 1 H), 6.78 (d, $J$ = 8.1 Hz, 1 H), 6.50 (s, 1 H), 2.47 (t, $J$ = 7.6 Hz, 2 H), 2.02 (s, 3 H), 1.50-1.56 (m, 2 H), 1.24-1.30 (m, 2 H), 0.79 (t, $J$ = 7.3 Hz, 3 H); $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ 156.8, 153.9, 142.1, 137.5, 131.7, 130.0, 129.2, 128.7, 128.4, 128.3, 126.6, 124.9, 121.0, 119.8, 119.7, 111.3, 110.0, 99.9, 99.2, 30.4, 26.6, 22.2, 16.9, 13.8; IR (KBr) 3050, 2955, 2928, 2859, 1602, 1581, 1550, 1498, 1483, 1457, 1392 $cm^{-1}$; HRMS m/z calcd for $C_{27}H_{26}NO$ ($[M+H]^+$): 380.2009, found 380.2023.

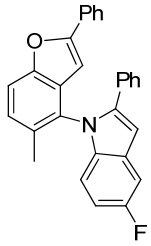



**5-methyl-1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-indole 7ae:** colorless solid; m.p. 227-229 °C; $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ 7.74 (d, $J$ = 7.4 Hz, 2 H), 7.52 (s, 1 H), 7.47 (d, $J$ = 8.2 Hz, 1 H), 7.37 (t, $J$ = 7.1 Hz, 2 H), 7.31 (d, $J$ = 6.9 Hz, 1 H), 7.25-7.28 (m, 2 H), 7.12-7.15 (m, 4 H), 6.95 (d, $J$ = 8.2 Hz, 1 H), 6.83 (s, 1 H), 6.78 (d, $J$ = 8.2 Hz, 1 H), 6.63 (s, 1 H), 2.47 (s, 3 H), 1.88 (s, 3 H); $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ 156.7, 153.7, 141.5, 137.1, 132.7,

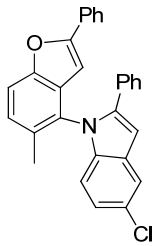
131.2, 130.0, 129.8, 129.5, 129.1, 128.7, 128.6, 128.2, 127.6, 127.3, 126.7, 124.9, 123.9, 120.2, 118.2, 111.0, 110.6, 102.3, 99.5, 21.5, 17.1; IR (KBr) 2963, 2922, 2850, 1591, 1468 $cm^{-1}$; HRMS m/z calcd for $C_{30}H_{24}NO$ ($[M+H]^+$): 414.1852, found 414.1866.



**5-isopropyl-1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-indole 7af:** colorless solid; m.p. 156-158 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.68 (d, $J$ = 7.3 Hz, 2 H), 7.51 (s, 1 H), 7.40 (d, $J$ = 8.2 Hz, 1 H), 7.31 (t, $J$ = 7.1 Hz, 2 H), 7.17-7.25 (m, 3 H), 7.05-7.08 (m, 4 H), 6.94 (dd, $J$ = 8.4 Hz, 1 H), 6.78 (s, 1 H), 6.73 (d, $J$ = 8.2 Hz, 1 H), 6.58 (s, 1 H), 2.93-3.00 (m, 1 H), 1.81 (s, 3 H), 1.27 (s, 3 H), 1.25 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 156.7, 153.7, 141.5, 141.2, 137.4, 132.8, 131.2, 130.0, 129.0, 128.7, 128.4, 128.2, 127.6, 127.2, 126.7, 124.9, 121.7, 117.2, 111.0, 110.7, 102.5, 99.6, 34.1, 24.6, 24.5, 17.2; IR (KBr) 3055, 3035, 2952, 2927, 2865, 1602, 1484, 1463, 1458 $cm^{-1}$; HRMS m/z calcd for $C_{32}H_{28}NO$ ($[M+H]^+$): 442.2165, found 442.2179.



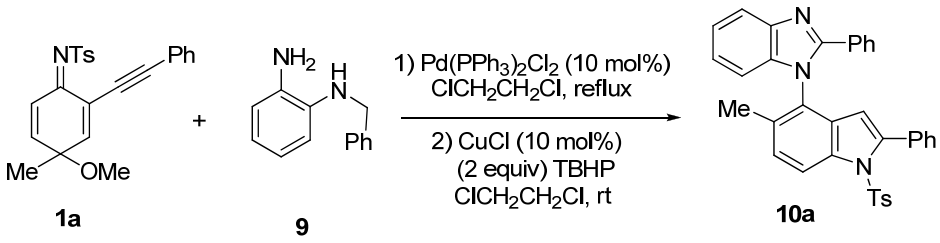
**5-fluoro-1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-indole 7ag:** colorless solid; m.p. 221-223 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.77 (d, $J$ = 7.4 Hz, 2 H), 7.49 (d, $J$ = 8.2 Hz, 1 H), 7.36-7.41 (m, 3 H), 7.32-7.34 (m, 1 H), 7.25-7.28 (m, 2 H), 7.13-7.17 (m, 4 H), 6.83-6.89 (m, 2 H), 6.76-6.80 (m, 1 H), 6.61 (s, 3 H), 1.87 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.0, 153.7, 143.0, 135.2, 132.3, 131.2, 129.9, 129.0, 128.9, 128.8, 128.3, 127.7,126.8, 125.0, 111.6, 111.5, 111.3, 110.7, 105.3, 105.1, 102.5, 99.2, 17.0; IR (KBr) 3060, 3025, 2952, 2922, 2850, 1602, 1478, 1463, 1448 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{21}FNO$ ($[M+H]^+$): 418.1602, found 418.1614.



**5-chloro-1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-indole 7ak:** colorless solid; m.p. 207-209 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.76 (d, $J$ = 7.3 Hz, 2 H), 7.70 (s, 1 H), 7.50 (d, $J$ = 7.8 Hz, 1 H), 7.39 (t, $J$ = 6.9 Hz, 2 H), 7.33 (d, $J$ = 6.4 Hz, 1 H), 7.25-7.27 (m, 2 H), 7.13-7.17 (m, 4 H), 7.07 (dd, $J$ = 8.7 Hz, 1 H), 6.84 (s, 1 H), 6.79 (d, $J$ = 8.2 Hz, 1 H), 6.59 (s, 1 H), 1.86 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.0, 153.7, 142.7, 137.0, 132.1, 131.2, 129.9,

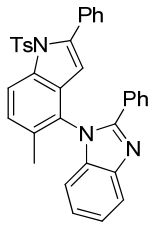
129.3, 128.9, 128.8, 128.3, 127.7, 126.8, 126.2, 125.0, 122.5, 119.8, 111.9, 111.4, 102.1, 99.1, 17.0; IR (KBr) 3059, 3020, 2958, 2916, 2850, 1607, 1555, 1478, 1443 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{21}ClNO$ ($[M+H]^+$): 434.1306, found 434.1311.

## 3. Synthesis of 1-(1*H*-indol-4-yl)-1*H*-benzo[*d*]imidazole



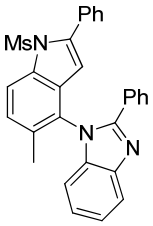

$Pd(PPh_3)_2Cl_2$ (7 mg, 0.01 mmol) was added into the solution of compound **1a** (39 mg, 0.1 mmol) and **9** (40 mg, 0.2 mmol) in DCE (2 mL) at 90 °C. After 3 hours, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 20:1) to afford the pure product **11a** (40 mg, 72% yield).

CuCl (1 mg, 10mol %) and *tert*-butyl hydroperoxide (13 mg, 0.14 mmol) was added into the solution of compound **11a** (40 mg, 0.07 mmol) in DCE (2 mL) at room temperature. Upon completion determined by TLC, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 10:1) to afford the pure product **10a** (37 mg, 94% yield).

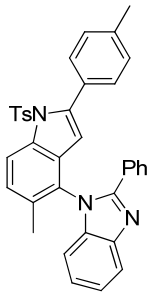



**1-(5-methyl-2-phenyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-benzo[d]imidazole 10a:** red solid; m.p. 187-189 °C; $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ 8.35 (d, $J$ = 8.3 Hz, 1 H), 7.88 (d, $J$ = 7.8 Hz, 1 H), 7.29-7.41 (m, 9 H), 7.24-7.27 (m, 3 H), 7.08-7.16 (m, 5 H), 6.69 (d, $J$ = 7.8 Hz, 1 H), 6.03 (s, 1 H), 2.37 (s, 3 H), 1.91 (s, 3 H); $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ 152.4, 144.7, 144.3, 143.1, 137.8, 136.5, 134.0, 132.0, 131.5, 130.1, 130.0, 129.5, 129.3, 129.1, 129.0, 128.2, 128.1, 127.7, 127.5, 127.2, 126.8, 123.3, 122.9, 119.9, 117.8, 110.5, 110.4, 21.6,

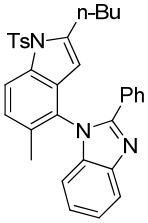
16.9; IR (KBr) 3065, 3024, 2957, 2911, 2855, 1597, 1473, 1443 $cm^{-1}$; HRMS m/z calcd for $C_{35}H_{28}N_3O_2S$ ($[M+H]^+$): 554.1897, found 554.1897.




**1-(5-methyl-1-(methylsulfonyl)-2-phenyl-1H-indol-4-yl)-2-phenyl-1H-benzo[d]imidazole 10c:** red solid; m.p. 186-188 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.16 (d, $J$ = 8.2 Hz, 1 H), 7.93 (d, $J$ = 7.8 Hz, 1 H), 7.56 (d, $J$ = 7.8 Hz, 2 H), 7.39-7.41 (m, 2 H), 7.33-7.37 (m, 4 H), 7.29-7.31 (m, 1 H), 7.24-7.26 (m, 4 H), 6.96 (d, $J$ = 7.8 Hz, 1 H), 6.14 (s, 1 H), 2.74 (s, 3 H), 2.05 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 152.6, 143.5, 143.1, 137.2, 136.5, 132.1, 130.9, 130.1, 129.6, 129.2, 128.9, 128.4, 128.3, 128.0, 127.7, 127.6, 123.5, 123.0, 120.0, 116.7, 110.5, 109.5, 39.7, 17.1; IR (KBr) 3060, 3035, 2952, 2922, 2845, 1607, 1494, 1478, 1437 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{24}N_3O_2S$ ($[M+H]^+$): 478.1584, found 478.1592.



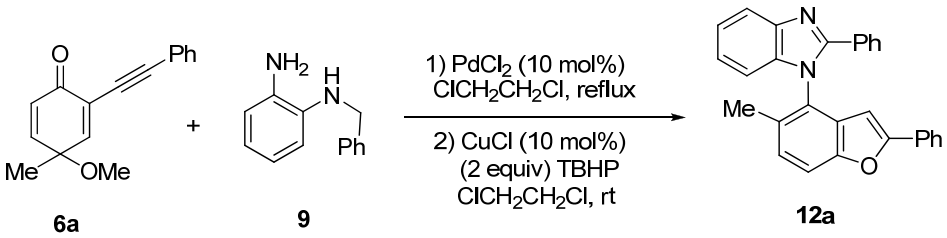

**1-(5-methyl-2-p-tolyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-benzo[d]imidazole 10g:** red solid; m.p. 216-218 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.33 (d, $J$ = 8.2 Hz, 1 H), 7.88 (d, $J$ = 8.3 Hz, 1 H), 7.38 (d, $J$ = 7.3 Hz, 2 H), 7.25-7.27 (m, 6 H), 7.09-7.17 (m, 8 H), 6.67 (d, $J$ = 8.2 Hz, 1 H), 6.01 (s, 1 H), 2.37 (s, 3 H), 1.89 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 152.4, 144.6, 144.5, 143.0, 139.1, 137.7, 136.5, 133.9, 132.0, 130.0, 129.3, 129.1, 128.6, 128.2, 128.1, 127.5, 126.8, 123.3, 122.9, 119.8, 117.9, 110.4, 110.1, 21.6, 21.4, 16.9; IR (KBr) 3055, 3029, 2952, 2916, 2855, 1648, 1602, 1484, 1437 $cm^{-1}$; HRMS m/z calcd for $C_{36}H_{30}N_3O_2S$ ($[M+H]^+$): 568.2053, found 568.2068.




**1-(2-butyl-5-methyl-1-tosyl-1H-indol-4-yl)-2-phenyl-1H-benzo[d]imidazole 10j:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 8.21 (d, $J$ = 8.2 Hz, 1 H), 7.92 (d, $J$ = 7.3 Hz, 1 H), 7.60 (d, $J$ = 7.3 Hz, 2 H), 7.45 (d, $J$ = 7.3 Hz, 2 H), 7.32 (t, $J$ = 7.3 Hz, 1 H), 7.19-7.25 (m, 4 H), 7.14-7.16 (m, 3 H), 6.83 (d, $J$ = 7.4 Hz, 1 H), 5.84 (s, 1 H), 2.86-2.84 (m, 2H), 2.40 (s, 3 H), 1.91 (s, 3H), 1.50-1.52 (m, 2H), 1.25-1.27 (m, 2H), 0.84 (t, $J$ = 6.4 Hz, 3H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 152.6, 144.8, 144.4, 143.0, 136.6, 136.5, 135.9, 130.9, 130.0, 129.8, 129.4, 128.5, 128.3, 128.2, 126.7, 126.6, 126.2, 123.2, 122.8, 119.8, 115.7, 110.6,

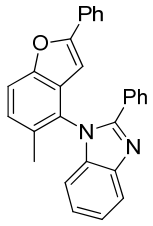
105.5, 30.6, 28.6, 22.2, 21.6, 16.9, 13.7; IR (KBr) 3060, 2952, 2932, 2865, 1597, 1561, 1489, 1458, 1443 $cm^{-1}$; HRMS m/z calcd for $C_{33}H_{32}N_3O_2S$ ($[M+H]^+$): 534.2210, found 534.2215.

## 4. Synthesis of 1-(benzofuran-4-yl)-1H-benzo[d]imidazole




$PdCl_2$ (2 mg, 0.01 mmol) was added into the solution of compound **6a** (24 mg, 0.1 mmol) and **9** (40 mg, 0.2 mmol) in DCE (2 mL) at 90 °C. After 10 hours, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 30:1) to afford the pure product **13a** (30 mg, 74% yield).

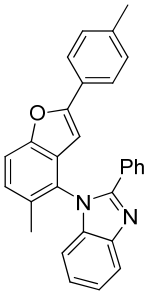
CuCl (1 mg, 10mol %) and *tert*-butyl hydroperoxide (13 mg, 0.14 mmol) was added into the solution of compound **13a** (30 mg, 0.07 mmol) in DCE (2 mL) at room temperature. Upon completion determined by TLC, the reaction mixture was quenched with saturated $NaHCO_3$ (25 mL), and extracted by ethyl acetate (25 mL x 3). The organic layer was dried over $Na_2SO_4$, and concentrated under vacuum. The residue was purified by flash column chromatography on silica gel (hexanes/ethyl acetate = 20:1) to afford the pure product **12a** (28 mg, 95% yield).



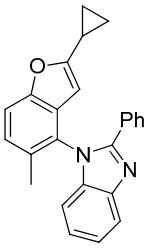

**1-(5-methyl-2-phenylbenzofuran-4-yl)-2-phenyl-1H-benzo[d]imidazole**

**12a:** red solid; m.p. 228-230 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.96 (d, $J$ = 7.8 Hz, 3 H), 7.74 (d, $J$ = 6.9 Hz, 2 H), 7.62 (d, $J$ = 6.9 Hz, 2 H), 7.57 (d, $J$ = 8.2 Hz, 1 H), 7.36-7.38 (m, 2 H), 7.29-7.33 (m, 2 H), 7.21-7.23 (m, 5 H), 6.95 (d, $J$ = 8.2 Hz, 1 H), 6.59 (s, 1 H), 1.92 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.5, 153.9, 152.6, 143.2, 136.7, 130.5, 130.1, 129.6, 129.1, 128.8, 128.4, 128.2, 127.4, 126.9, 125.0, 123.4, 122.9, 119.8, 112.0, 110.7, 98.7, 17.0; IR

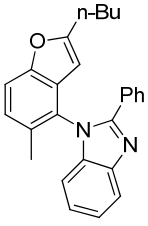
(KBr) 3060, 3028, 2963, 2916, 2845, 1597, 1484, 1437 $cm^{-1}$; HRMS m/z calcd for $C_{28}H_{21}N_2O$ ($[M+H]^+$): 401.1648, found 401.1666.



**1-(5-methyl-2-p-tolylbenzofuran-4-yl)-2-phenyl-1H-benzo[d]imidazole 12g:** red solid; m.p. 184-186 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.95 (d, $J$ = 7.8 Hz, 1 H), 7.60-7.65 (m, 4H), 7.56 (d, $J$ = 8.2 Hz, 1 H), 7.35 (t, $J$ = 7.6 Hz, 1 H), 7.28-7.29 (m, 1H), 7.19-7.25 (m, 6H), 6.96 (d, $J$ = 7.8 Hz, 1 H), 6.53 (s, 1 H), 2.36 (s, 3H), 1.91 (s, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 157.7, 153.8, 152.7, 143.2, 139.3, 136.7, 130.4, 130.1, 129.6, 129.5, 128.4, 128.3, 127.2, 126.9, 126.7, 125.0, 123.4, 122.9, 119.8, 111.9, 110.7, 98.0, 21.4, 17.0; IR (KBr) 3060, 3029, 2952, 2932, 2850, 1612, 1484, 1443 $cm^{-1}$; HRMS m/z calcd for $C_{29}H_{23}N_2O$ ($[M+H]^+$): 415.1805, found 415.1812.

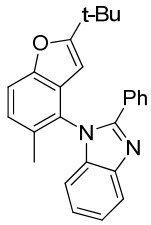


**1-(2-cyclopropyl-5-methylbenzofuran-4-yl)-2-phenyl-1H-benzo[d]imidazole 12i:** red solid; m.p. 178-180 °C; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.92 (d, $J$ = 7.8 Hz, 1 H), 7.58 (d, $J$ = 7.3 Hz, 2 H), 7.40 (d, $J$ = 8.2 Hz, 1 H), 7.28-7.33 (m, 2 H), 7.18-7.26 (m, 3 H), 7.10 (d, $J$ = 8.2 Hz, 1 H), 6.90 (d, $J$ = 8.3 Hz, 1 H), 5.92 (s, 1 H), 1.90-1.94 (m, 1 H), 1.88 (s, 3 H), 0.90-0.97 (m, 4 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 162.3, 153.3, 152.5, 143.1, 136.6, 130.2, 129.8, 129.5, 128.3, 128.2, 126.5, 125.5, 123.2, 122.8, 119.7, 111.4, 110.7, 97.9, 17.0, 9.4, 7.7; IR (KBr) 3070, 3019, 2952, 2921, 2850, 1586, 1494, 1458, 1443 $cm^{-1}$; HRMS m/z calcd for $C_{25}H_{21}N_2O$ ($[M+H]^+$): 365.1648, found 365.1665.

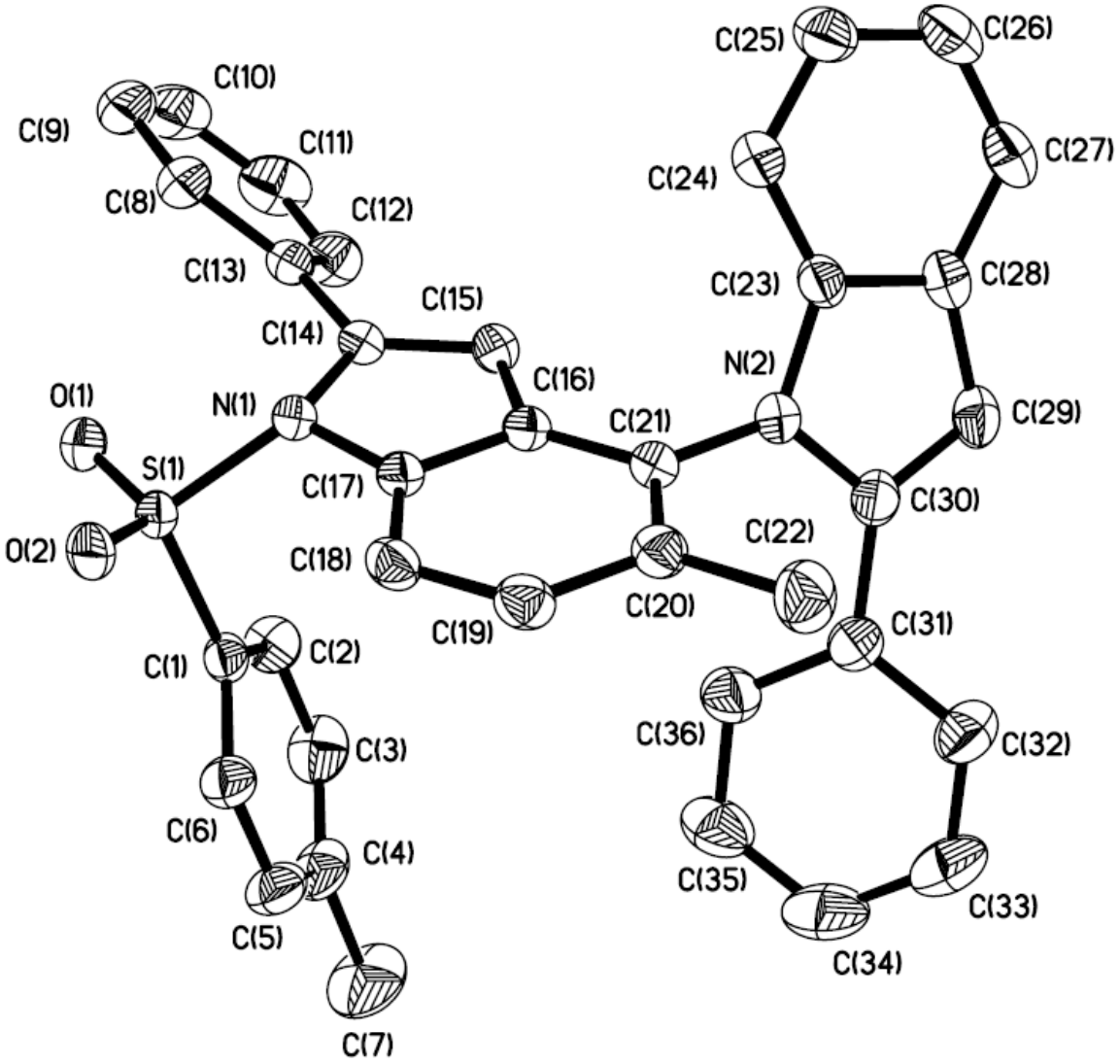


**1-(2-butyl-5-methylbenzofuran-4-yl)-2-phenyl-1 H-benzo[d]imidazole 12j:** yellow oil; $^1$H NMR (400 MHz, $CDCl_3$) $\delta$ 7.93 (d, $J$ = 7.8 Hz, 1 H), 7.57 (d, $J$ = 6.9 Hz, 2 H), 7.45 (d, $J$ = 8.3 Hz, 1 H), 7.34 (t, $J$ = 7.8 Hz, 1 H), 7.28 (d, $J$ = 7.3 Hz, 1 H), 7.21-7.24 (m, 3H), 7.14 (d, $J$ = 8.2 Hz, 1 H), 6.92 (d, $J$ = 7.8 Hz, 1 H), 5.93 (s, 1 H), 2.68 (t, $J$ = 7.3 Hz, 2 H), 1.91 (s, 3 H), 1.61-1.65 (m, 2H), 1.29-1.35 (m, 2H), 0.89 (t, $J$ = 6.8 Hz, 3 H); $^{13}$C NMR (100 MHz, $CDCl_3$) $\delta$ 161.5, 153.7, 152.6, 143.1, 136.6, 130.2, 129.7, 129.5, 128.3, 128.2, 127.9, 126.8, 125.7, 123.2, 122.8, 119.8, 111.5, 110.7, 99.5, 29.4, 28.1, 22.1, 17.0,

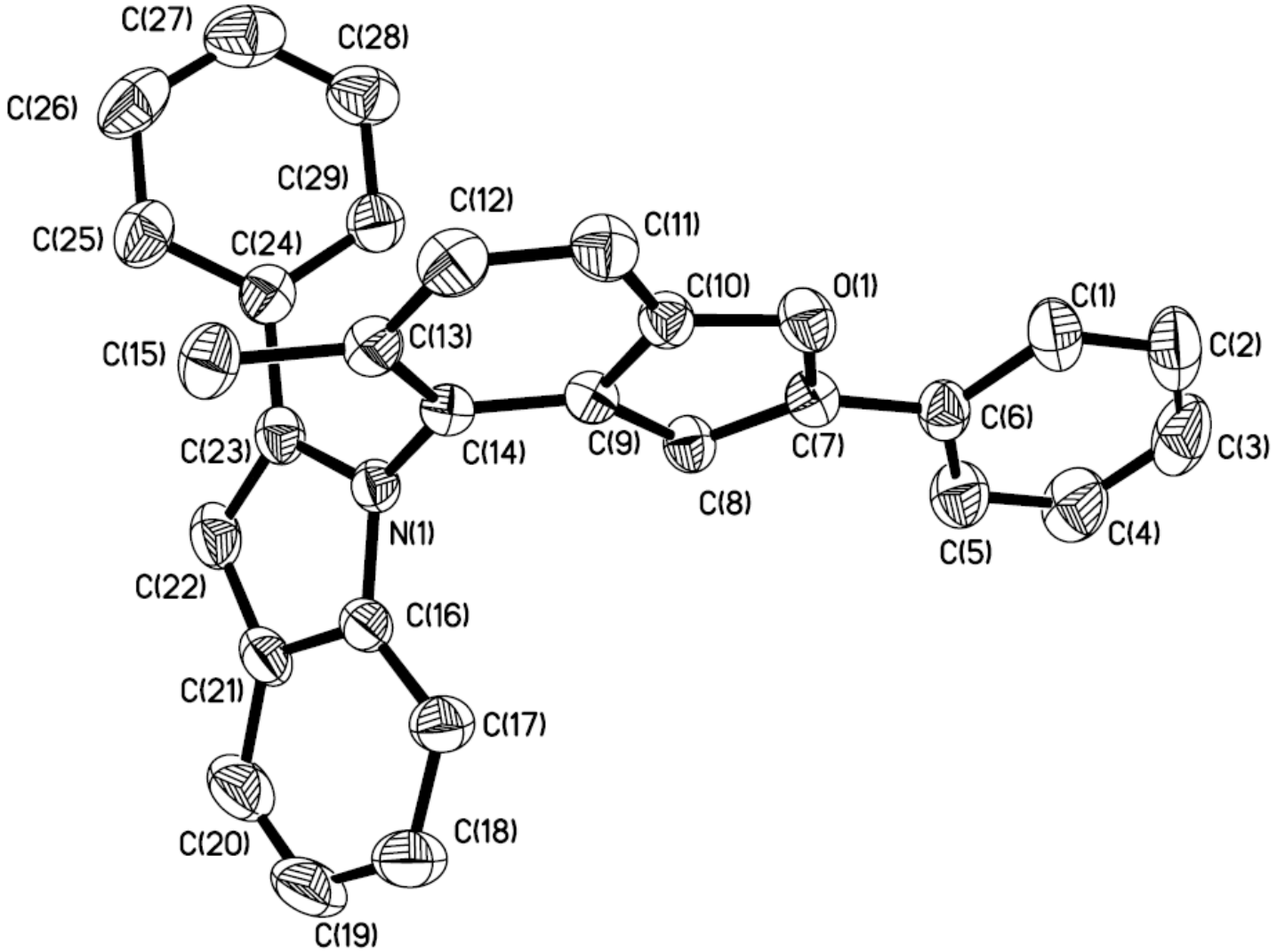
13.7; IR (KBr) 3060, 3029, 2957, 2927, 2865, 1586, 1489, 1453 $cm^{-1}$; HRMS m/z calcd for $C_{26}H_{25}N_2O$ ($[M+H]^+$): 381.1961, found 381.1974.



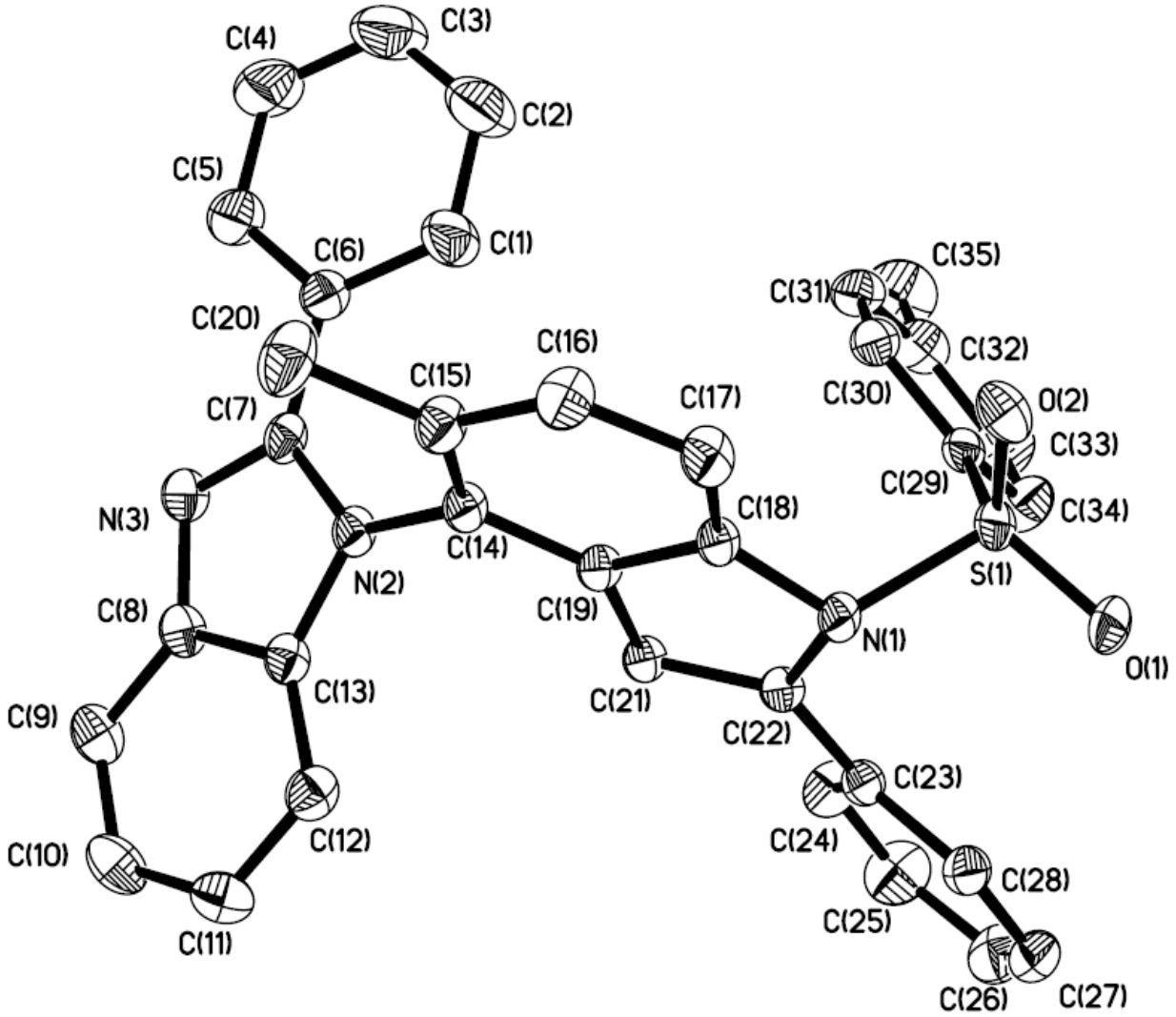

**1-(2-tert-butyl-5-methylbenzofuran-4-yl)-2-phenyl-1H-benzo[d]imidazole 12k:** yellow oil; $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ 7.94 (d, $J$ = 7.8 Hz, 1 H), 7.58 (d, $J$ = 7.3 Hz, 2 H), 7.46 (d, $J$ = 8.3 Hz, 1 H), 7.34 (t, $J$ = 7.8 Hz, 1 H), 7.28 (d, $J$ = 6.9 Hz, 1 H), 7.23-7.25 (m, 3 H), 7.14 (d, $J$ = 8.2 Hz, 1 H), 6.93 (d, $J$ = 7.8 Hz, 1 H), 5.90 (s, 1 H), 1.90 (s, 3 H), 1.29 (s, 9 H); $^{13}C$ NMR (100 MHz, $CDCl_3$) $\delta$ 169.1, 153.7, 152.6, 143.1, 136.7, 130.2, 129.6, 129.4, 128.3, 128.2, 127.8, 127.0, 125.7, 123.2, 122.8, 119.7, 111.6, 110.8, 96.7, 33.1, 28.7, 17.0; IR (KBr) 3065, 3035, 2968, 2927, 2865, 1602, 1581, 1489, 1453 $cm^{-1}$; HRMS m/z calcd for $C_{26}H_{25}N_2O$ ($[M+H]^+$): 381.1961, found 381.1977.



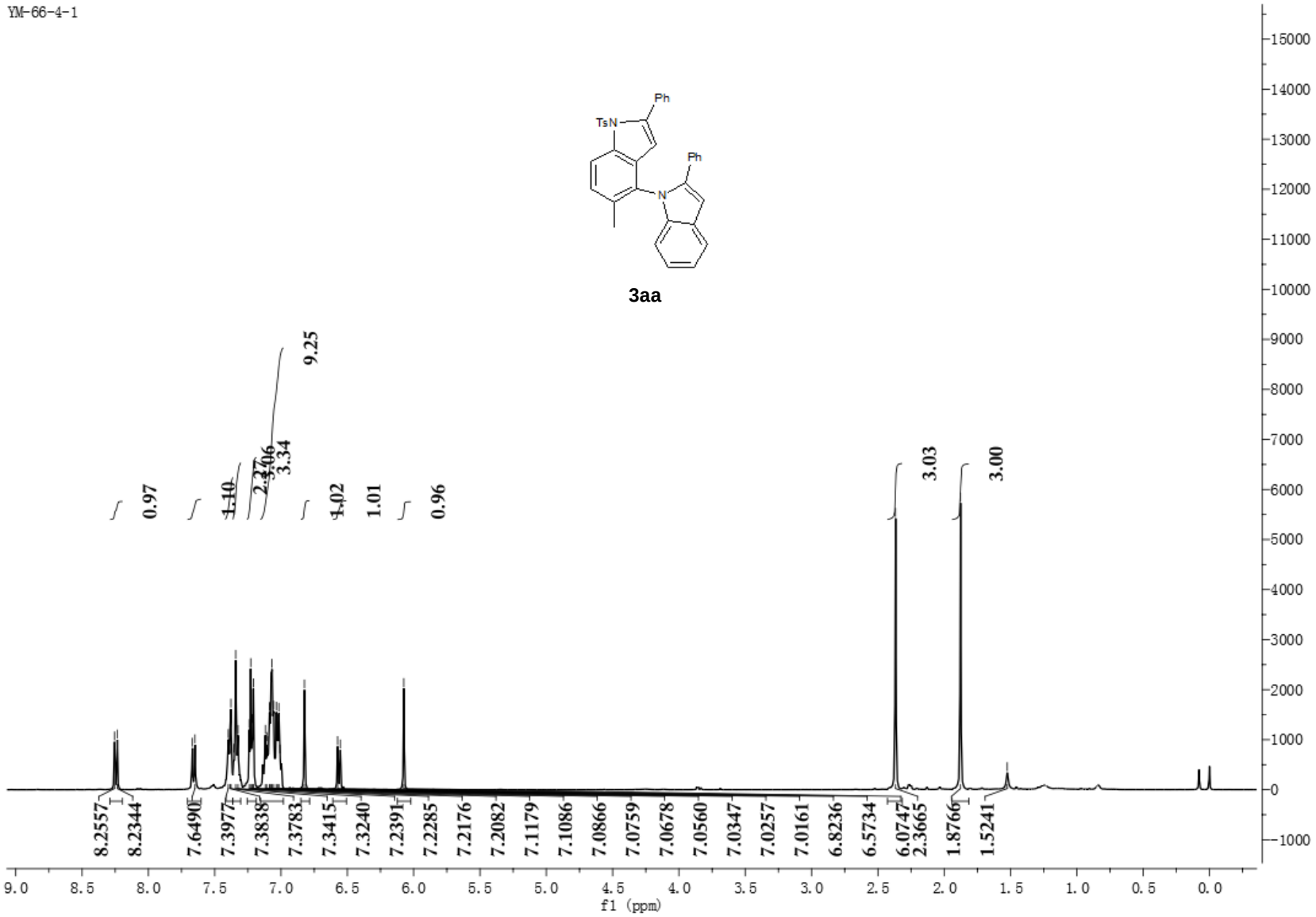

X-ray diffraction structure of compound **3aa**

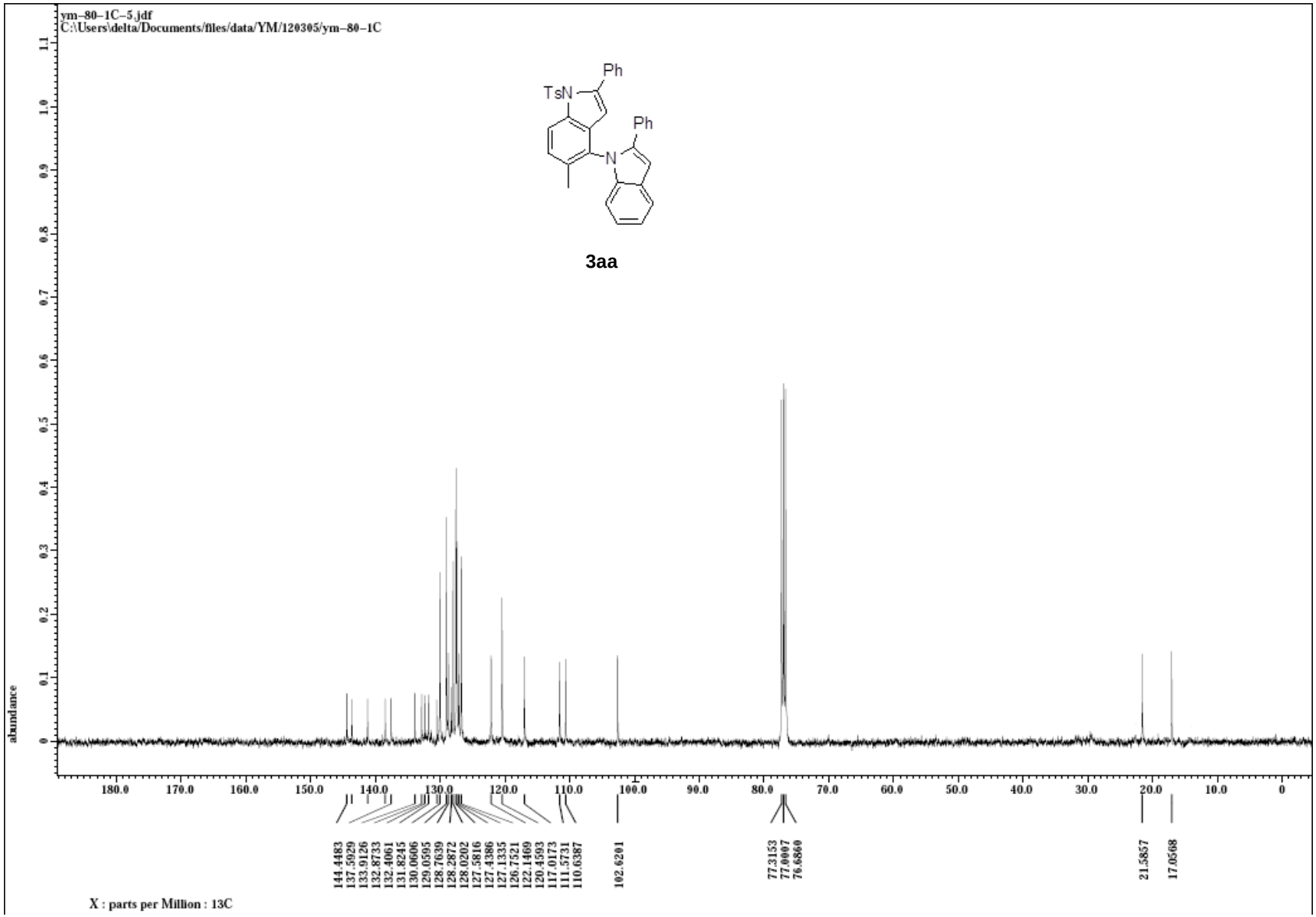


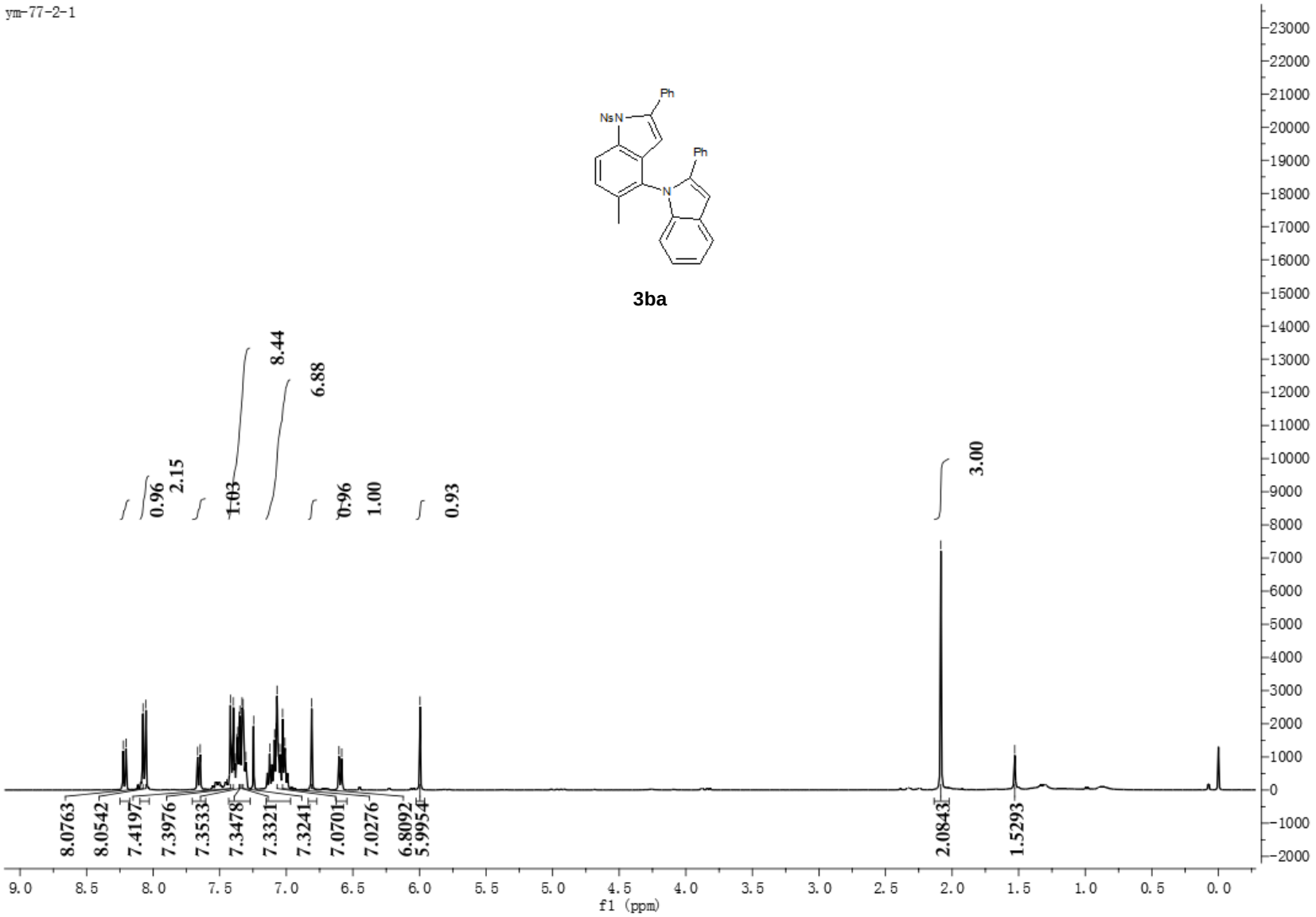

X-ray diffraction structure of compound **7aa**




X-ray diffraction structure of compound **10a**


YM-66-4-1
Ph
TsN
Ph
N
3aa
9.25
3.34
2.37
2.06
1.10
1.02
1.01
0.97
0.96
3.03
3.00
8.2557
8.2344
7.6490
7.3977
7.3838
7.3783
7.3415
7.3240
7.2391
7.2285
7.2176
7.2082
7.1179
7.1086
7.0866
7.0759
7.0678
7.0560
7.0347
7.0257
7.0161
6.8236
6.5734
6.0747
2.3665
1.8766
1.5241
f1 (ppm)


ym-80-1C-5.jdf
C:\Users\delta\Documents\files\data\YM\120305\ym-80-1C
Ph
TsN
Ph
N
3aa
abundance
144.4483
137.5929
133.9126
132.8733
132.4061
131.8245
130.0606
129.0595
128.7639
128.2872
128.0202
127.5816
127.4386
127.1335
126.7521
122.1469
120.4593
117.0173
111.5731
110.6387
102.6291
77.3153
77.0007
76.6860
21.5857
17.0568
X : parts per Million : 13C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NsN
Ph
N
3ba
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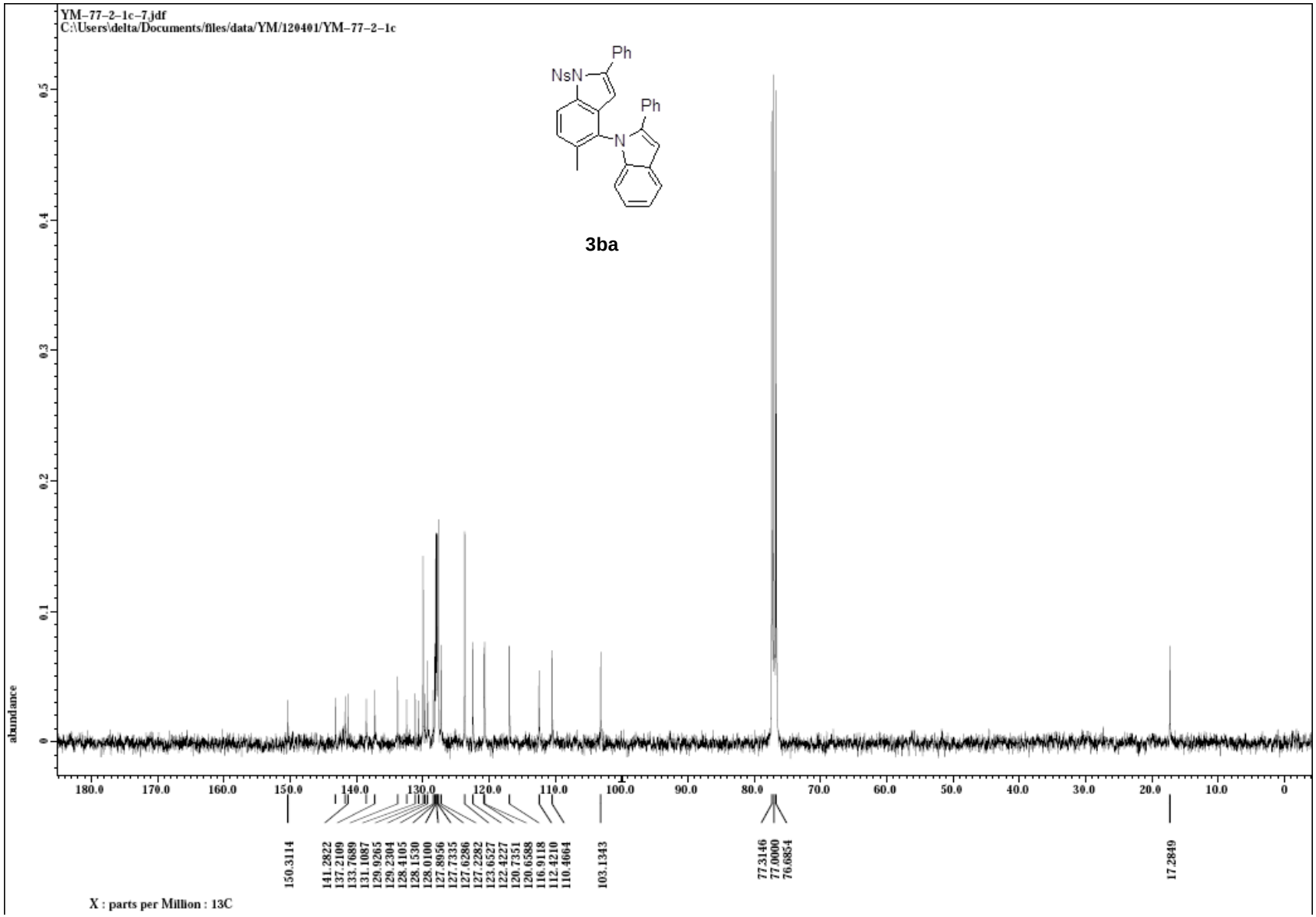
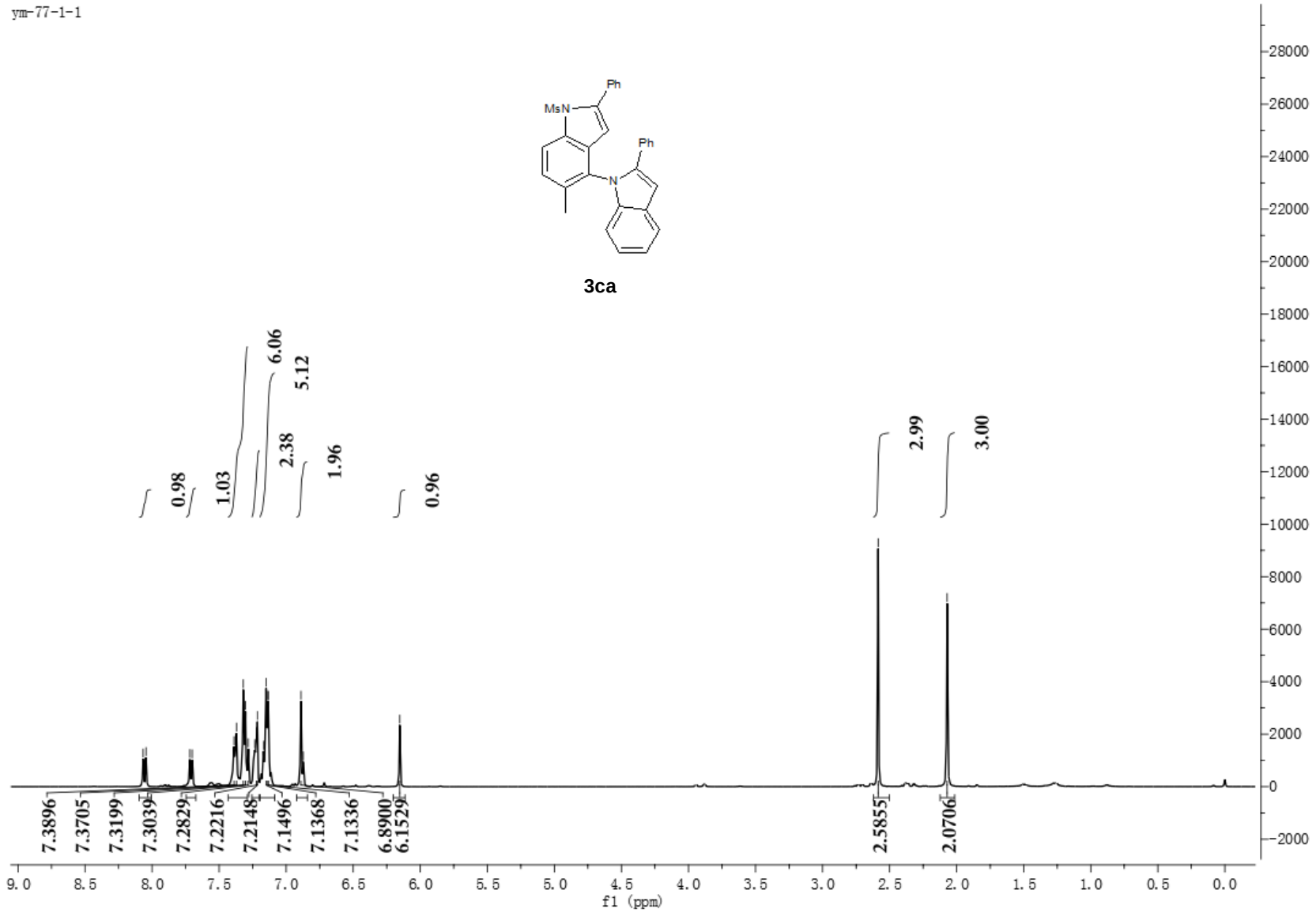
2.15
1.03
8.44
6.88
0.96
1.00
0.93
3.00
8.0763
8.0542
7.4197
7.3976
7.3533
7.3478
7.3321
7.3241
7.0701
7.0276
6.8092
5.9954
2.0843
1.5293
f1 (ppm)


YM–77–2–1c–7.jdf
C:\Users\delta/Documents/files/data/YM/120401/YM–77–2–1c
Ph
NsN
Ph
N
3ba
abundance
150.3114
141.2822
137.2109
133.7689
131.1087
129.9265
129.2304
128.4105
128.1530
128.0100
127.8956
127.7335
127.6286
127.2282
123.6527
122.4227
120.7351
120.6588
116.9118
112.4210
110.4664
103.1343
77.3146
77.0000
76.6854
17.2849
X : parts per Million : 13C


ym-77-1-1
Ph
MsN
Ph
N
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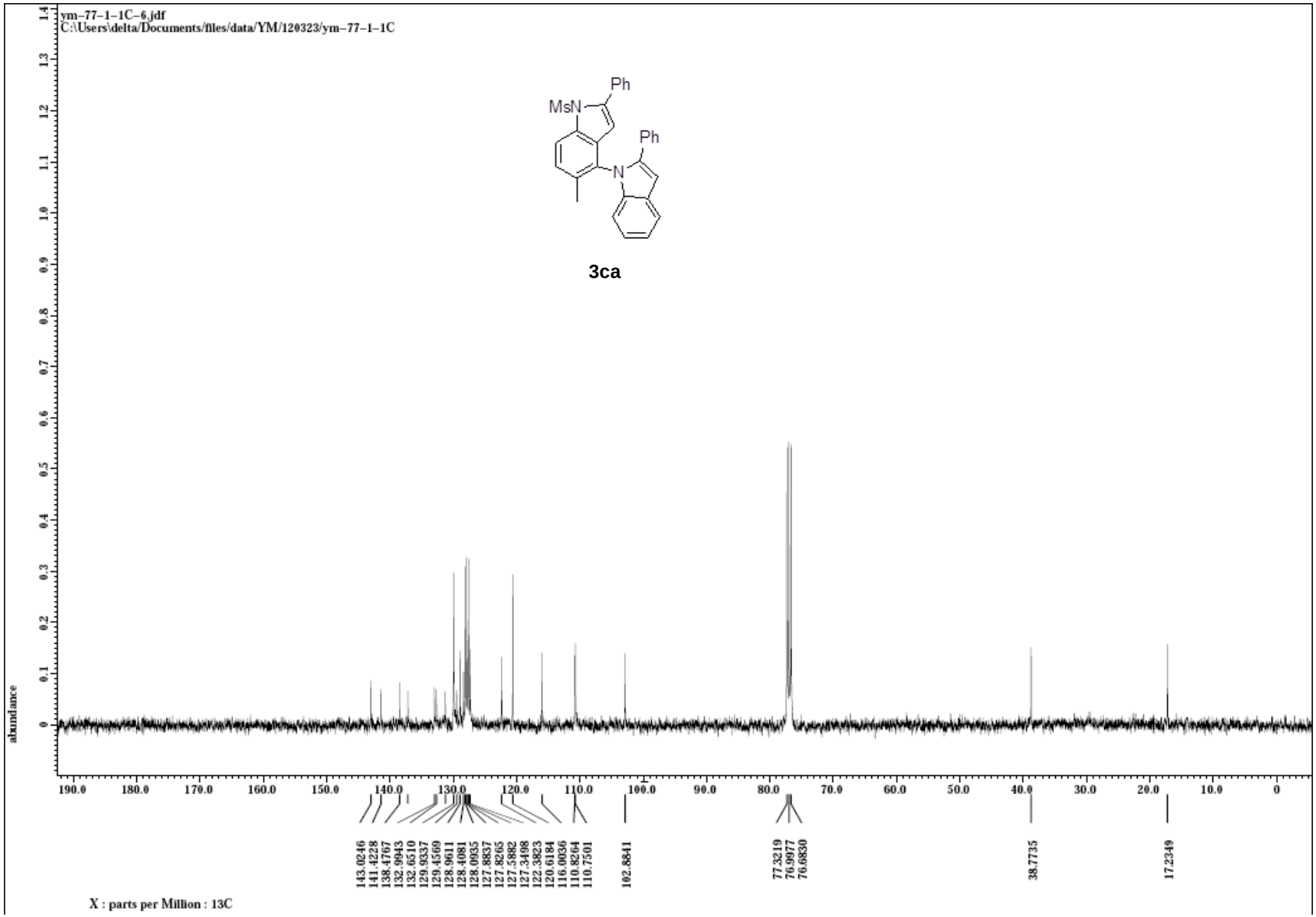
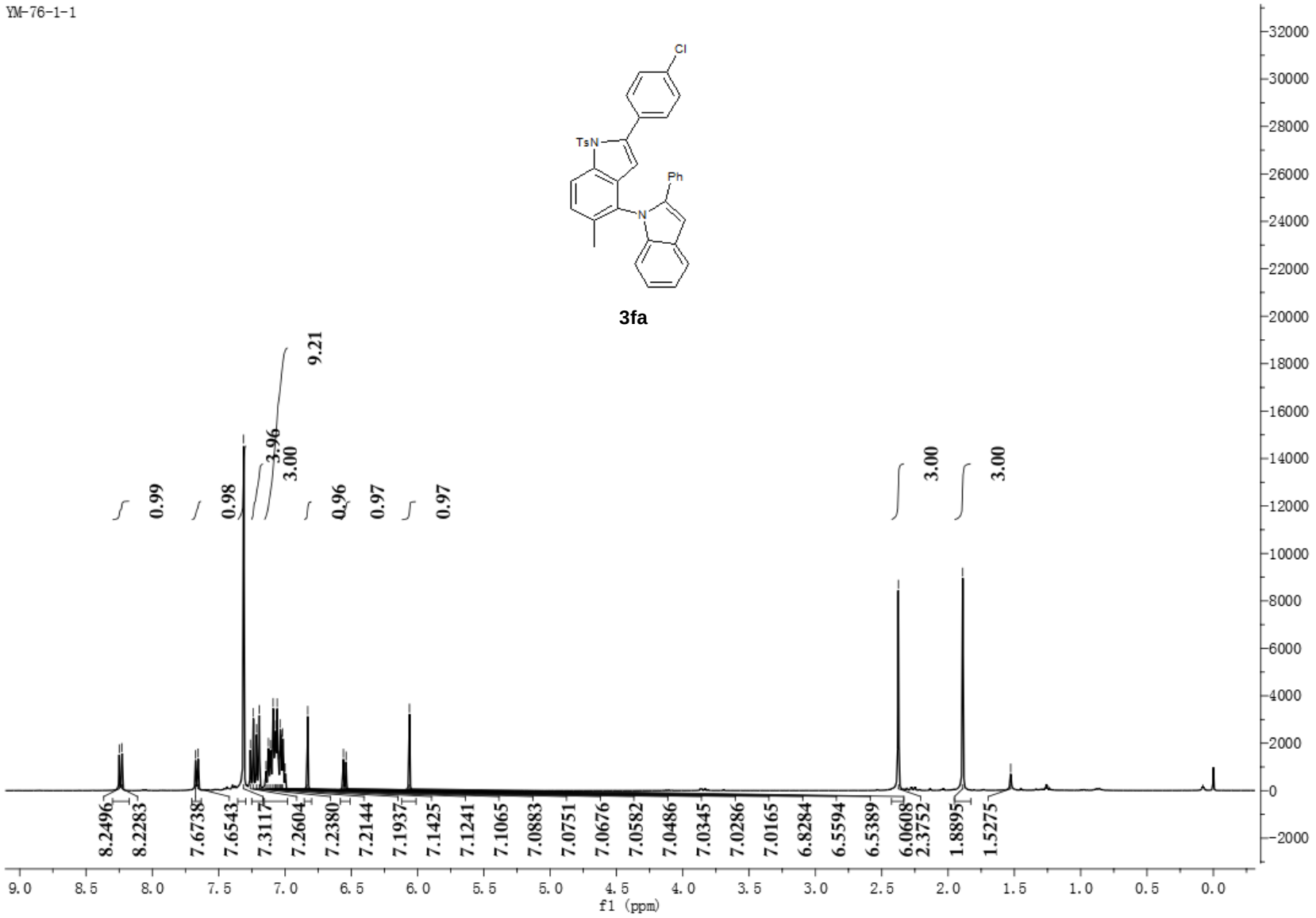
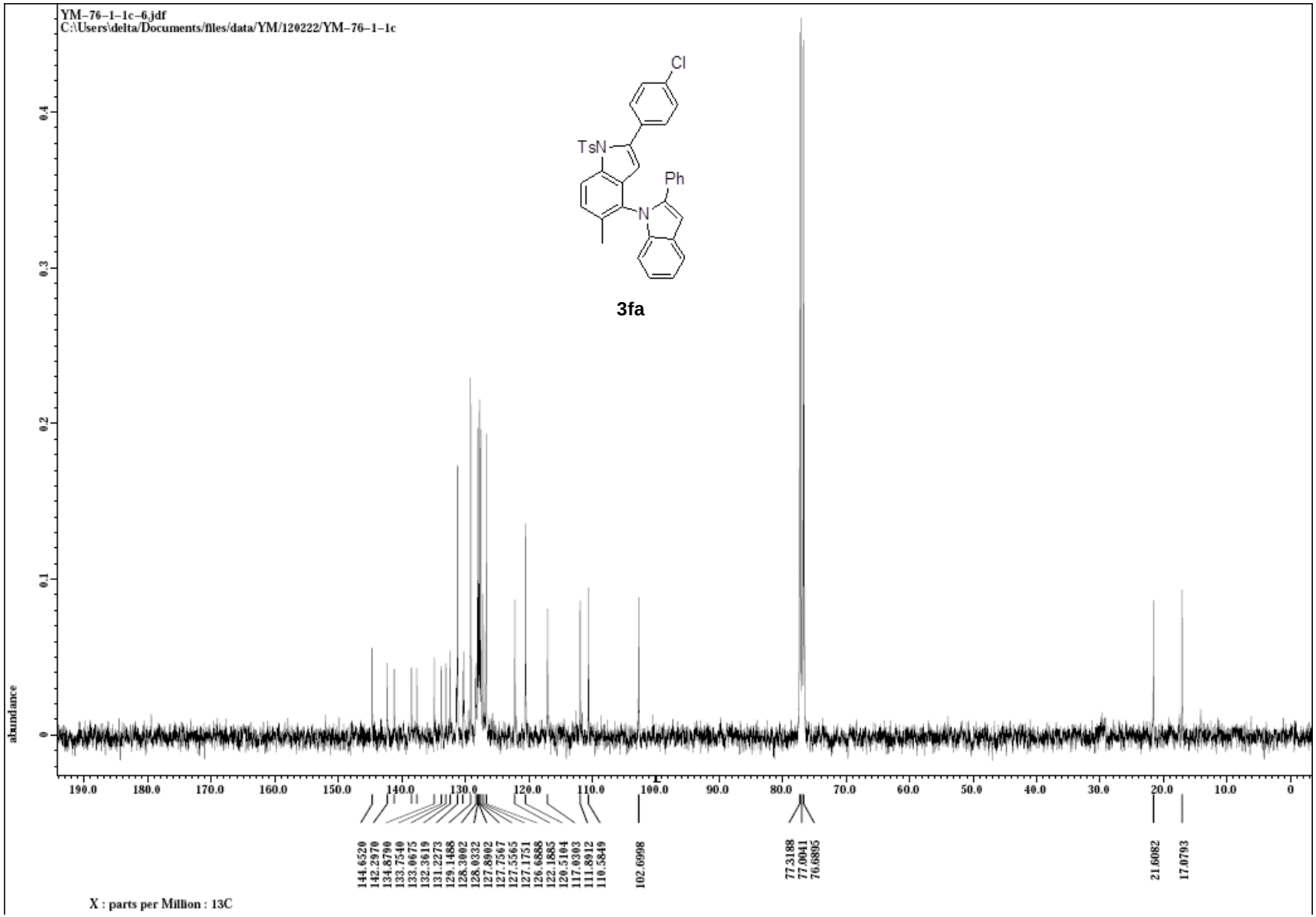
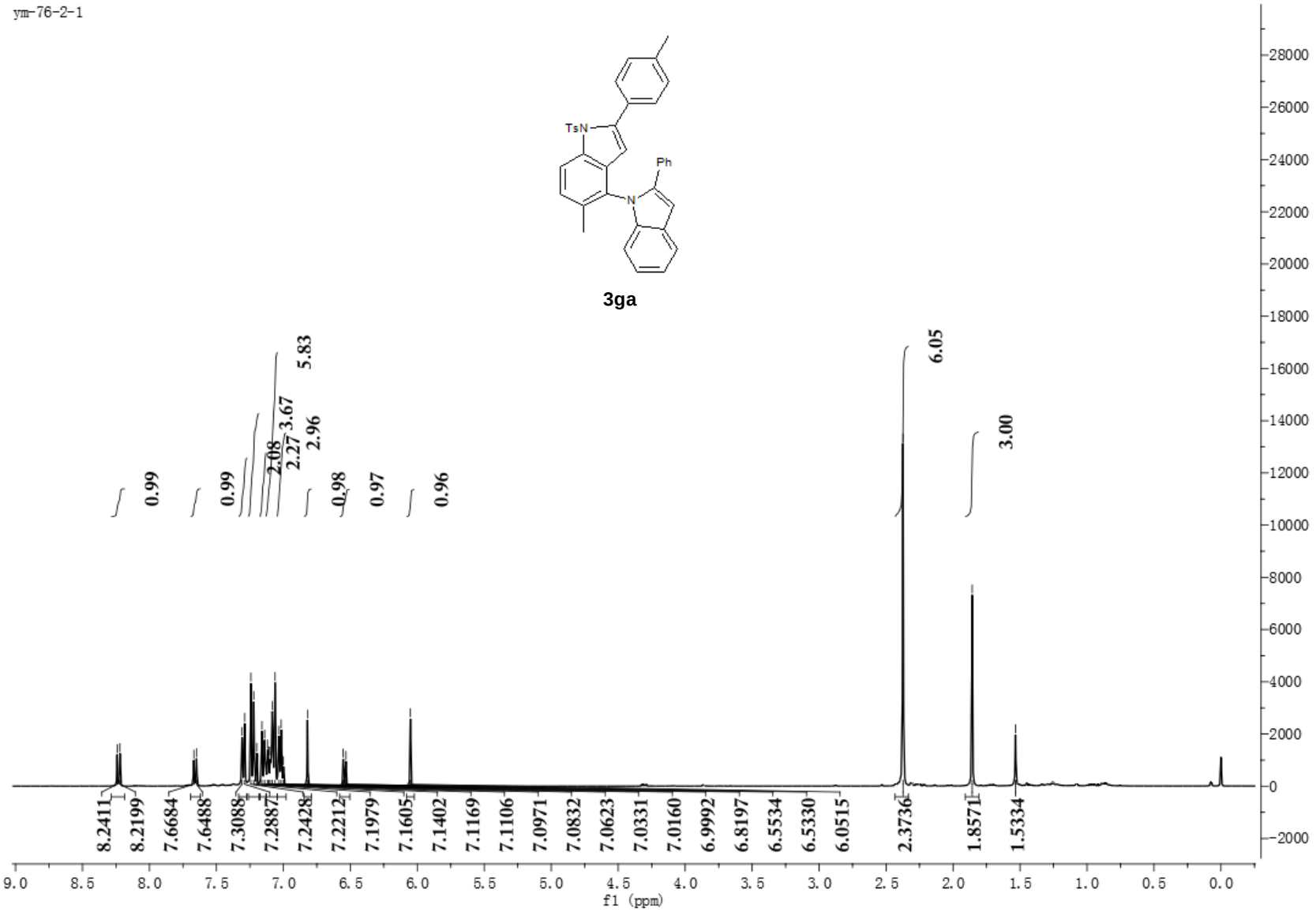
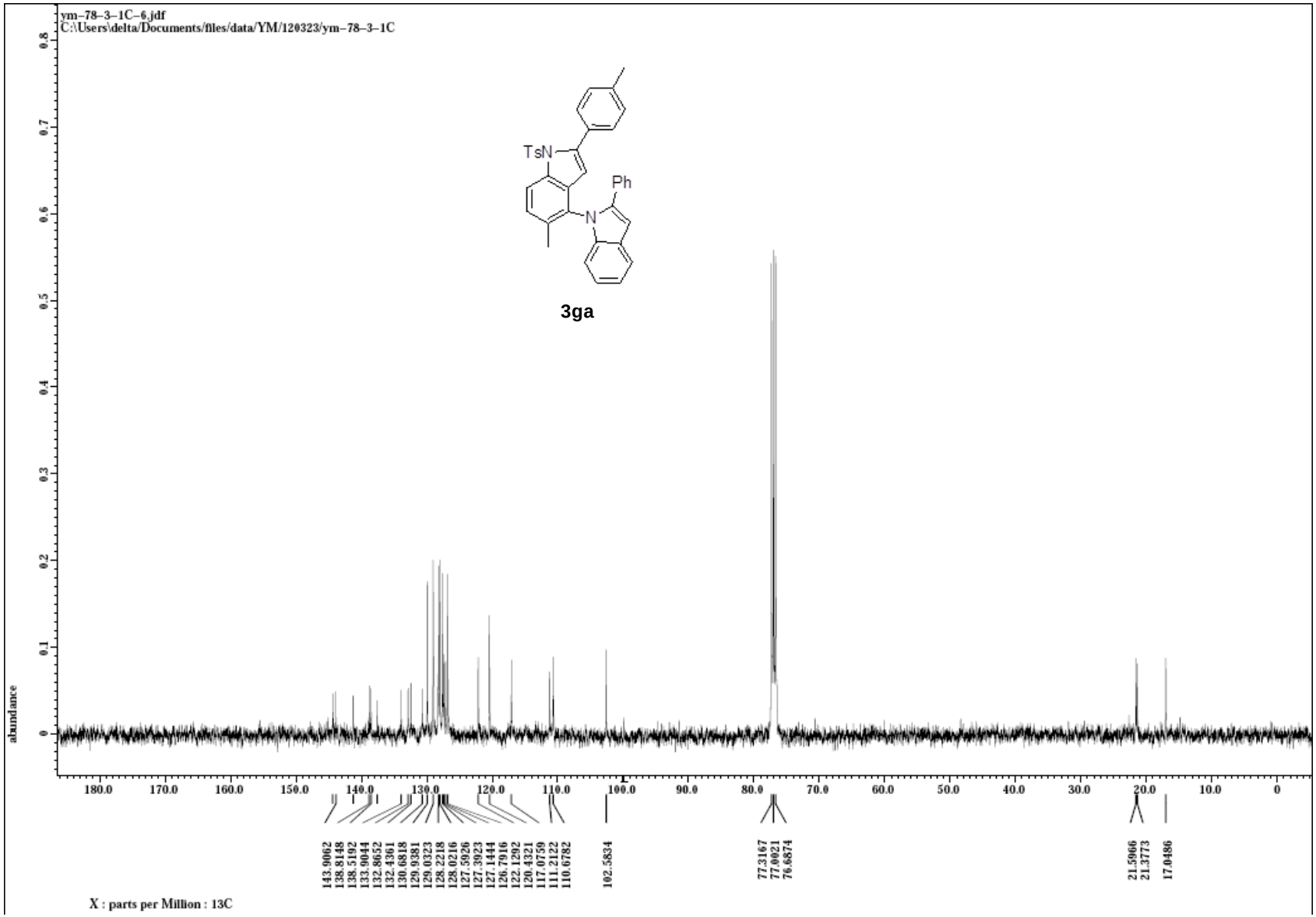
0.98
1.03
6.06
5.12
2.38
1.96
0.96
2.99
3.00
7.3896
7.3705
7.3199
7.3039
7.2829
7.2216
7.2148
7.1496
7.1368
7.1336
6.8900
6.1529
2.5855
2.0706
f1 (ppm)

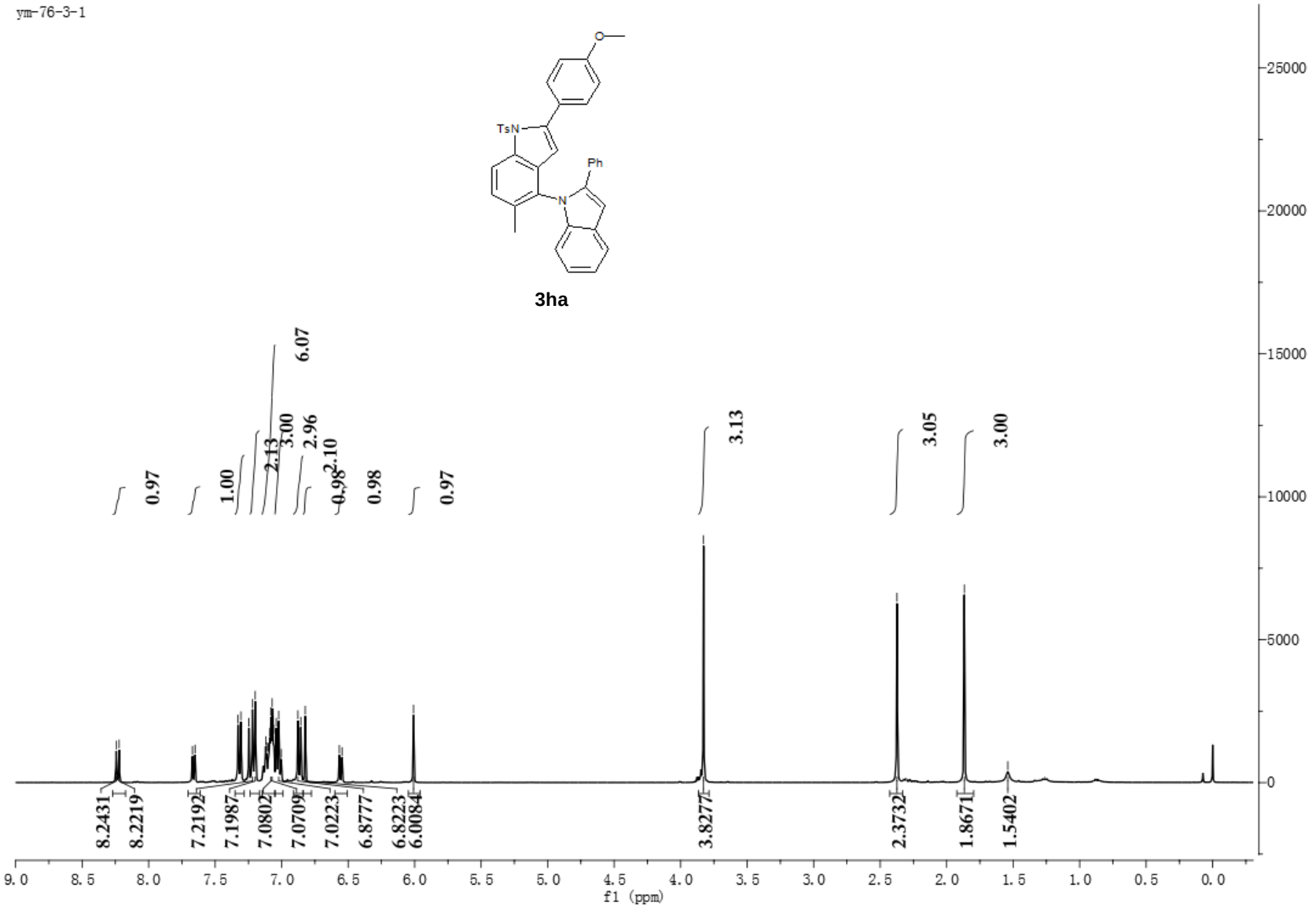

ym-77-1-1C-6.jdf
C:\Users\delta/Documents/files/data/YM/120323/ym-77-1-1C
Ph
MsN
Ph
N
3ca
abundance
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
143.0246
141.4228
138.4767
132.9943
132.6510
129.9337
129.4569
128.9611
128.4081
128.0935
127.8837
127.8265
127.5882
127.3498
122.3823
120.6184
116.0036
110.8264
110.7501
102.8841
77.3219
76.9977
76.6830
38.7735
17.2349
X : parts per Million : 13C


YM-76-1-1
Cl
TsN
Ph
N
3fa
0.99
0.98
9.21
3.96
3.00
0.96
0.97
0.97
3.00
3.00
8.2496
8.2283
7.6738
7.6543
7.3117
7.2604
7.2380
7.2144
7.1937
7.1425
7.1241
7.1065
7.0883
7.0751
7.0676
7.0582
7.0486
7.0345
7.0286
7.0165
6.8284
6.5594
6.5389
6.0608
2.3752
1.8895
1.5275
f1 (ppm)




ym-76-2-1
TsN
Ph
N
3ga
0.99
0.99
2.08
2.27
3.67
5.83
2.96
0.98
0.97
0.96
6.05
3.00
8.2411
8.2199
7.6684
7.6488
7.3088
7.2887
7.2428
7.2212
7.1979
7.1605
7.1402
7.1169
7.1106
7.0971
7.0832
7.0623
7.0331
7.0160
6.9992
6.8197
6.5534
6.5330
6.0515
2.3736
1.8571
1.5334
f1 (ppm)


ym-78-3-1C-6.jdf
C:\Users\delta/Documents/files/data/YM/120323/ym-78-3-1C
TsN
Ph
N
3ga
abundance
143.9062
138.8148
138.5192
133.9044
132.8652
132.4361
130.6818
129.9381
129.0323
128.2218
128.0216
127.5926
127.3923
127.1444
126.7916
122.1292
120.4321
117.0759
111.2122
110.6782
102.5834
77.3167
77.0021
76.6874
21.5966
21.3773
17.0486
X : parts per Million : 13C


ym-76-3-1
TsN
Ph
N
O
3ha
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1.00
2.13
3.00
2.96
2.10
0.98
0.98
0.97
6.07
3.13
3.05
3.00
8.2431
8.2219
7.2192
7.1987
7.0802
7.0709
7.0223
6.8777
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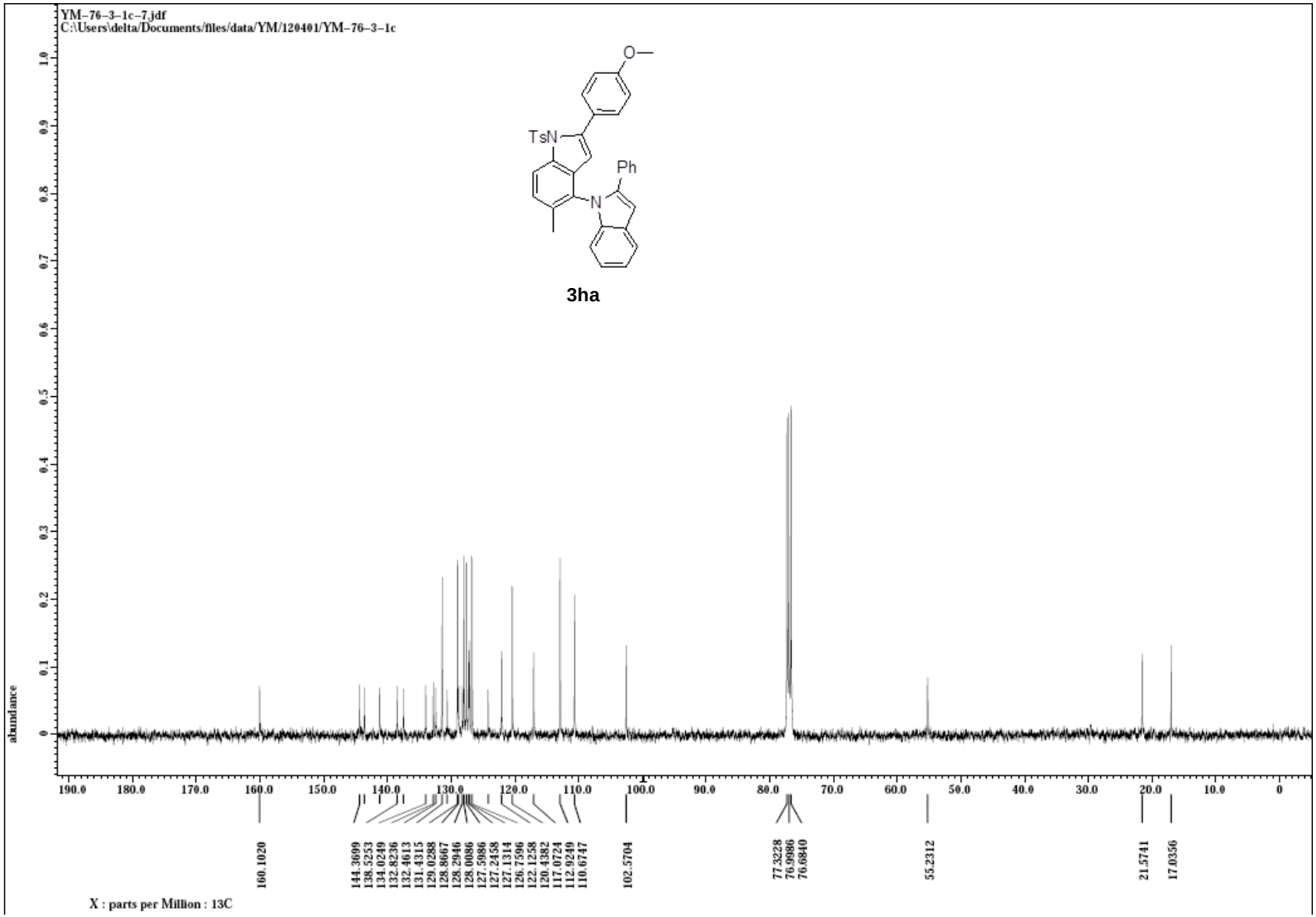
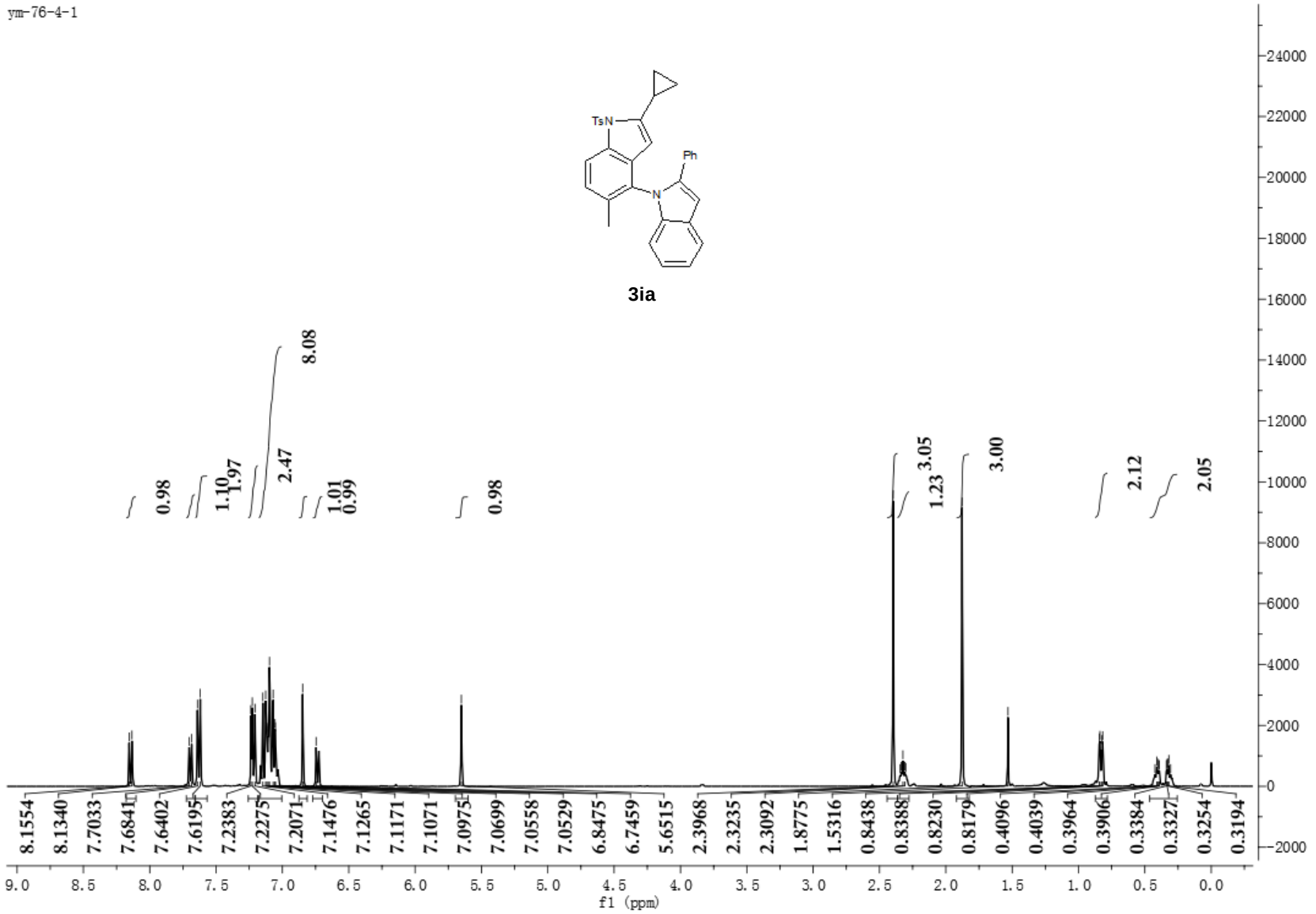
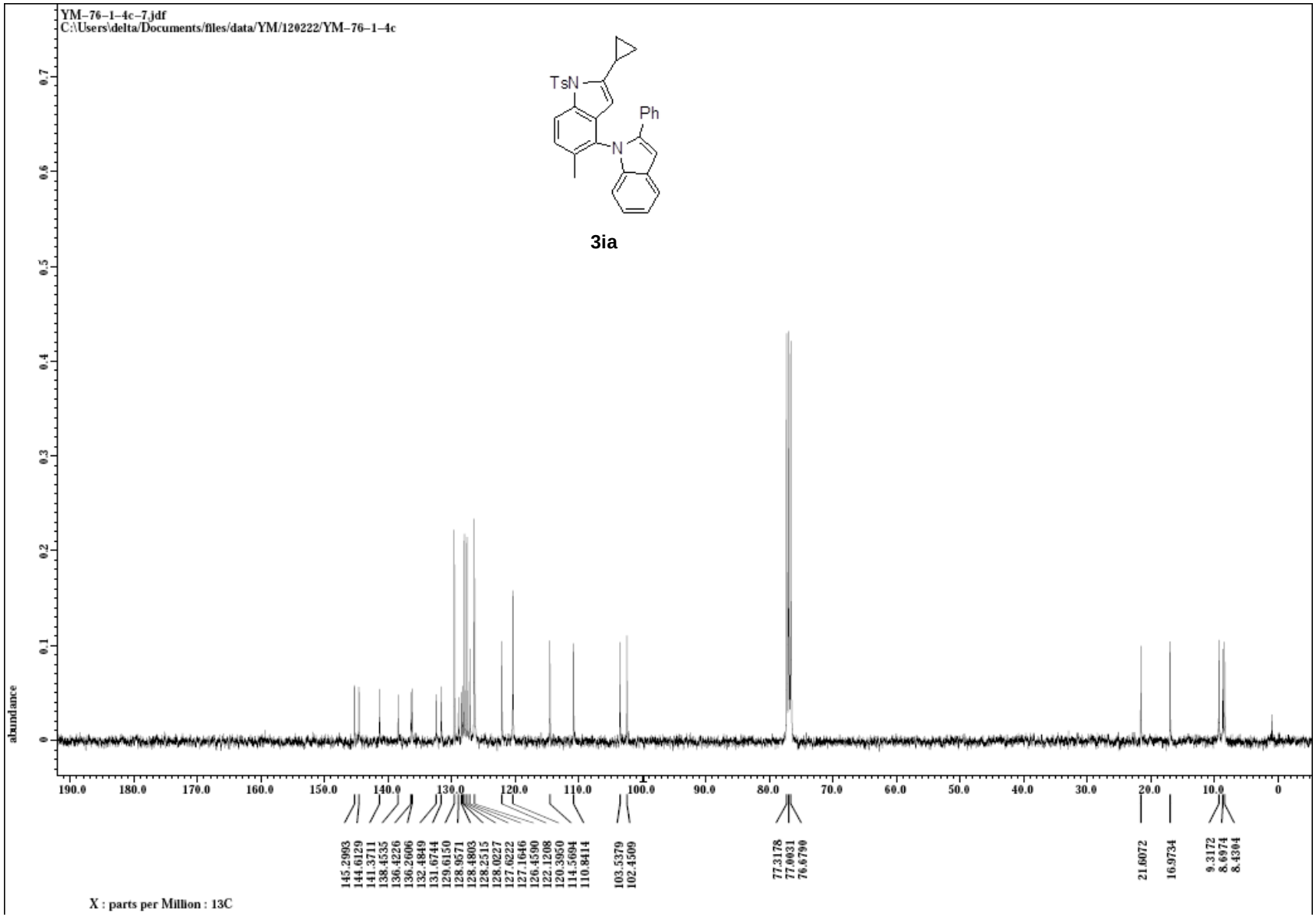
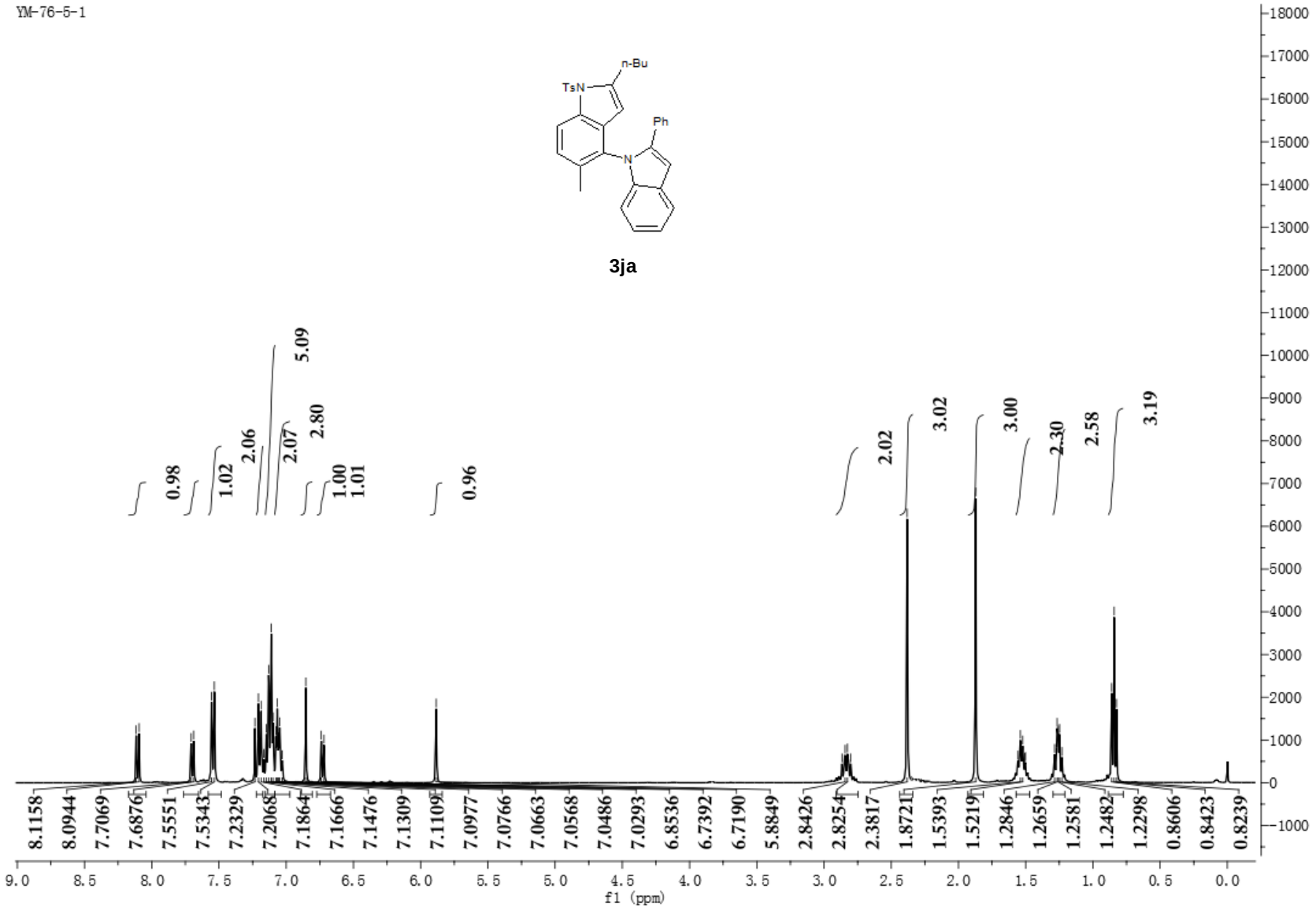
2.3732
1.8671
1.5402
f1 (ppm)


YM-76-3-1c-7.jdf
C:\Users\delta\Documents\files\data\YM\120401\YM-76-3-1c
O
TsN
Ph
N
abundance
160.1020
144.3699
138.5253
134.0249
132.8236
132.4613
131.4315
129.0288
128.8667
128.2946
128.0086
127.5986
127.2458
127.1314
126.7596
122.1258
120.4382
117.0724
112.9249
110.6747
102.5704
77.3228
76.9986
76.6840
55.2312
21.5741
17.0356
X : parts per Million : 13C

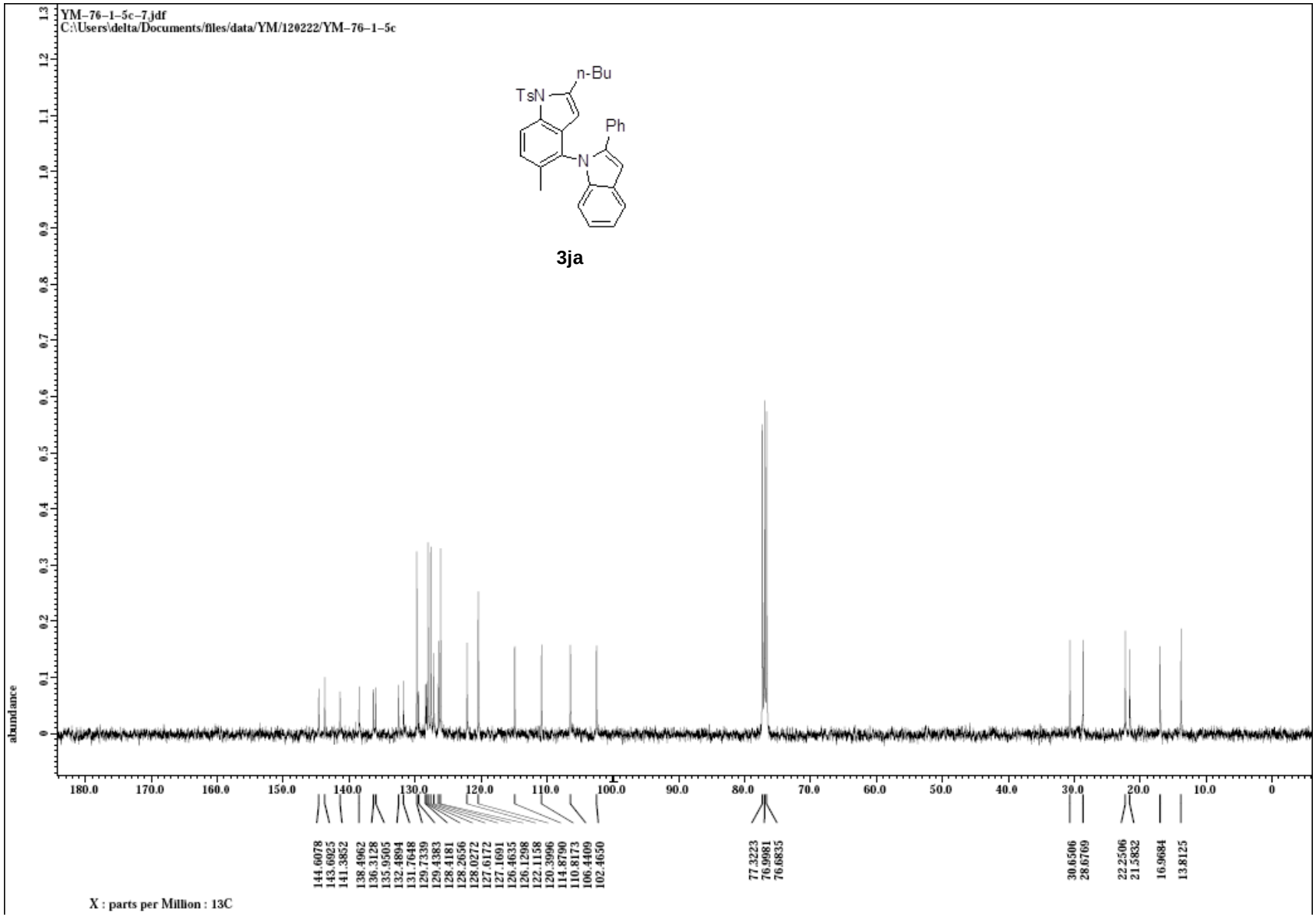
**3ha**


ym-76-4-1
TsN
Ph
N
3ia
0.98
1.10
1.97
2.47
8.08
1.01
0.99
0.98
3.05
1.23
3.00
2.12
2.05
8.1554
8.1340
7.7033
7.6841
7.6402
7.6195
7.2383
7.2275
7.2071
7.1476
7.1265
7.1171
7.1071
7.0975
7.0699
7.0558
7.0529
6.8475
6.7459
5.6515
2.3968
2.3235
2.3092
1.8775
1.5316
0.8438
0.8388
0.8230
0.8179
0.4096
0.4039
0.3964
0.3906
0.3384
0.3327
0.3254
0.3194
f1 (ppm)

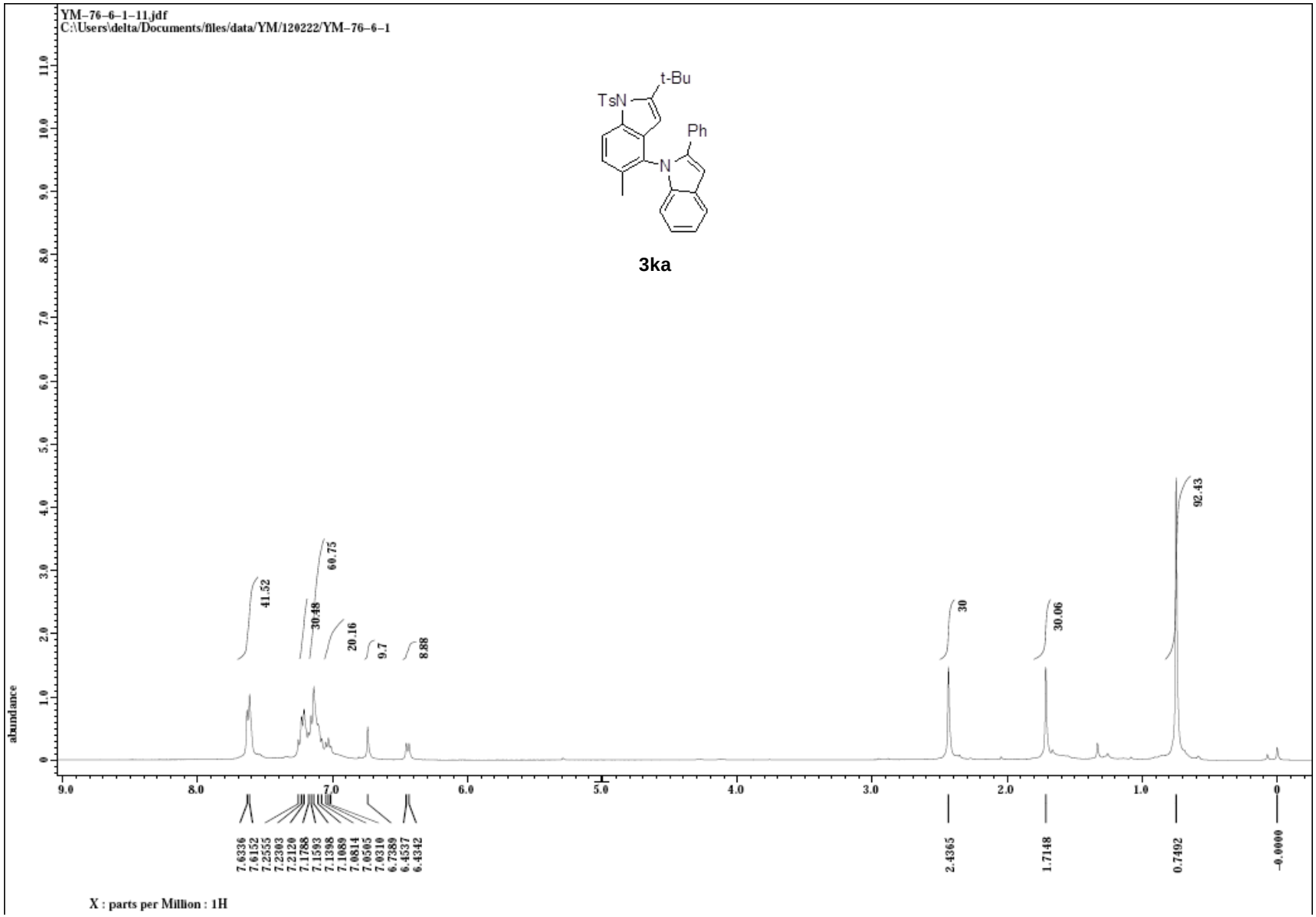


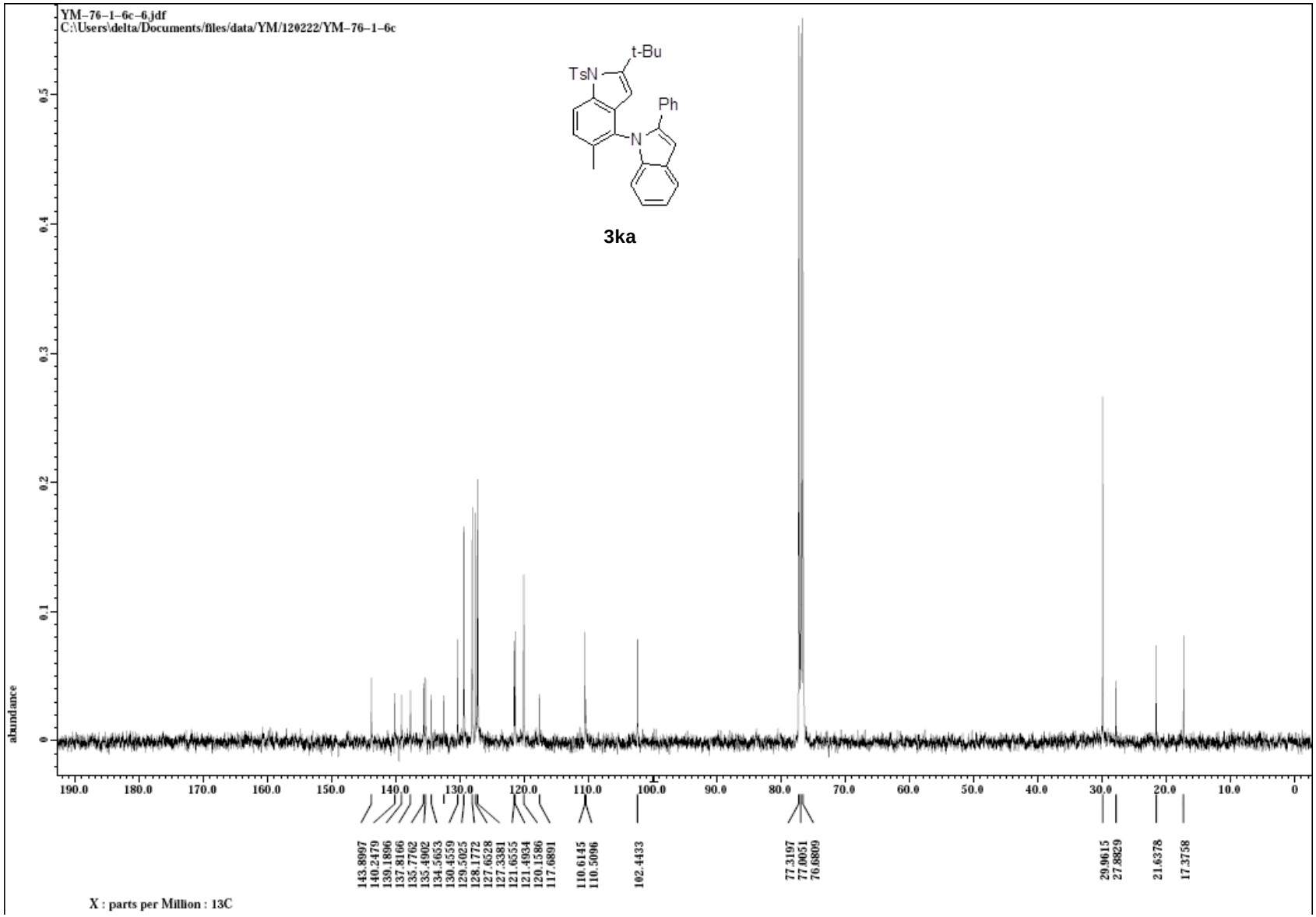

YM-76-5-1
n-Bu
TsN
Ph
N
0.98
1.02
2.06
2.07
5.09
2.80
1.00
1.01
0.96
2.02
3.02
3.00
2.30
2.58
3.19
8.1158
8.0944
7.7069
7.6876
7.5551
7.5343
7.2329
7.2068
7.1864
7.1666
7.1476
7.1309
7.1109
7.0977
7.0766
7.0663
7.0568
7.0486
7.0293
6.8536
6.7392
6.7190
5.8849
2.8426
2.8254
2.3817
1.8721
1.5393
1.5219
1.2846
1.2659
1.2581
1.2482
1.2298
0.8606
0.8423
0.8239
f1 (ppm)

**3ja**




**3ja**


YM-76-6-1-11.jdf
C:\Users\delta/Documents/files/data/YM/120222/YM-76-6-1
t-Bu
TsN
Ph
N
3ka
abundance
41.52
30.48
60.75
20.16
9.7
8.88
30
30.06
92.43
7.6336
7.6132
7.2555
7.2303
7.2120
7.1788
7.1593
7.1398
7.1089
7.0814
7.0565
7.0310
6.7389
6.4537
6.4342
2.4365
1.7148
0.7492
-0.0000
X : parts per Million : 1H


YM-76-1-6c-6.jdf
C:\Users\delta/Documents/files/data/YM/120222/YM-76-1-6c
t-Bu
TsN
Ph
N
3ka
abundance
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
143.8997
140.2479
139.1896
137.8166
135.7762
135.4902
134.5653
130.4559
129.5025
128.1772
127.6528
127.3381
121.6555
121.4934
120.1586
117.6891
110.6145
110.5096
102.4433
77.3197
77.0051
76.6809
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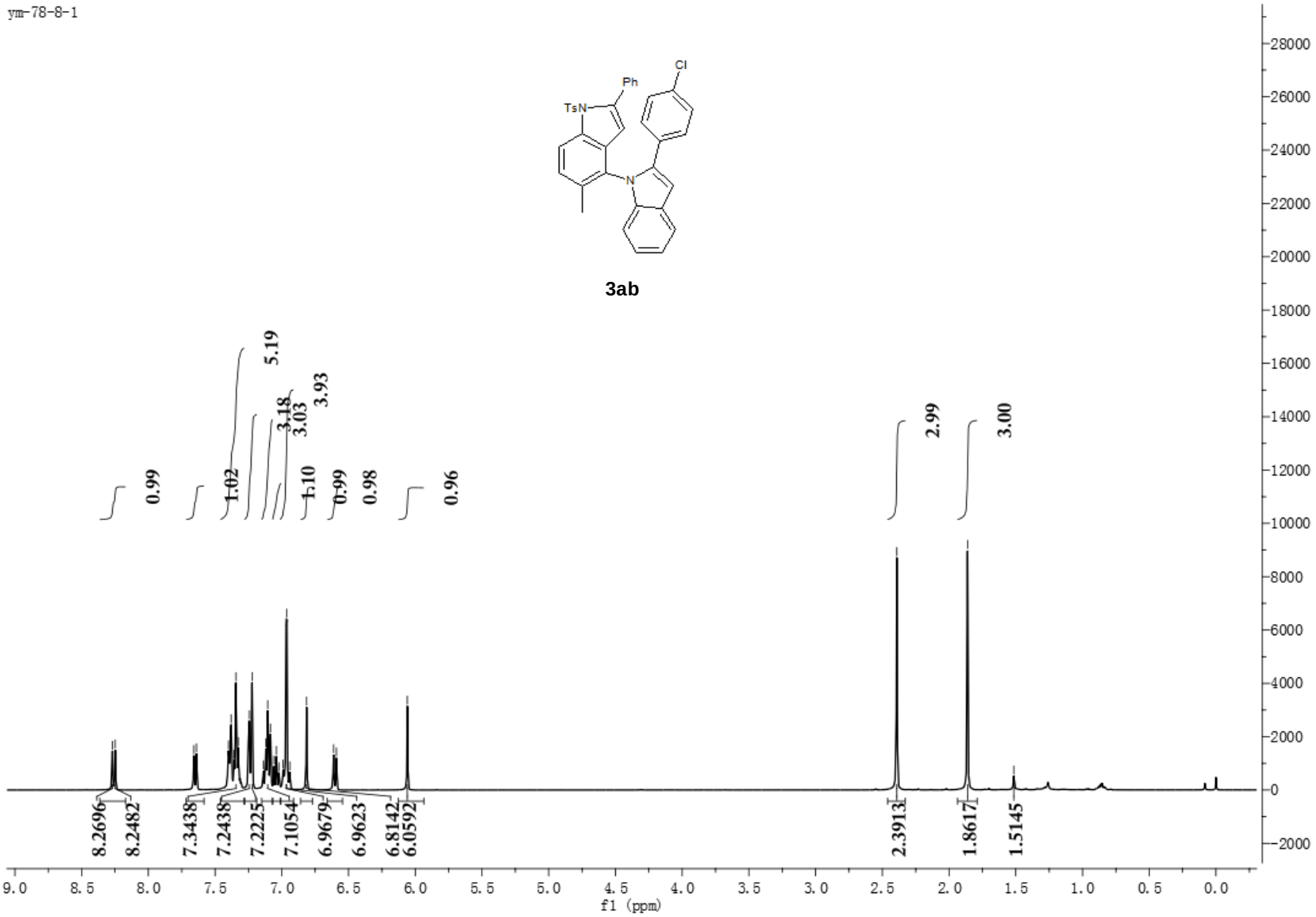
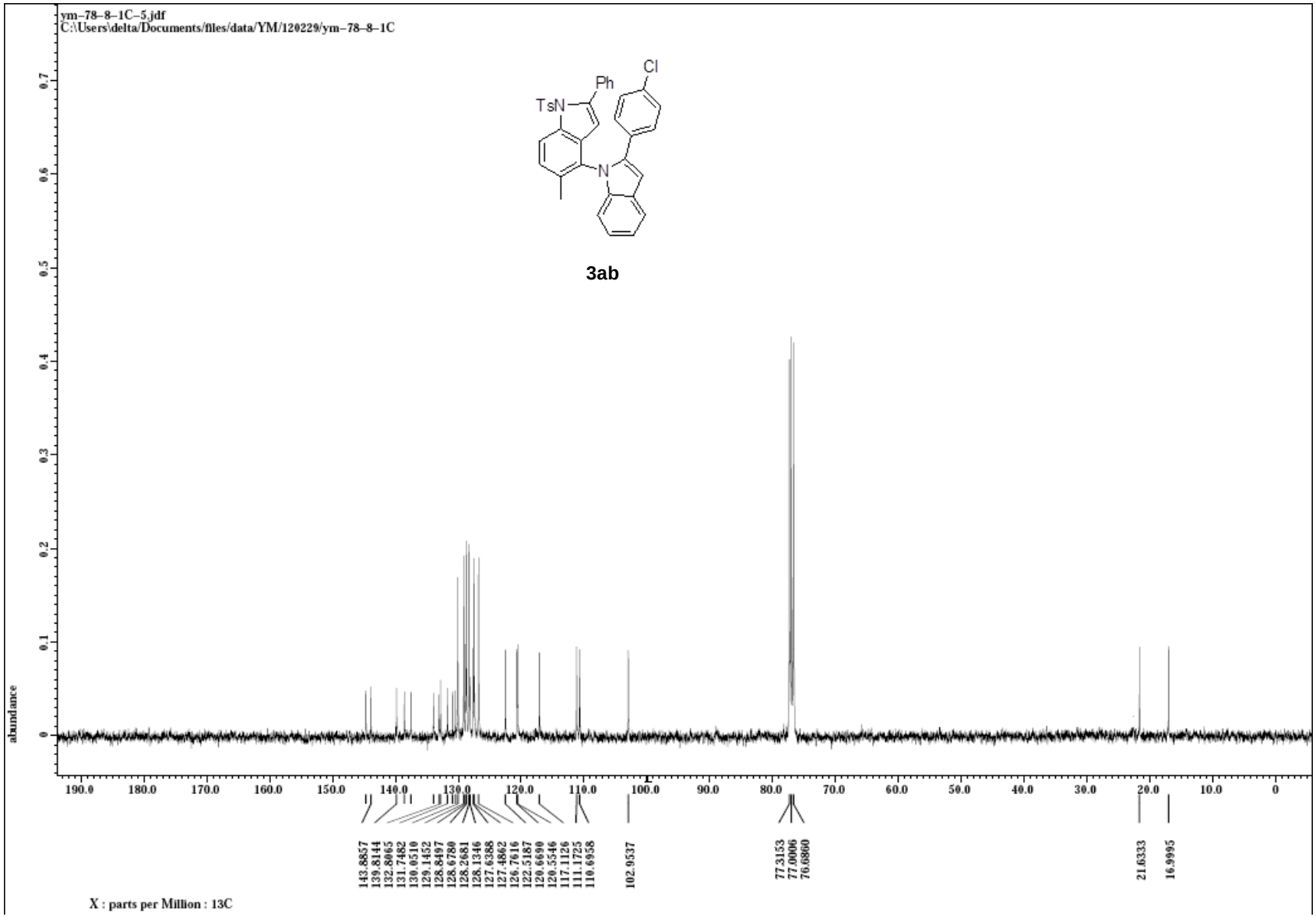
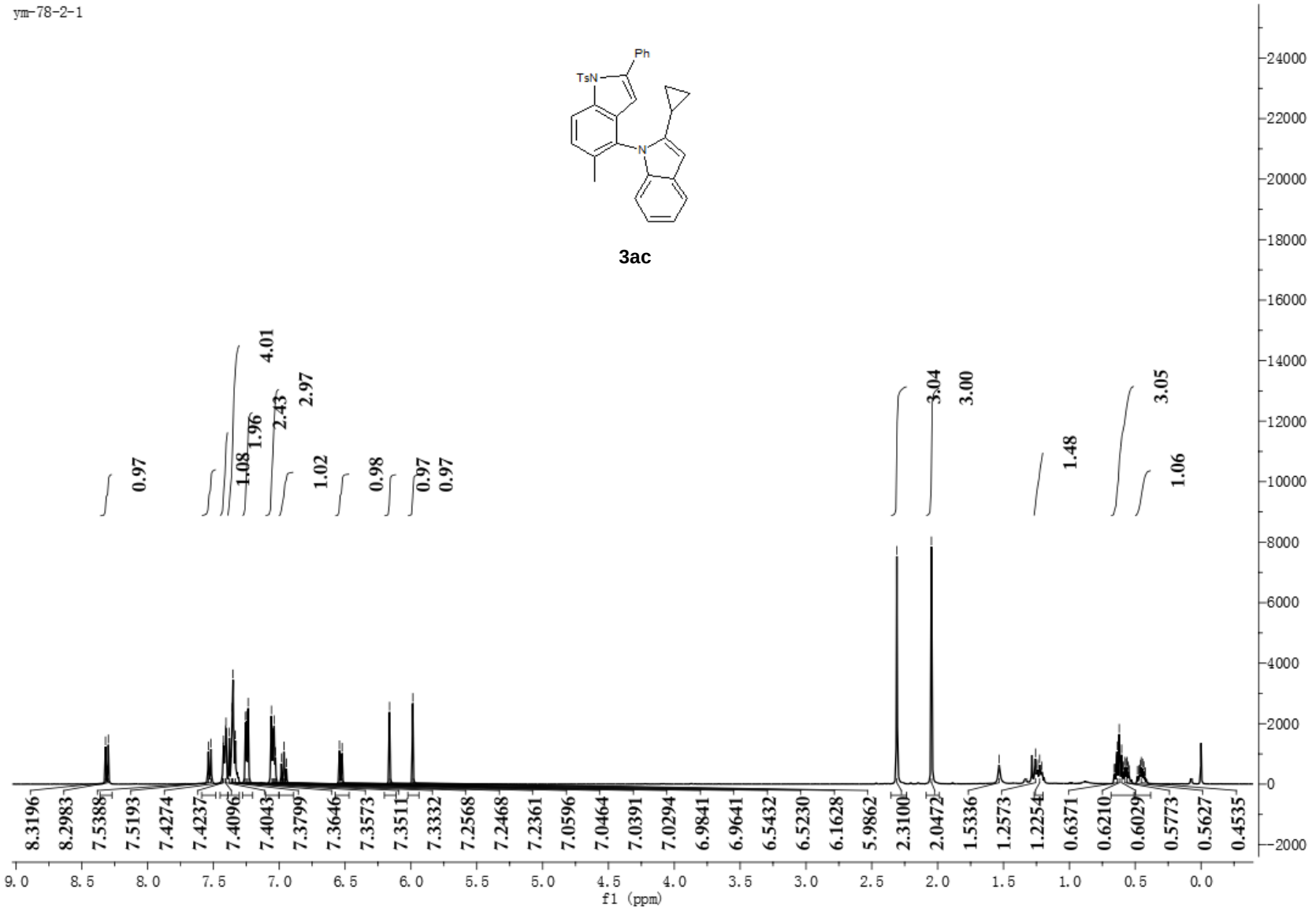
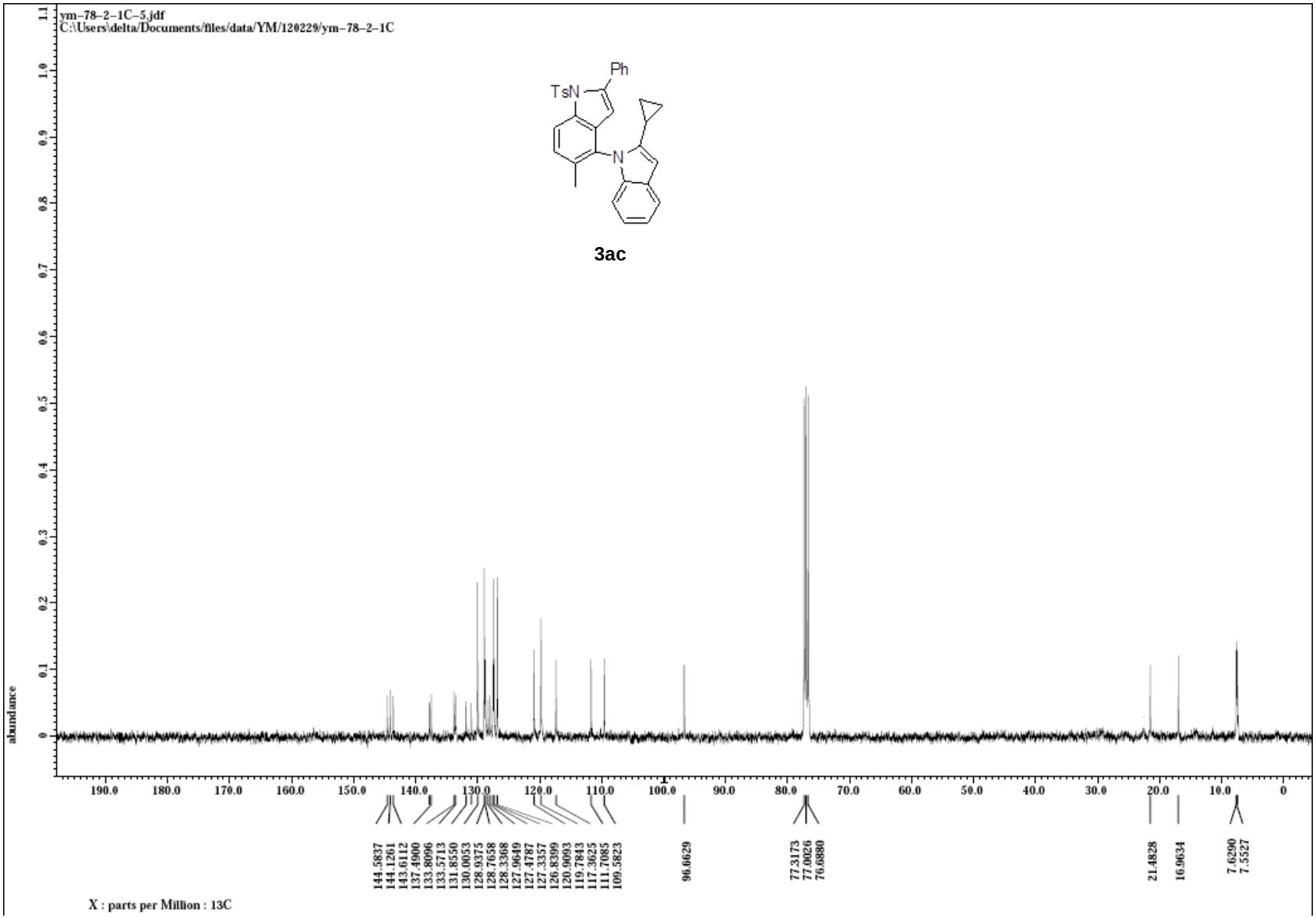
27.8829
21.6378
17.3758
X : parts per Million : 13C

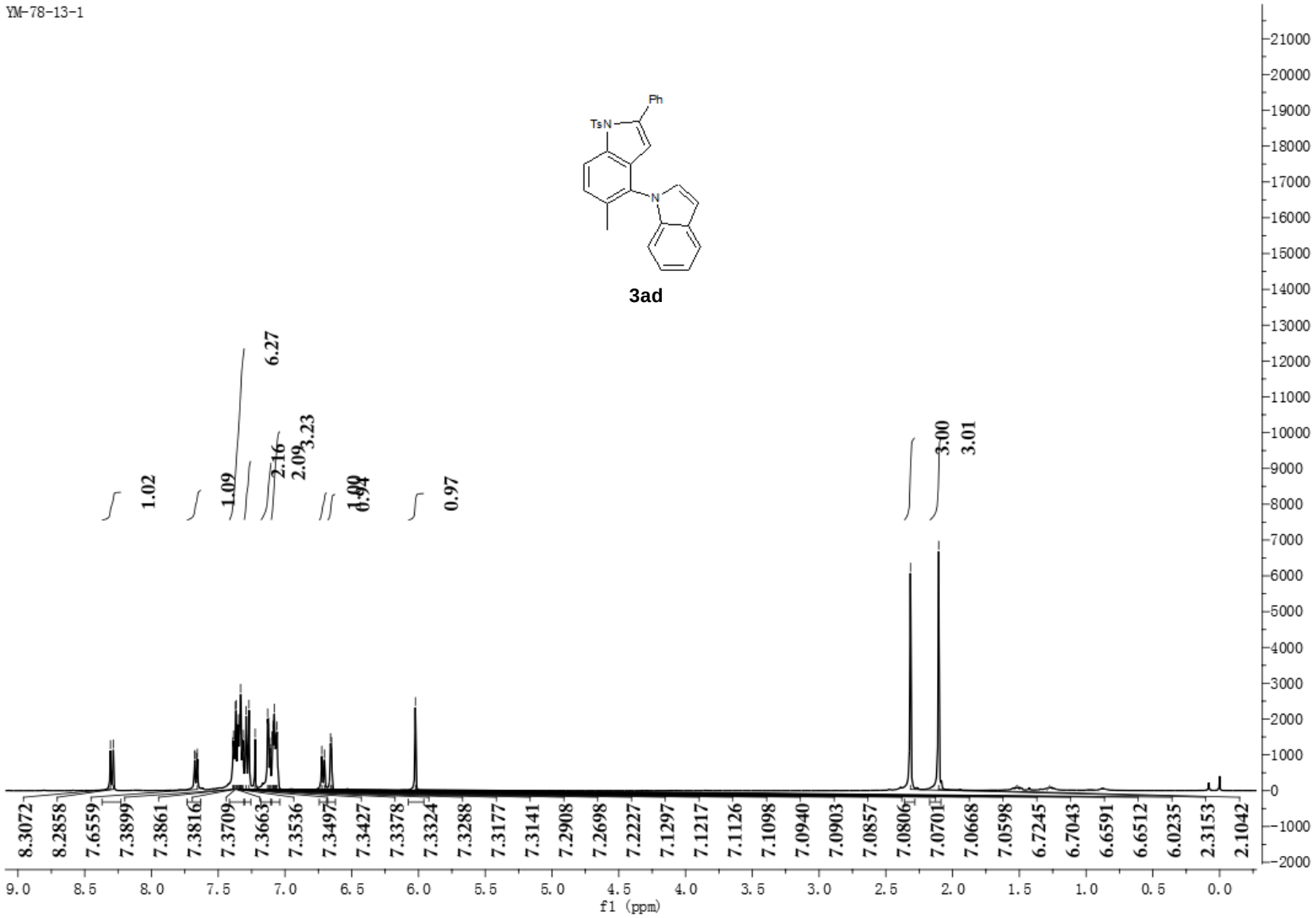


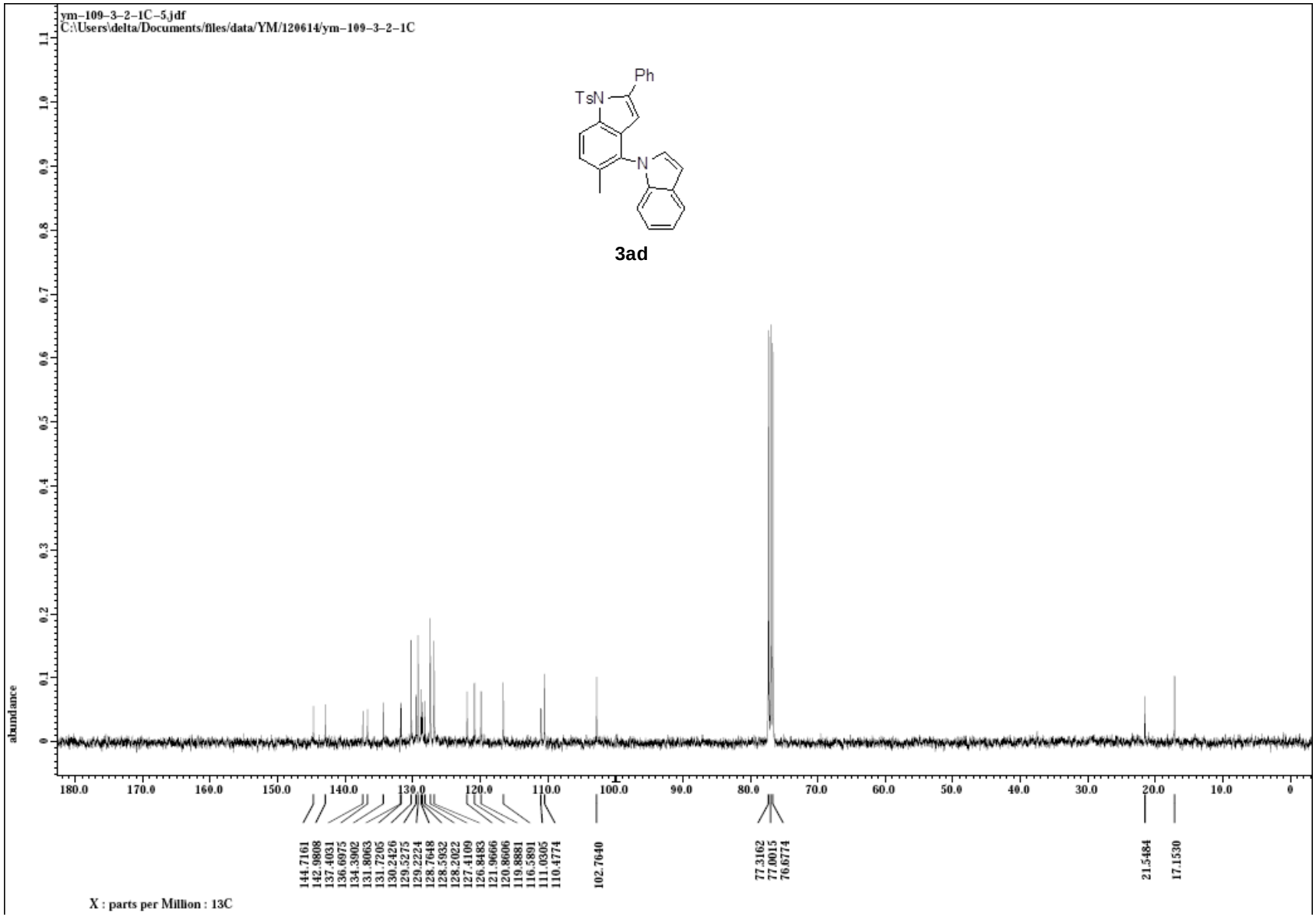

ym-78-8-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120229/ym-78-8-1C
Cl
Ph
TsN
N
3ab
abundance
143.8857
139.8144
132.8065
131.7482
130.0510
129.1452
128.8497
128.6780
128.2681
128.1346
127.6388
127.4862
126.7616
122.5187
120.6690
120.5546
117.1126
111.1725
110.6958
102.9537
77.3153
77.0006
76.6860
21.6333
16.9995
X : parts per Million : 13C

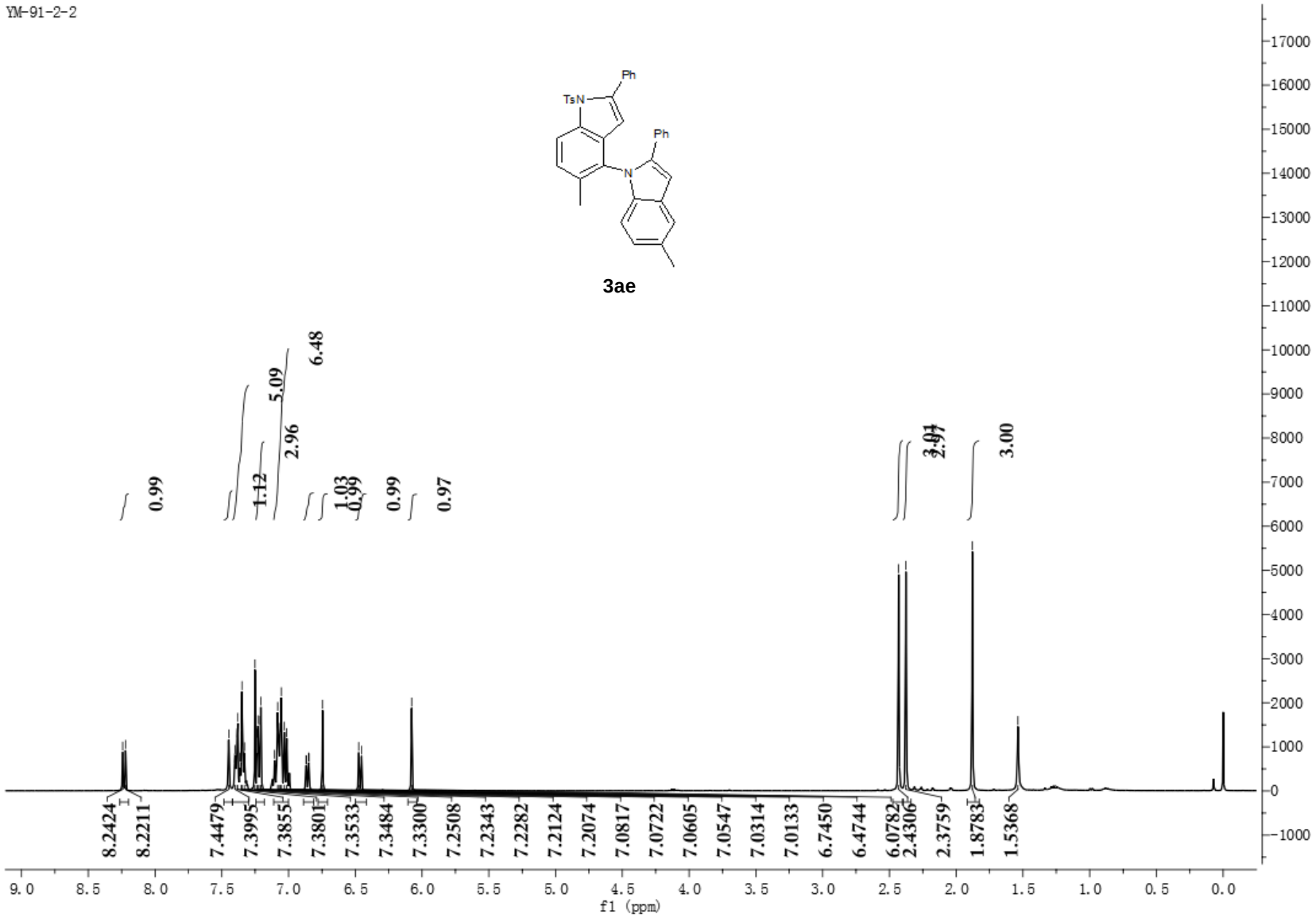

ym-78-2-1
Ph
TsN
N
0.97
1.08
1.96
4.01
2.43
2.97
1.02
0.98
0.97
0.97
3.04
3.00
1.48
3.05
1.06
8.3196
8.2983
7.5388
7.5193
7.4274
7.4237
7.4096
7.4043
7.3799
7.3646
7.3573
7.3511
7.3332
7.2568
7.2468
7.2361
7.0596
7.0464
7.0391
7.0294
6.9841
6.9641
6.5432
6.5230
6.1628
5.9862
2.3100
2.0472
1.5336
1.2573
1.2254
0.6371
0.6210
0.6029
0.5773
0.5627
0.4535
f1 (ppm)

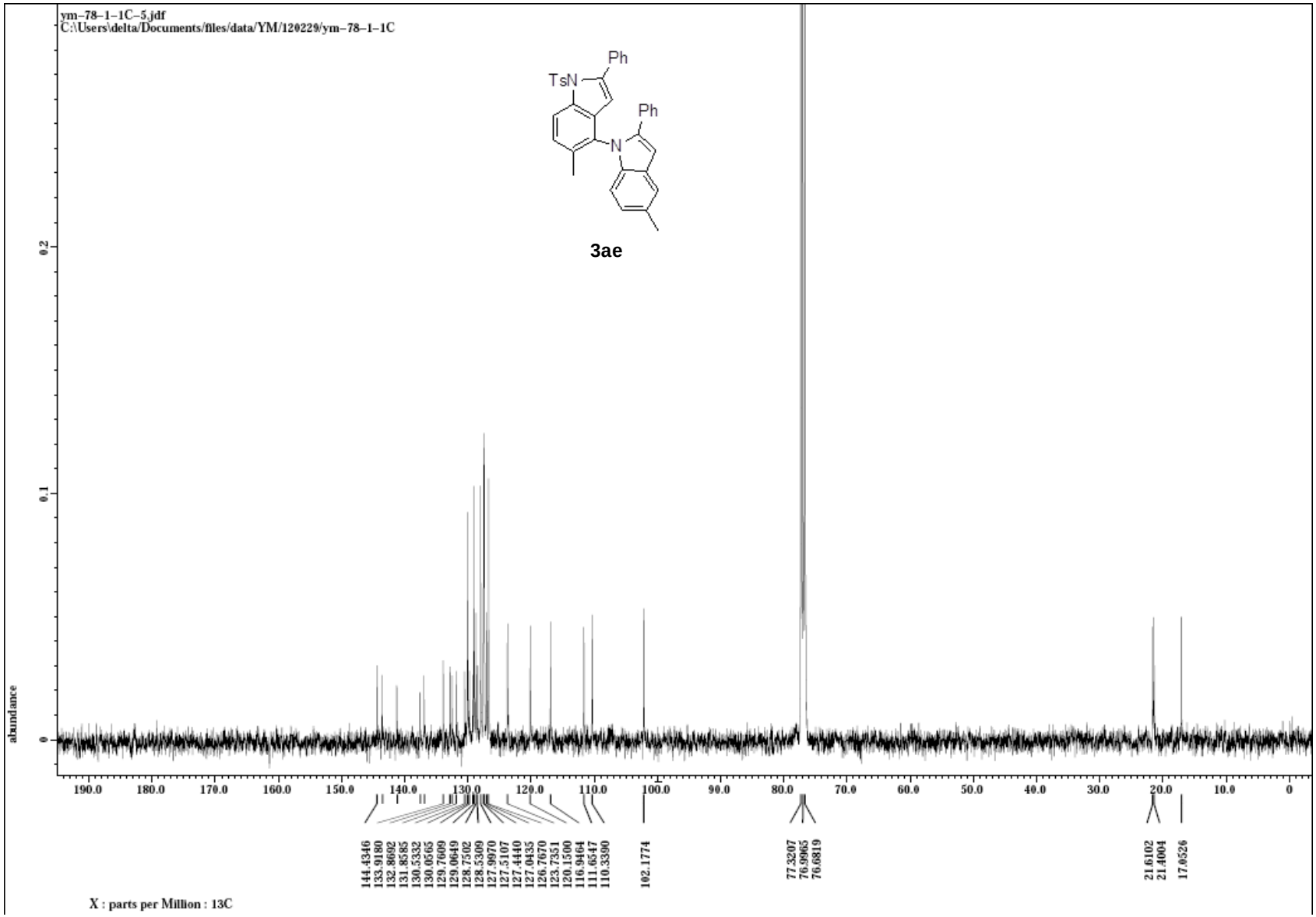
**3ac**

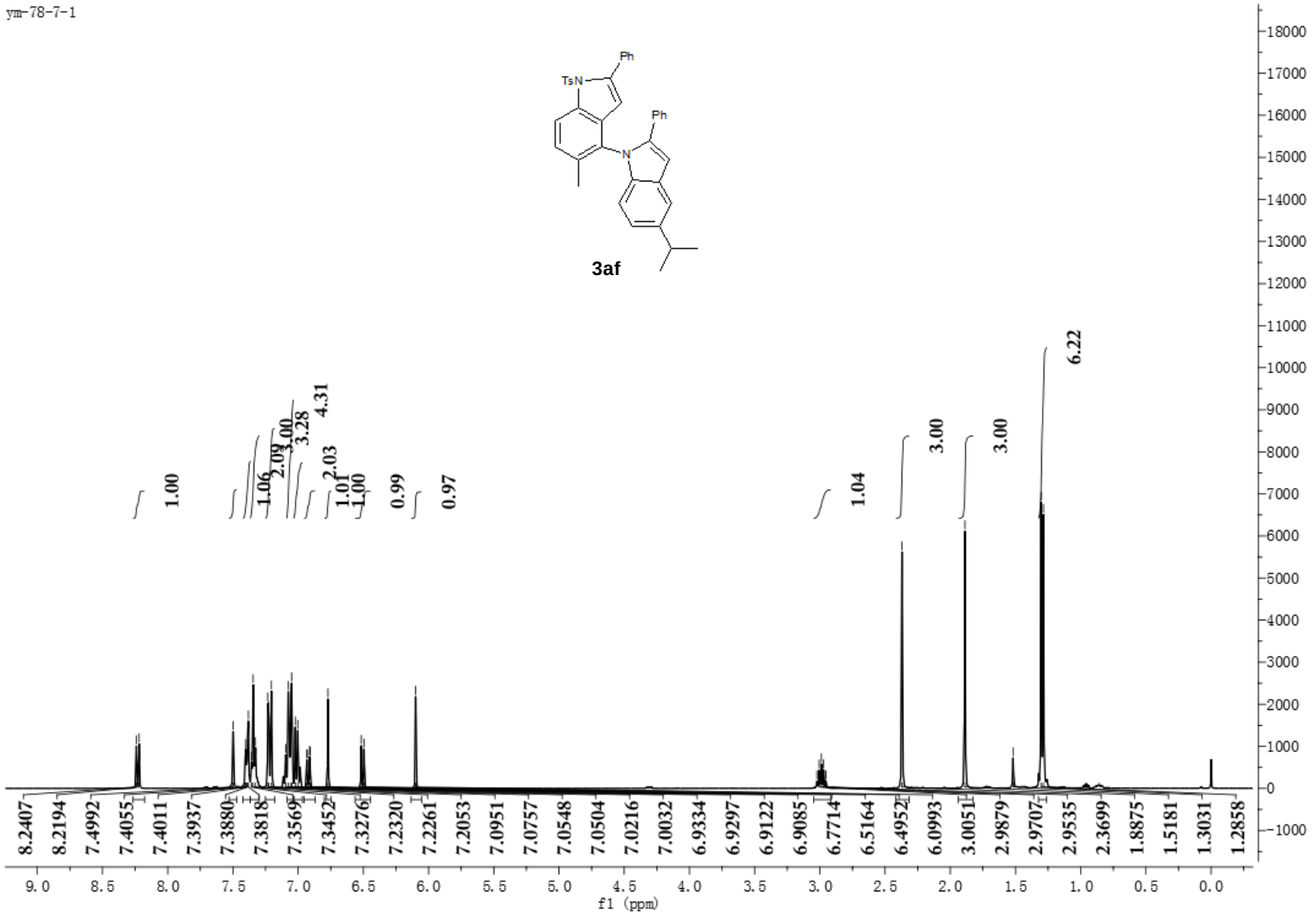


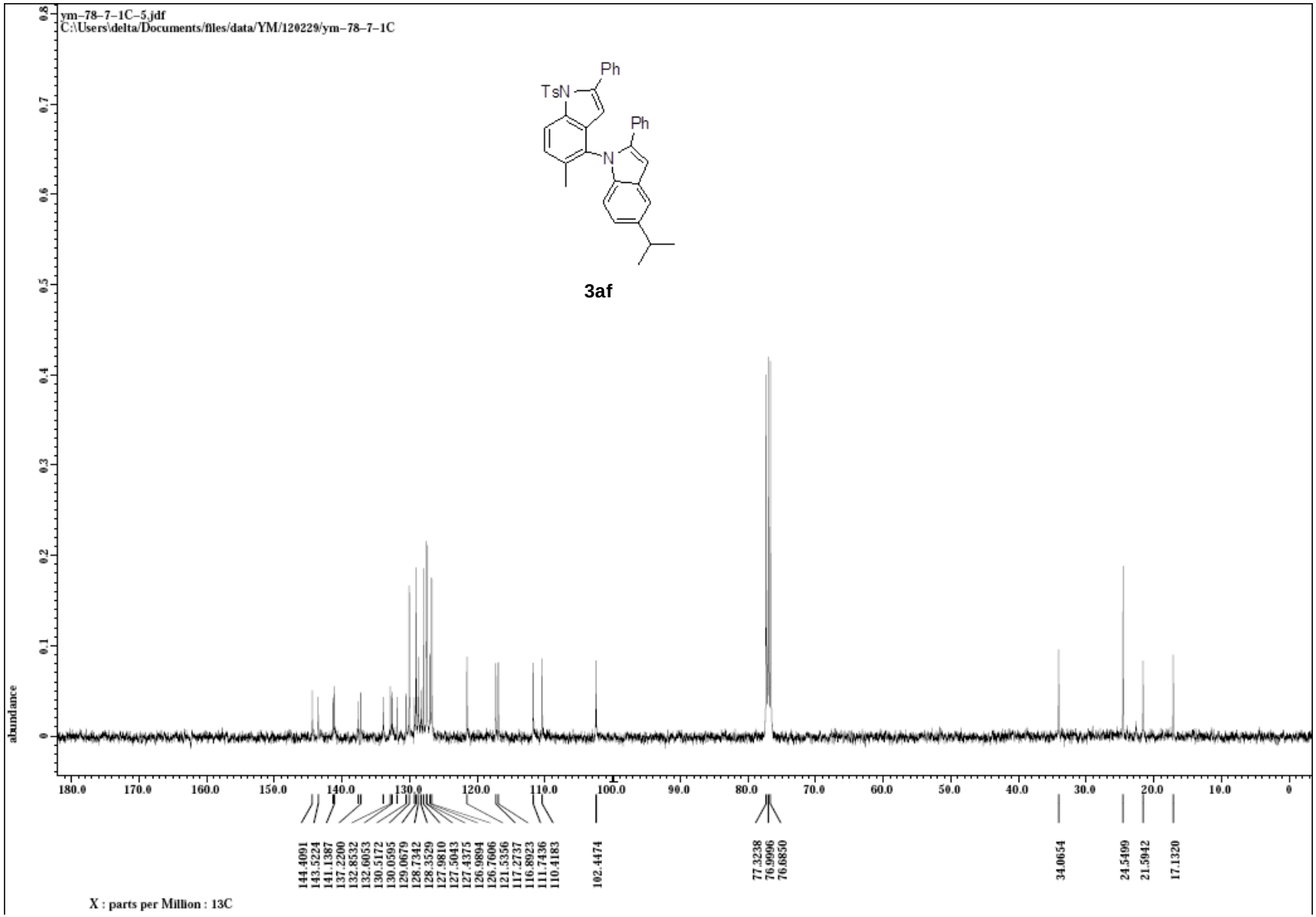


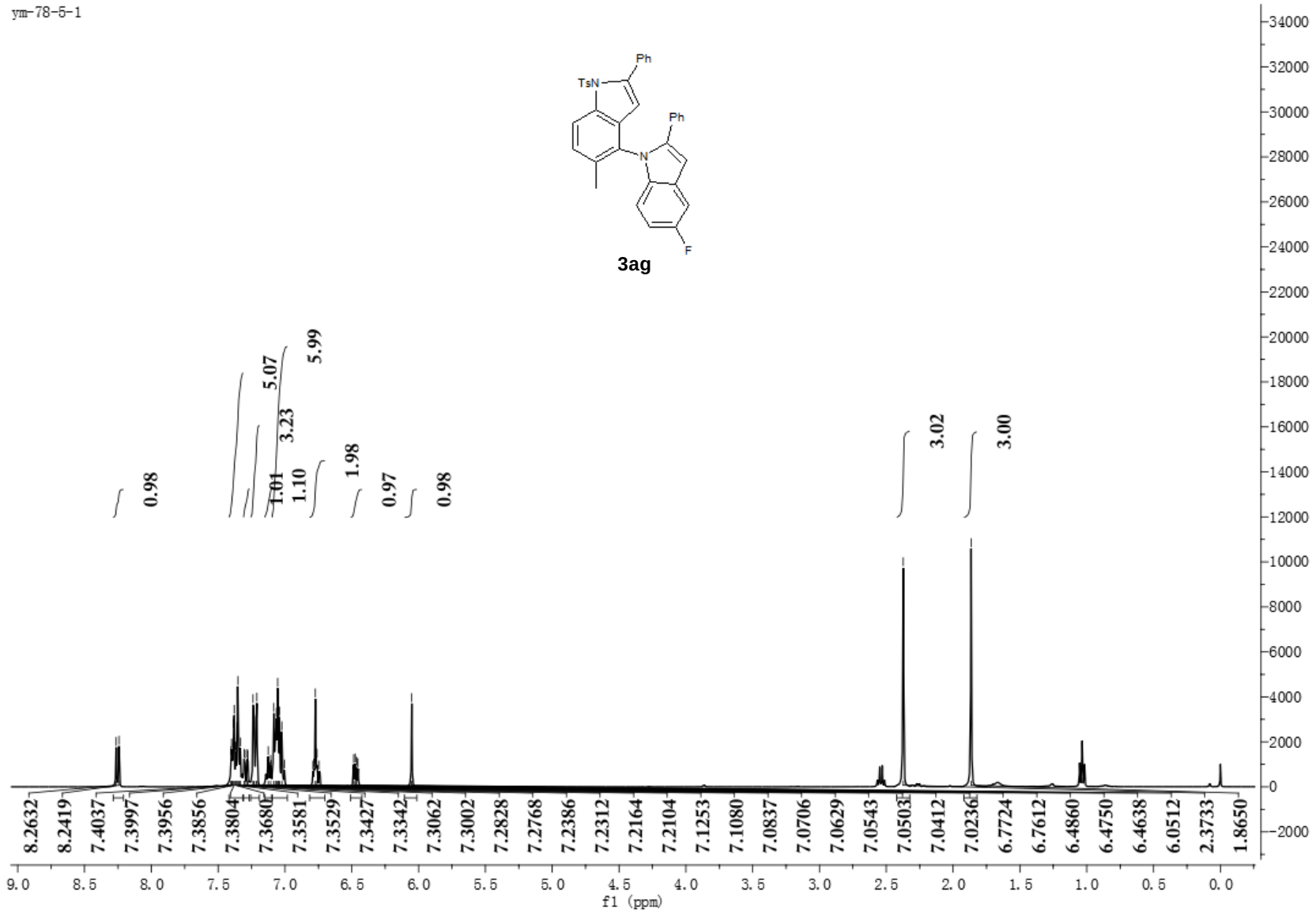

ym-109-3-2-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120614/ym-109-3-2-1C
Ph
TsN
N
3ad
abundance
144.7161
142.9808
137.4031
136.6975
134.3902
131.8063
131.7205
130.2426
129.5275
129.2224
128.7648
128.5932
128.2022
127.4109
126.8483
121.9666
120.8606
119.8881
116.5891
111.0305
110.4774
102.7640
77.3162
77.0015
76.6774
21.5484
17.1530
X : parts per Million : 13C

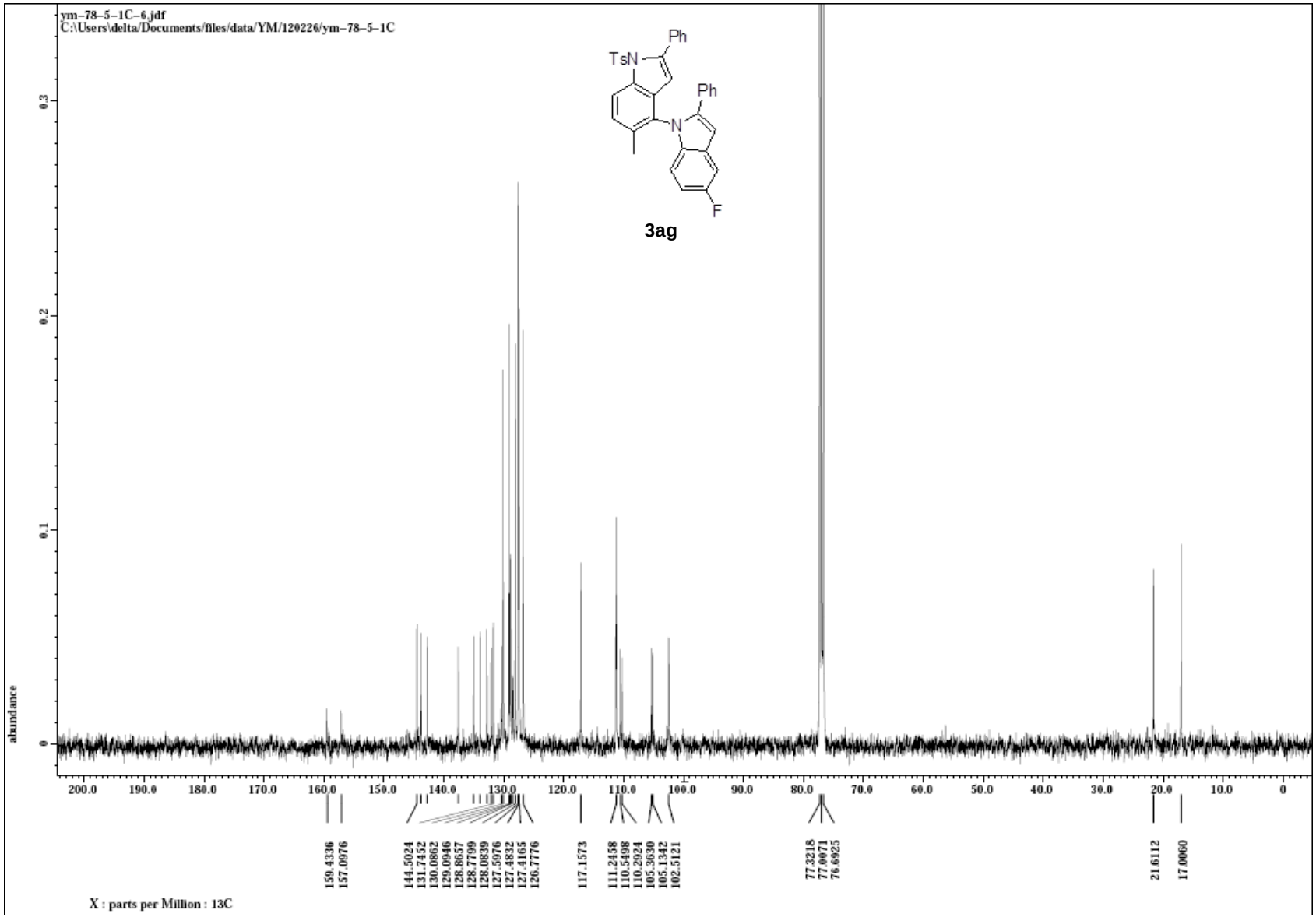

YM-91-2-2
Ph
TsN
Ph
N
3ae
0.99
1.12
2.96
5.09
6.48
1.03
0.99
0.99
0.97
3.01
2.97
3.00
8.2424
8.2211
7.4479
7.3995
7.3855
7.3801
7.3533
7.3484
7.3300
7.2508
7.2343
7.2282
7.2124
7.2074
7.0817
7.0722
7.0605
7.0547
7.0314
7.0133
6.7450
6.4744
6.0782
2.4306
2.3759
1.8783
1.5368
f1 (ppm)

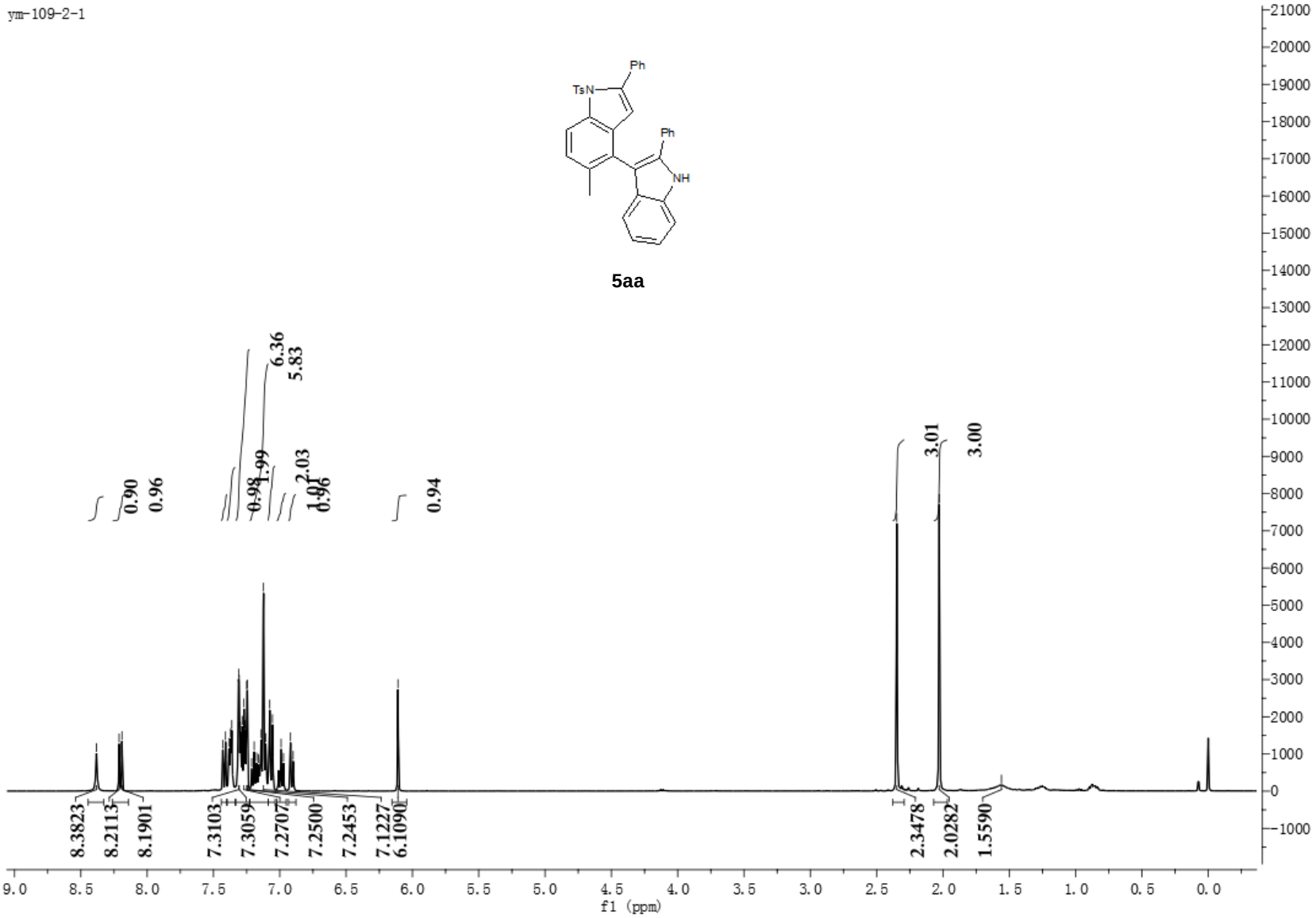


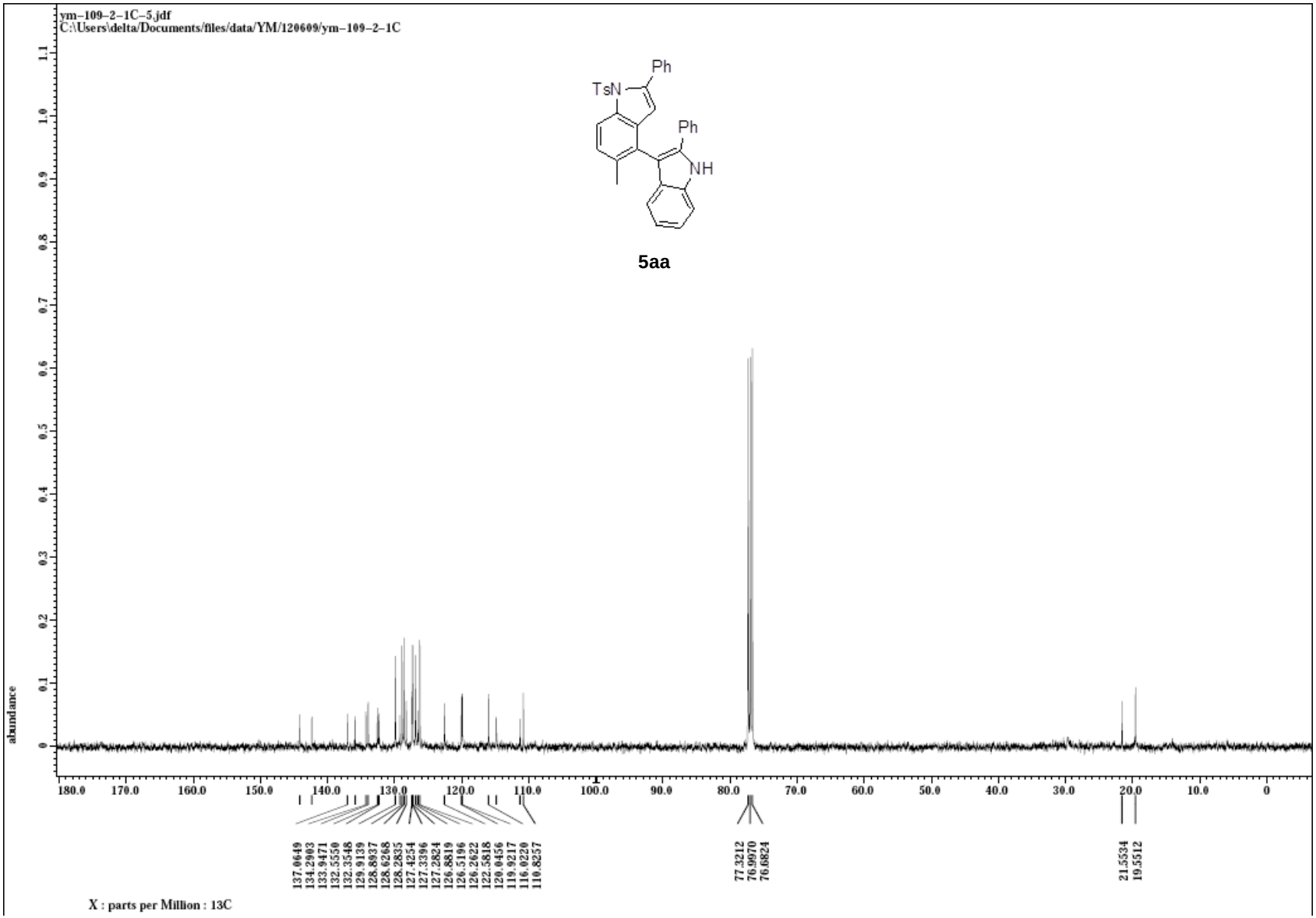

ym-78-7-1
Ph
TsN
Ph
N
3af
1.00
1.06
2.09
3.00
3.28
4.31
2.03
1.01
1.00
0.99
0.97
1.04
3.00
3.00
6.22
8.2407
8.2194
7.4992
7.4055
7.4011
7.3937
7.3880
7.3818
7.3569
7.3452
7.3276
7.2320
7.2261
7.2053
7.0951
7.0757
7.0548
7.0504
7.0216
7.0032
6.9334
6.9297
6.9122
6.9085
6.7714
6.5164
6.4952
6.0993
3.0051
2.9879
2.9707
2.9535
2.3699
1.8875
1.5181
1.3031
1.2858
f1 (ppm)

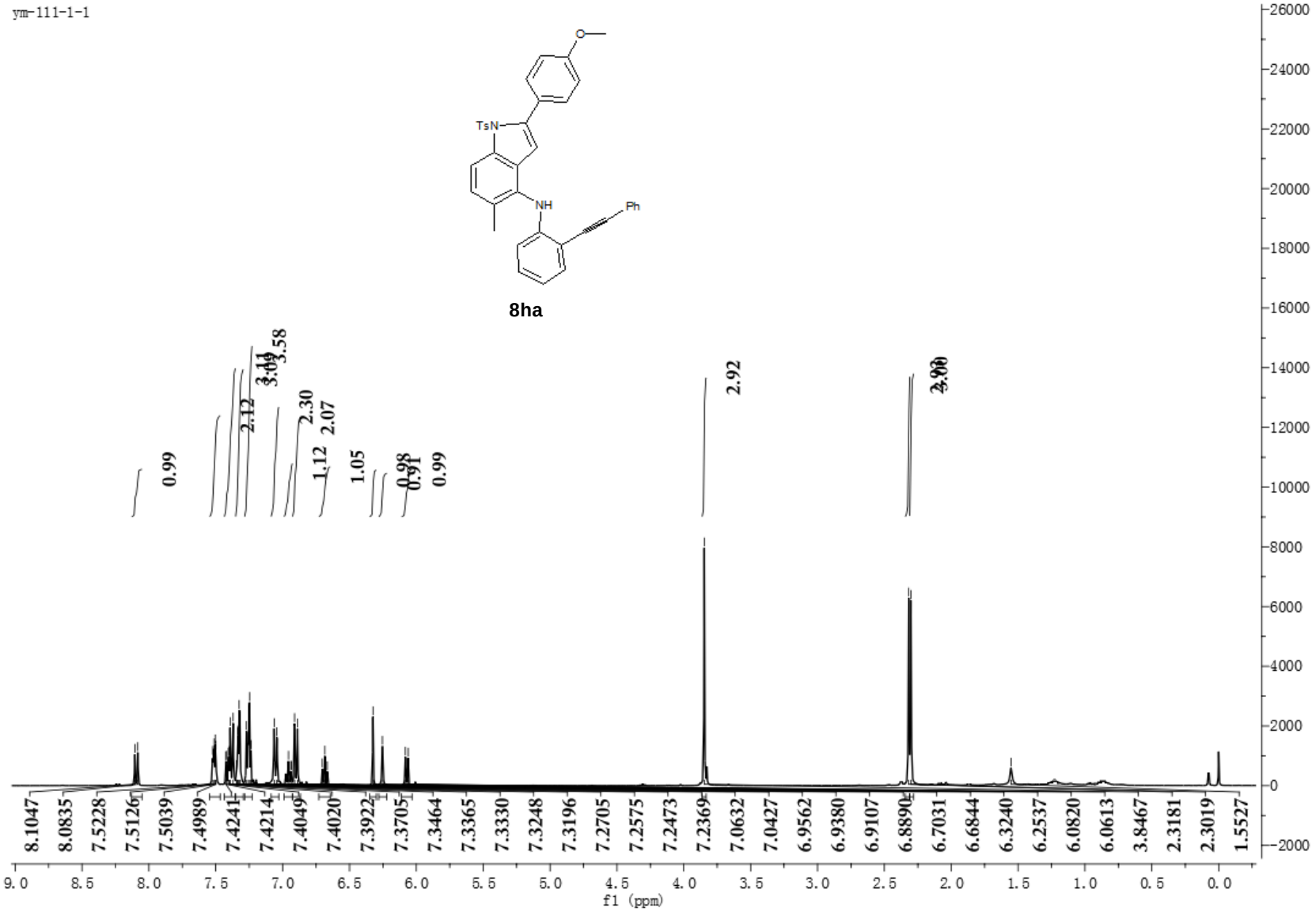

ym-78-7-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120229/ym-78-7-1C
Ph
TsN
Ph
N
3af
abundance
144.4091
143.5224
141.1387
137.2200
132.8532
132.6053
130.5172
130.0595
129.0679
128.7342
128.3529
127.9810
127.5043
127.4375
126.9894
126.7606
121.5356
117.2737
116.8923
111.7436
110.4183
102.4474
77.3238
76.9996
76.6850
34.0654
24.5499
21.5942
17.1320
X : parts per Million : 13C

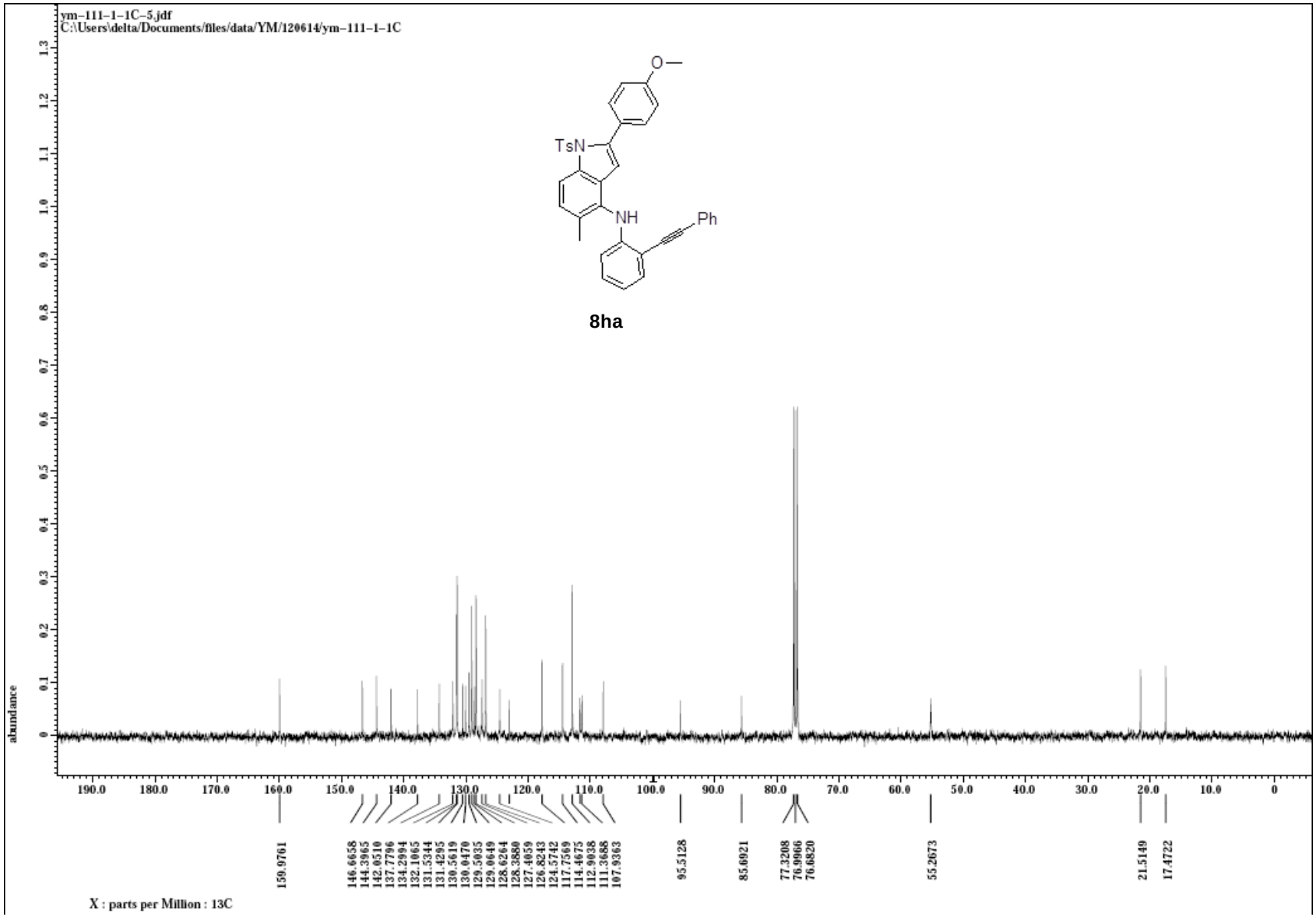

ym-78-5-1
Ph
TsN
Ph
N
F
3ag
0.98
5.07
3.23
5.99
1.01
1.10
1.98
0.97
0.98
3.02
3.00
8.2632
8.2419
7.4037
7.3997
7.3956
7.3856
7.3804
7.3680
7.3581
7.3529
7.3427
7.3342
7.3062
7.3002
7.2828
7.2768
7.2386
7.2312
7.2164
7.2104
7.1253
7.1080
7.0837
7.0706
7.0629
7.0543
7.0503
7.0412
7.0236
6.7724
6.7612
6.4860
6.4750
6.4638
6.0512
2.3733
1.8650
f1 (ppm)

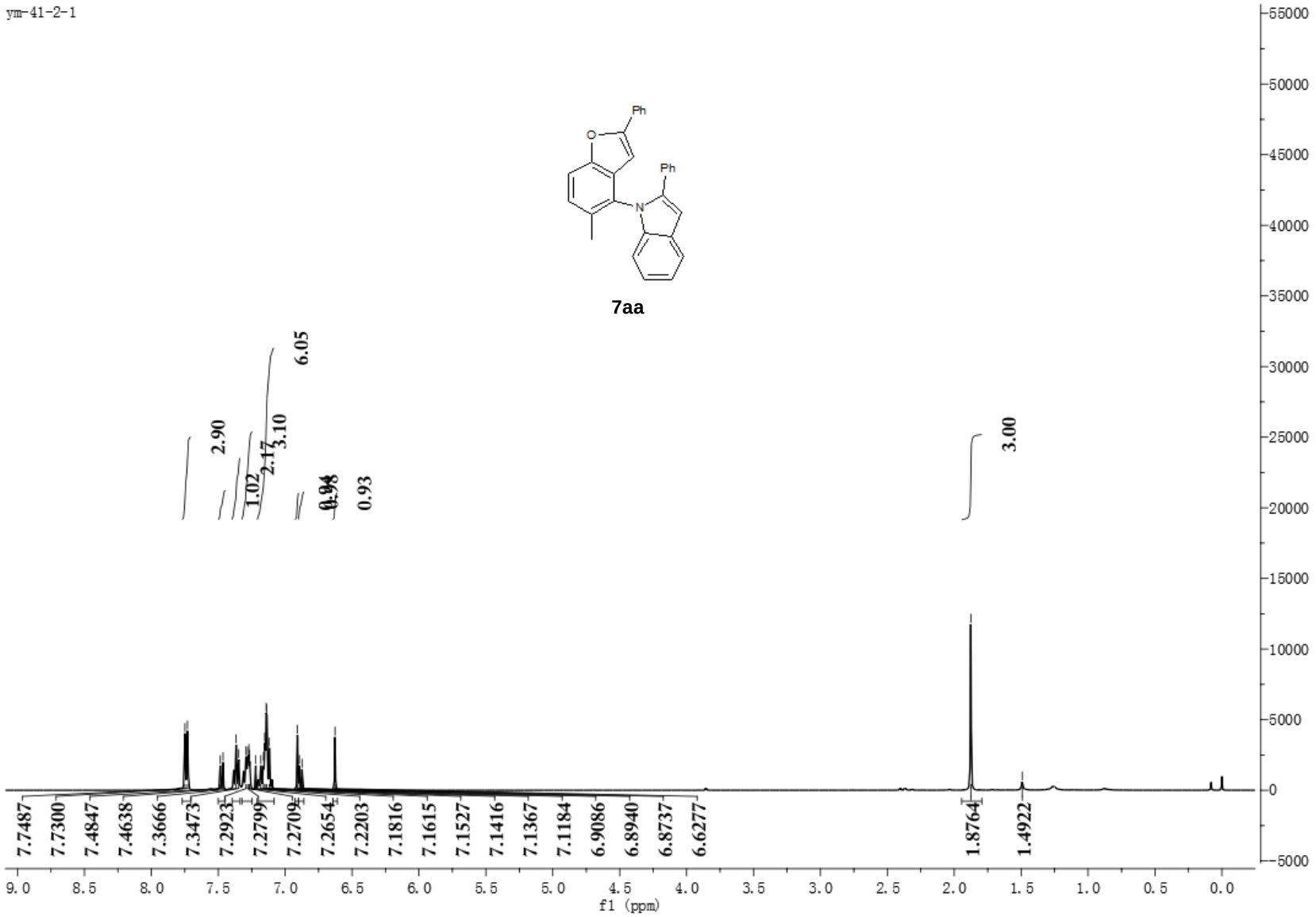


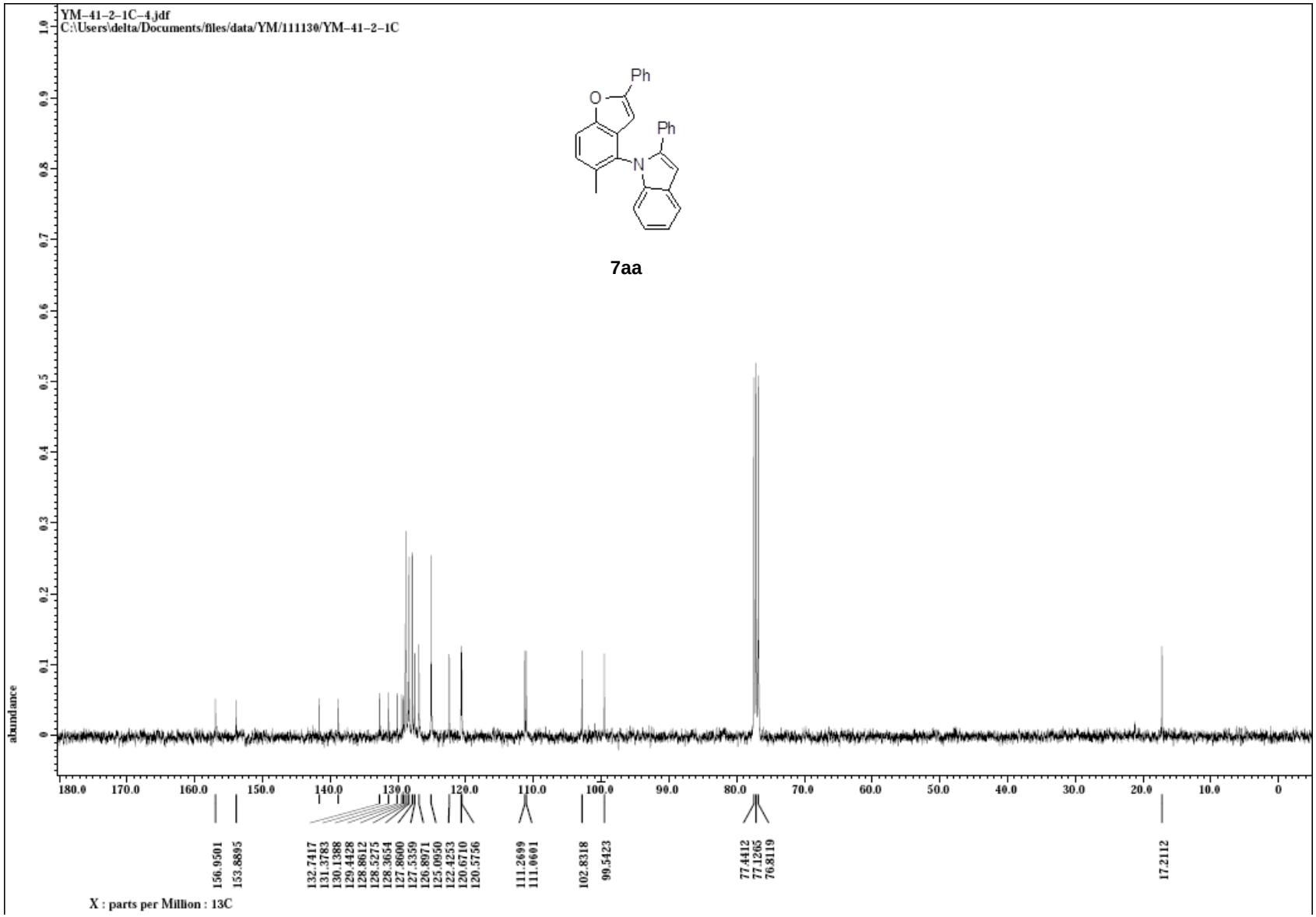

ym-109-2-1
Ph
TsN
Ph
NH
5aa
6.36
5.83
1.99
2.03
1.01
0.98
0.96
0.90
0.96
0.94
3.01
3.00
8.3823
8.2113
8.1901
7.3103
7.3059
7.2707
7.2500
7.2453
7.1227
6.1090
2.3478
2.0282
1.5590
f1 (ppm)


ym-109-2-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120609/ym-109-2-1C
Ph
TsN
Ph
NH
5aa
abundance
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
137.0649
134.2903
133.9471
132.5550
132.3548
129.9139
128.8937
128.6268
128.2835
127.4254
127.3396
127.2824
126.8819
126.5196
126.2622
122.5818
120.0456
119.9217
116.0220
110.8257
77.3212
76.9970
76.6824
21.5534
19.5512
X : parts per Million : 13C

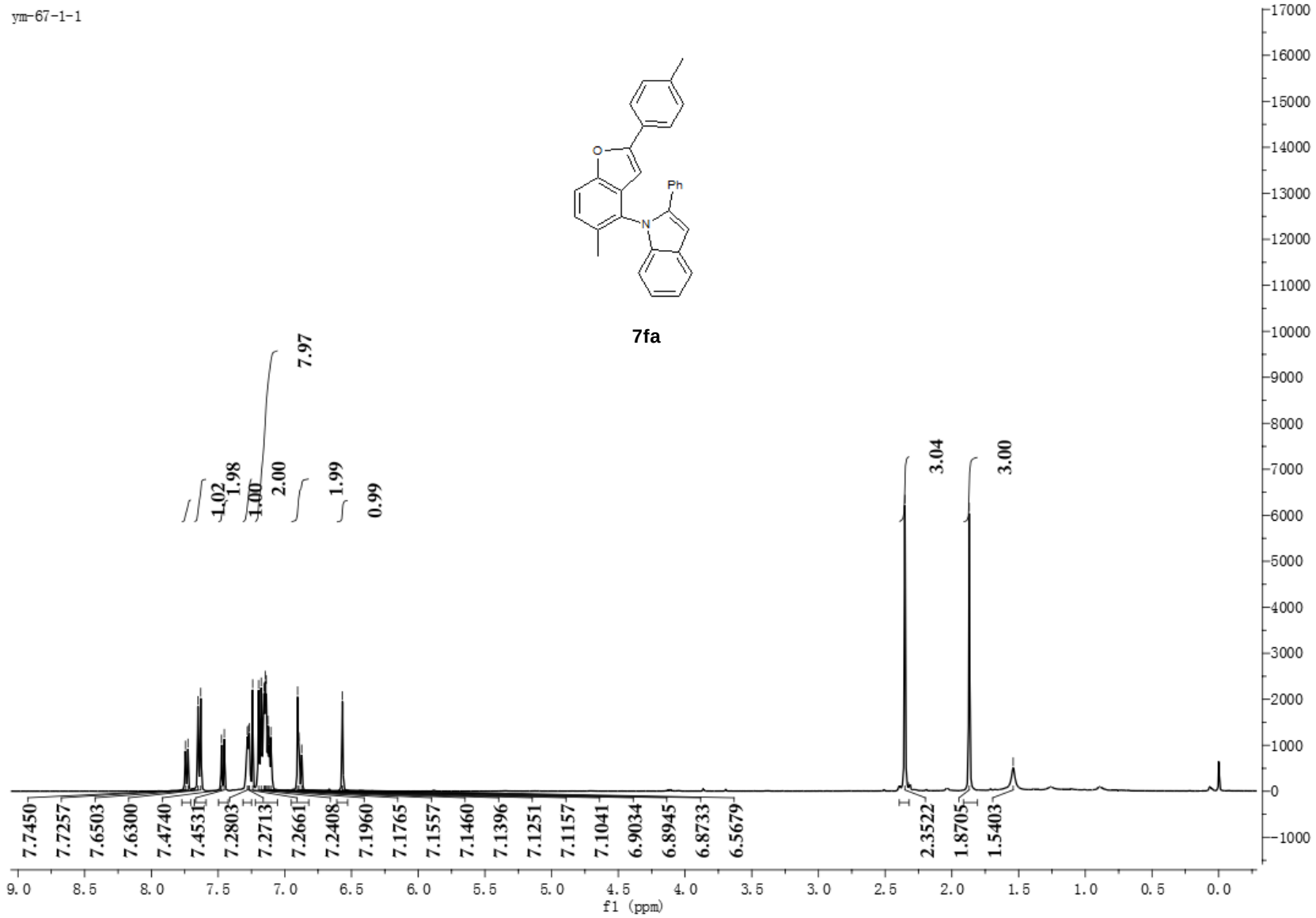

ym-111-1-1
TsN
NH
Ph
O
8ha
0.99
2.12
3.11
3.04
3.58
2.30
2.07
1.12
1.05
0.98
0.91
0.99
2.92
8.1047
8.0835
7.5228
7.5126
7.5039
7.4989
7.4241
7.4214
7.4049
7.4020
7.3922
7.3705
7.3464
7.3365
7.3330
7.3248
7.3196
7.2705
7.2575
7.2473
7.2369
7.0632
7.0427
6.9562
6.9380
6.9107
6.8890
6.7031
6.6844
6.3240
6.2537
6.0820
6.0613
3.8467
2.3181
2.3019
1.5527
f1 (ppm)

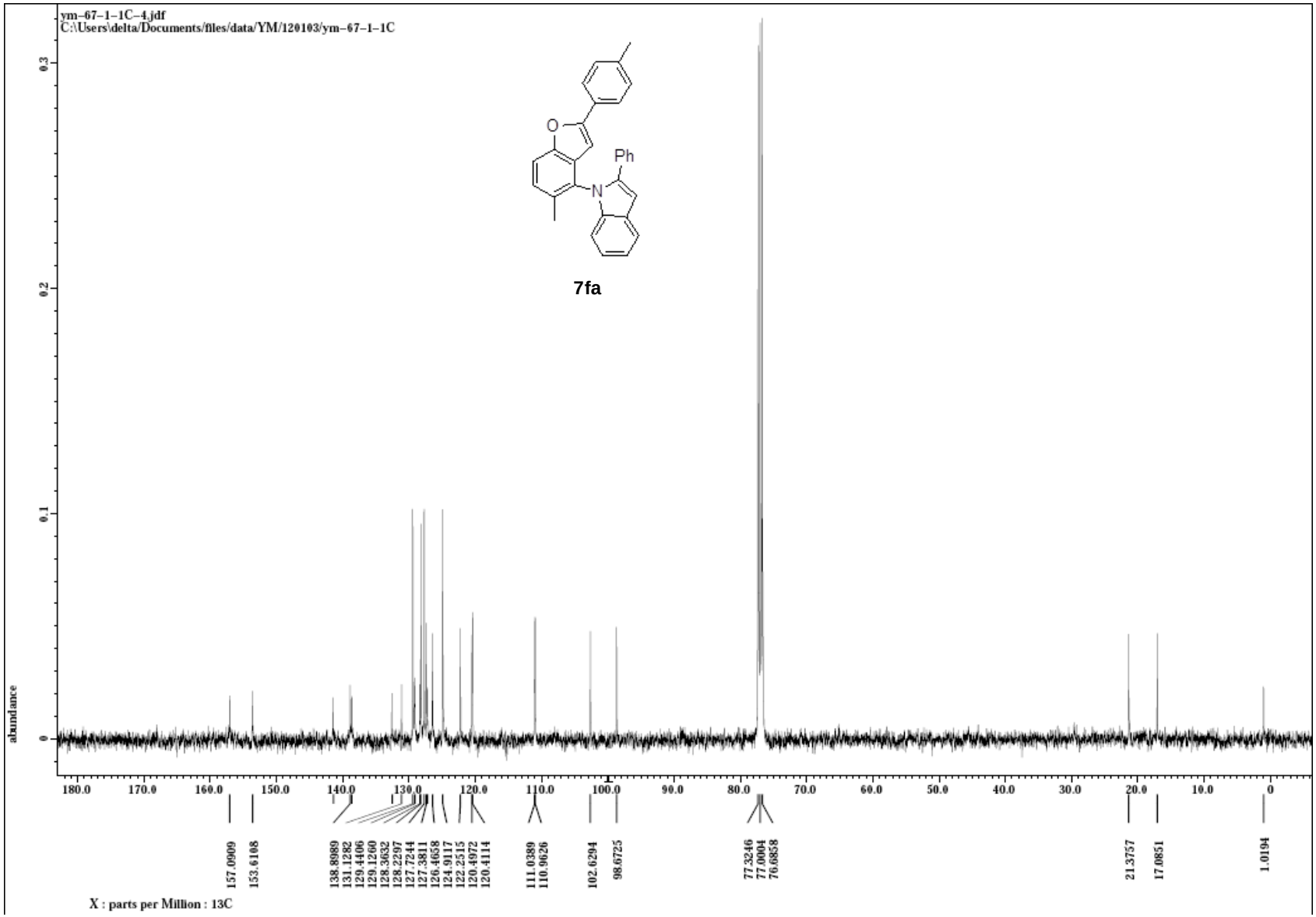

ym-111-1-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120614/ym-111-1-1C
O
TsN
NH
Ph
8ha
abundance
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
150.9761
146.6658
144.3965
142.0510
137.7796
134.2994
132.1065
131.5344
131.4295
130.5619
130.0470
129.5035
129.0649
128.6264
128.3880
127.4059
126.8243
124.5742
117.7569
114.4675
112.9038
111.3688
107.9363
95.5128
85.6921
77.3208
76.9966
76.6820
55.2673
21.5149
17.4722
X : parts per Million : 13C

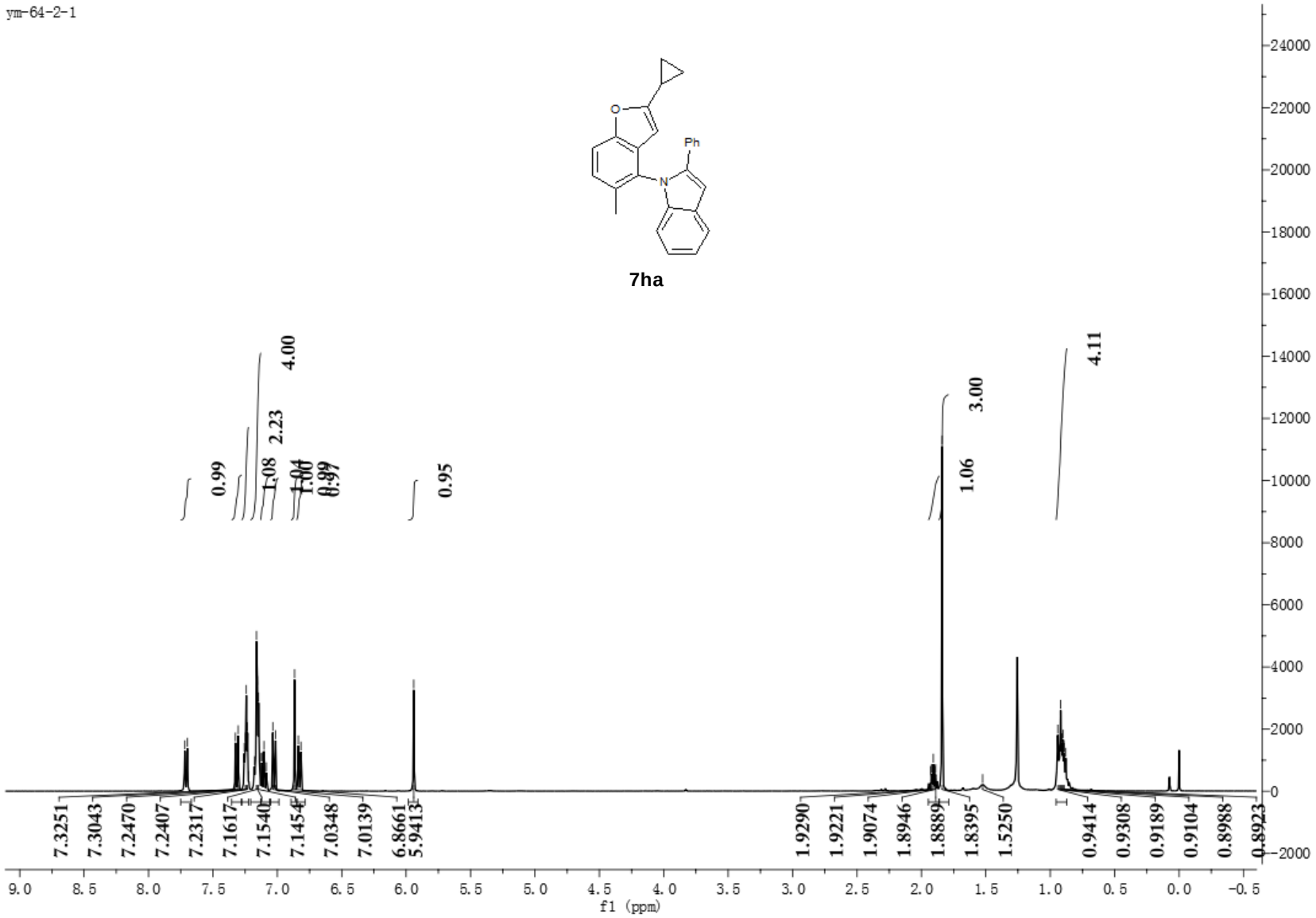

ym-41-2-1
Ph
O
Ph
N
7aa
2.90
1.02
2.17
3.10
6.05
0.93
3.00
7.7487
7.7300
7.4847
7.4638
7.3666
7.3473
7.2923
7.2799
7.2709
7.2654
7.2203
7.1816
7.1615
7.1527
7.1416
7.1367
7.1184
6.9086
6.8940
6.8737
6.6277
1.8764
1.4922
f1 (ppm)

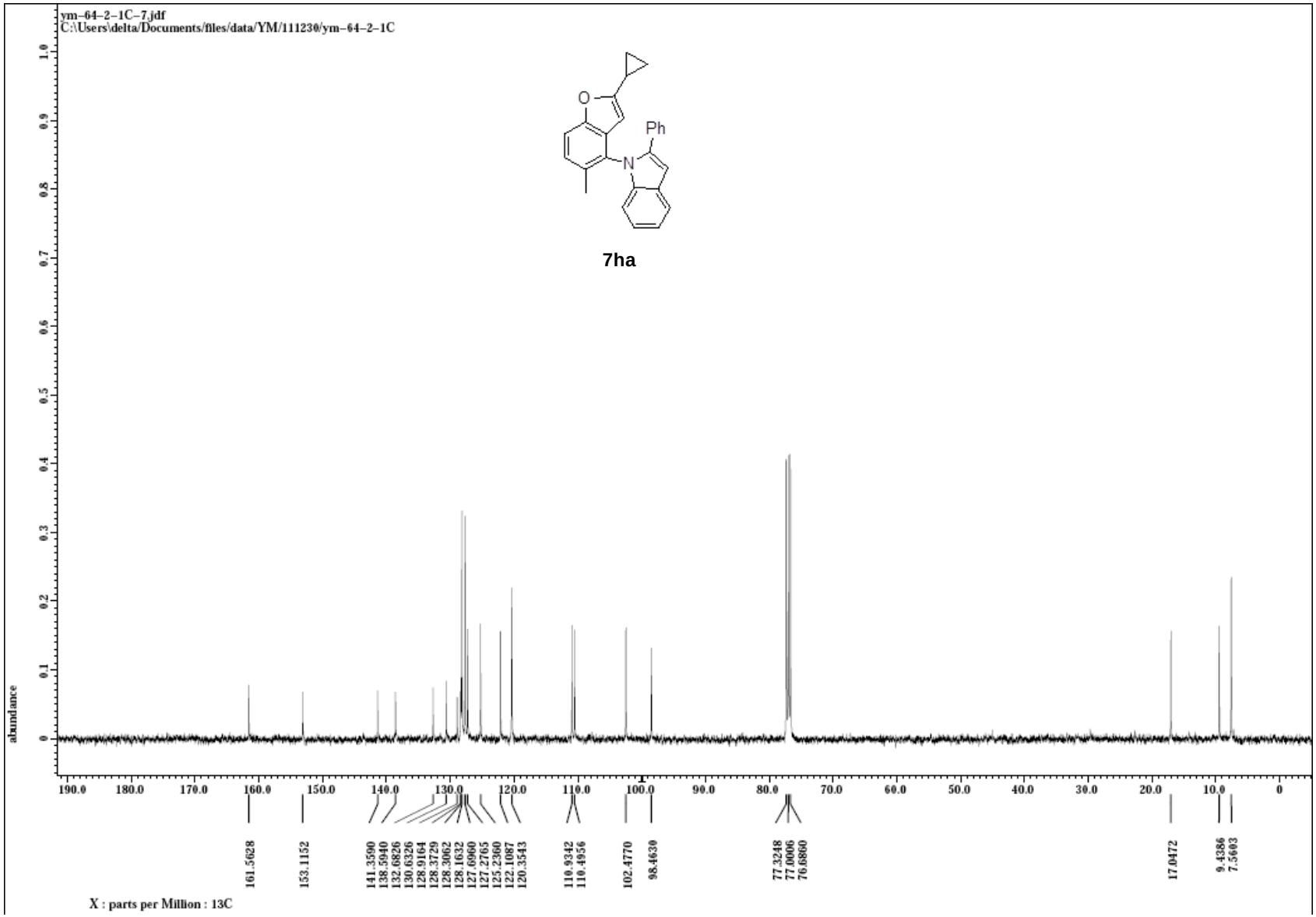



**7aa**

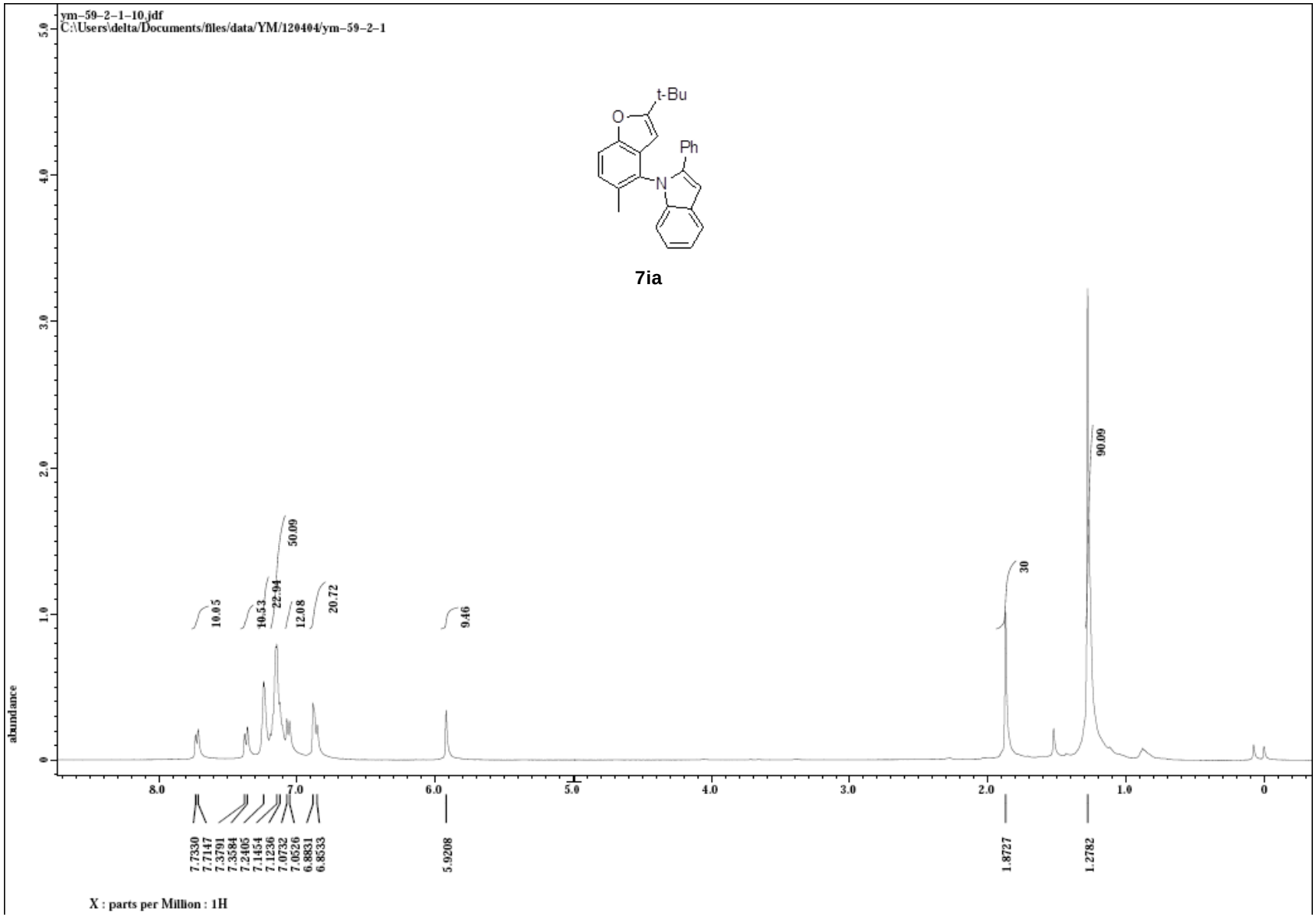

ym-67-1-1
O
Ph
N
7fa
1.02
1.98
1.00
2.00
7.97
1.99
0.99
3.04
3.00
7.7450
7.7257
7.6503
7.6300
7.4740
7.4531
7.2803
7.2713
7.2661
7.2408
7.1960
7.1765
7.1557
7.1460
7.1396
7.1251
7.1157
7.1041
6.9034
6.8945
6.8733
6.5679
2.3522
1.8705
1.5403
f1 (ppm)

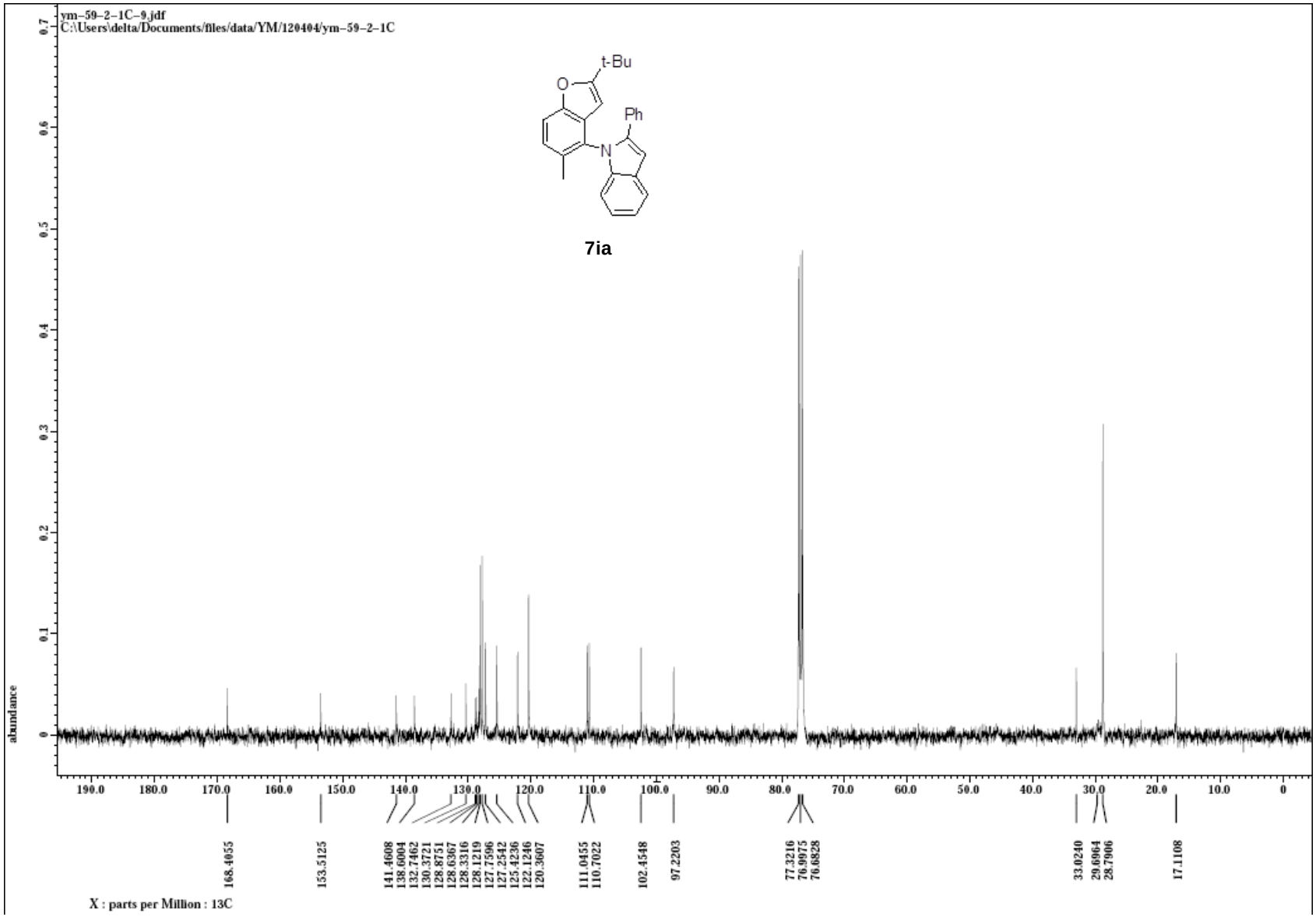

ym-67-1-1C-4.jdf
C:\Users\delta\Documents/files/data/YM/120103/ym-67-1-1C
O
Ph
N
7fa
abundance
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
157.0909
153.6108
138.8989
131.1282
129.4406
129.1260
128.3632
128.2297
127.7244
127.3811
126.4658
124.9117
122.2515
120.4972
120.4114
111.0389
110.9626
102.6294
98.6725
77.3246
77.0004
76.6858
21.3757
17.0851
1.0194
X : parts per Million : 13C

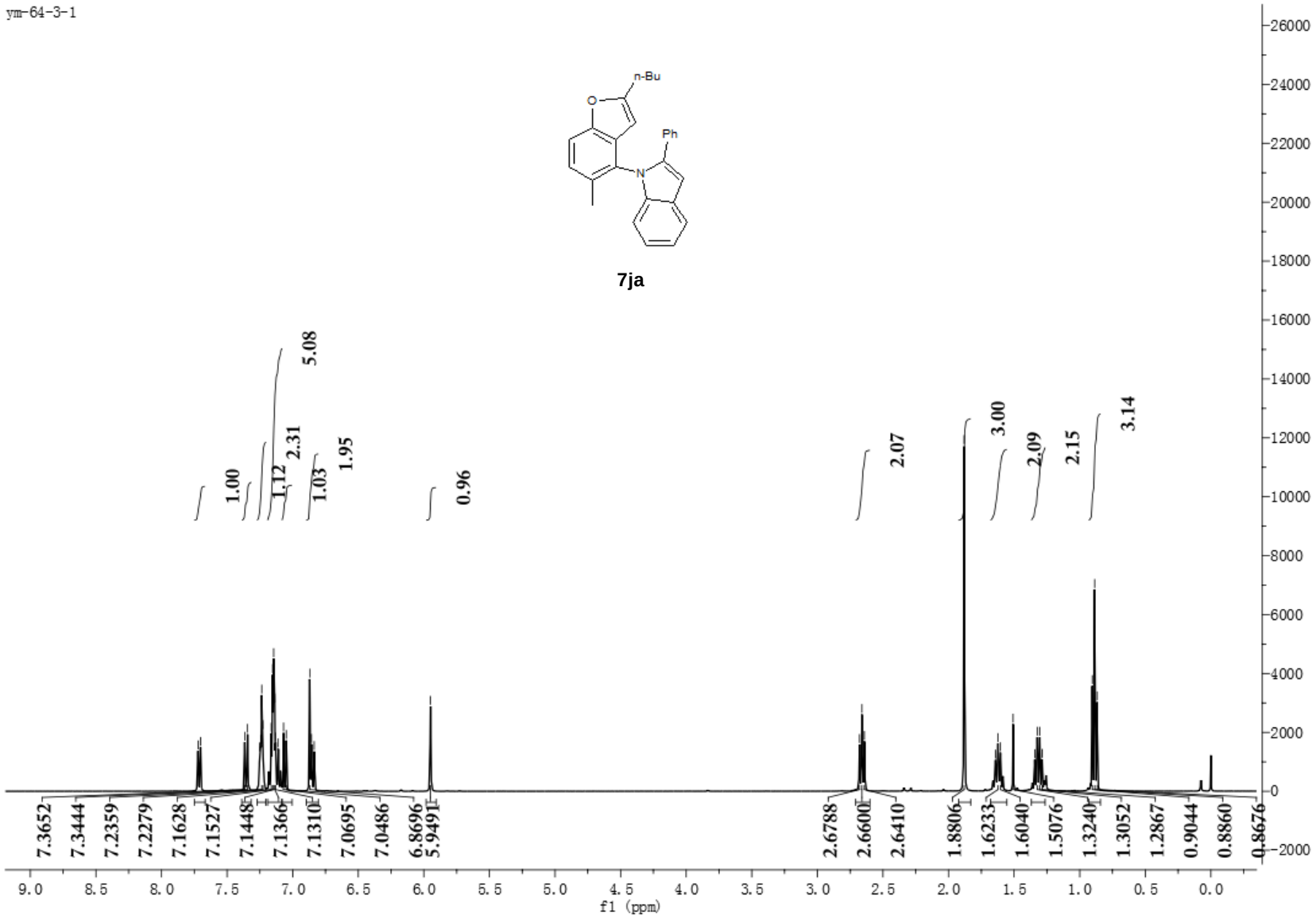

ym-64-2-1
O
Ph
N
7ha
4.00
2.23
1.08
1.04
1.00
0.99
0.97
0.99
0.95
3.00
1.06
4.11
7.3251
7.3043
7.2470
7.2407
7.2317
7.1617
7.1540
7.1454
7.0348
7.0139
6.8661
5.9413
1.9290
1.9221
1.9074
1.8946
1.8889
1.8395
1.5250
0.9414
0.9308
0.9189
0.9104
0.8988
0.8923
f1 (ppm)

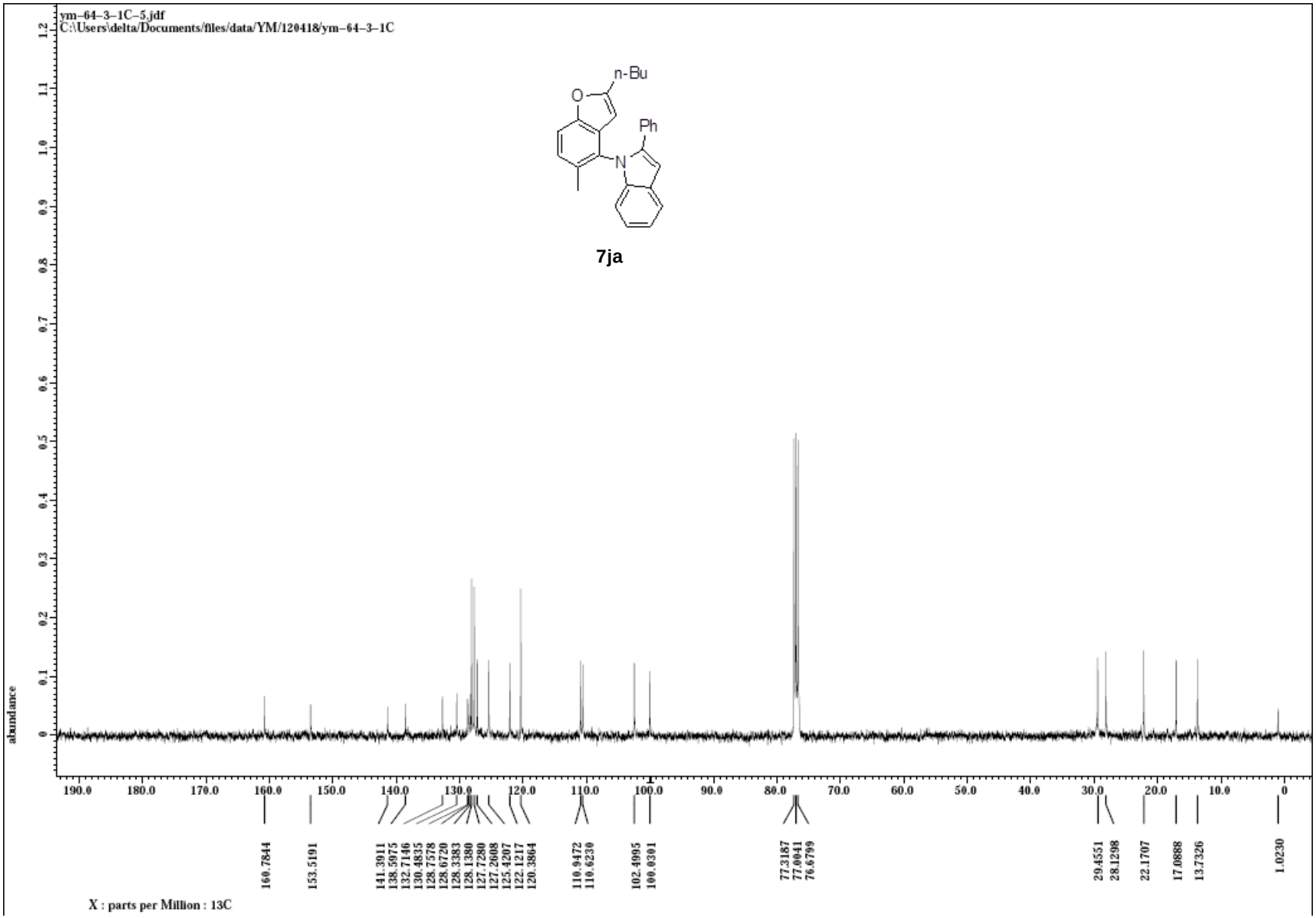

ym-64-2-1C-7.jdf
C:\Users\delta/Documents/files/data/YM/111230/ym-64-2-1C
O
Ph
N
abundance
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
161.5628
153.1152
141.3590
138.5940
132.6826
130.6326
128.9164
128.3729
128.3062
128.1632
127.6960
127.2765
125.2360
122.1087
120.3543
110.9342
110.4956
102.4770
98.4630
77.3248
77.0006
76.6860
17.0472
9.4386
7.5603
X : parts per Million : 13C

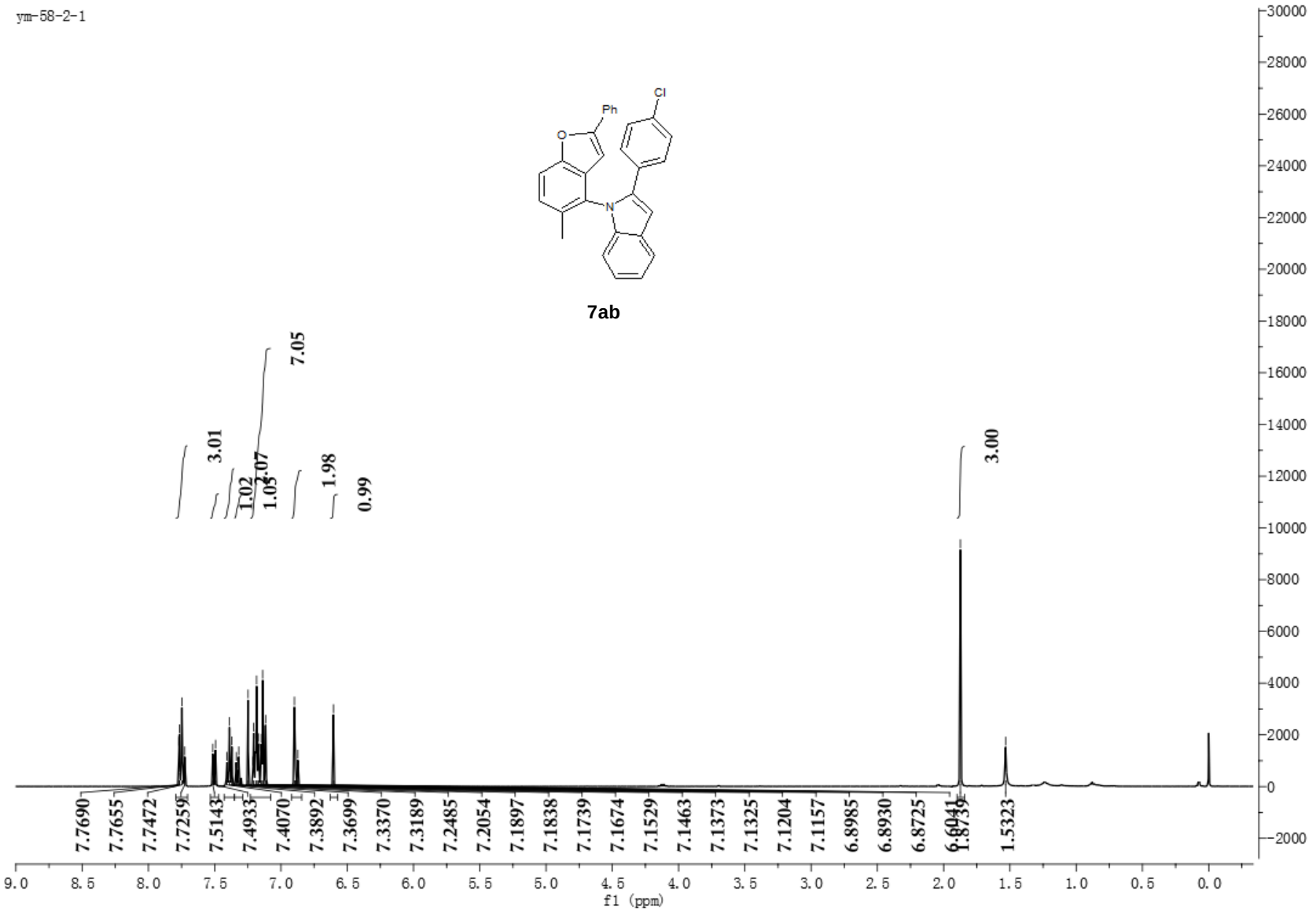
**7ha**

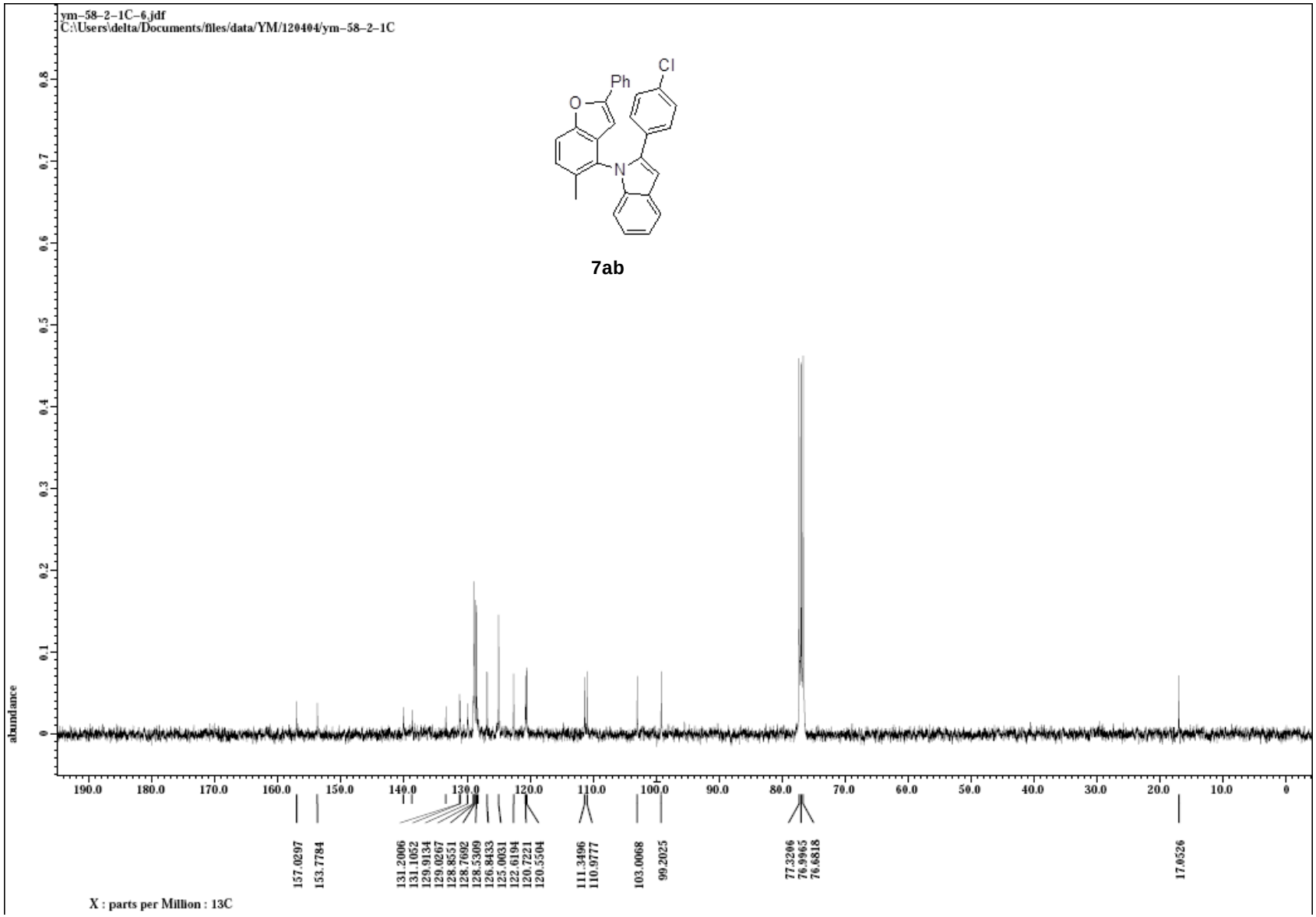


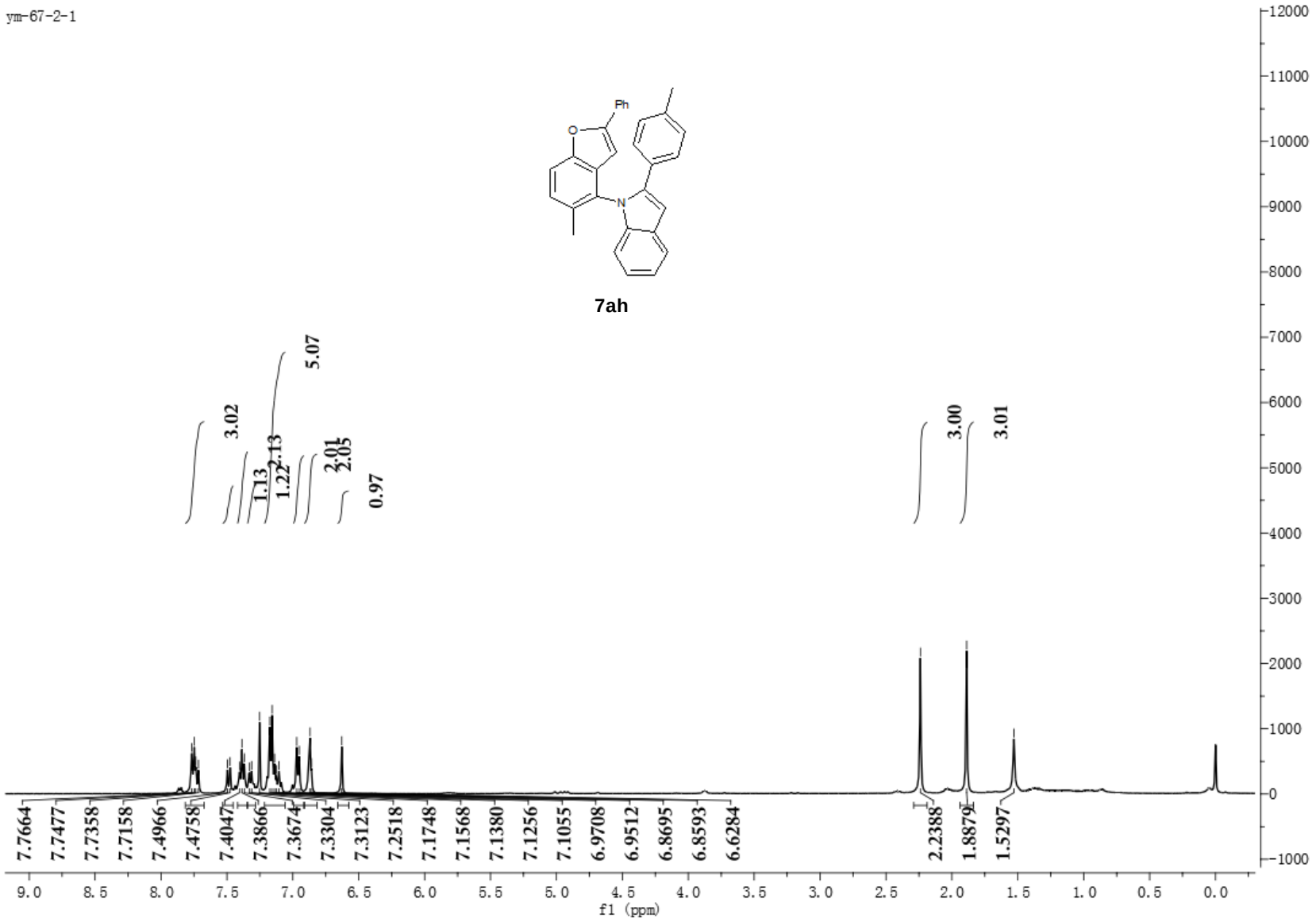

ym-59-2-1C-9.jdf
C:\Users\delta\Documents\files\data\YM\120404\ym-59-2-1C
t-Bu
O
Ph
N
7ia
abundance
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.4055
153.5125
141.4608
138.6004
132.7462
130.3721
128.8751
128.6367
128.3316
128.1219
127.7596
127.2542
125.4236
122.1246
120.3607
111.0455
110.7022
102.4548
97.2203
77.3216
76.9975
76.6828
33.0240
29.6964
28.7906
17.1108
X : parts per Million : 13C

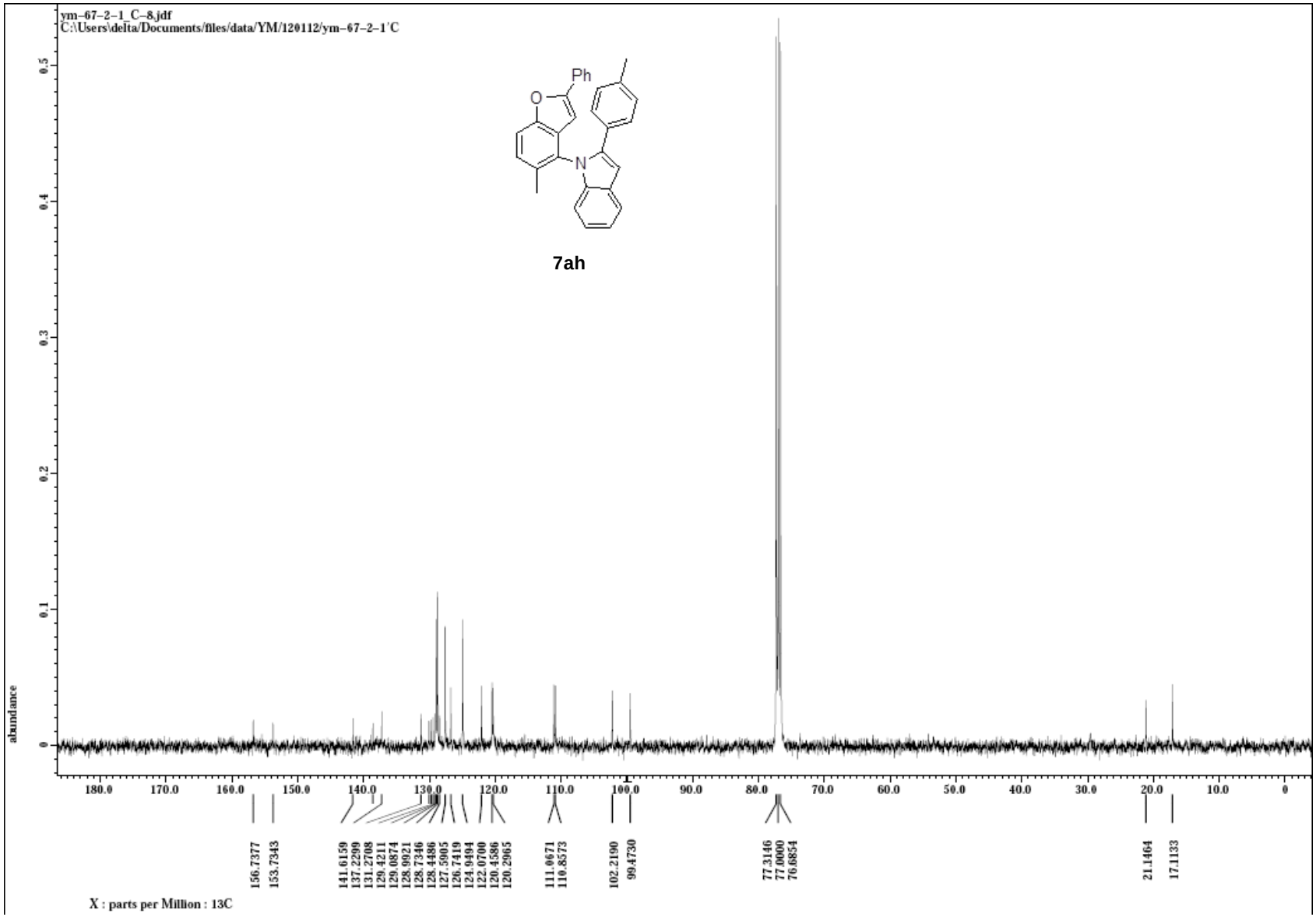

ym-64-3-1
n-Bu
O
Ph
N
7ja
1.00
1.12
2.31
5.08
1.03
1.95
0.96
2.07
3.00
2.09
2.15
3.14
7.3652
7.3444
7.2359
7.2279
7.1628
7.1527
7.1448
7.1366
7.1310
7.0695
7.0486
6.8696
5.9491
2.6788
2.6600
2.6410
1.8806
1.6233
1.6040
1.5076
1.3240
1.3052
1.2867
0.9044
0.8860
0.8676
f1 (ppm)

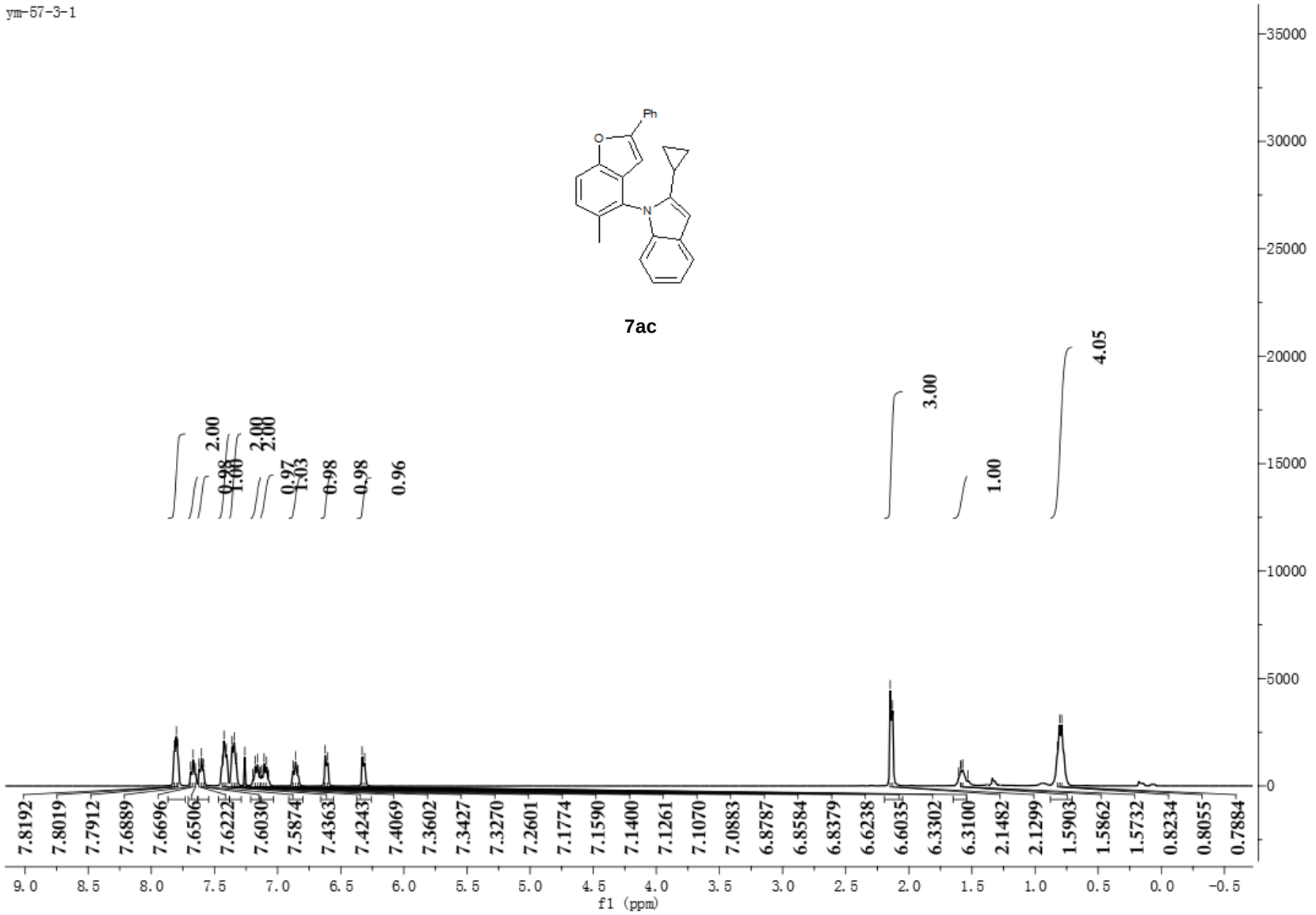

ym-64-3-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120418/ym-64-3-1C
n-Bu
O
Ph
N
7ja
abundance
X : parts per Million : 13C
160.7844
153.5191
141.3911
138.5975
132.7146
130.4835
128.7578
128.6720
128.3383
128.1380
127.7280
127.2608
125.4207
122.1217
120.3864
110.9472
110.6230
102.4995
100.0301
77.3187
77.0041
76.6799
29.4551
28.1298
22.1707
17.0888
13.7326
1.0230

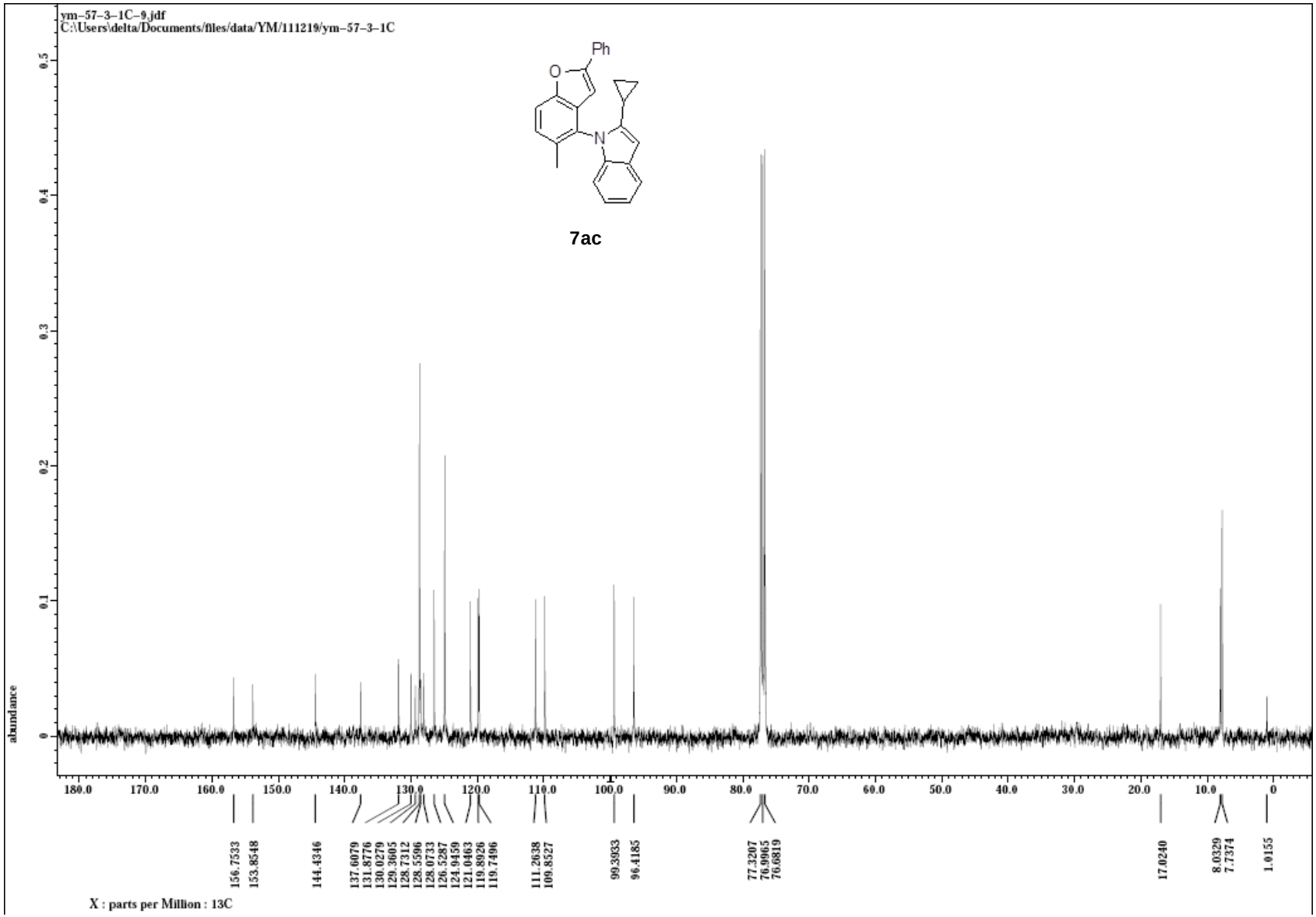

ym-58-2-1
Ph
Cl
O
N
7ab
3.01
1.02
1.05
2.07
7.05
1.98
0.99
3.00
7.7690
7.7655
7.7472
7.7259
7.5143
7.4933
7.4070
7.3892
7.3699
7.3370
7.3189
7.2485
7.2054
7.1897
7.1838
7.1739
7.1674
7.1529
7.1463
7.1373
7.1325
7.1204
7.1157
6.8985
6.8930
6.8725
6.6041
1.8739
1.5323
f1 (ppm)

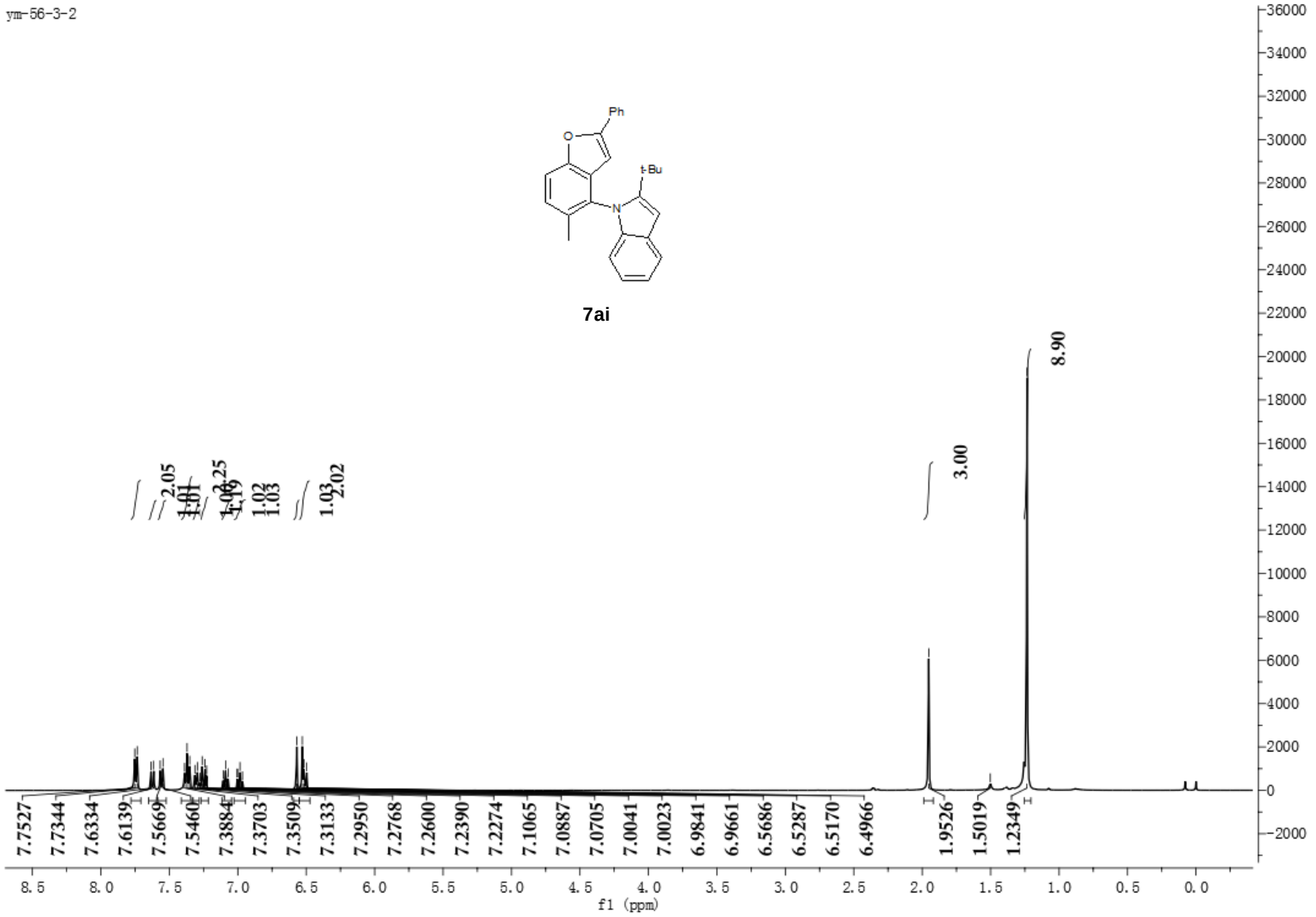

ym-58-2-1C-6.jdf
C:\Users\delta/Documents/files/data/YM/120404/ym-58-2-1C
Ph
Cl
O
N
7ab
abundance
157.0297
153.7784
131.2006
131.1052
129.9134
129.0267
128.8531
128.7692
128.5309
126.8433
125.0031
122.6194
120.7221
120.5504
111.3496
110.9777
103.0068
99.2025
77.3206
76.9965
76.6818
17.0526
X : parts per Million : 13C

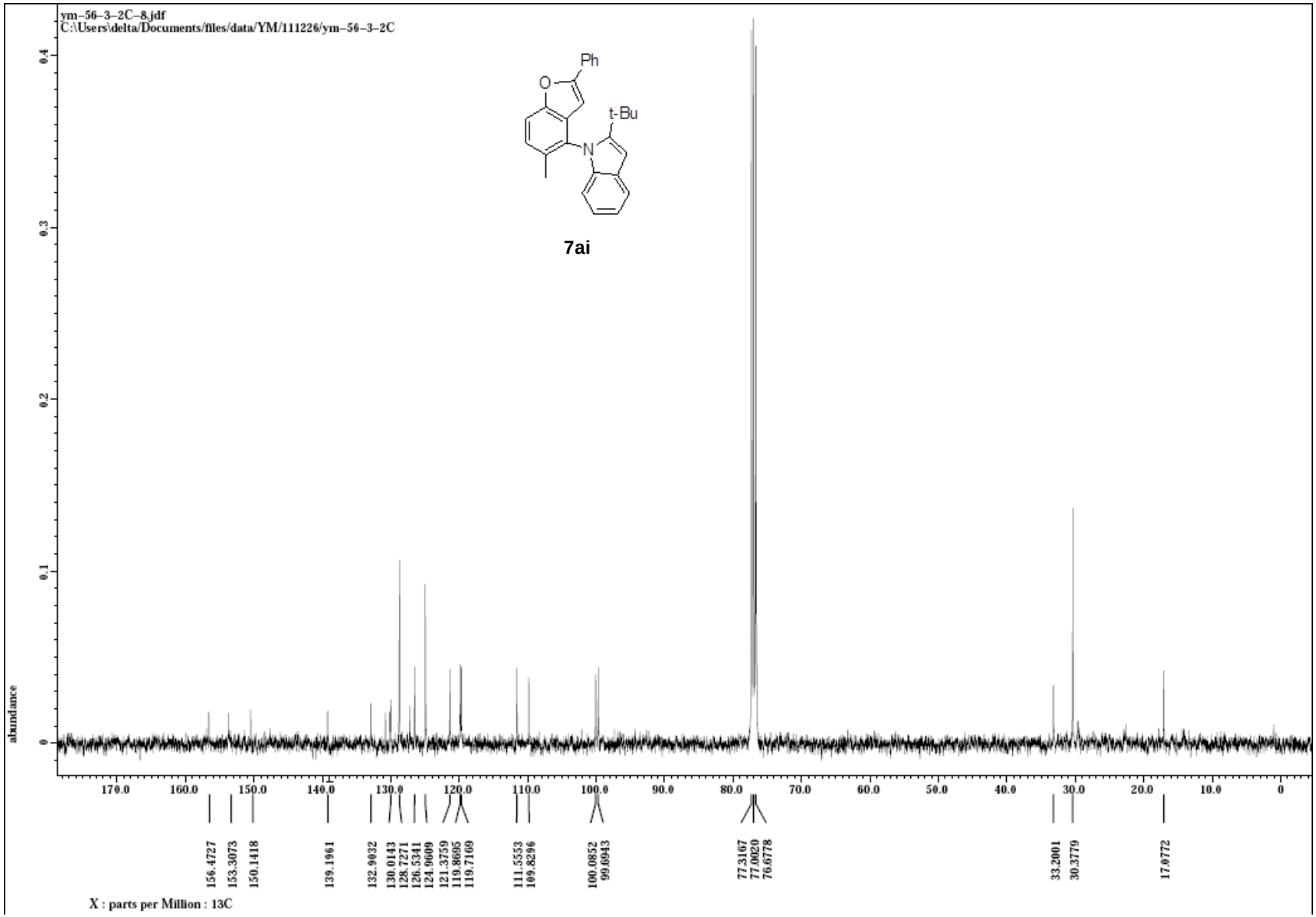

ym-67-2-1
Ph
O
N
7ah
3.02
1.13
1.22
2.13
5.07
2.01
2.05
0.97
3.00
3.01
7.7664
7.7477
7.7358
7.7158
7.4966
7.4758
7.4047
7.3866
7.3674
7.3304
7.3123
7.2518
7.1748
7.1568
7.1380
7.1256
7.1055
6.9708
6.9512
6.8695
6.8593
6.6284
2.2388
1.8879
1.5297
f1 (ppm)

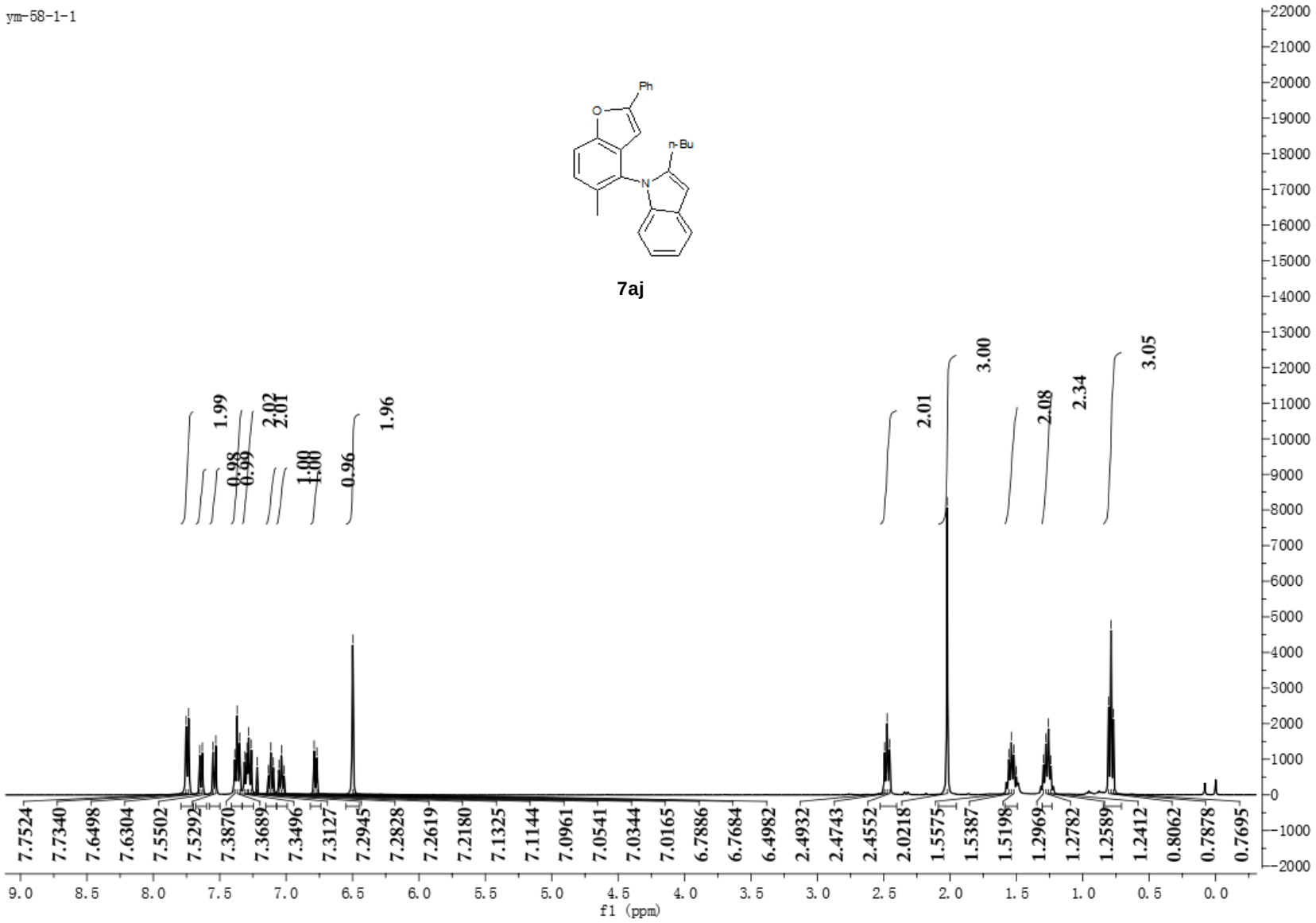

ym-67-2-1_C-8.jdf
C:\Users\delta/Documents/files/data/YM/120112/ym-67-2-1'C
Ph
O
N
7ah
abundance
0.5
0.4
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.7377
153.7343
141.6159
137.2299
131.2708
129.4211
129.0874
128.9921
128.7346
128.4486
127.5905
126.7419
124.9494
122.0700
120.4586
120.2965
111.0671
110.8573
102.2190
99.4730
77.3146
77.0000
76.6854
21.1464
17.1133
X : parts per Million : 13C

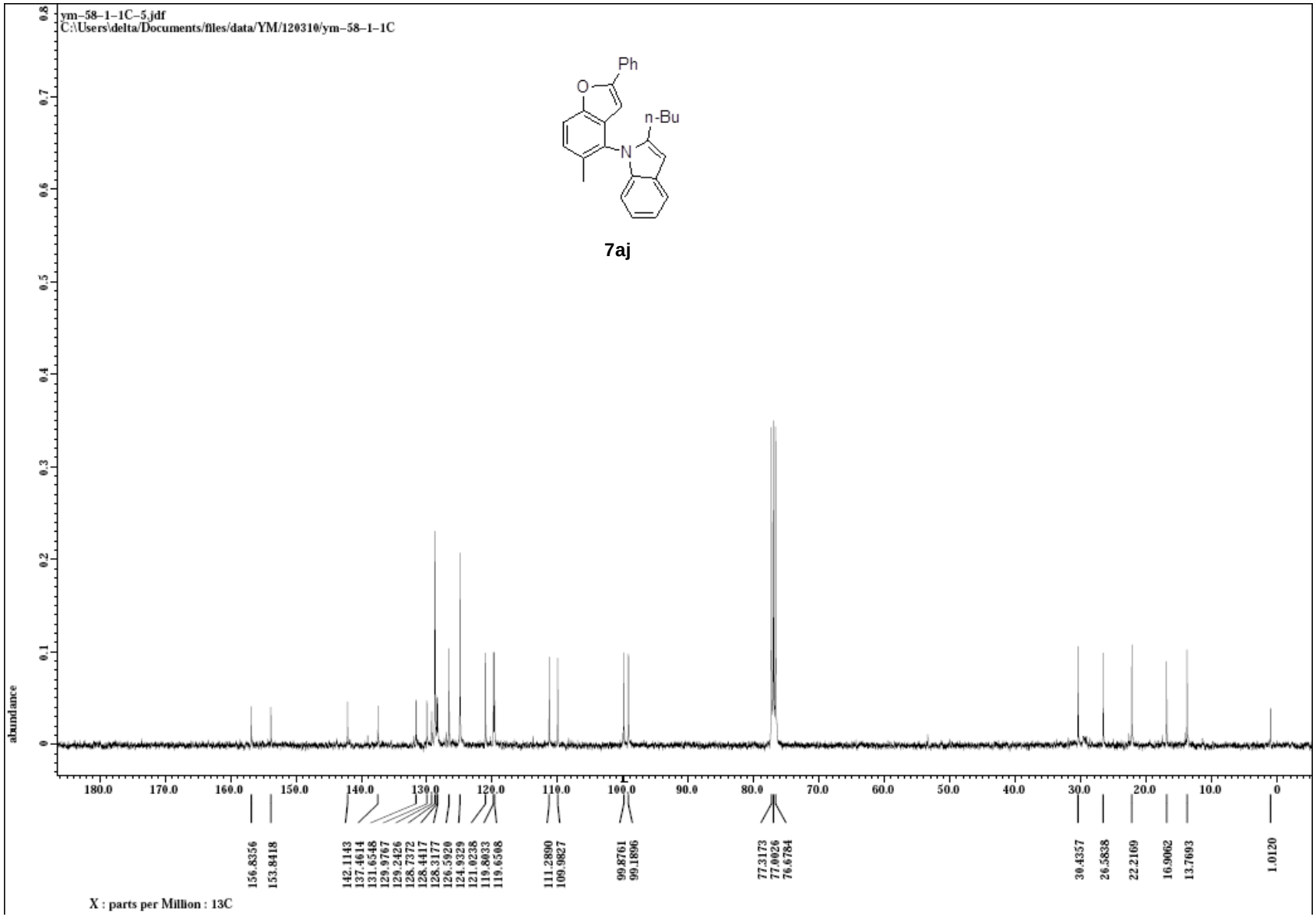

ym-57-3-1
Ph
O
N
7ac
2.00
0.98
1.00
2.00
2.00
0.97
1.03
0.98
0.98
0.96
3.00
1.00
4.05
7.8192
7.8019
7.7912
7.6889
7.6696
7.6506
7.6222
7.6030
7.5874
7.4363
7.4243
7.4069
7.3602
7.3427
7.3270
7.2601
7.1774
7.1590
7.1400
7.1261
7.1070
7.0883
6.8787
6.8584
6.8379
6.6238
6.6035
6.3302
6.3100
2.1482
2.1299
1.5903
1.5862
1.5732
0.8234
0.8055
0.7884
f1 (ppm)


ym-57-3-1C-9.jdf
C:\Users\delta\Documents\files\data\YM\111219\ym-57-3-1C
Ph
O
N
7ac
abundance
0.5
0.4
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.7533
153.8548
144.4346
137.6079
131.8776
130.0279
129.3605
128.7312
128.5596
128.0733
126.5287
124.9459
121.0463
119.8926
119.7496
111.2638
109.8527
99.3933
96.4185
77.3207
76.9965
76.6819
17.0240
8.0329
7.7374
1.0155
X : parts per Million : 13C

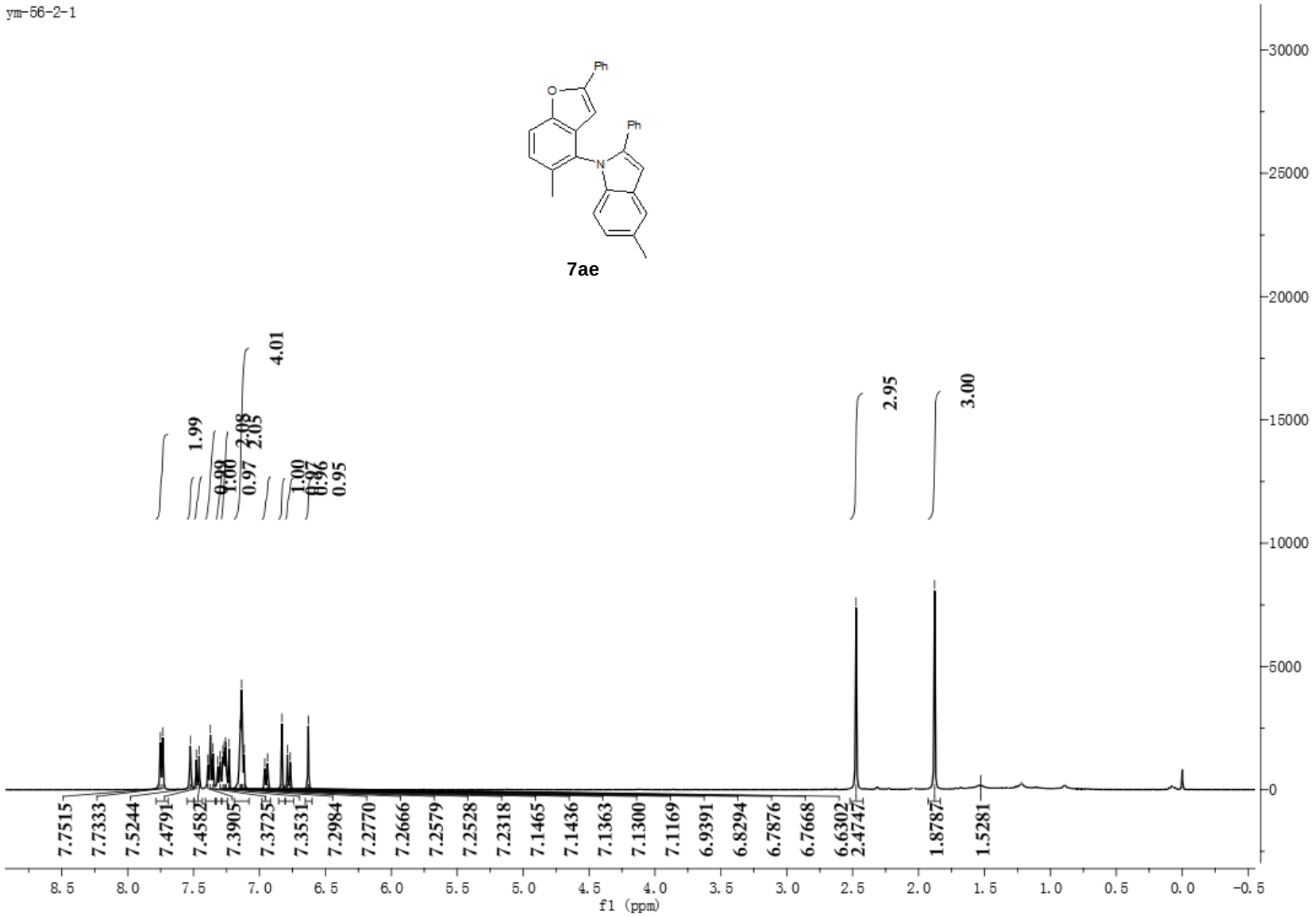

ym-56-3-2
Ph
O
t-Bu
N
7ai
2.05
1.01
3.25
1.08
1.19
1.02
1.03
1.03
2.02
3.00
8.90
7.7527
7.7344
7.6334
7.6139
7.5669
7.5460
7.3884
7.3703
7.3509
7.3133
7.2950
7.2768
7.2600
7.2390
7.2274
7.1065
7.0887
7.0705
7.0041
7.0023
6.9841
6.9661
6.5686
6.5287
6.5170
6.4966
1.9526
1.5019
1.2349
f1 (ppm)

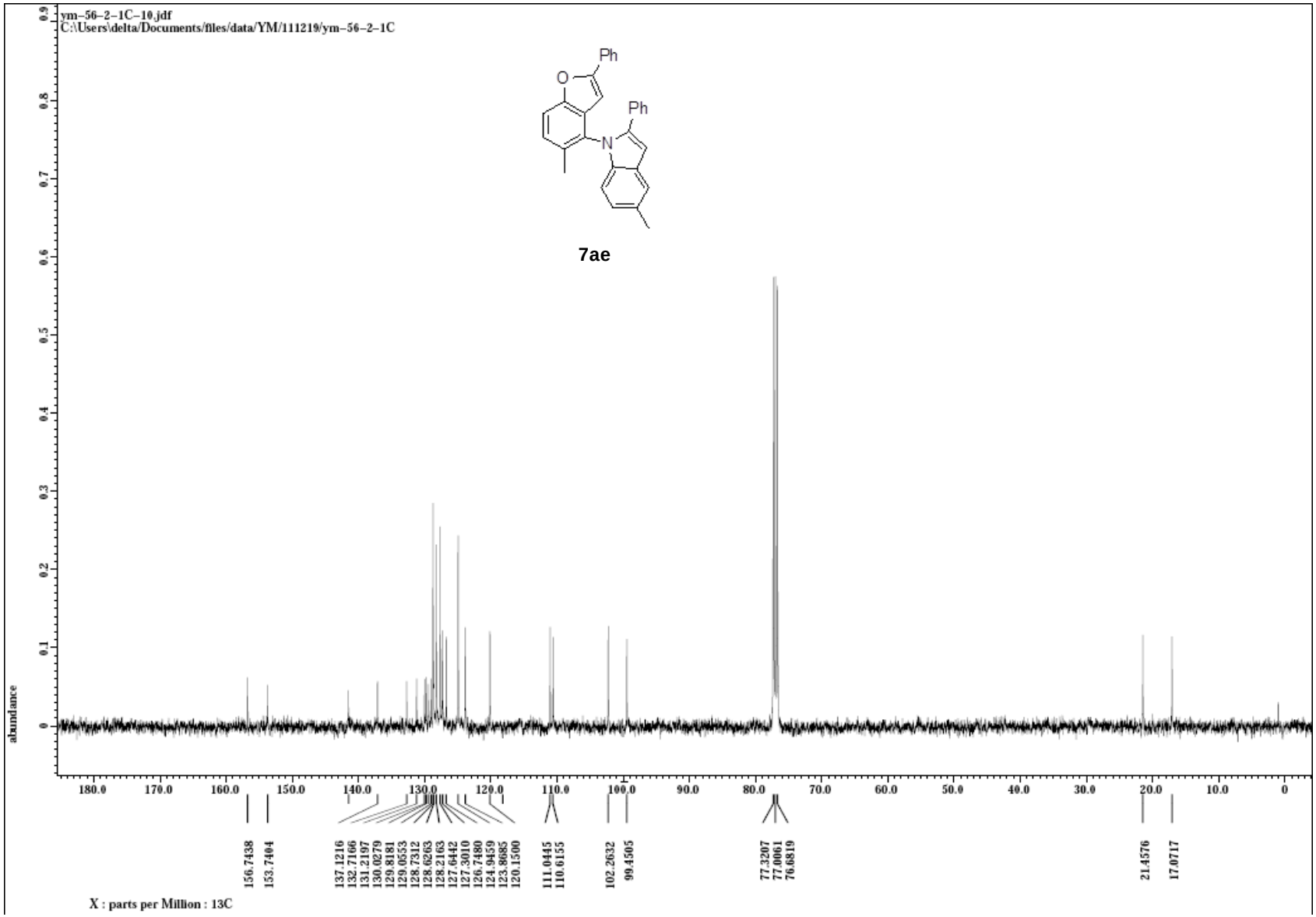

ym-56-3-2C-8.jdf
C:\Users\delta\Documents\files\data\YM\111226\ym-56-3-2C
Ph
O
t-Bu
N
7ai
abundance
0.4
0.3
0.2
0.1
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.4727
153.3073
150.1418
139.1961
132.9032
130.0143
128.7271
126.5341
124.9609
121.3759
119.8695
119.7169
111.5553
109.8296
100.0852
99.6943
77.3167
77.0020
76.6778
33.2001
30.3779
17.0772
X : parts per Million : 13C

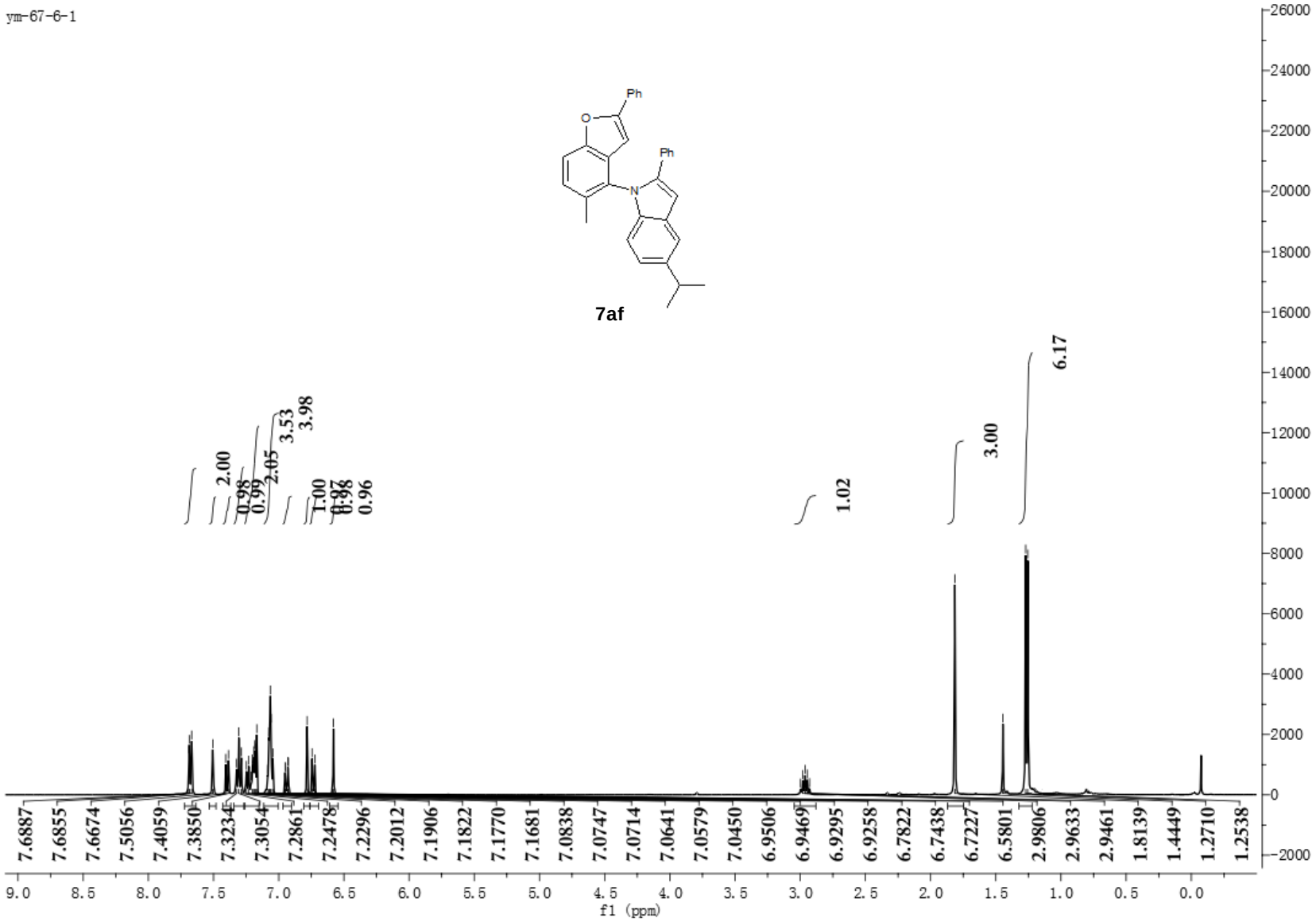

ym-58-1-1
Ph
O
n-Bu
N
7aj
1.99
0.98
0.99
2.02
2.01
1.00
1.00
0.96
1.96
2.01
3.00
2.08
2.34
3.05
7.7524
7.7340
7.6498
7.6304
7.5502
7.5292
7.3870
7.3689
7.3496
7.3127
7.2945
7.2828
7.2619
7.2180
7.1325
7.1144
7.0961
7.0541
7.0344
7.0165
6.7886
6.7684
6.4982
2.4932
2.4743
2.4552
2.0218
1.5575
1.5387
1.5198
1.2969
1.2782
1.2589
1.2412
0.8062
0.7878
0.7695
f1 (ppm)

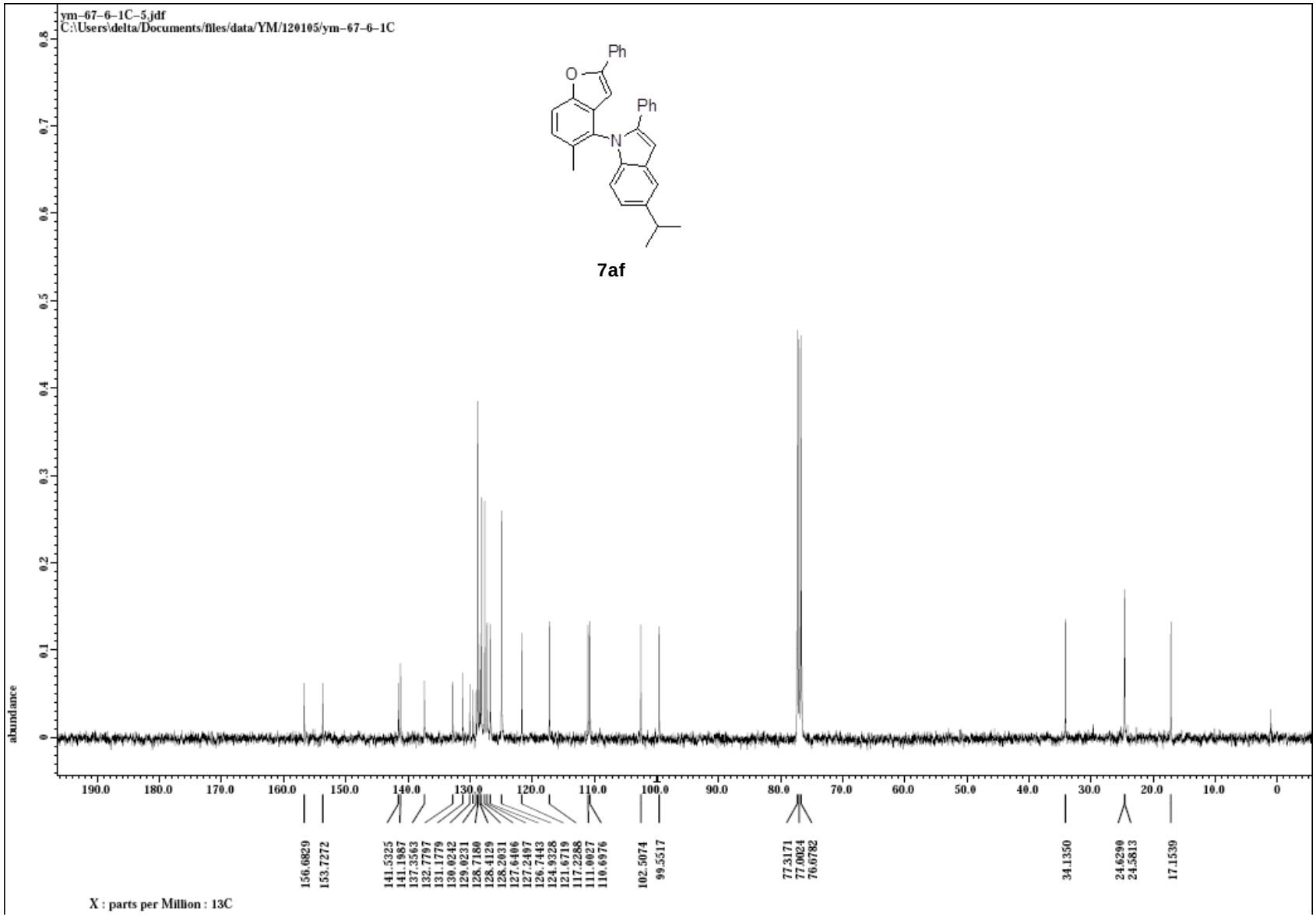

ym-58-1-1C-5.jdf
C:\Users\delta\Documents\files\data\YM\120310\ym-58-1-1C
Ph
O
n-Bu
N
abundance
X : parts per Million : 13C
156.8356
153.8418
142.1143
137.4614
131.6548
129.9767
129.2426
128.7372
128.4417
128.3177
126.5920
124.9329
121.0238
119.8033
119.6508
111.2890
109.9827
99.8761
99.1896
77.3173
77.0026
76.6784
30.4357
26.5838
22.2169
16.9062
13.7693
1.0120

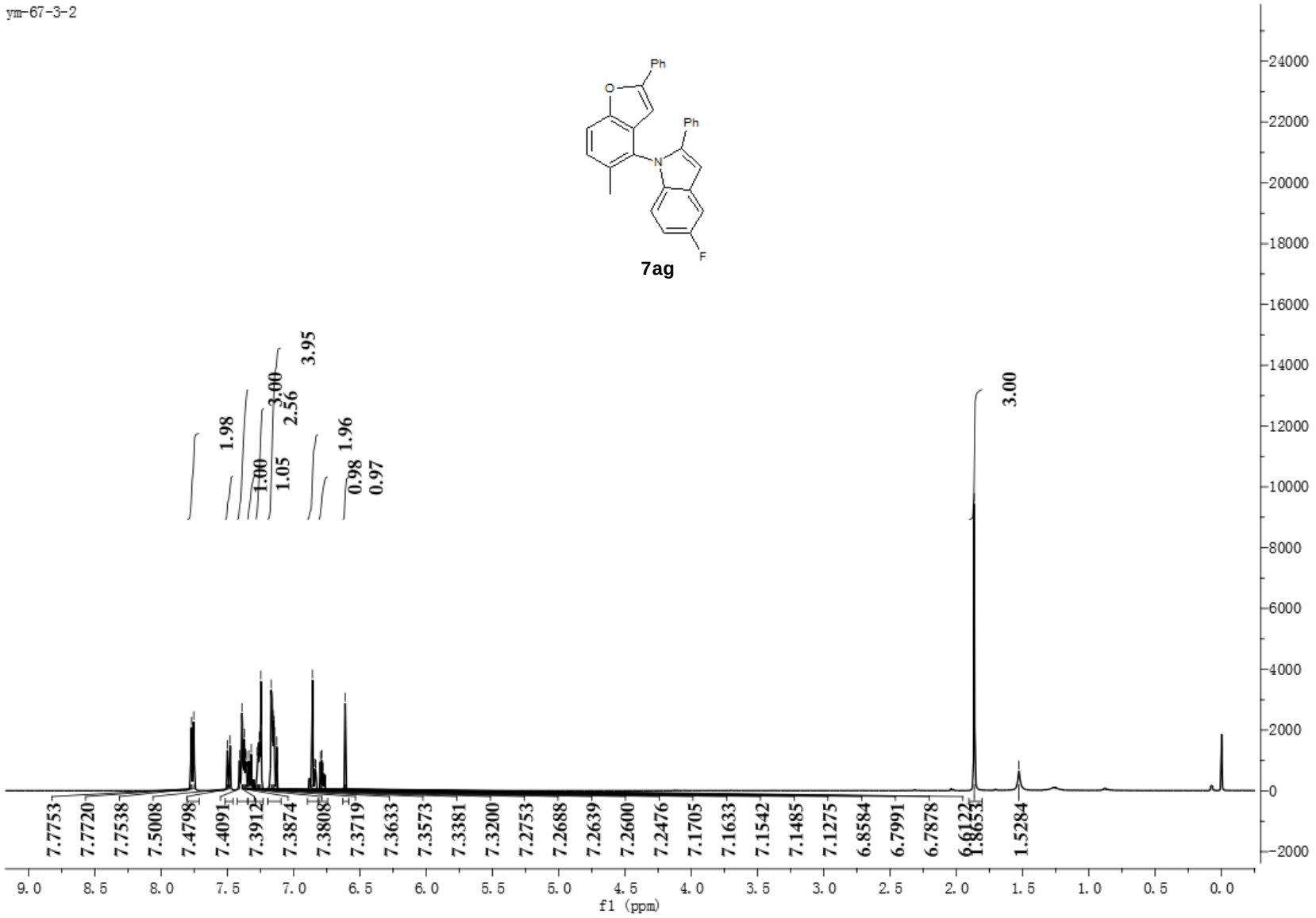
**7aj**

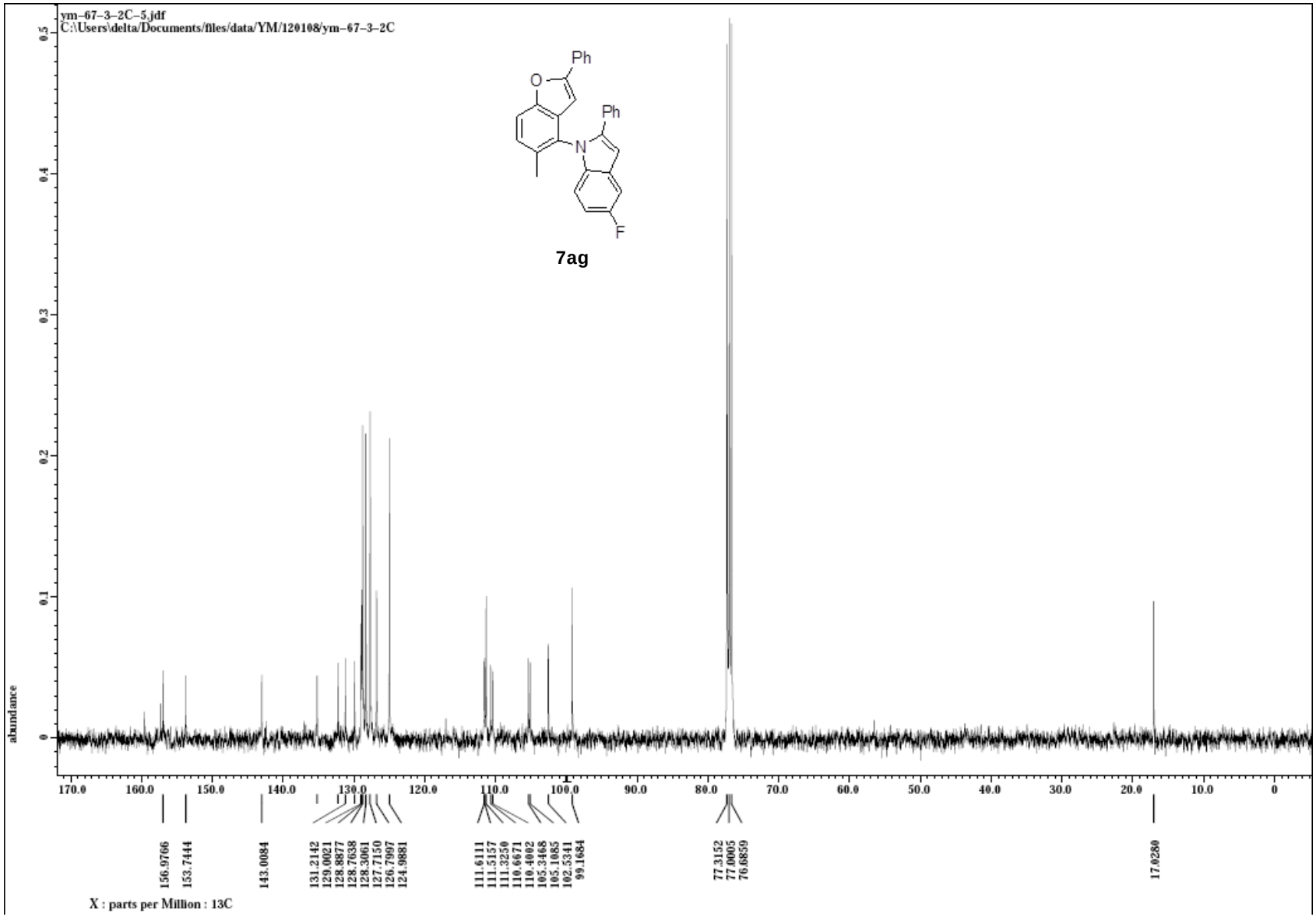

ym-56-2-1
Ph
O
Ph
N
7ae
4.01
1.99
2.08
2.05
0.97
1.00
0.96
0.95
2.95
3.00
7.7515
7.7333
7.5244
7.4791
7.4582
7.3905
7.3725
7.3531
7.2984
7.2770
7.2666
7.2579
7.2528
7.2318
7.1465
7.1436
7.1363
7.1300
7.1169
6.9391
6.8294
6.7876
6.7668
6.6302
2.4747
1.8787
1.5281
f1 (ppm)

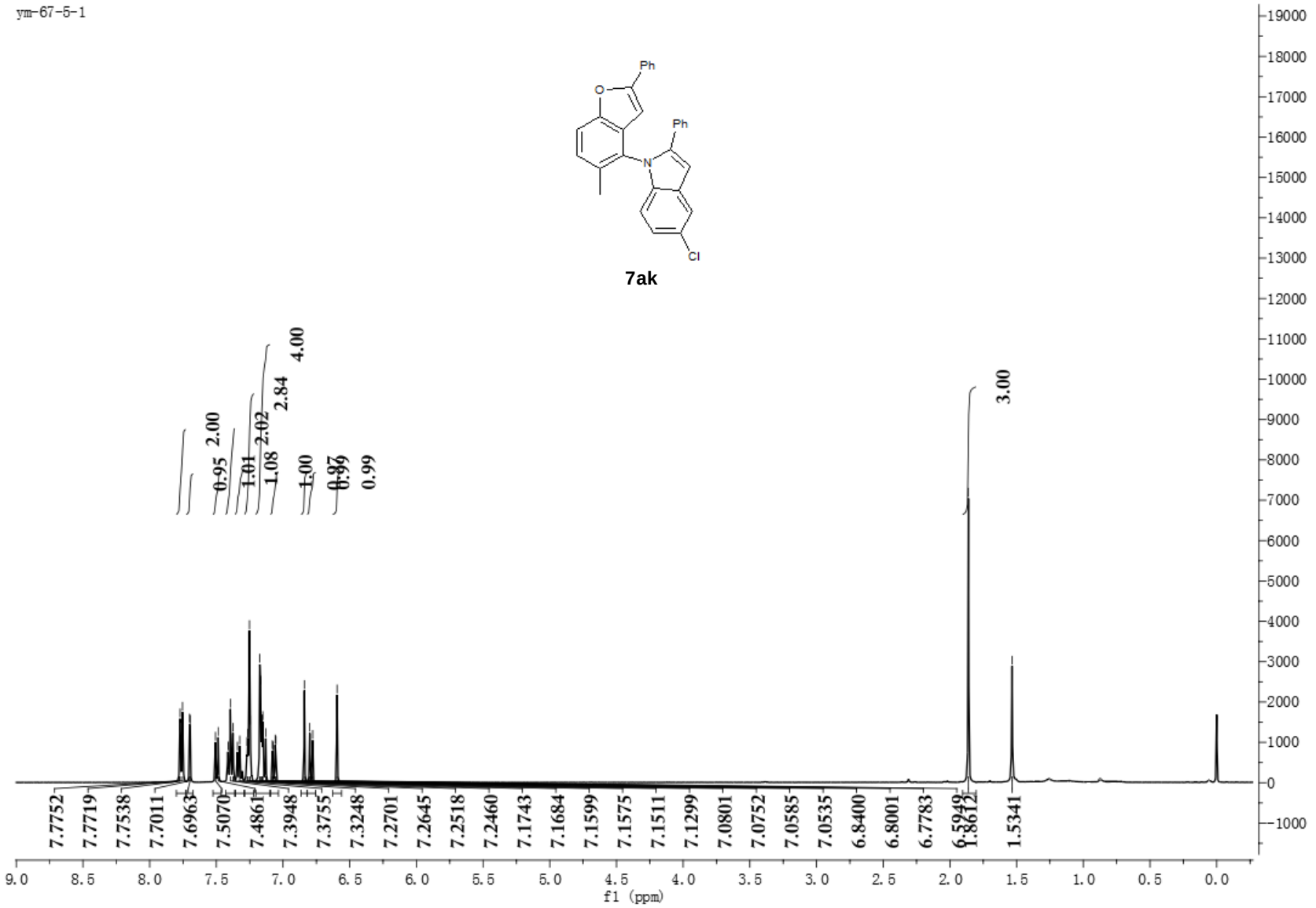


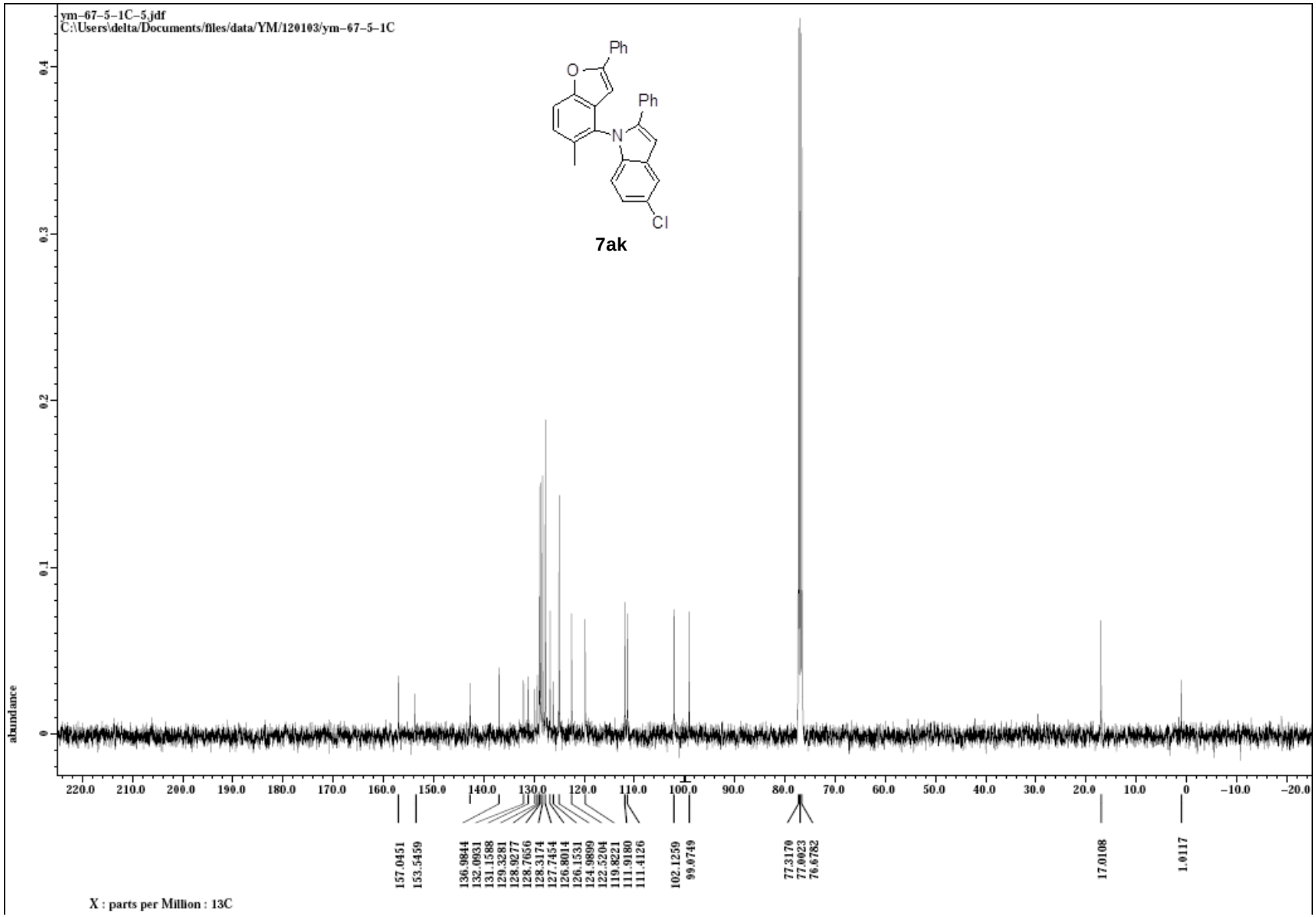

ym-67-6-1
Ph
O
Ph
N
7af
2.00
0.98
0.99
2.05
3.53
3.98
1.00
0.97
0.98
0.96
1.02
3.00
6.17
7.6887
7.6855
7.6674
7.5056
7.4059
7.3850
7.3234
7.3054
7.2861
7.2478
7.2296
7.2012
7.1906
7.1822
7.1770
7.1681
7.0838
7.0747
7.0714
7.0641
7.0579
7.0450
6.9506
6.9469
6.9295
6.9258
6.7822
6.7438
6.7227
6.5801
2.9806
2.9633
2.9461
1.8139
1.4449
1.2710
1.2538
f1 (ppm)

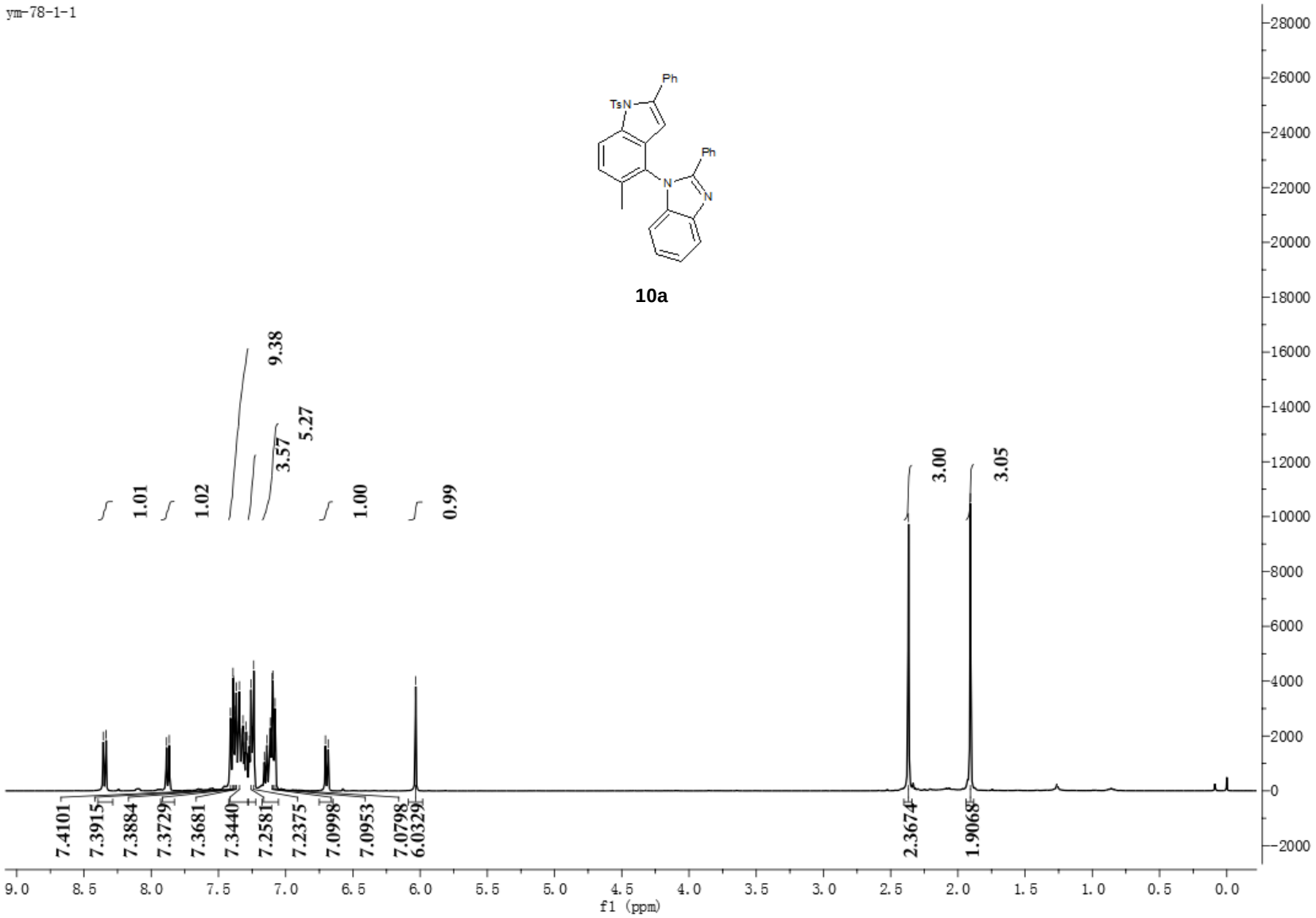

ym-67-6-1C-5.jdf
C:\Users\delta/Documents/files/data/YM/120105/ym-67-6-1C
Ph
O
Ph
N
7af
abundance
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.6829
153.7272
141.5325
141.1987
137.3563
132.7797
131.1779
130.0242
129.0231
128.7180
128.4129
128.2031
127.6406
127.2497
126.7443
124.9328
121.6719
117.2288
111.0027
110.6976
102.5074
99.5517
77.3171
77.0024
76.6782
34.1350
24.6290
24.5813
17.1539
X : parts per Million : 13C

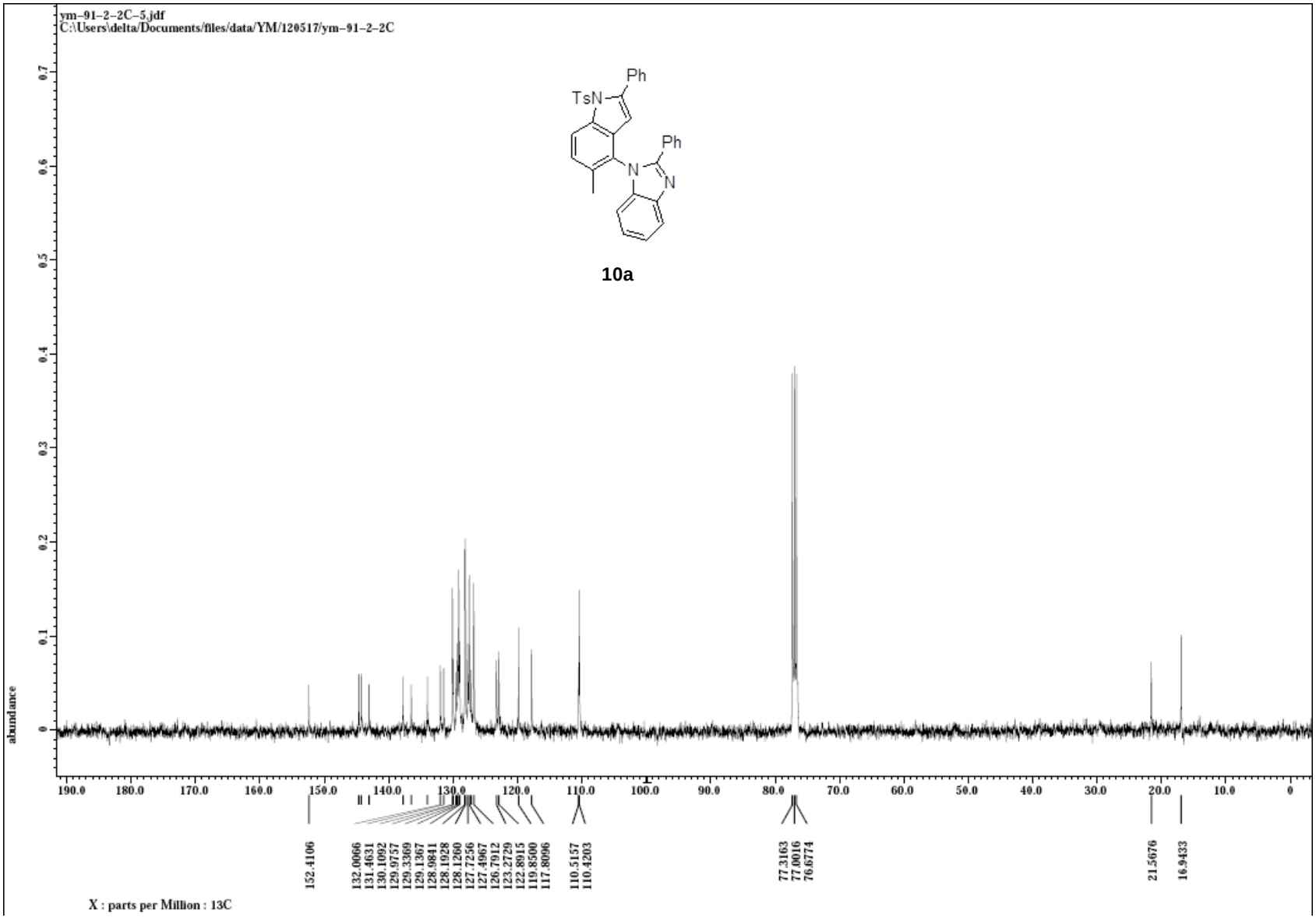

ym-67-3-2
Ph
O
Ph
N
F
7ag
1.98
1.00
1.05
3.00
2.56
3.95
1.96
0.98
0.97
3.00
7.7753
7.7720
7.7538
7.5008
7.4798
7.4091
7.3912
7.3874
7.3808
7.3719
7.3633
7.3573
7.3381
7.3200
7.2753
7.2688
7.2639
7.2600
7.2476
7.1705
7.1633
7.1542
7.1485
7.1275
6.8584
6.7991
6.7878
6.6122
1.8653
1.5284
f1 (ppm)

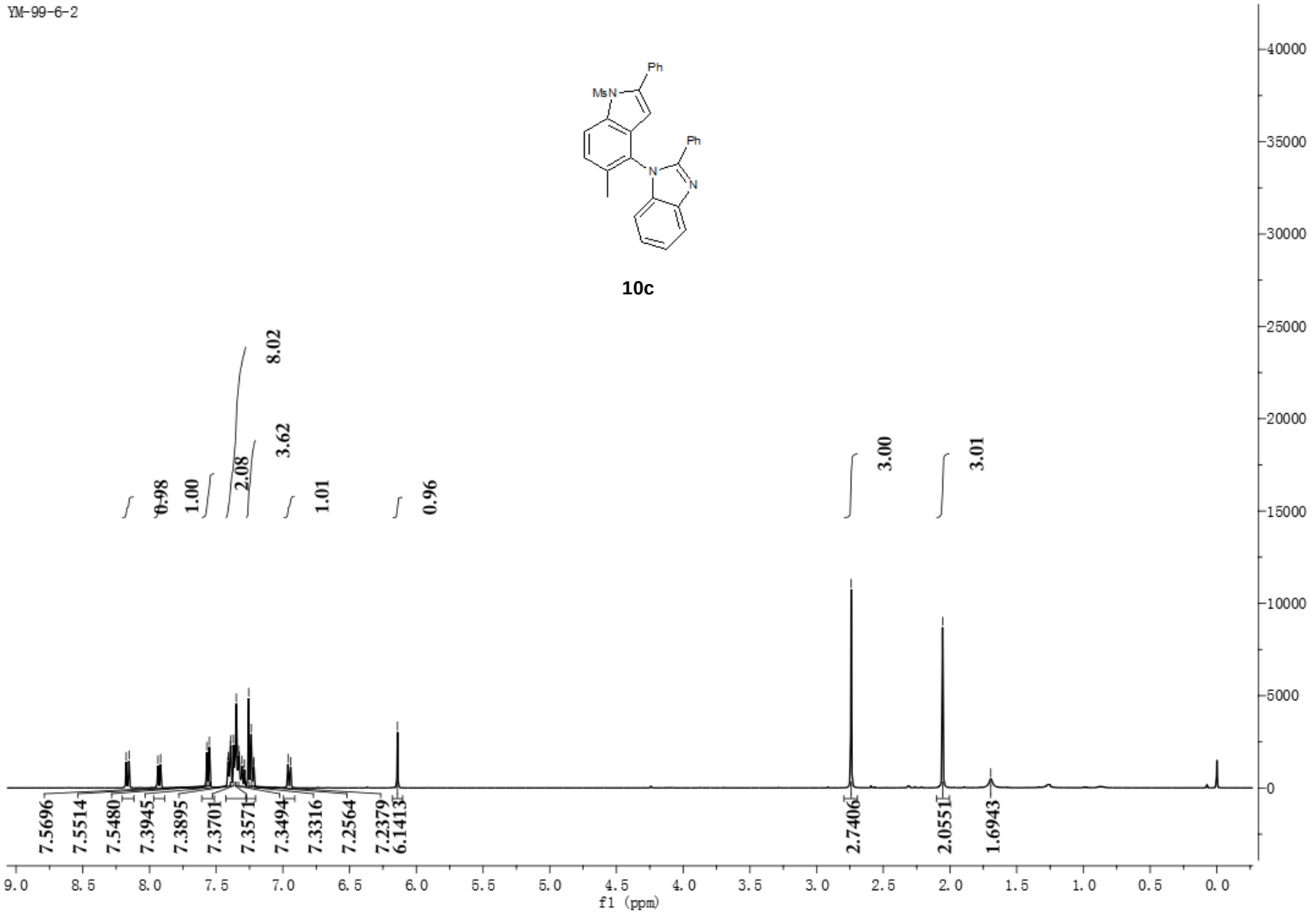

ym-67-3-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120108/ym-67-3-2C
Ph
O
Ph
N
F
7ag
abundance
0.5
0.4
0.3
0.2
0.1
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
156.9766
153.7444
143.0084
131.2142
129.0021
128.8877
128.7638
128.3061
127.7150
126.7997
124.9881
111.6111
111.5157
111.3250
110.6671
110.4002
105.3468
105.1085
102.5341
99.1684
77.3152
77.0005
76.6859
17.0280
X : parts per Million : 13C

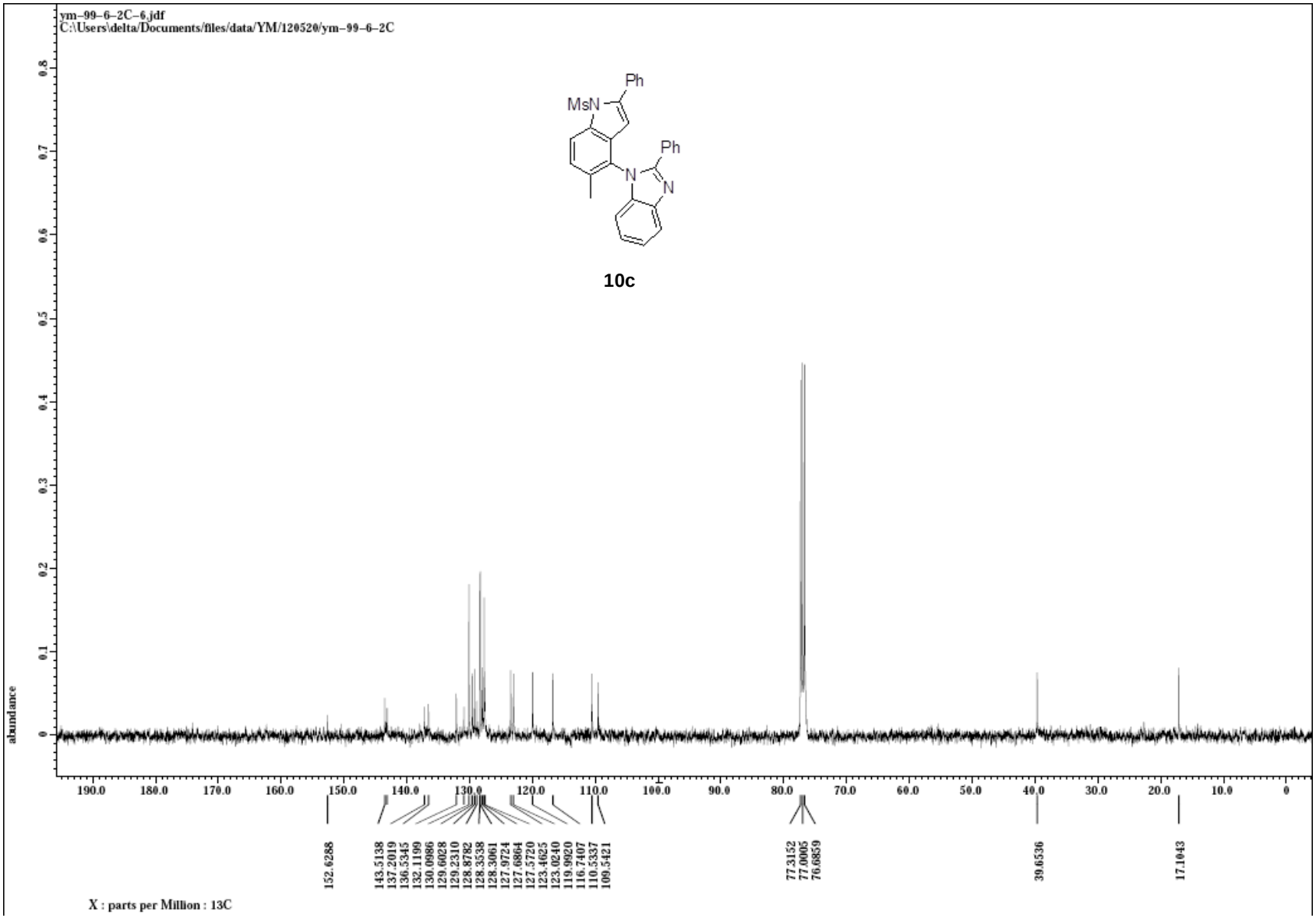

ym-67-5-1
Ph
O
Ph
N
Cl
7ak
4.00
2.84
2.02
2.00
1.08
1.01
1.00
0.95
0.99
3.00
7.7752
7.7719
7.7538
7.7011
7.6963
7.5070
7.4861
7.3948
7.3755
7.3248
7.2701
7.2645
7.2518
7.2460
7.1743
7.1684
7.1599
7.1575
7.1511
7.1299
7.0801
7.0752
7.0585
7.0535
6.8400
6.8001
6.7783
6.5949
1.8612
1.5341
f1 (ppm)


ym-67-5-1C-5.jdf
C:\Users\delta\Documents\files\data\YM\120103\ym-67-5-1C
Ph
O
Ph
N
Cl
7ak
abundance
0.4
0.3
0.2
0.1
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
157.0451
153.5459
136.9844
132.0931
131.1588
129.3281
128.9277
128.7656
128.3174
127.7454
126.8014
126.1531
124.9899
122.5204
119.8221
111.9180
111.4126
102.1259
99.0749
77.3170
77.0023
76.6782
17.0108
1.0117
X : parts per Million : 13C

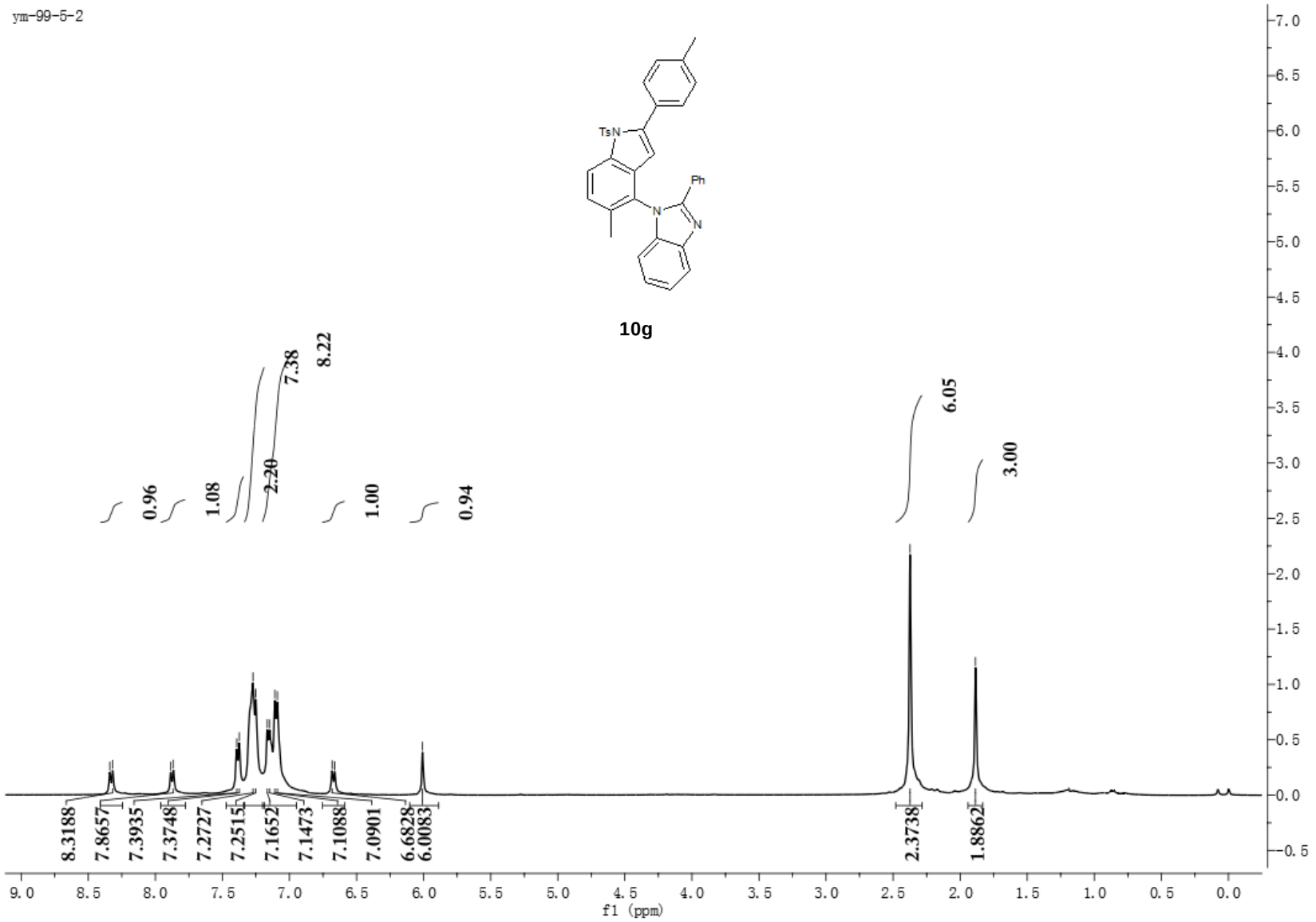

ym-78-1-1
Ph
TsN
Ph
N
N
10a
9.38
5.27
3.57
1.01
1.02
1.00
0.99
3.00
3.05
7.4101
7.3915
7.3884
7.3729
7.3681
7.3440
7.2581
7.2375
7.0998
7.0953
7.0798
6.0329
2.3674
1.9068
f1 (ppm)

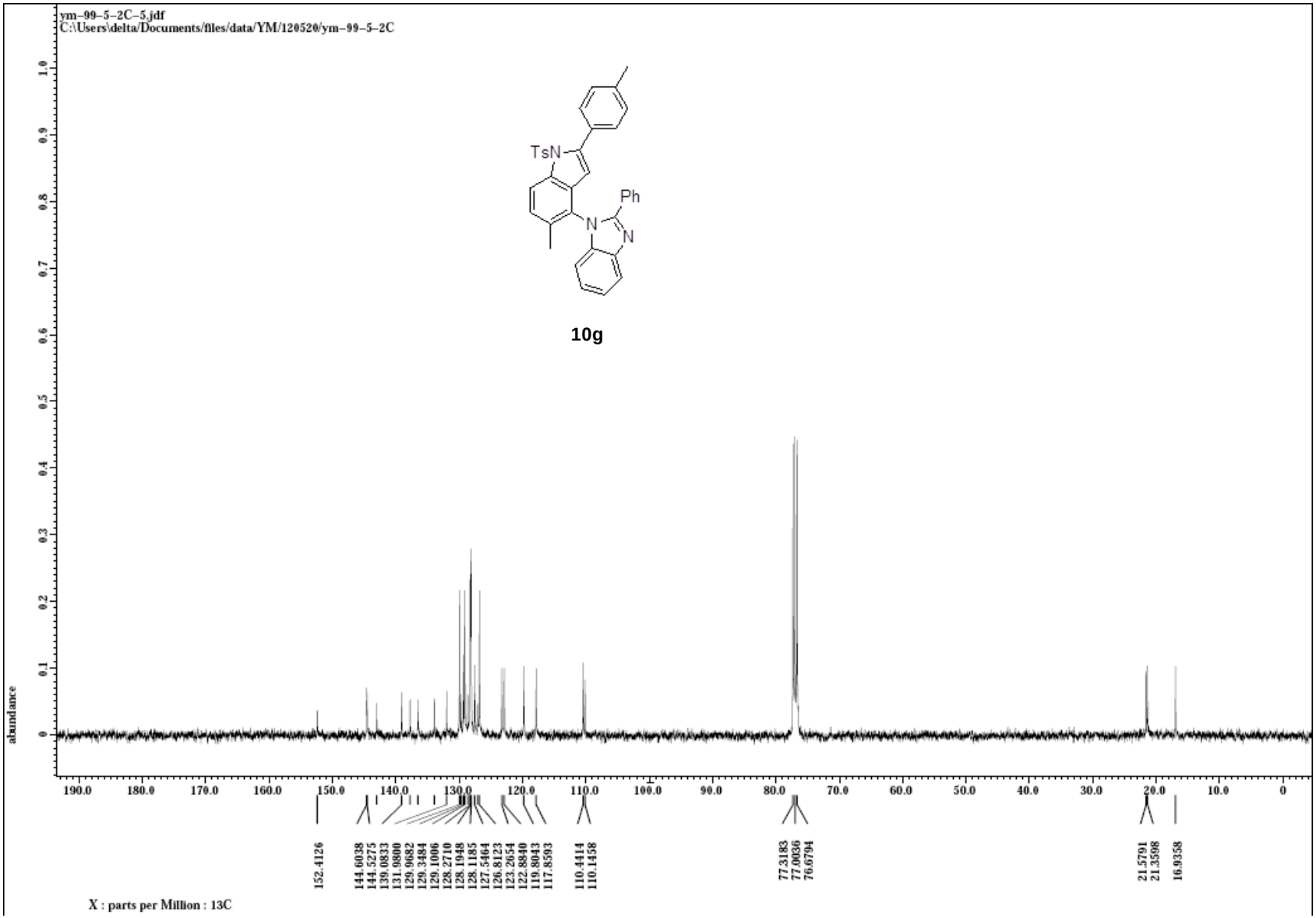

ym-91-2-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120517/ym-91-2-2C
Ph
TsN
Ph
N
N
10a
abundance
190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
152.4106
132.0066
131.4631
130.1092
129.9757
129.3369
129.1367
128.9841
128.1928
128.1260
127.7256
127.4967
126.7912
123.2729
122.8915
119.8500
117.8096
110.5157
110.4203
77.3163
77.0016
76.6774
21.5676
16.9433
X : parts per Million : 13C

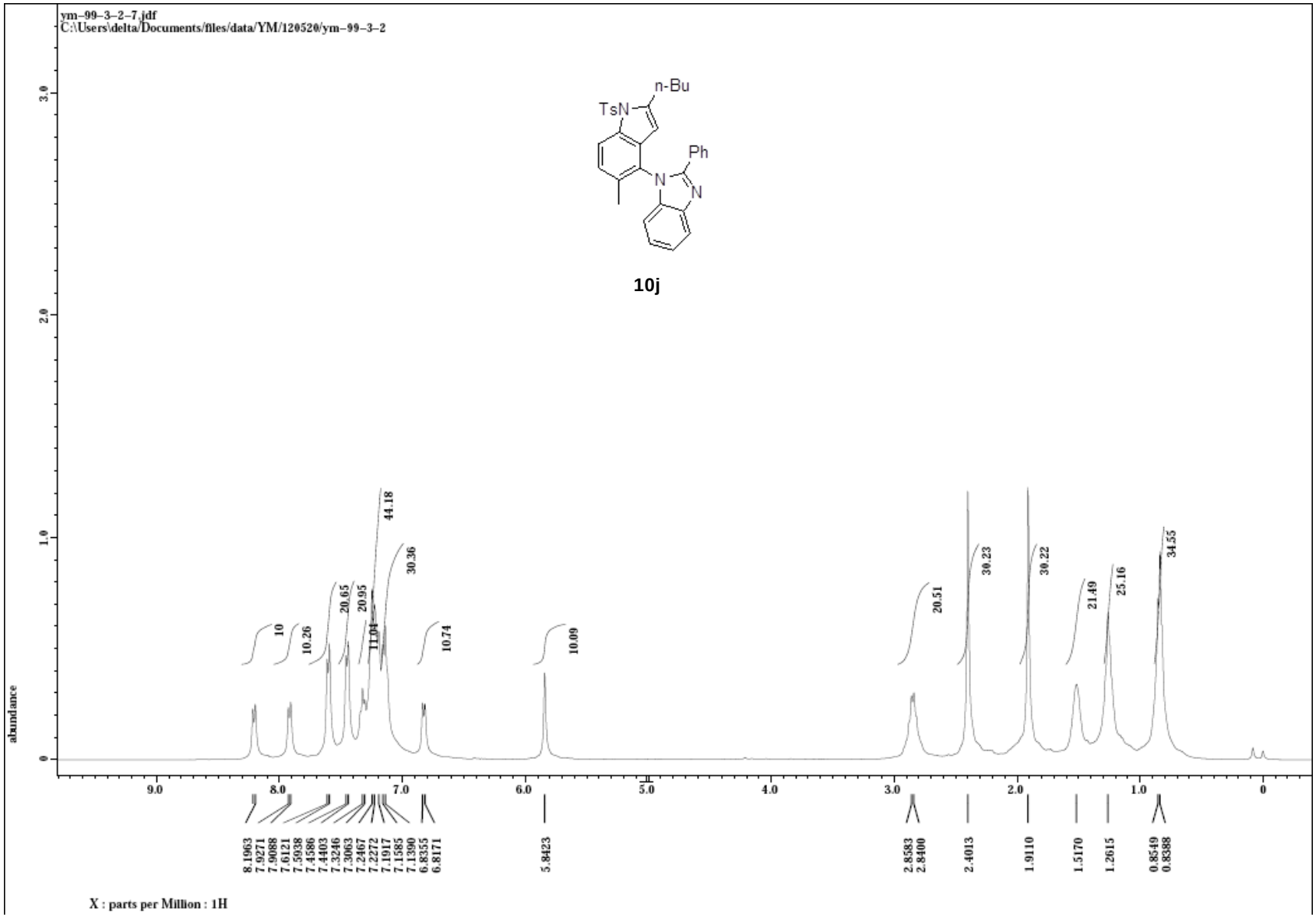

YM-99-6-2
Ph
MsN
Ph
N
N
10c
8.02
3.62
2.08
1.00
0.98
1.01
0.96
3.00
3.01
7.5696
7.5514
7.5480
7.3945
7.3895
7.3701
7.3571
7.3494
7.3316
7.2564
7.2379
6.1413
2.7406
2.0551
1.6943
f1 (ppm)



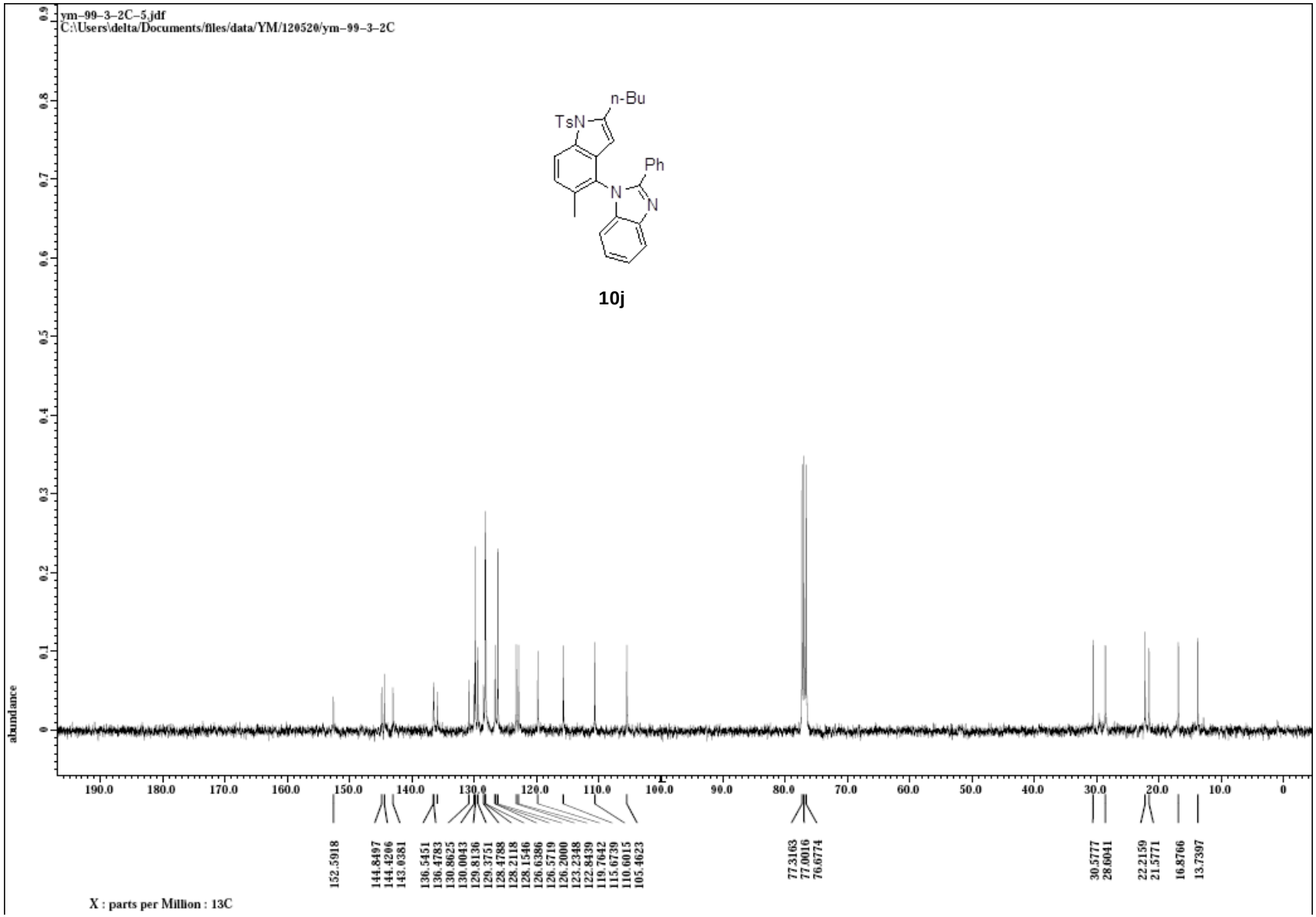

**10c**

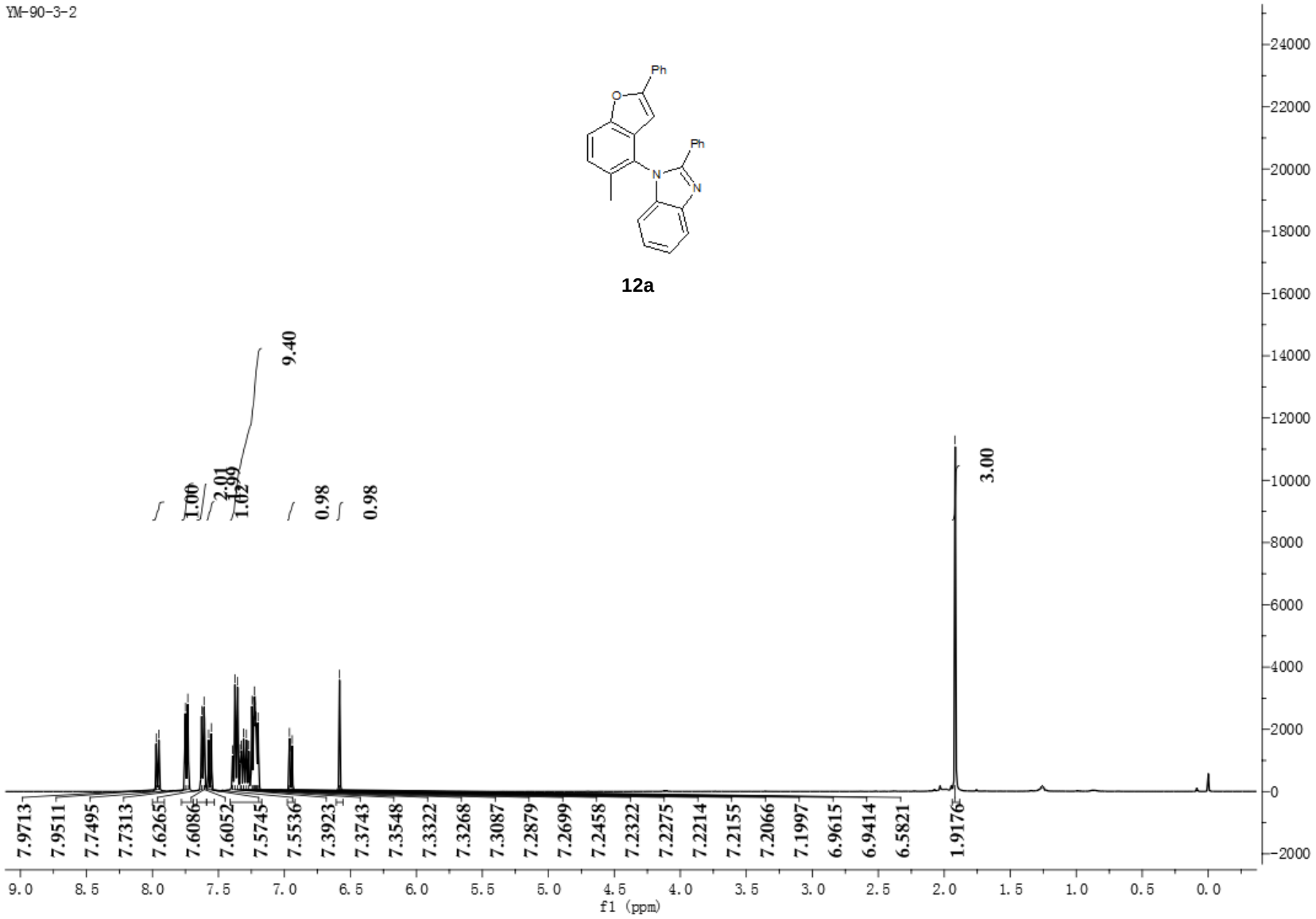

ym-99-5-2
TsN
Ph
N
N
10g
8.22
7.38
2.20
1.08
0.96
1.00
0.94
6.05
3.00
8.3188
7.8657
7.3935
7.3748
7.2727
7.2515
7.1652
7.1473
7.1088
7.0901
6.6828
6.0083
2.3738
1.8862
f1 (ppm)

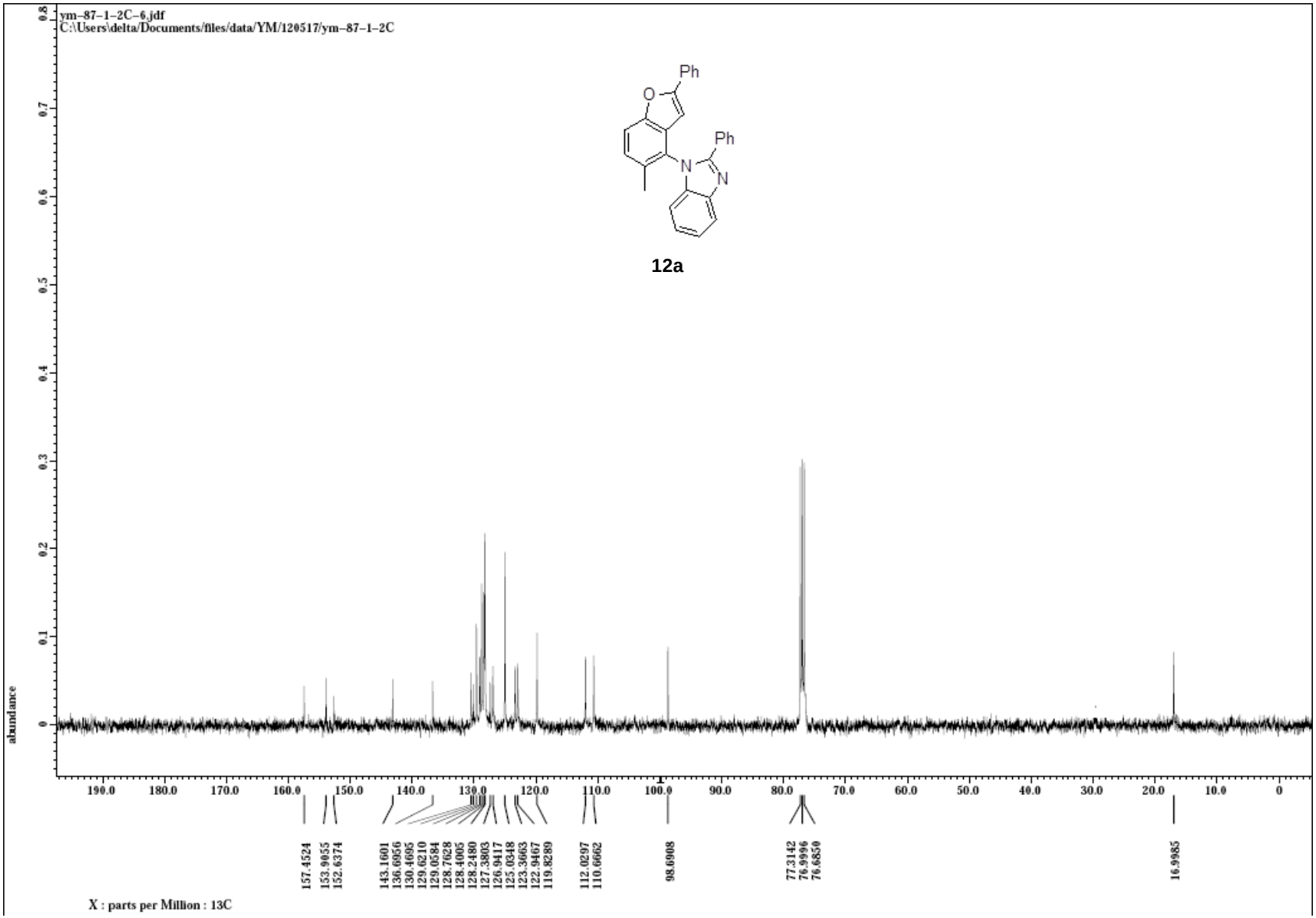


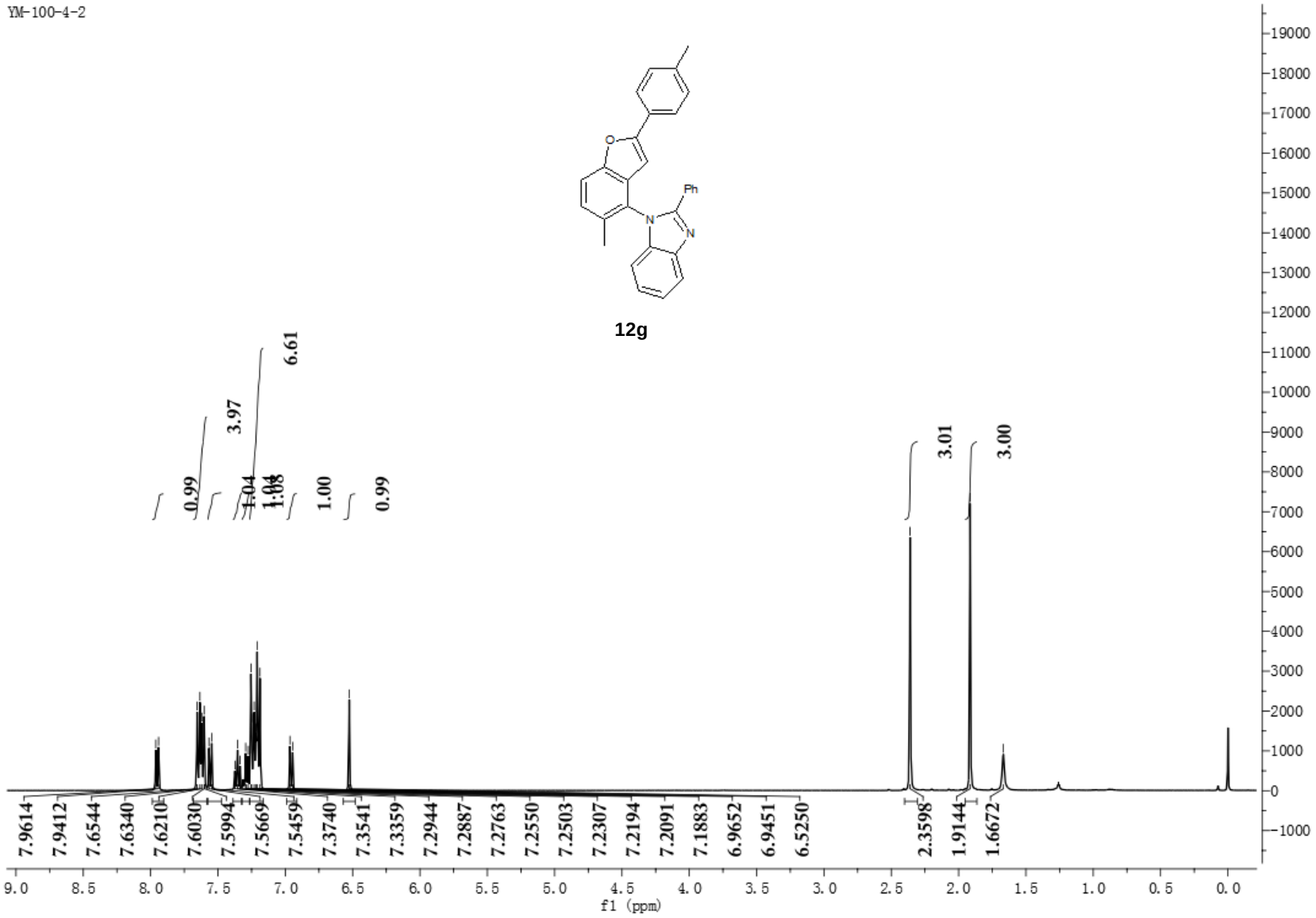


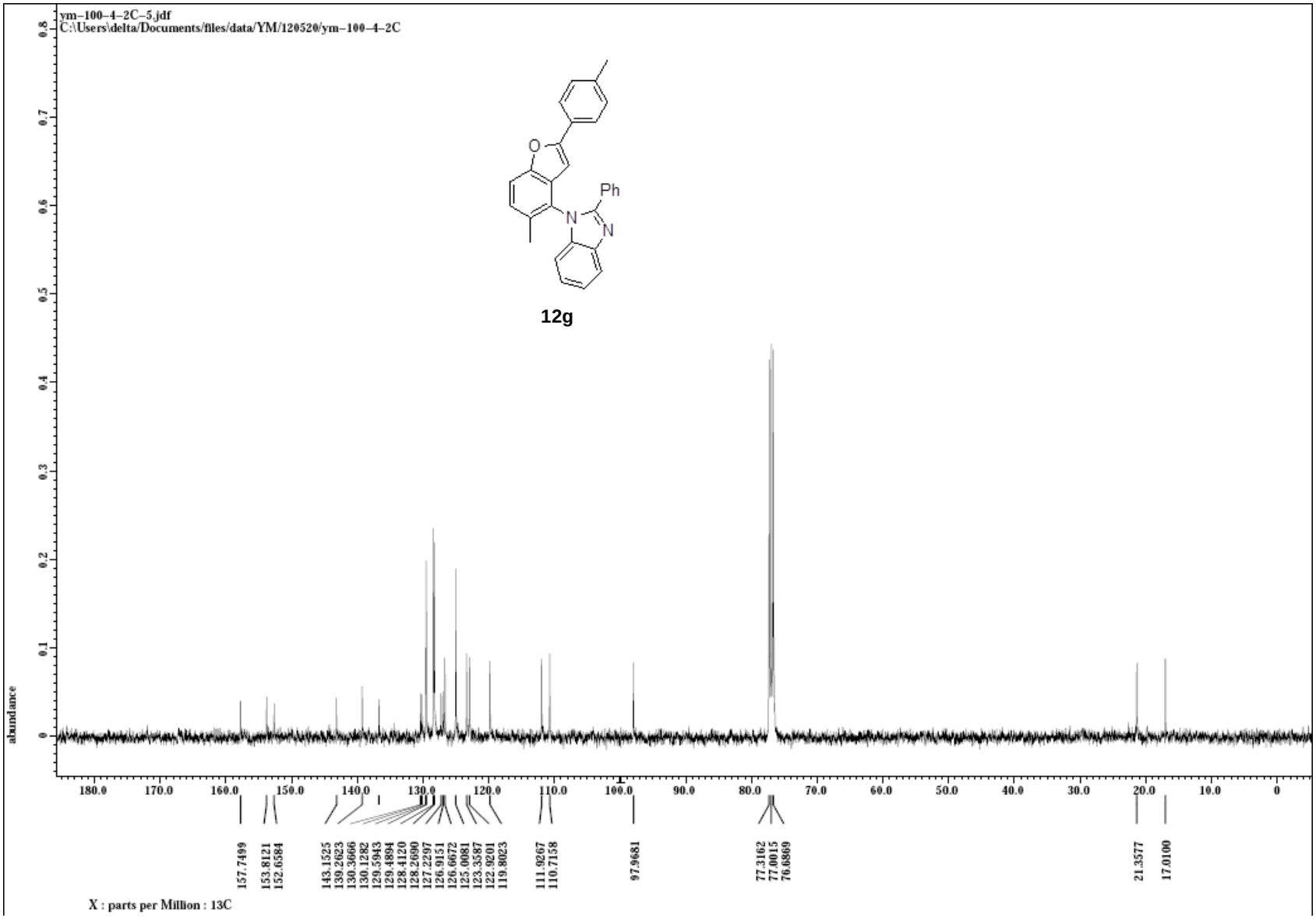

**10j**

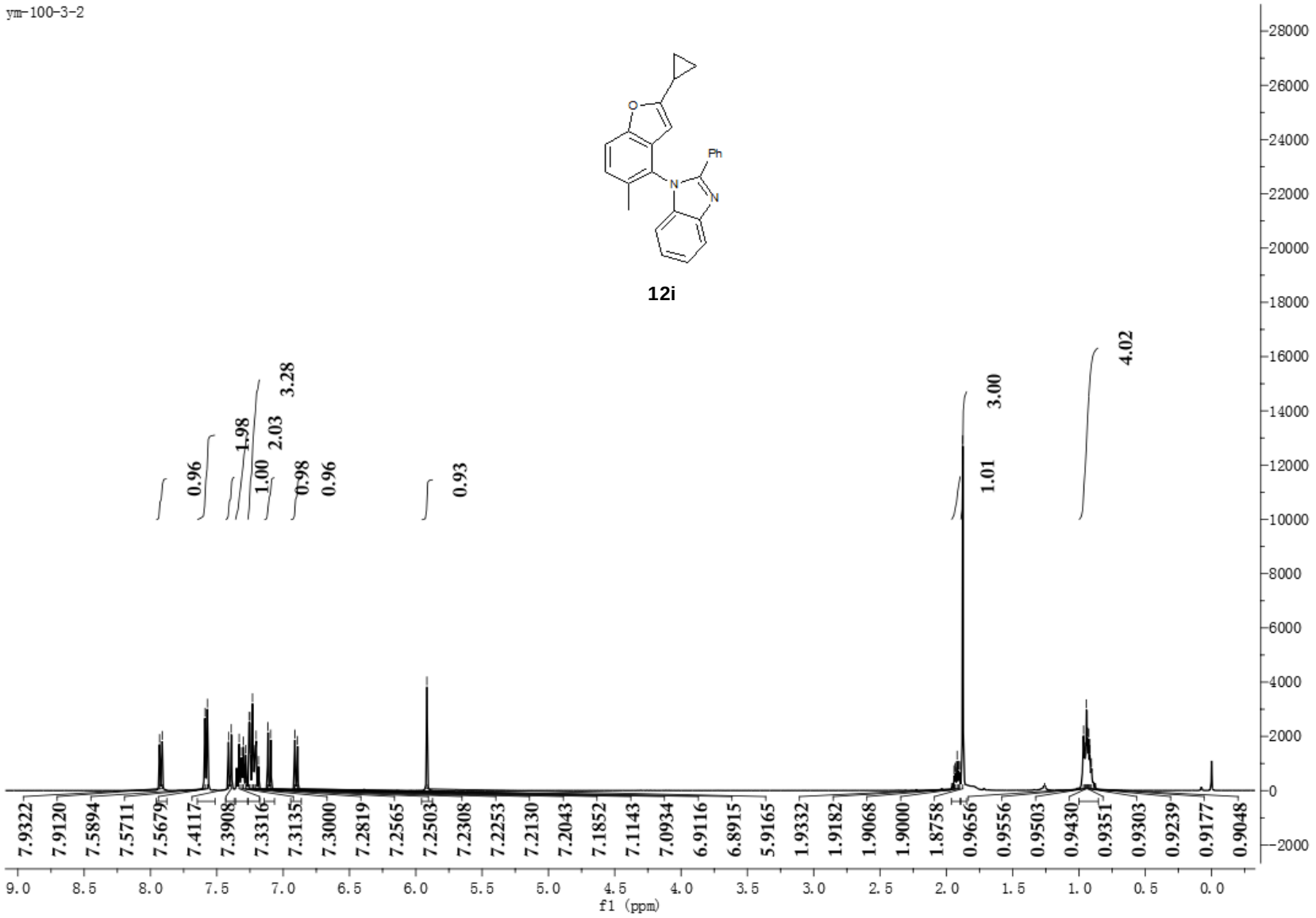

ym-99-3-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120520/ym-99-3-2C
n-Bu
TsN
Ph
N
N
10j
abundance
X : parts per Million : 13C
152.5918
144.8497
144.4206
143.0381
136.5451
136.4783
130.8625
130.0043
129.8136
129.3751
128.4788
128.2118
128.1546
126.6386
126.5719
126.2000
123.2348
122.8439
119.7642
115.6739
110.6015
105.4623
77.3163
77.0016
76.6774
30.5777
28.6041
22.2159
21.5771
16.8766
13.7397

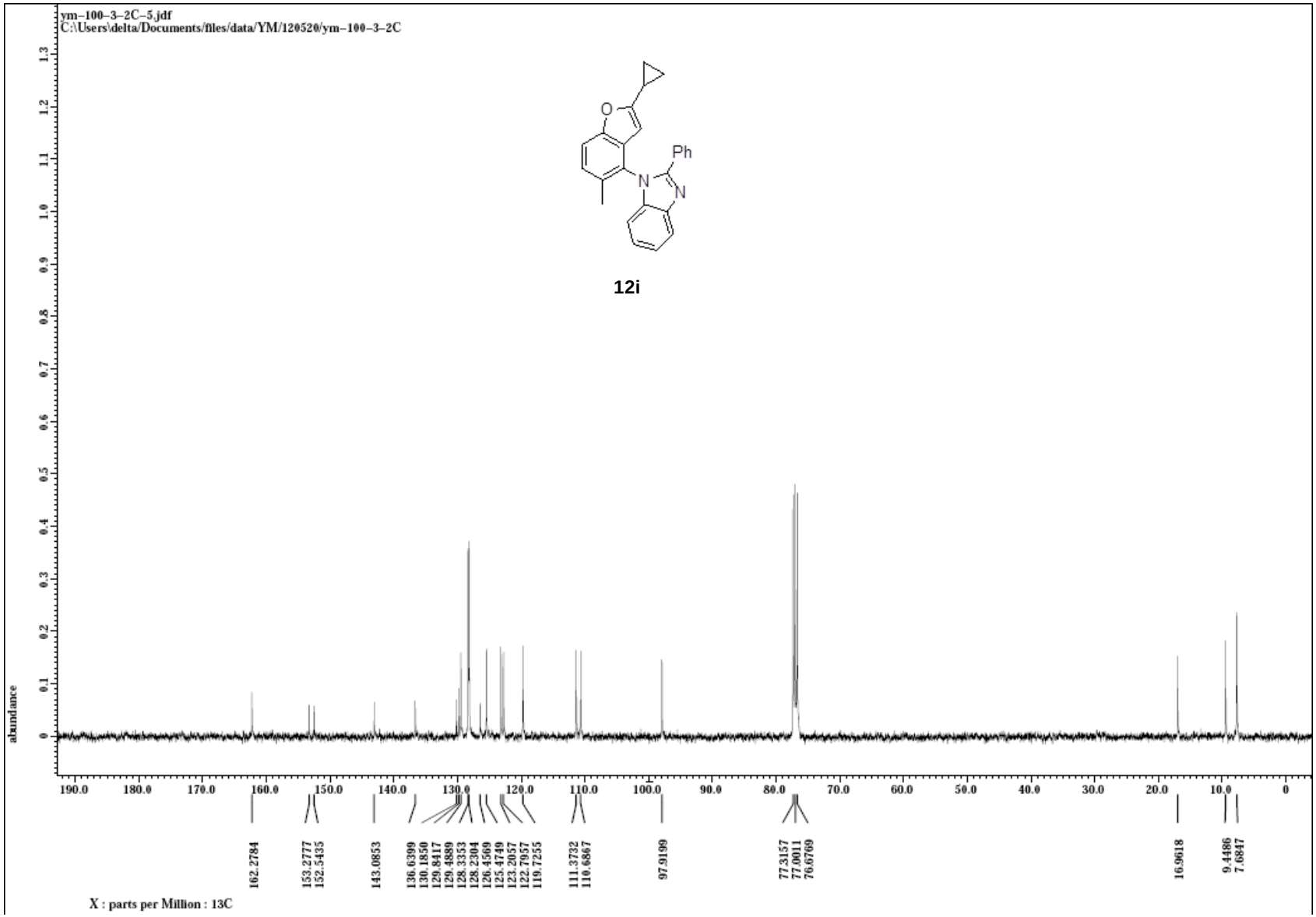

YM-90-3-2
Ph
O
Ph
N
N
12a
9.40
3.00
1.00
2.01
1.99
1.02
0.98
0.98
7.9713
7.9511
7.7495
7.7313
7.6265
7.6086
7.6052
7.5745
7.5536
7.3923
7.3743
7.3548
7.3322
7.3268
7.3087
7.2879
7.2699
7.2458
7.2322
7.2275
7.2214
7.2155
7.2066
7.1997
6.9615
6.9414
6.5821
1.9176
f1 (ppm)

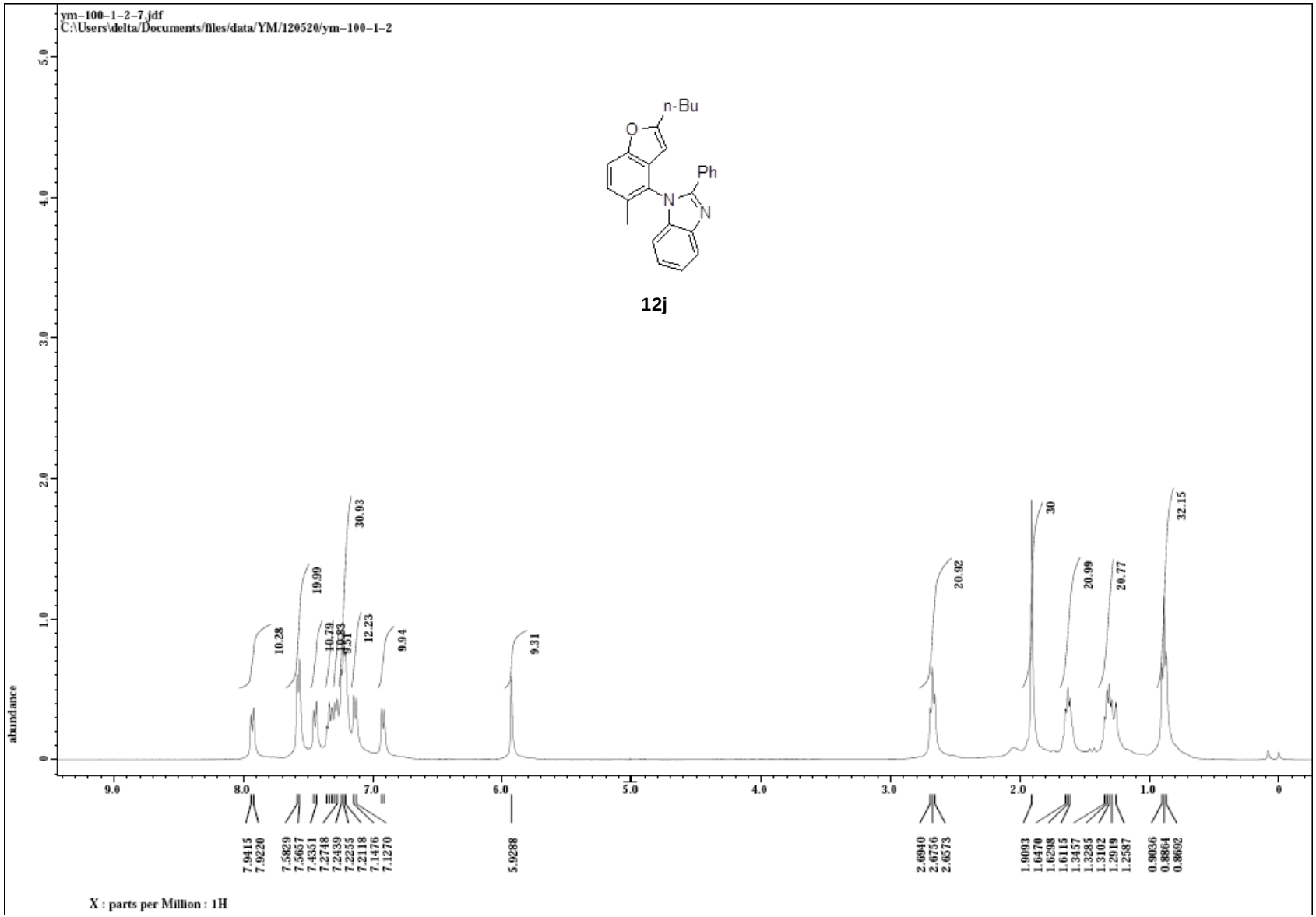


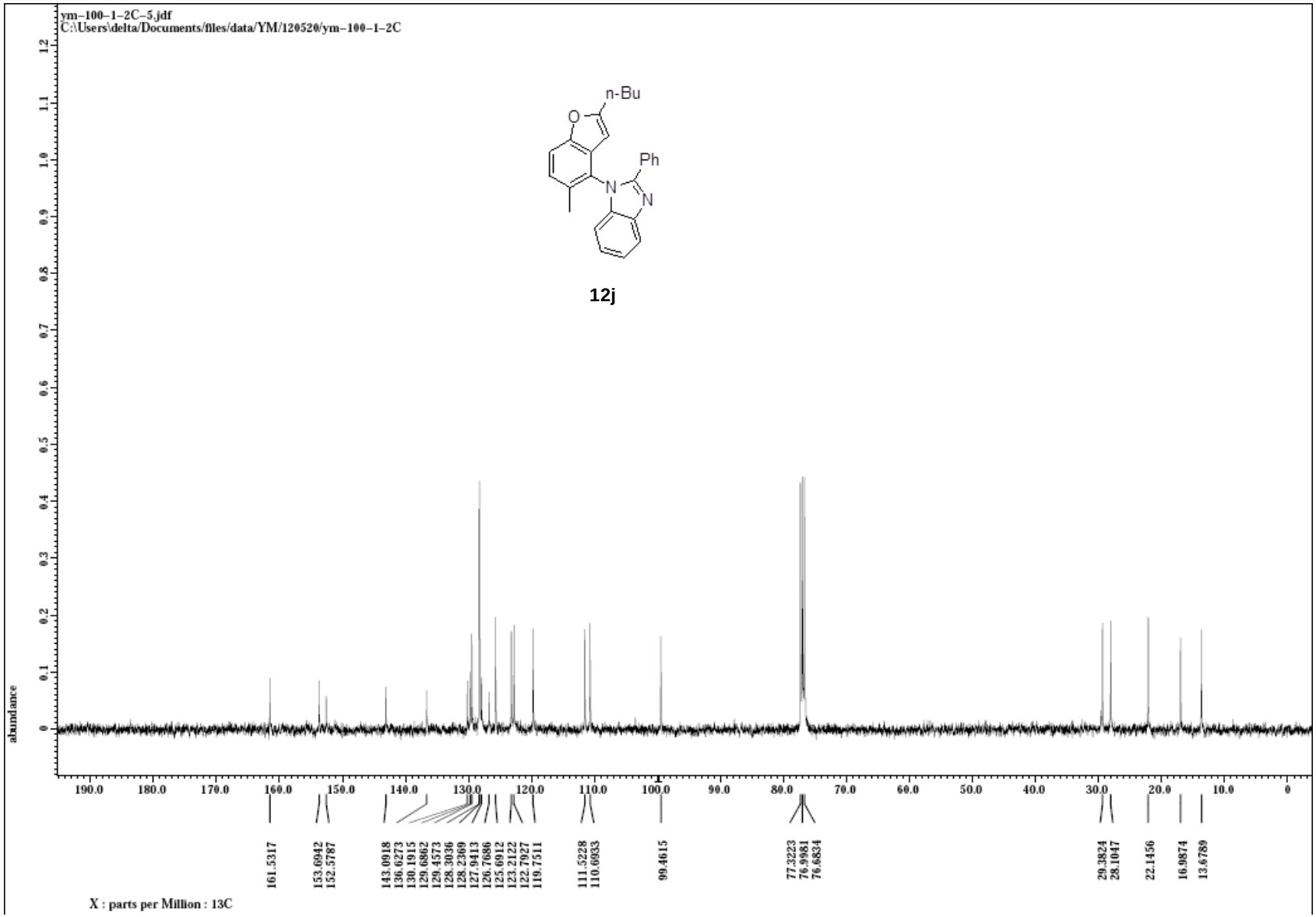

YM-100-4-2
Ph
N
N
O
12g
0.99
3.97
1.04
1.08
6.61
1.00
0.99
3.01
3.00
7.9614
7.9412
7.6544
7.6340
7.6210
7.6030
7.5994
7.5669
7.5459
7.3740
7.3541
7.3359
7.2944
7.2887
7.2763
7.2550
7.2503
7.2307
7.2194
7.2091
7.1883
6.9652
6.9451
6.5250
2.3598
1.9144
1.6672
f1 (ppm)

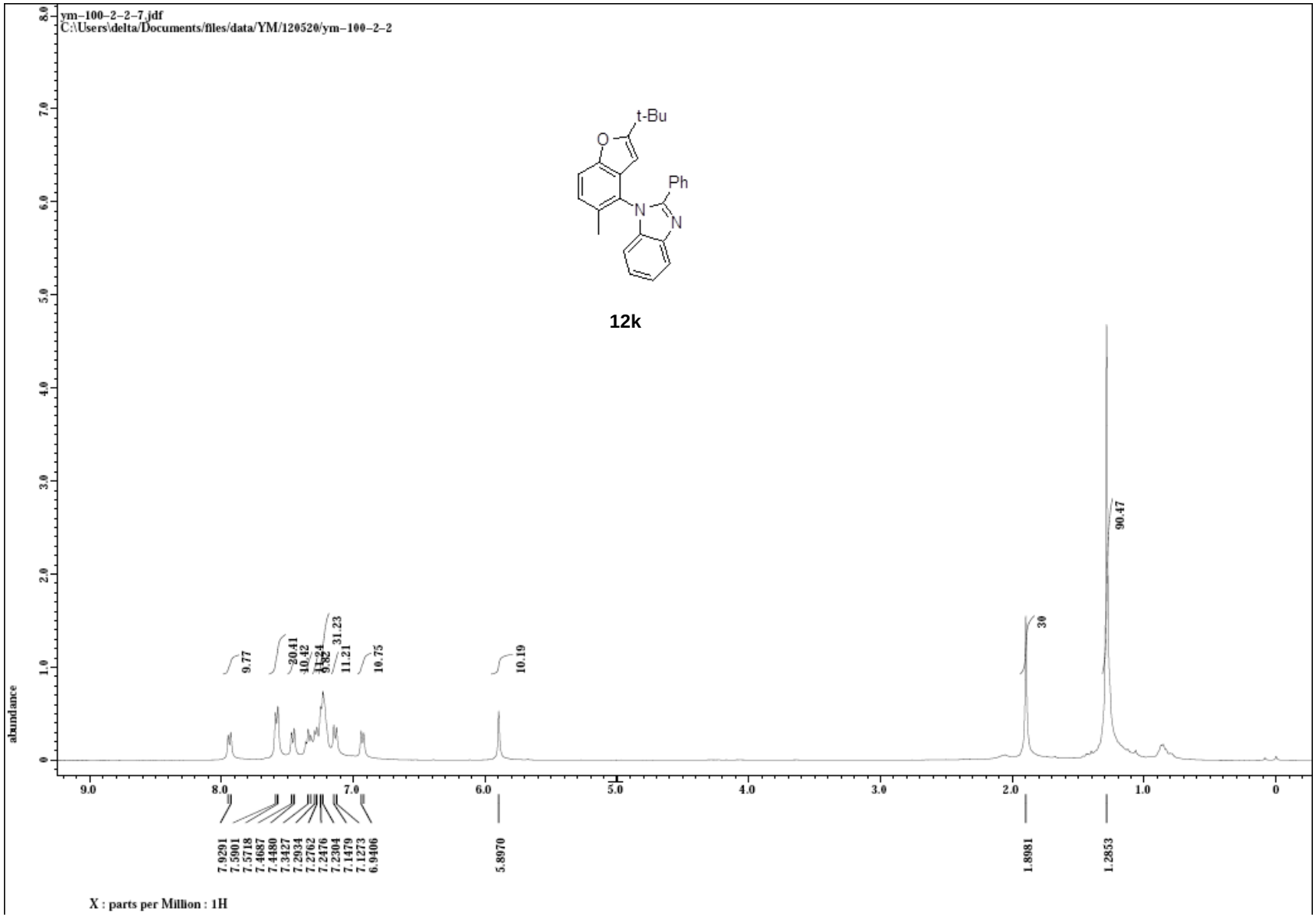


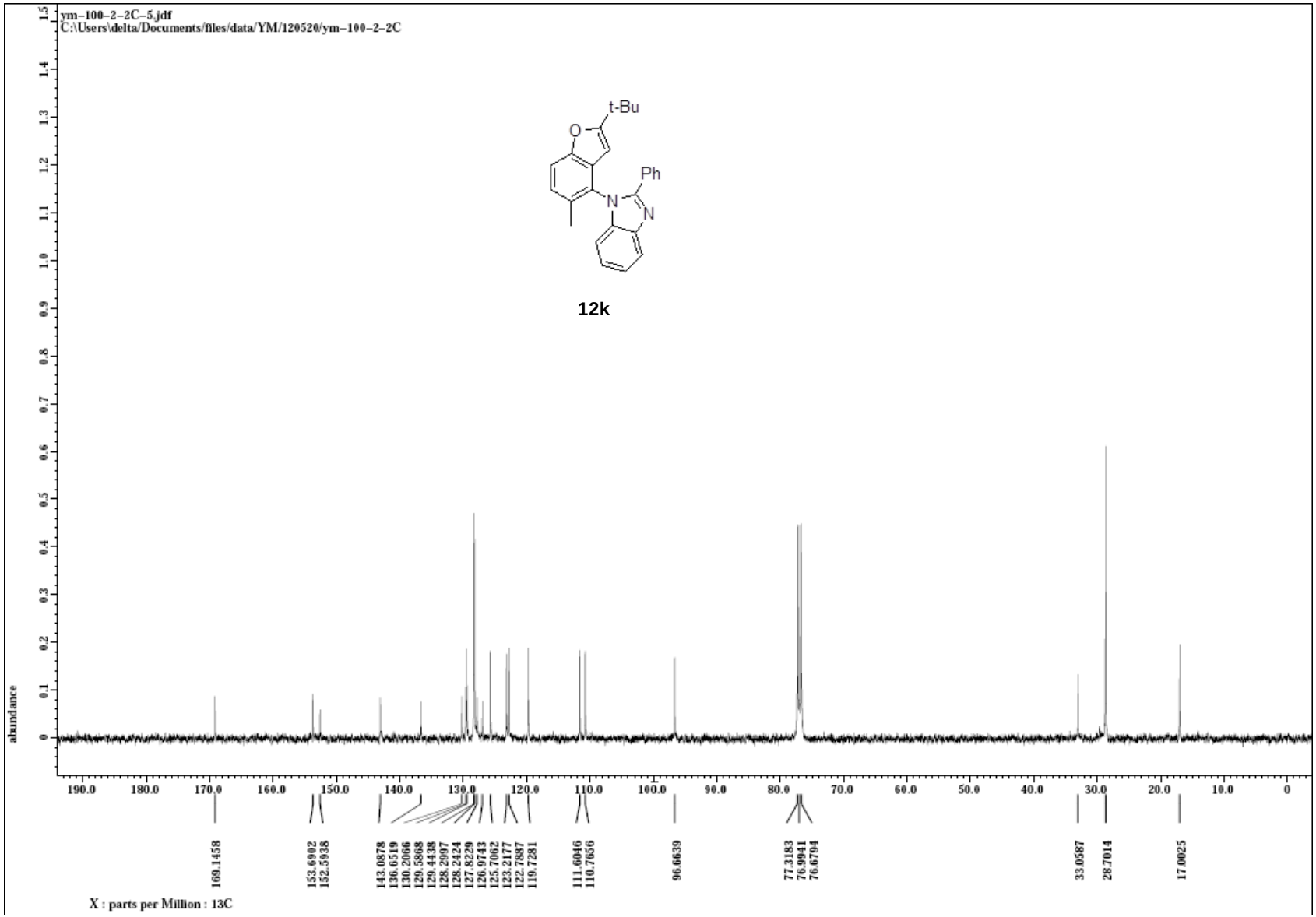

ym-100-3-2
O
Ph
N
N
12i
0.96
1.98
2.03
3.28
1.00
0.98
0.96
0.93
1.01
3.00
4.02
7.9322
7.9120
7.5894
7.5711
7.5679
7.4117
7.3908
7.3316
7.3135
7.3000
7.2819
7.2565
7.2503
7.2308
7.2253
7.2130
7.2043
7.1852
7.1143
7.0934
6.9116
6.8915
5.9165
1.9332
1.9182
1.9068
1.9000
1.8758
0.9656
0.9556
0.9503
0.9430
0.9351
0.9303
0.9239
0.9177
0.9048
f1 (ppm)


ym-100-3-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120520/ym-100-3-2C
O
Ph
N
N
12i
abundance
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
162.2784
153.2777
152.5435
143.0853
136.6399
130.1850
129.8417
129.4889
128.3353
128.2304
126.4569
125.4749
123.2057
122.7957
119.7255
111.3732
110.6867
97.9199
77.3157
77.0011
76.6769
16.9618
9.4486
7.6847
X : parts per Million : 13C




ym-100-1-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120520/ym-100-1-2C
n-Bu
O
Ph
N
N
12j
abundance
161.5317
153.6942
152.5787
143.0918
136.6273
130.1915
129.6862
129.4573
128.3036
128.2369
127.9413
126.7686
125.6912
123.2122
122.7927
119.7511
111.5228
110.6933
99.4615
77.3223
76.9981
76.6834
29.3824
28.1047
22.1456
16.9874
13.6789
X : parts per Million : 13C




ym-100-2-2C-5.jdf
C:\Users\delta/Documents/files/data/YM/120520/ym-100-2-2C
t-Bu
O
Ph
N
N
12k
abundance
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.1458
153.6902
152.5938
143.0878
136.6519
130.2066
129.5868
129.4438
128.2997
128.2424
127.8229
126.9743
125.7062
123.2177
122.7887
119.7281
111.6046
110.7656
96.6639
77.3183
76.9941
76.6794
33.0587
28.7014
17.0025
X : parts per Million : 13C