Oxidative Nucleophilic Cyclization of 2-Alkynylanilines with Thiophenols under Metal-Free Conditions

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Supporting Information

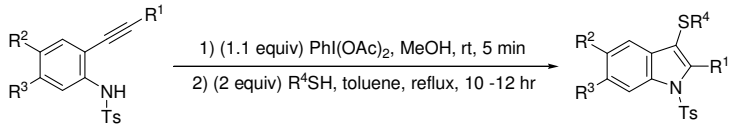
1. General experimental methods (S1)
2. General experimental procedure and characterization data. (S2-S9)
3. X-ray diffraction structure of compound **3** (S9)
4. Computational details and references (S10-S42)
5. Copies of ^{1}H, ^{13}C NMR spectra of products (S43-S86)

General experimental methods:

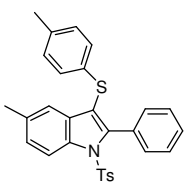
All reactions were performed in Schlenk tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated 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

Oxidative Nucleophilic Cyclization of 2-Alkynylanilines with Thiophenols

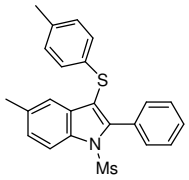


$PhI(OAc)_2$ (0.22 mmol) was added into the solution of 2-alkynylaniline (0.2 mmol) in MeOH (2 mL) at room temperature. After 5 minutes, MeOH was removed under a pressure-reducing condition. The crude product was mixed with toluene (2 mL) and thiophenol (0.4 mmol). The resulting mixture was stirred at reflux. 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 corresponding product.

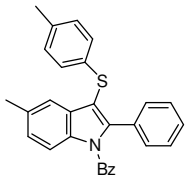


5-Methyl-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **3**: yellow solid; m.p. 126-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.4 Hz, 1 H), 7.43-7.33 (m, 5 H), 7.29 (d, J = 8.3 Hz, 2 H), 7.24-7.20 (m, 2 H), 7.08 (d, J

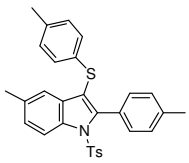
= 8.1 Hz, 2 H), 6.85 (d, *J* = 8.0 Hz, 2 H), 6.69 (d, *J* = 8.1 Hz, 2 H), 2.35 (s, 3 H), 2.34 (s, 3 H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 144.7, 135.7, 135.0, 134.8, 134.5, 133.2, 131.6, 131.4, 130.2, 129.5, 129.3, 129.1, 127.1, 126.9, 126.5, 120.0, 116.2, 113.8, 21.6, 21.3, 20.8; HRMS m/z calcd for $C_{29}H_{25}NO_2S_2$ ($[M+H]^+$): 484.1399, found 484.1392.



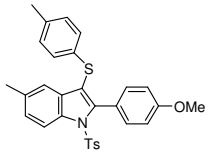
5-Methyl-1-(methylsulfonyl)-2-phenyl-3-(*p*-tolylthio)-1*H*-indole **6**: yellow solid; m.p. 166-167 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.5 Hz, 1 H), 7.45-7.41 (m, 5 H), 7.34 (s, 1 H), 7.22 (d, *J* = 8.6 Hz, 1 H), 6.95 (dd, *J* = 14.8 Hz, 8.3Hz, 4 H), 2.84 (s, 3 H), 2.40 (s, 3 H), 2.24 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 135.5, 135.0, 134.6, 132.8, 131.1, 131.0, 130.1, 129.6, 129.3, 128.8, 127.5, 127.3, 127.2, 120.3, 115.0, 113.6, 40.5, 21.3, 20.9; HRMS m/z calcd for $C_{23}H_{21}NO_2S_2$ ($[M+H]^+$): 408.1086, found 408.1084.



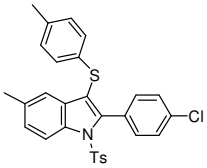
(5-Methyl-2-phenyl-3-(*p*-tolylthio)-1*H*-indol-1-yl)(phenyl)methanone **7**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58-7.54 (m, 3 H), 7.41-7.36 (m, 2 H), 7.30-7.22 (m, 5 H), 7.15-7.11 (m, 4 H), 7.01 (s, 3 H), 2.40 (s, 3 H), 2.26 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 144.4, 135.6, 135.0, 134.8, 134.1, 133.5, 133.3, 132.8, 131.2, 130.6, 130.4, 130.2, 130.1, 129.7, 128.3, 128.2, 127.8, 126.5, 119.9, 113.6, 21.4, 20.9; HRMS m/z calcd for $C_{29}H_{23}NOS$ ($[M+H]^+$): 434.1573, found 434.1584.



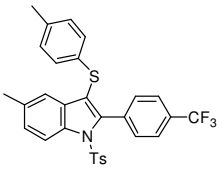
5-Methyl-2-(p-tolyl)-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **9**: yellow solid; m.p. 145-146°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, *J* = 8.4 Hz, 1 H), 7.31-7.18 (m, 8 H), 7.07 (d, *J* = 8.1 Hz, 2 H), 6.85 (d, *J* = 8.0 Hz, 2 H), 6.68 (d, *J* = 8.1Hz, 2 H), 2.40 (s, 3 H), 2.33 (s, 6 H), 2.22 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.7, 139.1, 135.6, 134.8, 134.7, 134.4, 133.4, 131.7, 131.2, 129.5, 129.3, 127.9, 127.2, 127.0, 126.8, 126.3, 119.9, 116.2, 113.5, 21.5, 21.2, 20.8; HRMS m/z calcd for $C_{30}H_{27}NO_2S_2$ ($[M+H]^+$): 498.1556, found4 98.1569.



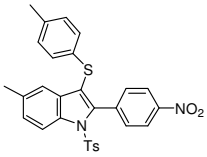
2-(4-Methoxyphenyl)-5-methyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **10**: yellow solid; m.p. 173-174°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.4 Hz, 1 H), 7.28 (dd, J = 8.5, 2.0 Hz, 4 H), 7.10 (d, J = 10.0 Hz, 2 H), 7.08 (d, J = 8.1 Hz, 2 H), 6.92-6.86 (m, 4 H), 6.67 (d, J = 8.2 Hz, 2 H), 3.84 (s, 3 H), 2.35 (s, 3 H), 2.34 (s, 3H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.2, 145.3, 144.7, 135.6, 134.8, 134.5, 133.4, 132.8, 131.8, 129.5, 129.3, 127.0, 126.8, 126.3, 122.3, 119.8, 116.3, 113.2, 112.9, 112.6, 55.2, 21.6, 21.3, 20.8; HRMS m/z calcd for $C_{30}H_{27}NO_3S_2$ ([M+H]$^+$): 514.1505, found 514.1522.



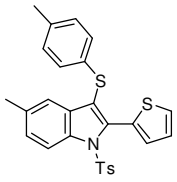
2-(4-Chlorophenyl)-5-methyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **11**: yellow solid; m.p. 147-148°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 8.5 Hz, 1 H), 7.35 (d, J = 8.5 Hz, 2 H), 7.28 (dd, J = 8.3, 1.4 Hz, 4 H), 7.23-7.20 (m, 2 H), 7.09 (d, J = 8.2 Hz, 2 H), 6.87 (d, J = 8.1 Hz, 2 H), 6.66 (d, J = 8.2 Hz, 2 H), 2.35 (s, 3 H), 2.34 (s, 3 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 143.8, 135.7, 135.3, 135.2, 134.7, 134.6, 132.9, 132.6, 131.6, 129.6, 129.4, 128.6, 127.5, 127.4, 126.8, 126.4, 120.0, 116.2, 114.4, 21.6, 21.3, 20.8; HRMS m/z calcd for $C_{29}H_{24}ClNO_2S_2$ ([M+Na]$^+$): 540.0829, found 540.0826.



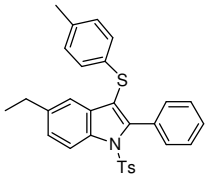
5-Methyl-3-(*p*-tolylthio)-1-tosyl-2-(4-(trifluoromethyl)phenyl)-1*H*-indole **12**: yellow solid; m.p. 187-188 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.24 (d, J = 8.5 Hz, 1 H), 7.63 (d, J = 8.1 Hz, 2 H), 7.48 (d, J = 8.0 Hz, 2 H), 7.29-7.22 (m, 4 H), 7.10 (d, J = 8.1 Hz, 2 H), 6.88 (d, J = 8.0 Hz, 2 H), 6.67 (d, J = 8.2 Hz, 2 H), 2.36 (s, 3 H), 2.35 (s, 3 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.1, 143.2, 135.8, 135.4, 134.8, 134.5, 134.0, 132.7, 131.7, 131.6, 130.9, 130.6, 130.3, 129.6, 129.5, 127.7, 126.8, 126.6, 124.5, 124.1, 120.2, 116.3, 115.3, 21.6, 21.3, 20.8; HRMS m/z calcd for $C_{30}H_{24}F_3NO_2S_2$ ([M+H]$^+$): 552.1273, found 552.1265.



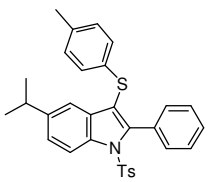
5-Methyl-2-(4-nitrophenyl)-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **13**: yellow solid; m.p. 178-179 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.22 (m, 2 H), 7.56 (d, J = 8.5 Hz, 2 H), 7.29-7.22 (m, 4 H), 7.12 (d, J = 8.0 Hz, 2 H), 6.88 (d, J = 7.8 Hz ,2 H), 6.65 (d, J = 7.9 Hz, 2 H), 2.37 (s, 6 H), 2.24(s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.8, 145.3, 142.2, 137.0, 136.0, 135.6, 135.1, 134.2, 132.4, 132.2, 131.6, 129.7, 129.6, 128.1, 126.7, 126.6, 123.9, 123.4, 120.4, 116.3, 21.6, 21.3, 20.9; HRMS m/z calcd for $C_{29}H_{24}N_2O_4S_2$ ($[M+H]^+$): 529.1250, found 529.1259.



5-Methyl-2-(thiophen-2-yl)-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **14**: yellow solid; m.p. 143-144 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 9.0 Hz, 1 H), 7.47 (d, J = 5.0 Hz, 1 H), 7.35 (d, J = 8.3 Hz, 2 H), 7.24-7.21 (m, 2 H), 7.15 (d, J = 2.6 Hz, 1 H), 7.10-7.08 (m, 3 H), 6.89 (d, J = 8.0 Hz ,2 H), 6.74 (d, J = 8.1 Hz, 2 H), 2.35 (s, 3 H), 2.34 (s, 3 H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.8, 137.7, 135.8, 135.2, 134.8, 134.5, 133.0, 132.1, 131.3, 129.8, 129.5, 129.4, 128.6, 127.5, 126.9, 126.8, 126.3, 120.0, 116.2, 115.8, 21.6, 21.3, 20.9; HRMS m/z calcd for $C_{27}H_{23}NO_2S_3$ ($[M+H]^+$): 490.0964, found 490.0962.

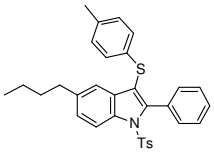


5-Ethyl-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **17**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.5 Hz, 1 H), 7.45-7.29 (m, 7 H), 7.25-7.21 (m, 2 H), 7.08 (d, J = 8.1 Hz, 2 H), 6.87 (d, J = 8.1 Hz, 2 H), 6.71 (d, J = 8.2 Hz, 2 H), 2.65 (q, J = 7.6 Hz, 2 H), 2.34 (s, 3 H), 2.23 (s, 3 H), 1.18 (t, J = 7.6 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 144.7, 141.0, 135.7, 135.0, 134.9, 133.3, 131.4, 130.2 129.5, 129.3, 129.1, 127.1, 126.9, 126.7, 126.0, 118.8, 116.2, 114.0, 28.6, 21.6, 20.8, 15.8; HRMS m/z calcd for $C_{30}H_{27}NO_2S_2$ ($[M+Na]^+$): 520.1375, found 520.1378.

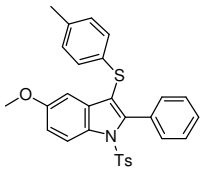


5-Isopropyl-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **18**: yellow solid; m.p. 130-131°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, J = 8.6 Hz, 1 H), 7.42-7.35 (m, 3 H), 7.33-7.27 (m, 5 H), 7.22 (s, 1 H), 7.08 (d, J = 8.1 Hz, 2

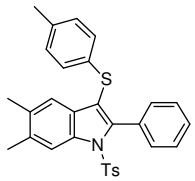
H), 6.87 (d, J = 8.0 Hz, 2 H), 6.74 (d, J = 8.2 Hz, 2 H), 2.95-2.88 (m, 1 H), 2.33 (s, 3 H), 2.22 (s, 3 H), 1.20 (s, 3 H), 1.18 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.7, 144.5, 135.7, 135.1, 135.0, 133.0, 131.5, 131.2, 130.3, 129.4, 129.3, 129.0, 127.1, 127.0, 126.9, 124.6, 117.4, 116.1, 114.2, 33.8, 24.1, 21.5, 20.8; HRMS m/z calcd for $C_{31}H_{29}NO_2S_2$ ([M+Na]$^+$): 534.1537, found 534.1541.



5-Butyl-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **19**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.6 Hz, 1 H), 7.43-7.33 (m, 5 H), 7.29 (d, J = 8.4 Hz, 2 H), 7.23-7.21 (m, 1 H), 7.16 (s, 1 H), 7.07 (d, J = 8.1 Hz, 2 H), 6.87 (d, J = 8.0 Hz, 2 H), 6.72 (d, J = 8.2 Hz, 2 H), 2.60 (t, J = 7.6 Hz, 2 H), 2.33 (s, 3 H), 2.22 (s, 3 H), 1.56-1.48 (m, 2 H), 1.29-1.22 (m, 2 H), 0.85 (t, J = 7.4 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 139.5, 135.7, 135.0, 134.9, 133.0, 131.4, 131.3, 130.3, 129.4, 129.3, 129.1, 127.1, 126.9, 126.8, 126.5, 119.4, 116.2, 114.1, 35.3, 33.7, 22.1, 21.5, 20.8, 13.9; HRMS m/z calcd for $C_{32}H_{31}NO_2S_2$ ([M+Na]$^+$): 548.1688, found 548.1683.

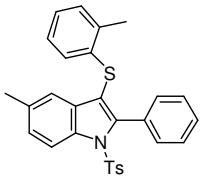


5-Methoxy-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **20**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 9.1 Hz, 1 H), 7.44-7.35 (m, 5 H), 7.27 (d, J = 8.3 Hz, 2 H), 7.08 (d, J = 8.1 Hz, 2 H), 6.99 (dd, J = 9.1, 2.6 Hz, 1 H), 6.87 (d, J = 8.0 Hz, 2 H), 6.81 (d, J = 2.5 Hz, 1 H), 6.70 (d, J = 8.2 Hz, 2 H), 3.71 (s, 3 H), 2.35 (s, 3 H), 2.23 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 145.6, 144.8, 135.2, 134.6, 132.9, 132.8, 131.8, 131.4, 130.2, 129.5, 129.3, 129.2, 127.1, 126.9, 126.8, 117.6, 114.6, 114.4, 102.3, 55.5, 21.6, 20.8; HRMS m/z calcd for $C_{29}H_{25}NO_3S_2$ ([M+H]$^+$): 500.1349, found 500.1354.

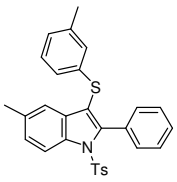


5,6-Dimethyl-2-phenyl-3-(*p*-tolylthio)-1-tosyl-1*H*-indole **21**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (s, 1 H), 7.42-7.31 (m, 5 H), 7.28 (d, J = 8.3 Hz, 2 H), 7.15 (s, 1 H), 7.08 (d, J = 8.1 Hz, 2 H), 6.86 (d, J = 8.0 Hz, 2 H), 6.69 (d, J = 8.2 Hz, 2 H), 2.42 (s, 3 H), 2.34 (s, 3 H), 2.24 (s, 3 H), 2.22

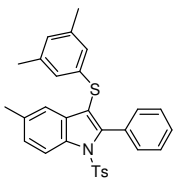
(s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 144.1, 136.2, 135.0, 134.9, 133.7, 133.4, 131.4, 130.3, 130.2, 129.5, 129.4, 129.3, 129.0, 127.1, 126.8, 126.5, 120.3, 117.0, 113.7, 21.6, 20.8, 20.7, 19.9; HRMS m/z calcd for $C_{30}H_{27}NO_2S_2$ ([M+Na]$^+$): 520.1375, found 520.1388.



5-Methyl-2-phenyl-3-(*o*-tolylthio)-1-tosyl-1*H*-indole **23**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.5 Hz, 1 H), 7.42-7.32 (m, 5 H), 7.29 (d, *J* = 8.3 Hz, 2 H), 7.22 (d, *J* = 9.1 Hz, 1 H), 7.12-7.06 (m, 4 H), 6.96 (t, *J* = 7.2 Hz, 1 H), 6.75 (t, *J* = 7.5 Hz ,1 H), 6.27 (d, *J* = 7.8 Hz,1 H), 2.34 (s, 6 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.8, 136.2, 135.8, 135.1, 134.7, 134.6, 131.7, 131.3, 130.2, 129.9, 129.3, 129.1, 127.2, 127.1, 126.9, 126.1, 125.4, 124.9, 119.9, 116.3, 113.3, 21.6, 21.3, 19.9; HRMS m/z calcd for $C_{29}H_{25}NO_2S_2$ ([M+H]$^+$): 484.1399, found 484.1392.

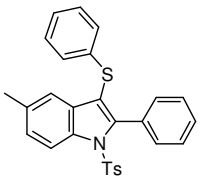


5-Methyl-2-phenyl-3-(*m*-tolylthio)-1-tosyl-1*H*-indole **24**: yellow solid; m.p. 143-144°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25(d, *J* = 8.6 Hz, 1 H), 7.44-7.33 (m, 5 H), 7.31 (d, *J* = 8.3 Hz, 2 H), 7.24-7.22 (m, 2 H), 7.09 (d, *J* = 8.1 Hz, 2 H), 6.92 (t, *J* = 7.6 Hz, 1 H), 6.84 (d, *J* = 7.5 Hz, 1 H), 6.72 (s, 1H), 6.50 (d, *J* = 7.8 Hz ,1 H), 2.36 (s, 3 H), 2.32 (s, 3 H), 2.16 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.3, 144.8, 138.5, 136.7, 135.6, 134.9, 134.5, 131.6, 131.4, 130.2, 129.3, 129.1, 128.6, 127.1, 126.9, 126.0, 123.2, 120.0, 116.1, 113.3, 21.6, 21.3; HRMS m/z calcd for $C_{29}H_{25}NO_2S_2$ ([M+H]$^+$): 484.1399, found484.1391.

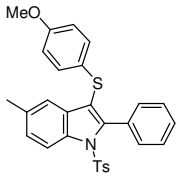


3-((3,5-Dimethylphenyl)thio)-5-methyl-2-phenyl-1-tosyl-1*H*-indole **25**: yellow solid; m.p. 155-156°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 9.1 Hz,1 H), 7.42-7.31 (m, 7 H), 7.22 (d, *J* = 7.3 Hz, 2 H), 7.08 (d, *J* = 8.1 Hz, 2 H), 6.66 (s, 1 H), 6.45 (s, 2 H), 2.36 (s, 3 H), 2.30 (s, 3 H), 2.10 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.2, 144.7, 138.3, 136.5, 135.5, 135.0, 134.4, 131.6, 131.4, 130.2, 129.4, 129.1, 127.4, 127.1, 126.9, 123.9, 120.0,

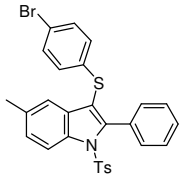
116.0, 113.2, 21.6, 21.3, 21.2; HRMS m/z calcd for $C_{30}H_{27}NO_2S_2$ ([M+Na]$^+$): 520.1375, found 520.1372.



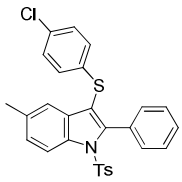
5-Methyl-2-phenyl-3-(phenylthio)-1-tosyl-1*H*-indole **26**: yellow solid; m.p. 169-170°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.5 Hz,1 H), 7.43-7.32 (m, 5 H), 7.30 (d, J = 8.4 Hz, 2 H), 7.23-7.19 (m, 2 H), 7.09-7.03 (m, 5 H), 6.79-6.77 (m, 2 H), 2.35 (s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.4, 144.8 137.0, 135.7, 134.8, 134.6, 131.5, 131.4, 130.1, 129.3, 129.2, 128.7, 127.2, 127.1, 126.9, 126.2, 125.1, 120.0, 116.2, 113.2, 21.6, 21.3; HRMS m/z calcd for $C_{28}H_{23}NO_2S_2$ ([M+Na]$^+$): 492.1062, found 492.1064.



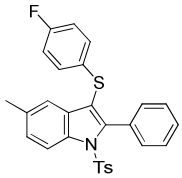
3-((4-Methoxyphenyl)thio)-5-methyl-2-phenyl-1-tosyl-1*H*-indole **27**: yellow solid; m.p. 120-121°C;^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, J = 9.1 Hz, 1 H), 7.46-7.34 (m, 5 H), 7.29 (d, J = 8.2 Hz, 2 H), 7.25-7.19 (m, 2 H), 7.08 (d, J = 8.0 Hz, 2 H), 6.79 (d, J = 8.7 Hz, 2 H), 6.62 (d, J = 8.7 Hz, 2 H), 3.71 (s, 3 H), 2.36 (s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 144.7, 144.5, 135.6, 134.9, 134.4, 131.5, 130.3, 129.3, 129.1, 129.0, 128.8, 127.1, 127.0, 126.9, 120.0, 116.1, 114.8, 114.5, 55.2, 21.6, 21.3; HRMS m/z calcd for $C_{29}H_{25}NO_3S_2$ ([M+Na]$^+$): 522.1168, found 522.1162.



3-((4-Bromophenyl)thio)-5-methyl-2-phenyl-1-tosyl-1H-indole **28**: yellow solid; m.p. 161-162°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.5 Hz, 1 H), 7.44-7.36 (m, 3 H), 7.31-7.28 (m, 4 H), 7.25-7.22 (m, 1 H), 7.17-7.14 (m, 3 H), 7.09 (d, J = 8.1 Hz, 2 H), 6.63 (d, J = 8.6 Hz, 2 H), 2.36 (s, 3 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 144.9, 136.4, 135.6, 134.8, 134.7, 131.7, 131.3, 131.1, 130.2, 129.9, 129.4, 129.3, 127.6, 127.4, 127.2, 126.9, 119.7, 118.7, 116.2, 112.5, 21.6, 21.3; HRMS m/z calcd for $C_{28}H_{22}BrNO_2S_2$ ([M+H]$^+$): 548.0348, found 548.0357.

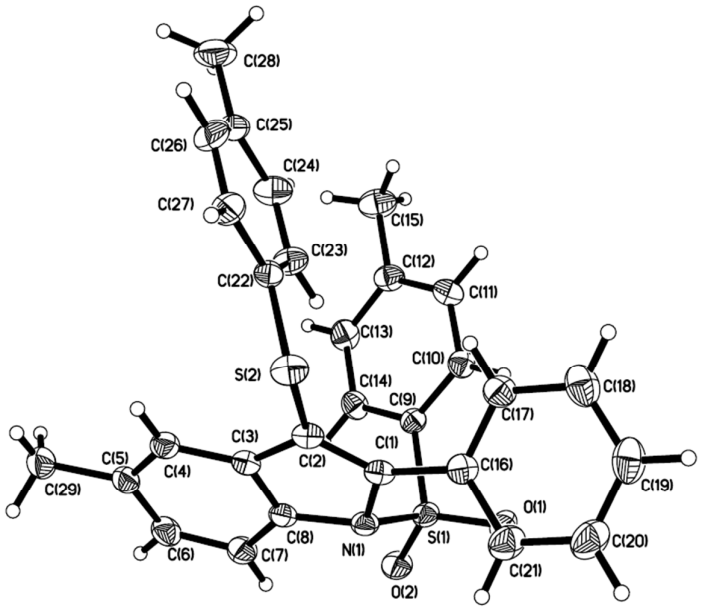


3-((4-Chlorophenyl)thio)-5-methyl-2-phenyl-1-tosyl-1*H*-indole **29**: yellow solid; m.p. 163-164°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (d, J = 8.6 Hz, 1 H), 7.46-7.36 (m, 3 H), 7.31-7.28 (m, 4 H), 7.25-7.22 (m, 1 H), 7.17 (s, 1 H), 7.09 (d, J = 8.2 Hz, 2 H), 7.01 (d, J = 8.6 Hz, 2 H), 6.70 (d, J = 8.6 Hz, 2 H), 2.37 (s, 3 H), 2.34 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 144.9, 135.6, 134.8, 134.7, 131.3, 131.1, 131.0, 130.2, 129.9, 129.4, 129.3, 128.8, 127.4, 127.2, 126.9, 119.7, 116.2, 112.7, 21.6, 21.3; HRMS m/z calcd for $C_{28}H_{22}ClNO_2S_2$ ([M+Na]$^+$): 526.0673, found 526.0662.



3-((4-Fluorophenyl)thio)-5-methyl-2-phenyl-1-tosyl-1*H*-indole **30**: yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 8.5 Hz,1 H), 7.46-7.37 (m, 3 H), 7.30 (t, J = 8.5 Hz, 4 H), 7.24-7.20 (m, 2 H), 7.08 (d, J = 8.1 Hz, 2 H), 6.77 (d, J = 6.8 Hz, 4 H), 2.37(s, 3 H), 2.33 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.2, 159.8, 145.1, 144.9, 135.6, 134.9, 134.6, 131.7, 131.4, 131.2, 130.1, 129.4, 129.2, 128.5, 128.4, 127.3, 127.2, 126.9, 119.8, 116.1, 115.9, 115.7, 113.7, 21.6, 21.3; HRMS m/z calcd for $C_{28}H_{22}FNO_2S_2$ ([M+H]$^+$): 488.1349, found 488.1130.

X-Ray diffraction structure of compound 3



Computational details

The B3LYP density functional theory calculations were performed with the Gaussian09 package using 6-31G(d) basis set[1, 2] B3LYP calculations utilize Becke's three parameter hybrid exchange functional together with the correlation functional of Lee, Yang and Parr. The NBO program in Gaussian 09, Version 5.9, was used to obtain more information about some special bonds.[3] The geometry optimizations were performed without symmetry constraints, and the nature of the extrema was checked by analytical frequency calculations. The intrinsic reaction coordinate (IRC)[4] pathways have been traced to verify two desired minima connected by the transition states.

Solvent effects including contributions of non electrostatic terms have been considered at B3LYP/6-31++G(d,p) level using using toluene as a solvent. Single point energies were calculated on the structures obtained in the gas-phase using a simple self-consistent reaction field (SCRF) method[5-7] based on the polarizable continuum model (PCM)[8-10] with UFF cavities.[11]

Table S1. Cartesian coordinates and absolute energies for DFT optimized structures.

PhSH -630.4341230 a.u.

6	0.201220	-1.210406	-0.000040
6	1.596883	-1.202759	-0.000001
6	2.300608	0.004896	0.000033
6	1.592258	1.209046	-0.000009
6	0.195552	1.211772	-0.000005
6	-0.508830	-0.000447	-0.000005
16	-2.294944	-0.083457	0.000027
1	-0.334813	-2.155269	-0.000089
1	2.133935	-2.146966	-0.000002
1	3.386186	0.007381	0.000074
1	2.125207	2.155694	-0.000038

1	-0.339689	2.157051	-0.000020
1	-2.517861	1.244802	-0.000187

AcOH -229.0817872 a.u.

C	0.09227000	0.12595500	0.00003000
O	0.64511800	1.20231000	-0.00000500
C	-1.39726800	-0.11028600	0.00000900
O	0.77895200	-1.04662200	0.00000300
H	-1.68425900	-0.69152600	-0.88247000
H	-1.91782900	0.84749100	0.00069100
H	-1.68415900	-0.69285200	0.88163000
H	1.72367200	-0.80262900	-0.00006900

MeOH -115.7144073 a.u.

6	0.046544	0.666944	0.000000
8	0.046544	-0.758304	0.000000
1	1.093388	0.977867	0.000000
1	-0.439733	1.080111	0.894525
1	-0.439733	1.080111	-0.894525
1	-0.865543	-1.073319	0.000000

A -1567.5421587 a.u.

C	-2.73077800	-1.78676200	-0.14488300
C	-4.02316300	-1.43084200	-0.20463100
C	-4.50252200	-0.00826500	-0.32069100
C	-3.37209800	0.98058500	-0.23176400
C	-2.05912300	0.64844900	-0.17173500

C	-1.65344900	-0.78683300	-0.14549400
N	-0.37752300	-1.02064100	-0.11160100
C	-1.04365500	1.64664300	-0.12678500
C	-0.19248400	2.51492700	-0.09537100
C	0.82725700	3.51113600	-0.05584700
C	0.49701900	4.88197500	-0.04834700
C	1.50150000	5.84752500	-0.01096800
C	2.84643200	5.46515400	0.01922500
C	3.18325700	4.10745800	0.01211200
C	2.18624800	3.13443800	-0.02481800
C	-5.24383200	0.17624500	-1.66151000
O	-5.50581100	0.27429900	0.67682100
C	-5.08612100	0.17743200	2.03834400
S	0.20293100	-2.62698100	-0.07128300
O	-0.09878700	-3.28463000	-1.35438500
O	-0.20501700	-3.26429800	1.19317200
C	1.96469400	-2.31144400	0.00229100
C	2.69214600	-2.20461600	-1.18348100
C	4.06469400	-1.96487200	-1.11514500
C	4.71950700	-1.83458200	0.11945200
C	3.95933800	-1.94862600	1.29393900
C	2.58614300	-2.18857100	1.24550000
C	6.21232500	-1.61400500	0.18374300
H	-2.45385800	-2.83243100	-0.08722100
H	-4.80126200	-2.19113100	-0.19006200
H	-3.66011700	2.02872800	-0.23871400
H	-0.54747500	5.17603700	-0.07218000

H	1.23461100	6.90033000	-0.00561900
H	3.62665800	6.22005300	0.04794400
H	4.22646100	3.80592300	0.03535000
H	2.44167400	2.07994000	-0.03065500
H	-5.62442600	1.19938600	-1.72912300
H	-6.09216000	-0.51293100	-1.70675600
H	-4.57661300	-0.01727000	-2.50534700
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H	-4.28362900	0.88926200	2.26912500
H	-4.74694500	-0.83511100	2.29045600
H	2.19124500	-2.31733700	-2.13888500
H	4.63574300	-1.88249100	-2.03625800
H	4.44798500	-1.85324100	2.26013800
H	2.00385000	-2.28914100	2.15496700
H	6.74574500	-2.57184100	0.22825800
H	6.49422100	-1.04166500	1.07267700
H	6.57608700	-1.07806200	-0.69802000

TSAB -2197.9194889 a.u.

6	-0.270436	2.971369	-1.927264
6	0.701279	3.895417	-1.884252
6	1.654801	4.087282	-0.732668
6	1.513361	3.006598	0.298514
6	0.554179	2.027028	0.265632
6	-0.473080	2.017138	-0.830126
7	-1.436694	1.169327	-0.678158
6	-3.167092	-0.663650	-1.526323

6	-3.717967	-1.084193	-0.313079
6	-4.052532	-2.423981	-0.154144
6	-3.853563	-3.350783	-1.190561
6	-3.305310	-2.897590	-2.396184
6	-2.959674	-1.558122	-2.573819
6	-4.244272	-4.797252	-1.008908
6	-2.756759	1.059216	-1.758481
8	-2.370291	1.240554	-3.168510
8	-3.814482	1.896061	-1.177976
6	1.415543	5.466800	-0.082745
8	3.012352	4.147136	-1.196877
6	3.504386	2.960095	-1.823162
6	0.513376	1.047394	1.250264
6	0.509513	0.177638	2.193973
6	2.330804	-1.270732	0.384394
6	3.455223	-2.444385	-0.271670
6	4.846500	-2.328090	-0.048663
6	5.734036	-3.261434	-0.574720
6	5.258646	-4.333131	-1.337335
6	3.885630	-4.465045	-1.569052
6	2.993962	-3.535495	-1.043551
6	-0.189210	0.110552	3.489578
6	-1.142713	1.072709	3.863838
6	0.105528	-0.940490	4.369782
6	-1.779478	0.983723	5.097484
6	-0.534081	-1.024624	5.605567
6	-1.476455	-0.063540	5.973040

1	-0.937848	2.901414	-2.776897
1	0.830832	4.589074	-2.712025
1	2.250619	3.005733	1.096172
1	-3.878047	-0.372118	0.488744
1	-4.475328	-2.759274	0.789091
1	-3.144072	-3.600926	-3.208431
1	-2.536565	-1.204153	-3.506885
1	-3.786229	-5.434756	-1.769600
1	-5.331386	-4.922354	-1.083123
1	-3.943126	-5.170696	-0.025096
1	2.130769	5.615171	0.730565
1	0.398531	5.546433	0.307924
1	1.576534	6.247767	-0.831174
1	4.534081	3.180190	-2.110446
1	2.930096	2.701253	-2.721480
1	3.498298	2.098719	-1.143558
1	1.185068	-0.716644	1.964979
1	5.209755	-1.494725	0.544086
1	6.799980	-3.156112	-0.392085
1	5.953219	-5.060275	-1.748032
1	3.512910	-5.296419	-2.161132
1	1.927397	-3.631774	-1.218945
1	-1.384229	1.879997	3.179060
1	0.838449	-1.687434	4.079096
1	-2.516386	1.730898	5.376906
1	-0.296575	-1.841876	6.279965
1	-1.975813	-0.129776	6.935041

B -2198.0196274 a.u.

C	-2.97168300	-2.64596100	0.66942500
C	-2.64631200	-3.94563100	0.62808900
C	-1.29683100	-4.46254400	0.21193300
C	-0.32661800	-3.34340700	-0.05867900
C	-0.62533300	-2.02793200	-0.05025000
C	-1.99442800	-1.59207900	0.35232200
N	-2.19430900	-0.31141800	0.43105200
C	-3.52880600	1.99104900	0.28302800
C	-4.05994200	2.21376600	-0.98764100
C	-3.97448500	3.48904800	-1.54089900
C	-3.37611200	4.54628000	-0.84052200
C	-2.85493100	4.29224600	0.43585900
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C	-3.32266800	5.93329200	-1.43580100
S	-3.64590600	0.36098800	1.01091800
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C	-1.44679100	-5.32575600	-1.05928900
O	-0.77126500	-5.37683900	1.18691900
C	-0.54285000	-4.83741400	2.48686800
C	0.42010300	-1.00488600	-0.35038500
C	0.39758400	-0.09066000	-1.34844700
S	1.94189600	-1.07261300	0.60375700
C	1.39711000	-1.09349000	2.31391200
C	2.14951500	-1.83992300	3.23137200

C	1.79477300	-1.84490100	4.58148500
C	0.67502900	-1.13407100	5.01874300
C	-0.07841000	-0.39887500	4.10093900
C	0.28968400	-0.35899500	2.75570900
H	-3.97148800	-2.33457100	0.94542500
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H	-4.53214300	1.40143600	-1.52928800
H	-4.38197400	3.66687000	-2.53306600
H	-2.38849600	5.10027400	0.99421200
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H	-4.23625200	6.49662200	-1.20351600
H	-3.23250200	5.89827900	-2.52662100
H	-2.47763600	6.50713800	-1.04184100
H	-0.46948100	-5.72680500	-1.34486500
H	-1.85288700	-4.74036200	-1.88923400
H	-2.11659600	-6.16586000	-0.85057700
H	-0.14661700	-5.66205900	3.08411900
H	-1.46963700	-4.47300900	2.94951200
H	0.18748500	-4.01908200	2.47363800
H	3.00468900	-2.41633500	2.88855400
H	2.38663100	-2.42088500	5.28826400
H	0.39053100	-1.15492300	6.06719200
H	-0.95951100	0.14971800	4.42214500
H	-0.29121300	0.22722200	2.05222200
C	-0.54780200	0.09531600	-2.45556100
C	-1.44018000	-0.88851900	-2.92244300

C	-0.53067600	1.33563500	-3.12300100
C	-2.29476900	-0.62917300	-3.99099600
H	-1.44998500	-1.86945000	-2.46124200
C	-1.38801500	1.59716200	-4.18835500
H	0.16260500	2.10373600	-2.78875200
C	-2.27811300	0.61492500	-4.62672800
H	-2.97201800	-1.40630500	-4.33550900
H	-1.35606000	2.56538900	-4.68100200
H	-2.94448000	0.81143900	-5.46233600
H	1.21492300	0.62797500	-1.34769900

TSBC -2197.9573922 a.u.

C	0.16662700	-3.19012500	-0.88777100
C	1.31889200	-3.87400500	-0.75490600
C	2.67148900	-3.25747400	-0.50615000
C	2.59892200	-1.78003600	-0.27806100
C	1.45808500	-1.04555900	-0.46159300
C	0.19407500	-1.74276000	-0.76019200
N	-0.81692500	-0.90068100	-0.89011400
C	-3.24152800	-0.74372600	0.37145300
C	-3.93579100	0.46545800	0.41081400
C	-4.54934300	0.84941100	1.60302400
C	-4.47691300	0.04793500	2.74999700
C	-3.78127700	-1.16990000	2.67338600
C	-3.16701000	-1.57506000	1.49315500
C	-5.11685700	0.48560800	4.04504600
S	-2.49272400	-1.27312200	-1.16273300

O	-2.66187100	-2.72510300	-1.27873200
O	-2.91769100	-0.38191500	-2.23575500
C	3.58406000	-3.59111600	-1.70984800
O	3.30089500	-3.96428200	0.59055300
C	2.73030400	-3.74636600	1.87194000
C	1.23419400	0.36584300	-0.53729200
C	-0.17291500	0.71957700	-0.42723400
S	2.48333400	1.49312400	-1.00418900
C	3.24431300	2.04570100	0.53728800
C	4.28393200	2.98182300	0.44079000
C	4.91984300	3.44467500	1.59164500
C	4.53021800	2.98144900	2.85108000
C	3.49617600	2.04850200	2.94539000
C	2.85422200	1.58124700	1.79726400
H	-0.77105500	-3.68685100	-1.09332000
H	1.31285600	-4.95968800	-0.83485100
H	3.53150800	-1.27563800	-0.04217800
H	-3.99653000	1.08436500	-0.47724300
H	-5.09869500	1.78661900	1.63863700
H	-3.72945300	-1.81297100	3.54828400
H	-2.65329200	-2.52934400	1.43593900
H	-5.90780400	1.22186900	3.87331300
H	-4.37566100	0.94762700	4.71034900
H	-5.55081000	-0.36312300	4.58411600
H	4.58037900	-3.18335300	-1.51545300
H	3.19234100	-3.14868500	-2.62988100
H	3.67048800	-4.67638800	-1.83319000

H	3.33642800	-4.32532300	2.57366000
H	1.68903300	-4.09856900	1.92990000
H	2.75567900	-2.68671100	2.15596300
H	4.59176300	3.34847000	-0.53589700
H	5.72309100	4.17232100	1.50332400
H	5.02739700	3.34346700	3.74690200
H	3.18509600	1.67877900	3.91998100
H	2.05050100	0.85352100	1.86753700
C	-0.74090000	1.86270400	-1.19443300
C	-0.50754700	1.99868700	-2.57038000
C	-1.51197300	2.82941300	-0.53530500
C	-1.03249800	3.08141500	-3.26958900
H	0.07980900	1.24388500	-3.08392400
C	-2.02380700	3.92499500	-1.23119200
H	-1.69306900	2.73104500	0.53254700
C	-1.78827400	4.04908500	-2.60124100
H	-0.85271500	3.17334000	-4.33709500
H	-2.60406700	4.67887100	-0.70573500
H	-2.19332500	4.89622600	-3.14848200
H	-0.63415800	0.65695800	0.56730300

C -2197.97068845 a.u.

C	0.46918900	-0.84728400	2.71629100
C	-0.64761800	-1.36118200	3.30660600
C	-2.04784300	-1.29315000	2.75940700
C	-2.15978100	-0.34260000	1.62279900
C	-1.04374900	0.18921700	1.02136800

C	0.29156100	-0.07267700	1.53805400
N	1.25916900	0.57934100	0.82117200
C	2.85054300	-1.37847500	-0.36687600
C	3.04556300	-1.23274100	-1.74275400
C	2.97437200	-2.35984600	-2.55769000
C	2.70789700	-3.62873900	-2.02263200
C	2.52897000	-3.74500400	-0.63604800
C	2.59892500	-2.63198900	0.19821900
C	2.60145200	-4.83840500	-2.91899300
S	2.91825600	0.06965300	0.68035400
O	3.32958500	-0.33834500	2.02081100
O	3.58246300	1.14273200	-0.04815600
C	-3.06240600	-1.00993600	3.87639800
O	-2.35636700	-2.72102000	2.43287000
C	-1.83361700	-3.21245600	1.21632000
C	-0.82893900	1.09401400	-0.06093000
C	0.63317500	1.36765900	-0.27819300
S	-2.01845700	2.01932200	-0.92935200
C	-3.21574800	0.80418200	-1.49431900
C	-4.53303200	1.24163000	-1.68782700
C	-5.49115700	0.36301800	-2.19196700
C	-5.15068700	-0.95941000	-2.48571700
C	-3.84023500	-1.39497700	-2.28036100
C	-2.86995800	-0.51900500	-1.79290300
H	1.45252900	-0.97073600	3.15188300
H	-0.53530500	-1.92374400	4.23181000
H	-3.15085800	-0.06794000	1.27990000

H	3.27464700	-0.25690400	-2.15764500
H	3.13716700	-2.25305100	-3.62706800
H	2.34161300	-4.72303000	-0.20037300
H	2.48314700	-2.73594300	1.27113300
H	3.20577000	-4.72113200	-3.82398700
H	1.56287400	-4.99803100	-3.23766500
H	2.92719200	-5.74838600	-2.40509000
H	-4.07247000	-1.01537000	3.45436200
H	-2.87687500	-0.03002200	4.32711500
H	-3.01212500	-1.78096100	4.65348800
H	-2.17548400	-4.24953700	1.13698400
H	-0.73110100	-3.20771100	1.19193900
H	-2.19839300	-2.64304200	0.35246000
H	-4.80489600	2.26425100	-1.44006200
H	-6.50922400	0.71155900	-2.34459400
H	-5.90136400	-1.64530300	-2.86818400
H	-3.56677200	-2.42272600	-2.50561800
H	-1.84830700	-0.85395000	-1.64506600
C	1.03484500	2.84109700	-0.23721700
C	0.81476100	3.60766000	0.91398200
C	1.57986000	3.44909400	-1.36962500
C	1.15125400	4.95894800	0.93217800
H	0.38034000	3.14318200	1.79511000
C	1.90669300	4.80649800	-1.35617200
H	1.75448900	2.85908000	-2.26589700
C	1.69633000	5.56327500	-0.20452100
H	0.98411200	5.54313200	1.83306000

H	2.32995100	5.26772400	-2.24436600
H	1.95395200	6.61884400	-0.19013300
H	0.97526900	0.94330400	-1.23320200

C-2AcOH -2656.1667417 a.u.

C	-0.60505400	-0.53313800	-3.02989400
C	-1.96616600	-0.52327800	-3.30461900
C	-2.99119500	-0.47277700	-2.22665400
C	-2.53971500	0.55049400	-1.26686200
C	-1.18975300	0.53797300	-0.90330800
C	-0.20969600	-0.13077500	-1.75805400
N	1.06824800	-0.13886400	-1.18843900
C	-0.45057200	1.06123200	0.15492800
C	-4.41251700	-0.24297100	-2.74452800
C	-3.06486000	-3.01424200	-2.22717300
S	1.92178900	-1.68101300	-1.23693800
O	2.03006000	-1.98953300	-2.66508400
O	1.29912500	-2.64738500	-0.32406800
C	3.53668700	-1.24973000	-0.61140700
C	4.46900700	-0.69546100	-1.49239600
C	5.74333100	-0.39742100	-1.02183900
C	6.10018300	-0.64807400	0.31243800
C	5.14558500	-1.21622000	1.16593600
C	3.86100900	-1.52285700	0.71839900
C	7.47710200	-0.29017200	0.81753200
O	-3.01511900	-1.81897300	-1.45902300
C	-3.51585000	2.93051600	1.69968300

C	-2.34739400	2.97748800	0.93109700
C	-2.27342700	3.81277300	-0.19075900
C	-3.37983200	4.57987300	-0.55189700
C	-4.54882500	4.53585300	0.21239300
C	-4.61262400	3.71551800	1.33976500
S	-0.91383100	2.05777000	1.49395500
C	0.99382000	0.58738900	0.10569900
C	2.01501900	1.71350900	0.20066900
C	2.71403000	1.90626700	1.39558900
C	2.22865200	2.58802100	-0.87188800
C	3.61650900	2.96554300	1.51941500
C	3.13243500	3.64137400	-0.74830200
C	3.82749400	3.83453200	0.44941400
H	0.12767900	-0.77024300	-3.79183400
H	-2.29822300	-0.59220800	-4.33929400
H	-3.25244400	1.24191500	-0.83832300
H	-5.11748000	-0.21152900	-1.90807400
H	-4.72582600	-1.04166200	-3.42507900
H	-4.47523200	0.70690800	-3.28552500
H	-2.92595100	-3.84506900	-1.52910700
H	-2.25346700	-3.04222000	-2.96423600
H	-4.02518000	-3.14643700	-2.74829300
H	4.19919000	-0.51855700	-2.52783600
H	6.47595300	0.03133500	-1.70115900
H	5.40812000	-1.42448900	2.20004500
H	3.12339200	-1.94608300	1.39268400
H	8.24378700	-0.47399600	0.05720300

H	7.73873200	-0.86354300	1.71229800
H	7.53057300	0.77429800	1.08159300
H	-3.56661700	2.27897400	2.56682900
H	-1.35930500	3.85573900	-0.77420500
H	-3.32463700	5.22078400	-1.42757500
H	-5.40580000	5.14122000	-0.06952600
H	-5.51932200	3.67693900	1.93715200
H	1.14715500	-0.11054900	0.94173100
H	2.55318400	1.22199400	2.22462000
H	1.69393400	2.43188000	-1.80489200
H	4.15599600	3.10606100	2.45236100
H	3.29546100	4.31348600	-1.58690700
H	4.53076900	4.65774800	0.54444100
C	0.19942800	-2.13428100	2.45177300
O	1.21992300	-1.51912900	2.71884800
C	0.04024000	-3.62325800	2.66916100
O	-0.83517300	-1.49123900	1.90251900
H	-0.96994900	-3.87940300	2.99958300
H	0.78184400	-3.96741200	3.39176300
H	0.22148800	-4.12324600	1.71058000
H	-1.60331900	-2.08496100	1.71331500
C	-4.27713900	-2.73126300	1.58891800
O	-3.10026500	-2.98950400	1.82915800
C	-5.40021600	-3.11140200	2.52664200
O	-4.70894200	-2.11269900	0.50574700
H	-5.96594200	-2.21722700	2.80844600
H	-4.99688600	-3.59407400	3.41727400

H	-6.09593500	-3.78708400	2.01809800
H	-3.96186500	-1.93385100	-0.16536100

TSCD -2656.16617189 a.u.

C	0.60108700	-0.70748700	2.98236400
C	1.95723600	-0.69005000	3.24706100
C	2.97467600	-0.38822900	2.22508400
C	2.48151100	0.58793500	1.27850500
C	1.12729100	0.54566800	0.93225200
C	0.17726200	-0.18501400	1.75669300
N	-1.10498900	-0.18058900	1.21151000
C	0.37196600	1.06958700	-0.12036600
C	4.37839600	-0.13959300	2.76273400
C	3.29166900	-3.03918100	2.02542800
S	-1.99815400	-1.70266300	1.30524400
O	-2.18747400	-1.91901800	2.74183500
O	-1.33779400	-2.72482500	0.48793600
C	-3.56797100	-1.28936700	0.56753500
C	-4.55012000	-0.69584600	1.36504300
C	-5.79192500	-0.41902800	0.80344500
C	-6.06752400	-0.73091500	-0.53715800
C	-5.06465400	-1.33844400	-1.30434600
C	-3.81072300	-1.62395100	-0.76590800
C	-7.41004900	-0.39685700	-1.14107400
O	3.17859300	-1.81839900	1.32334800
C	3.39321300	3.00181300	-1.67379400
C	2.23180400	3.02759100	-0.89384700

C	2.15405300	3.85609900	0.23251700
C	3.25148700	4.63892300	0.58692600
C	4.41385900	4.61655800	-0.18826300
C	4.48064400	3.80234500	-1.31987100
S	0.80875500	2.08642800	-1.44889500
C	-1.05670100	0.56143200	-0.07401800
C	-2.10508500	1.66313700	-0.15593100
C	-2.80613900	1.85879700	-1.34897300
C	-2.33796800	2.51822400	0.92839800
C	-3.73041100	2.90060200	-1.45924400
C	-3.26364000	3.55396000	0.81856800
C	-3.96123900	3.74941700	-0.37720900
H	-0.11559300	-1.06353000	3.71187900
H	2.29572600	-0.95672200	4.24662100
H	3.17846100	1.23635700	0.76501900
H	5.07936700	0.01020800	1.93652900
H	4.73434600	-0.98408900	3.36157100
H	4.39538000	0.75587500	3.39488500
H	3.23203100	-3.85795400	1.29784400
H	2.46398700	-3.16611200	2.73748200
H	4.24190800	-3.13794900	2.57753200
H	-4.34397500	-0.47193600	2.40594200
H	-6.56336100	0.04093200	1.41597600
H	-5.26469400	-1.59475400	-2.34161500
H	-3.03201400	-2.07509600	-1.37255200
H	-8.22277500	-0.55143200	-0.42327400
H	-7.61536200	-1.00645300	-2.02641700

H	-7.44623900	0.65608000	-1.45037600
H	3.44685000	2.35355500	-2.54315200
H	1.24483900	3.88202700	0.82458500
H	3.19457000	5.27458600	1.46626200
H	5.26390300	5.23369300	0.08894200
H	5.38266200	3.78009700	-1.92499400
H	-1.18754500	-0.13910800	-0.91491600
H	-2.63093800	1.19095800	-2.18821600
H	-1.80028000	2.36143100	1.85958400
H	-4.27078700	3.04355200	-2.39125800
H	-3.44113700	4.21076000	1.66623600
H	-4.68137800	4.55901000	-0.46170900
C	-0.00277900	-2.18474100	-2.27496500
O	-1.05308300	-1.60967400	-2.52462100
C	0.21682500	-3.65940300	-2.53261700
O	1.00078300	-1.51321600	-1.71018200
H	1.23426100	-3.86265500	-2.87654900
H	-0.51655400	-4.01624800	-3.25743000
H	0.06563900	-4.19276400	-1.58648600
H	1.81391200	-2.06636500	-1.57216200
C	4.48157000	-2.52061000	-1.63706400
O	3.32123800	-2.86886200	-1.86488000
C	5.60437900	-2.79715700	-2.61352000
O	4.88491300	-1.89715000	-0.55434400
H	6.11794800	-1.86303500	-2.86334900
H	5.21090100	-3.26185100	-3.51830700
H	6.34408000	-3.45758900	-2.14832900

H	4.12774700	-1.80770900	0.16299900

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C	-0.64283500	-1.47258700	-2.72662000
C	-1.93143000	-1.27317600	-3.18577100
C	-2.75591400	-0.18397400	-2.78053200
C	-2.24930700	0.71710000	-1.86775200
C	-0.94300000	0.53700900	-1.34120300
C	-0.13079900	-0.54801300	-1.79923200
N	1.13192700	-0.48605900	-1.23551000
C	-0.17267000	1.26584500	-0.41521700
C	-4.16228800	-0.06132700	-3.31269600
C	-5.11655800	-3.40759500	-1.41194300
S	1.98845400	-2.01466700	-0.96416500
O	2.14219900	-2.57023900	-2.31128100
O	1.27400500	-2.75718800	0.07119300
C	3.58708400	-1.52908900	-0.35373000
C	4.63002200	-1.37540100	-1.27130200
C	5.90468300	-1.09260700	-0.79156000
C	6.14939900	-0.96698000	0.58453300
C	5.08121800	-1.13986500	1.47572300
C	3.79431400	-1.42342800	1.02370100
C	7.53006500	-0.62839700	1.09145600
O	-5.68893200	-2.15646700	-1.08129800
C	-3.05989900	2.01560500	1.11508500
C	-2.23183900	2.94957900	0.48127800
C	-2.75138600	4.12335200	-0.07585200

C	-4.12602600	4.35692500	-0.00962700
C	-4.96599500	3.41980700	0.59641100
C	-4.43365500	2.25305000	1.15132500
S	-0.45291700	2.70483100	0.48148600
C	1.14730400	0.59788500	-0.22947100
C	2.34807400	1.53387200	-0.29984600
C	2.93357900	1.99077100	0.88620000
C	2.82305300	1.99883700	-1.53318600
C	3.98278700	2.91172100	0.83486900
C	3.87658200	2.90995700	-1.57889600
C	4.45611200	3.37189300	-0.39389800
H	-0.04039600	-2.29944900	-3.07802500
H	-2.33496300	-1.97951600	-3.90770800
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C	5.30166900	-1.30261100	-3.37510700
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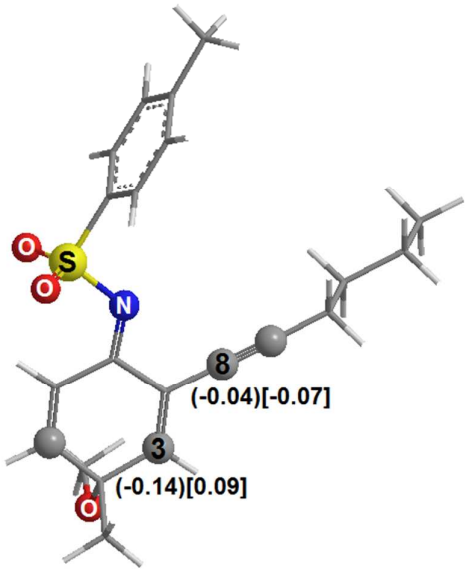

Figure S1. Optimized structure of **G**. The numbers in the parenthesis are the NBO charges on atoms and the numbers in square brackets are the condensed Fukui functions.

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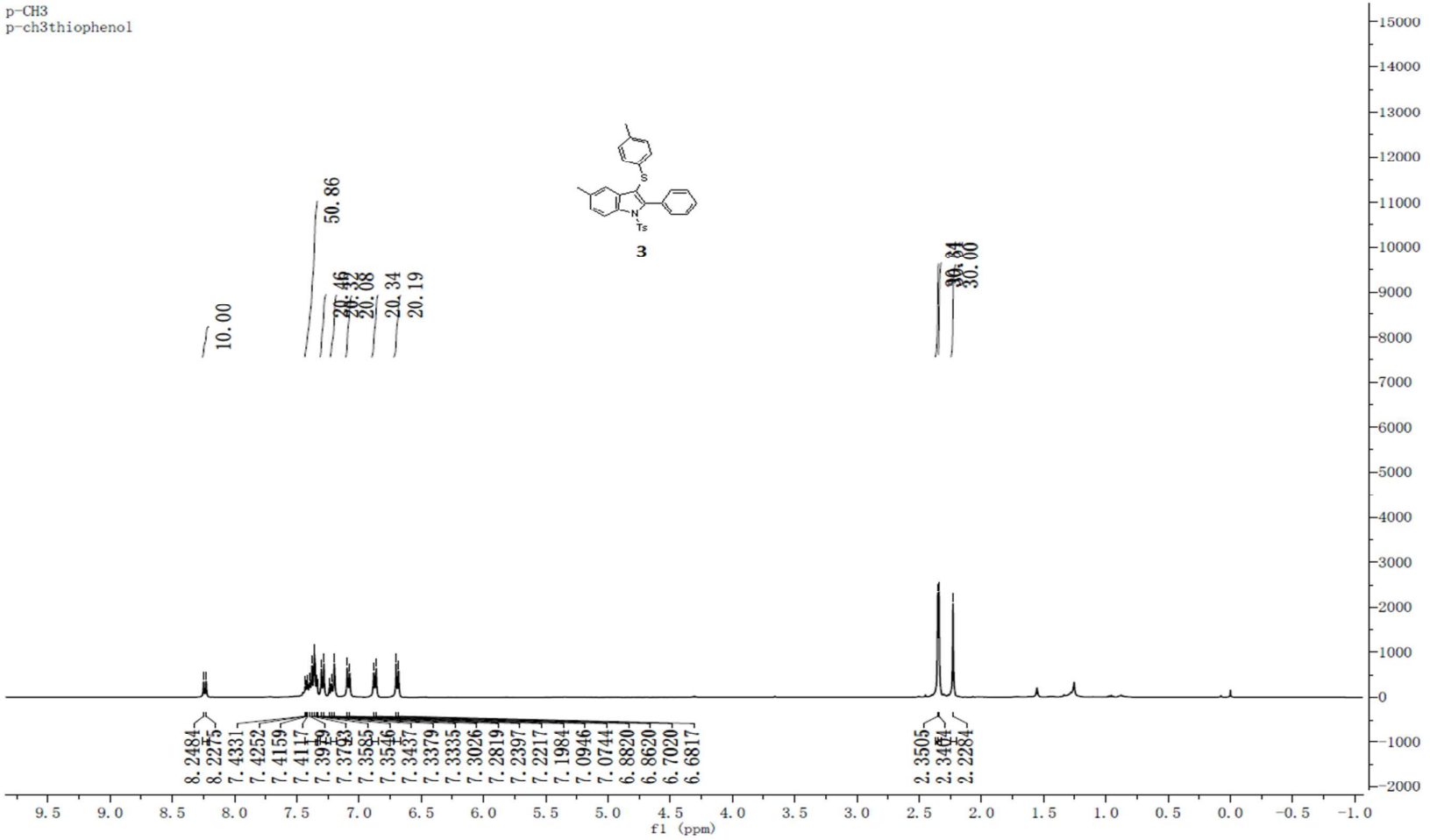
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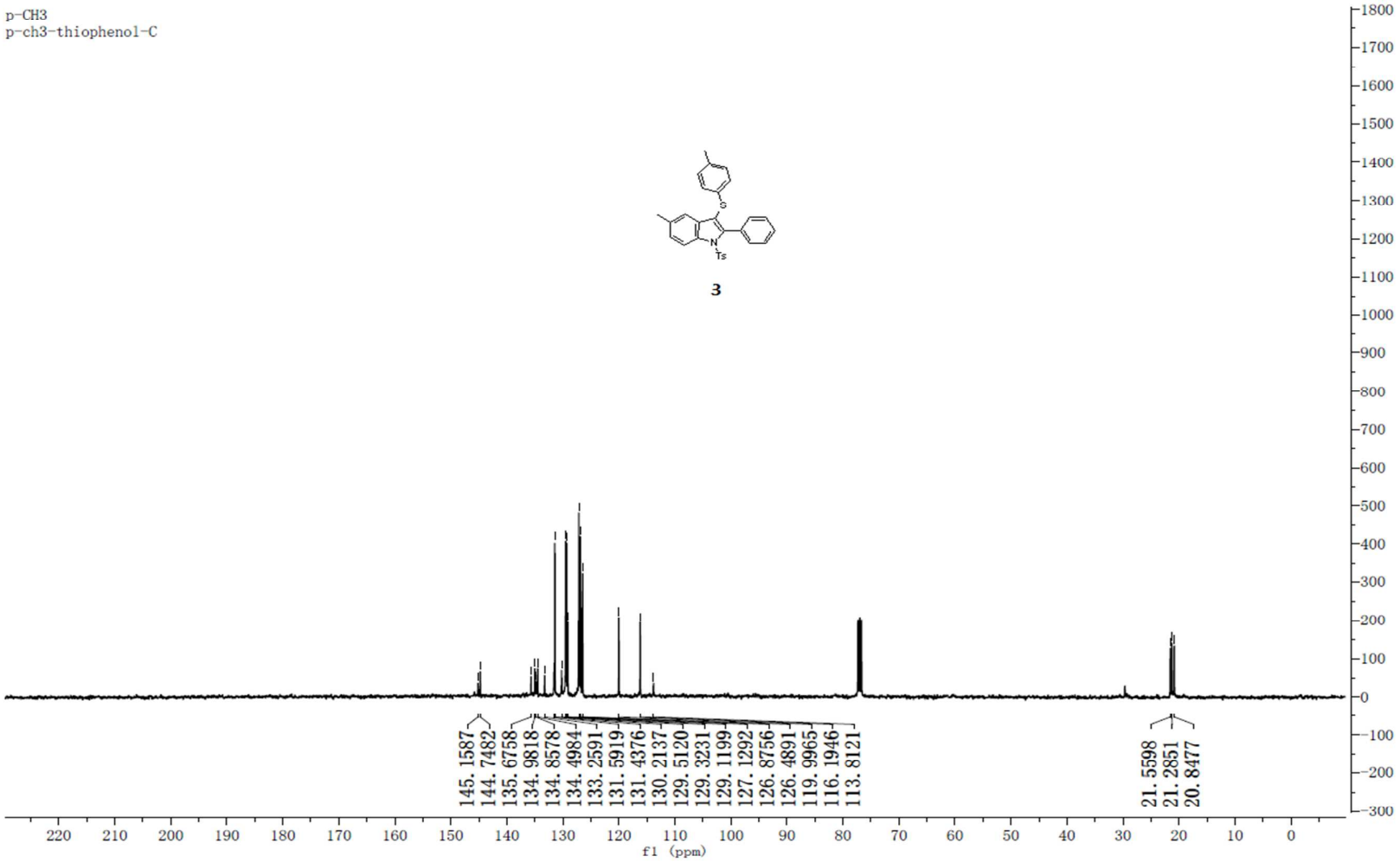
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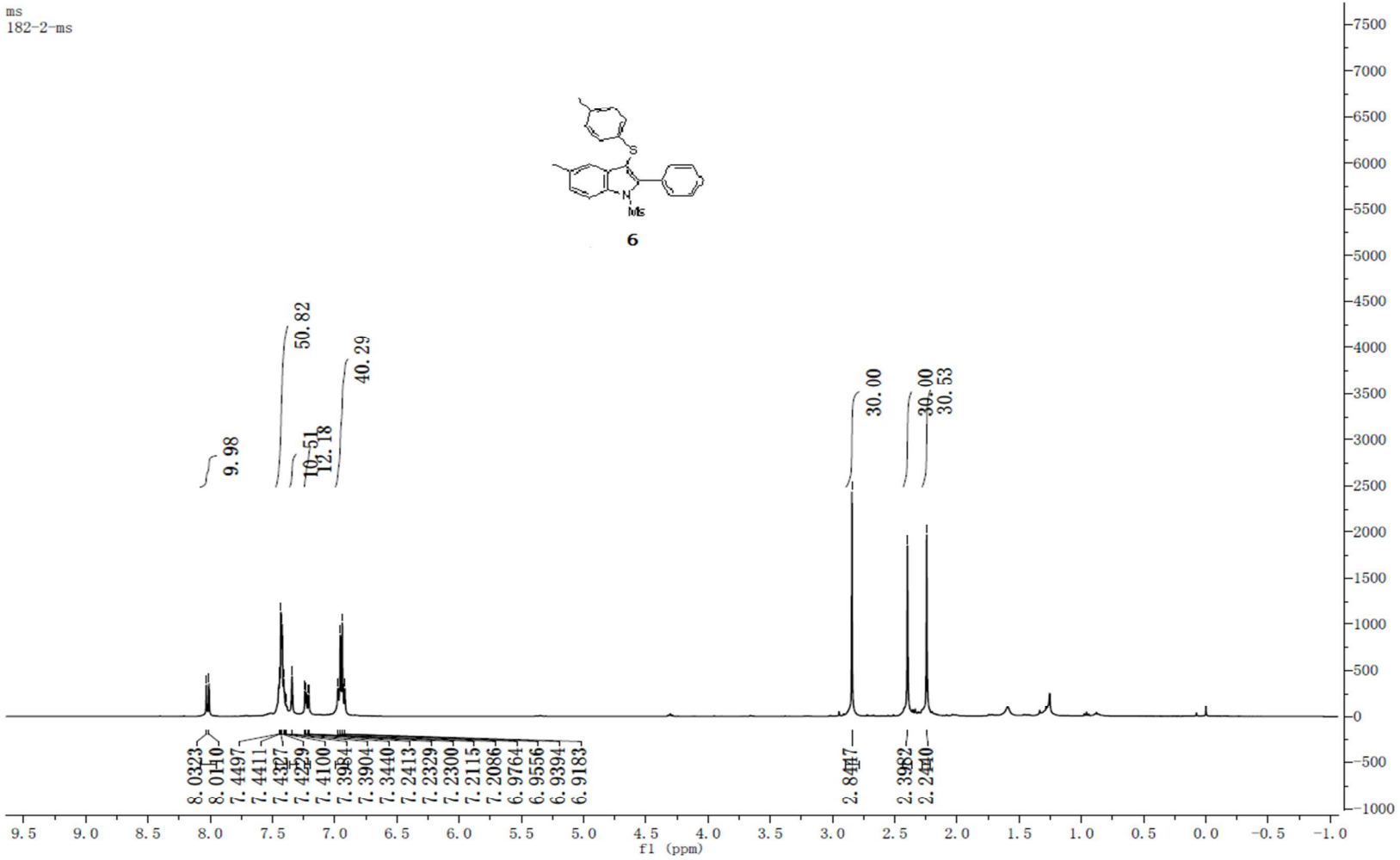
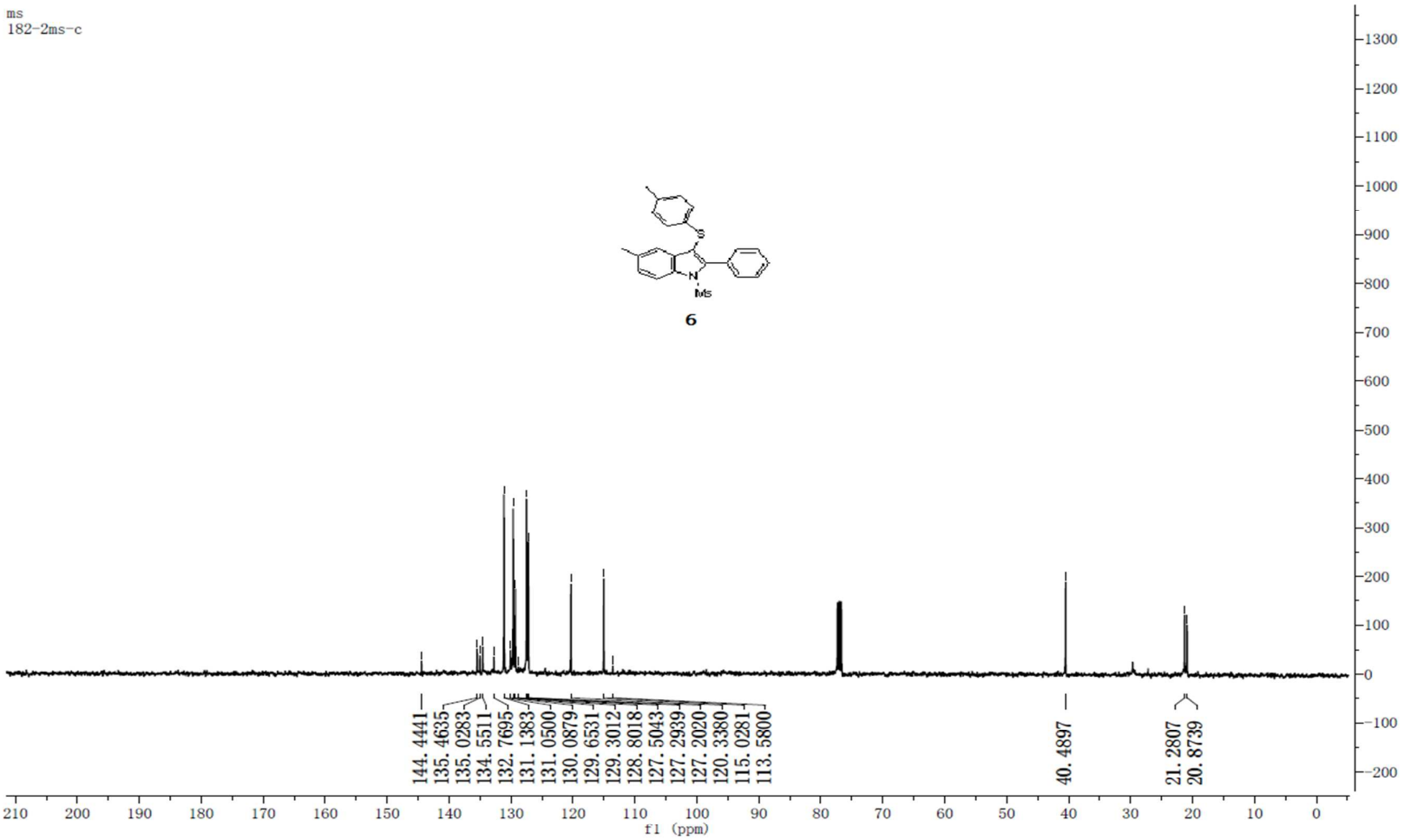
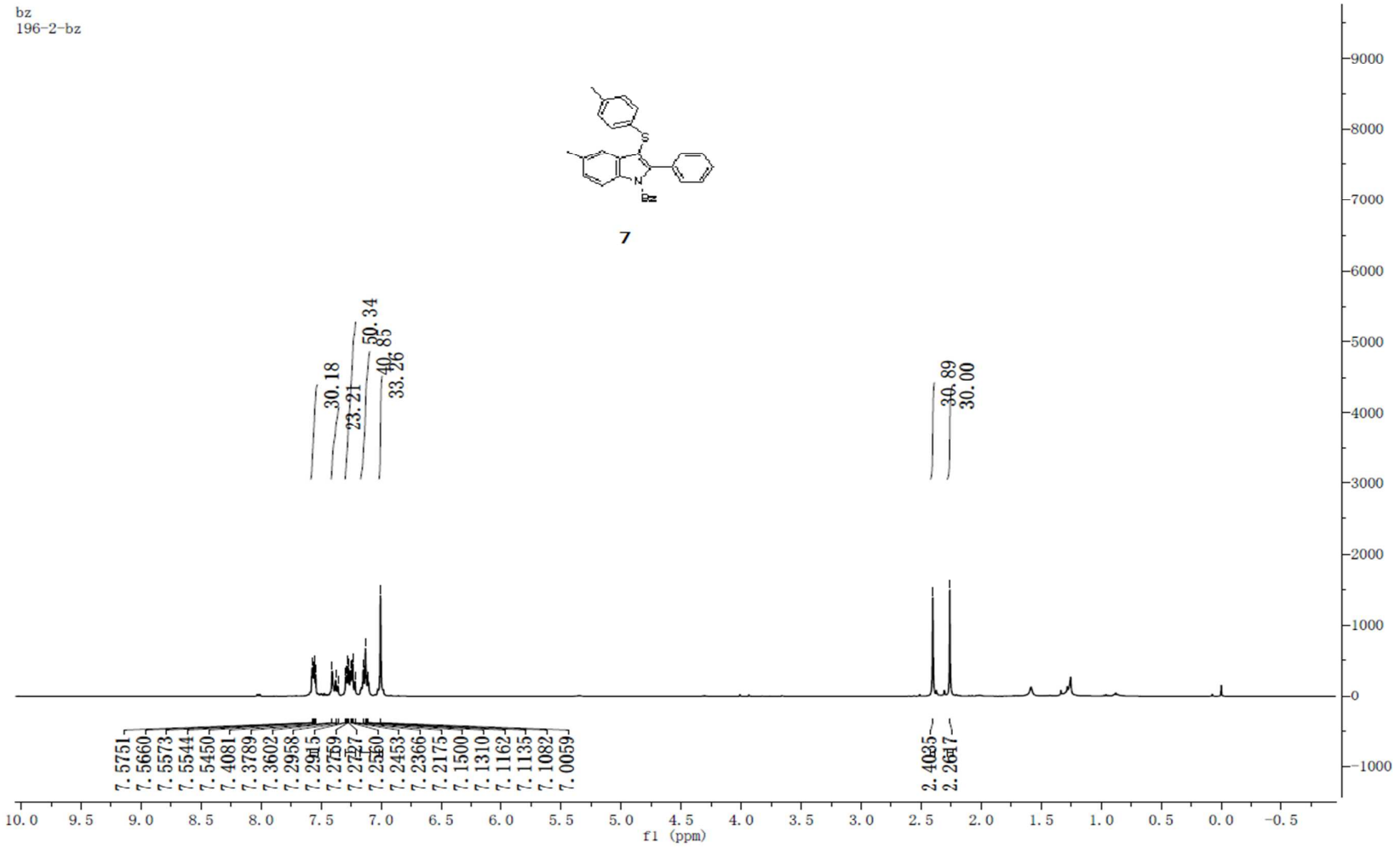
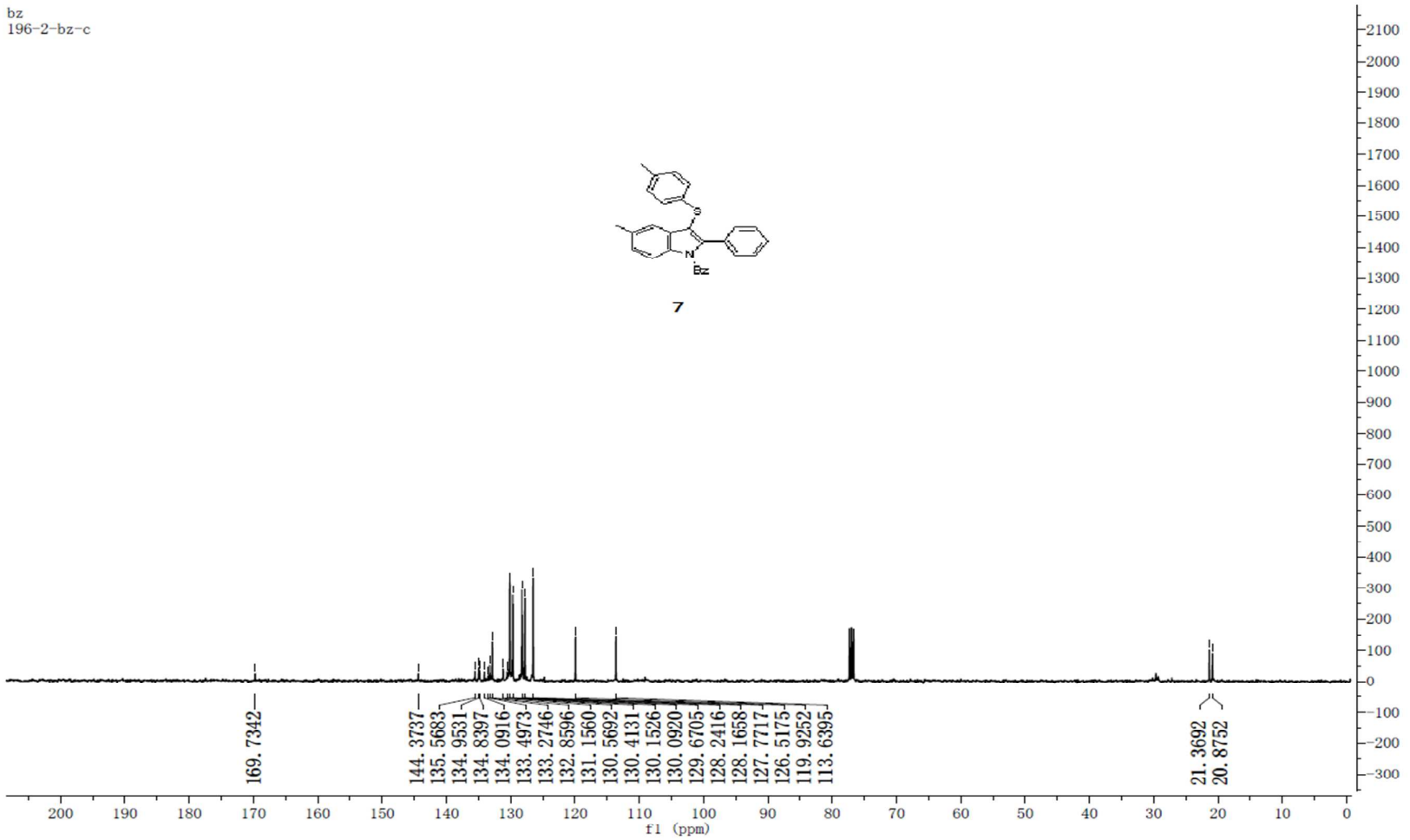
133.2591
131.5919
131.4376
130.2137
129.5120
129.3231
129.1199
127.1292
126.8756
126.4891
119.9965
116.1946
113.8121
21.5598
21.2851
20.8477
f1 (ppm)

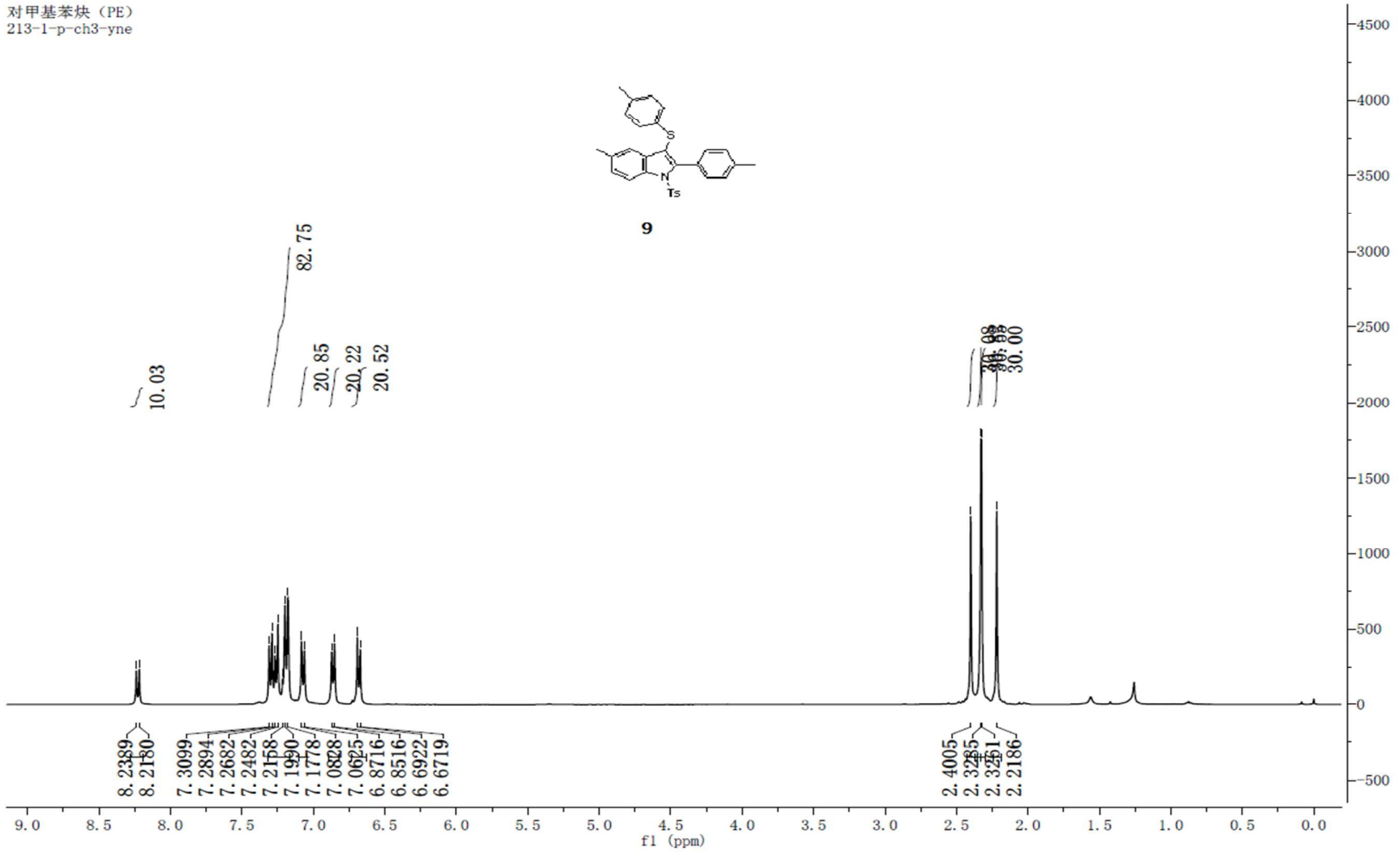

ms
182-2-ms
6
9.98
50.82
10.51
12.18
40.29
30.00
30.00
30.53
f1 (ppm)

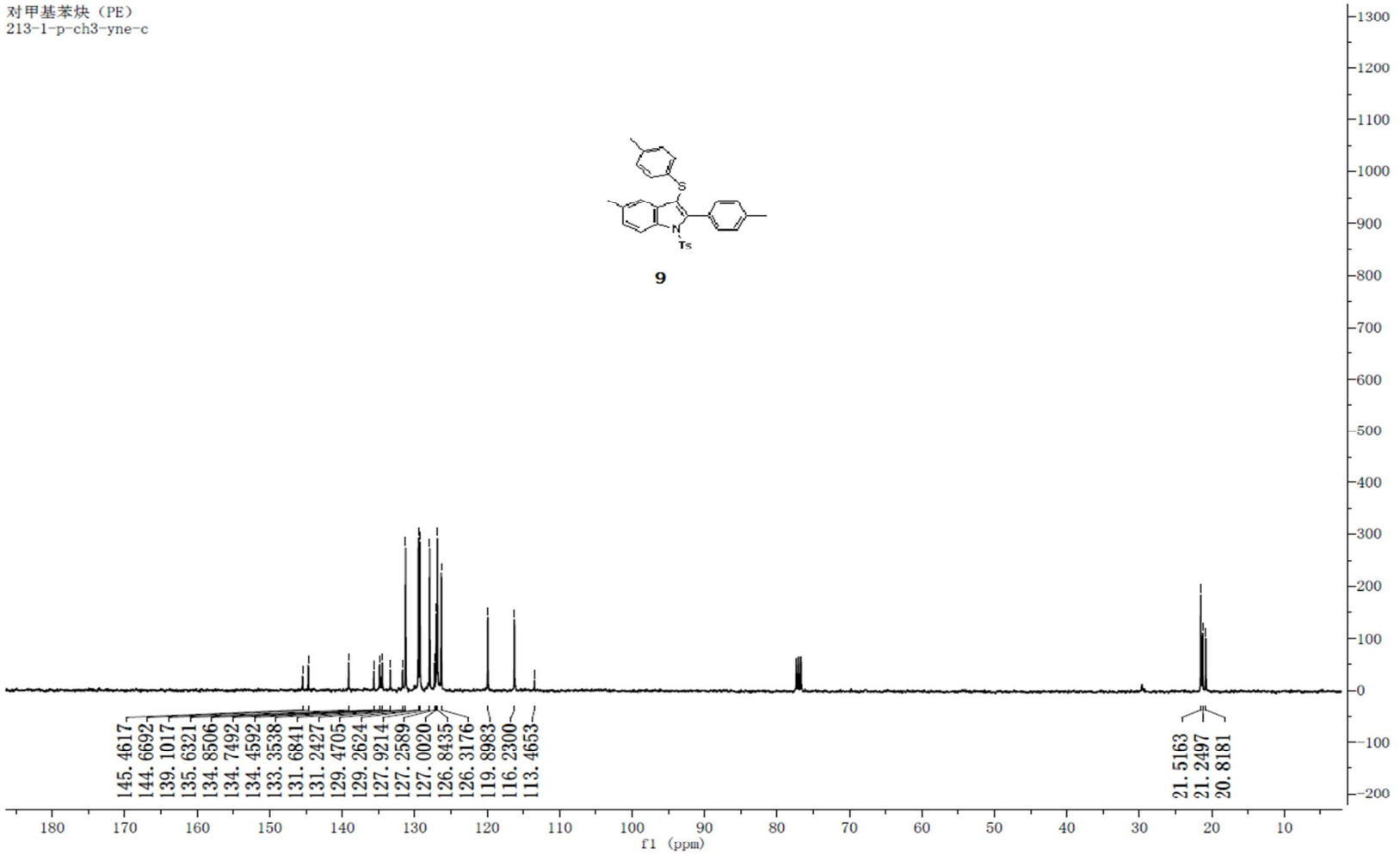

ms
182-2ms-c
S
N
Ms
144.4441
135.4635
135.0283
134.5511
132.7695
131.1383
131.0500
130.0879
129.6531
129.3012
128.8018
127.5043
127.2939
127.2020
120.3380
115.0281
113.5800
40.4897
21.2807
20.8739
f1 (ppm)

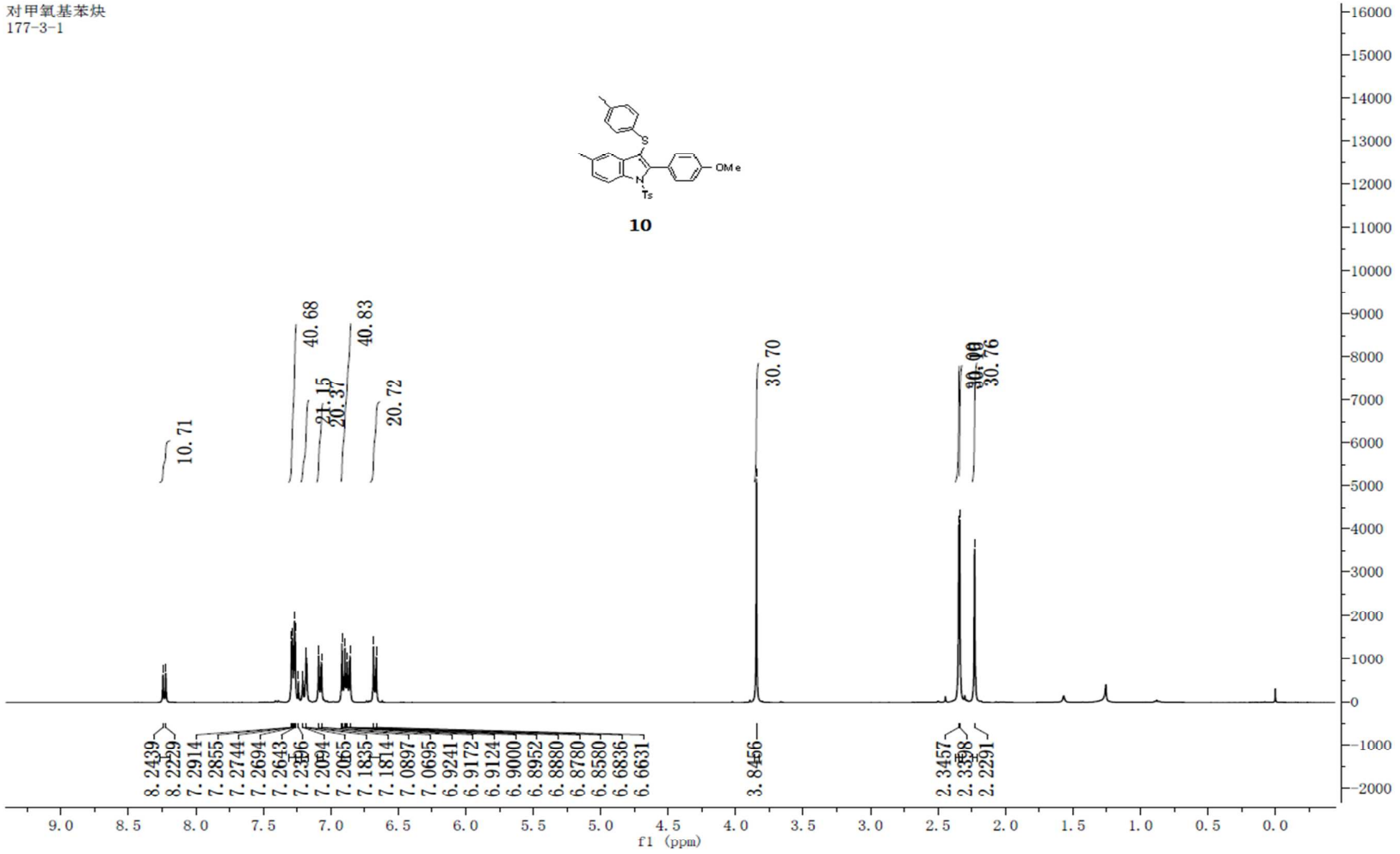
6

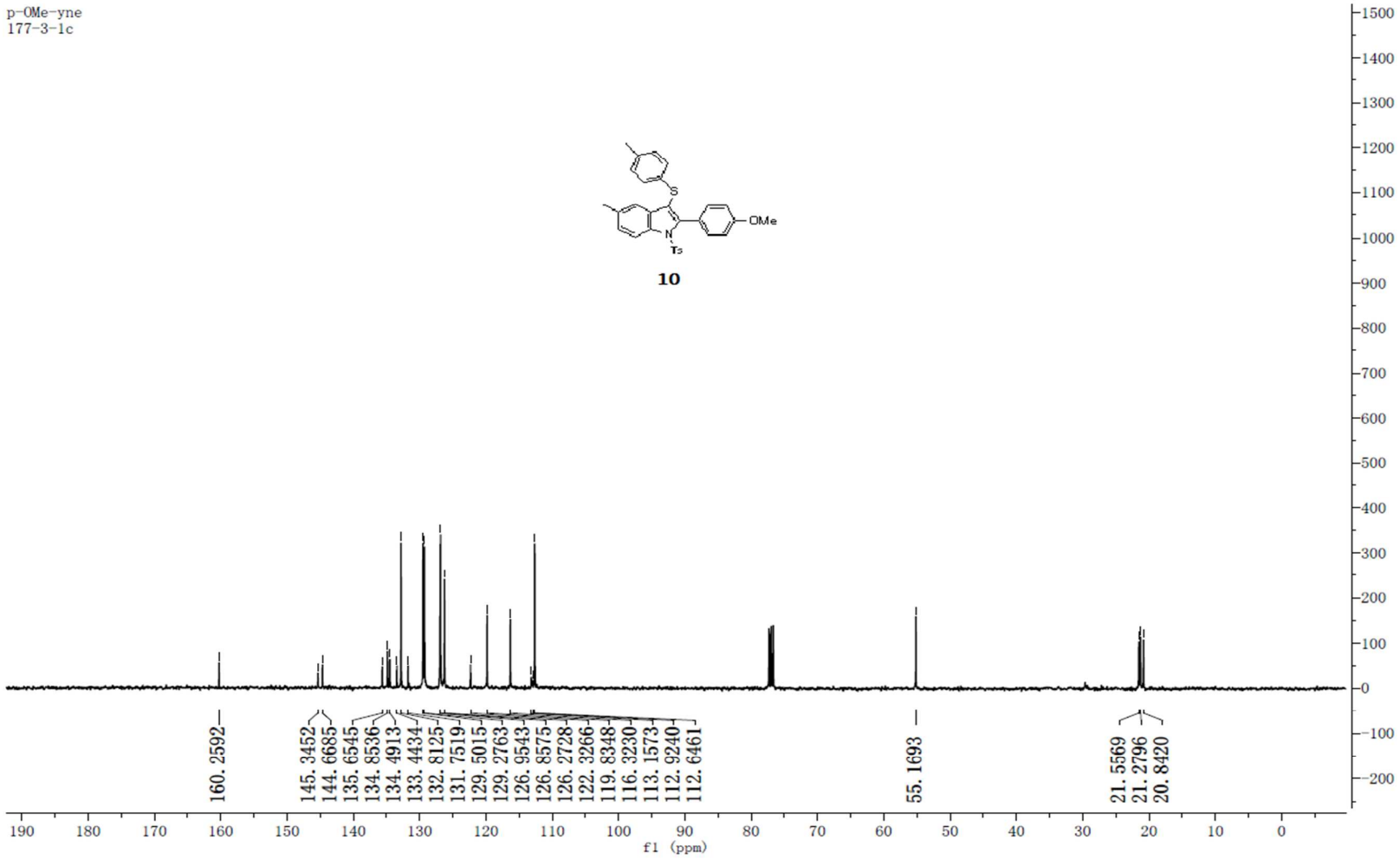

bz
196-2-bz
7
30.18
23.21
50.34
40.85
33.26
30.89
30.00
7.5751
7.5660
7.5573
7.5544
7.5450
7.4081
7.3789
7.3602
7.2958
7.2759
7.2727
7.2360
7.2453
7.2366
7.2175
7.1500
7.1310
7.1162
7.1135
7.1082
7.0059
2.4035
2.2647
f1 (ppm)

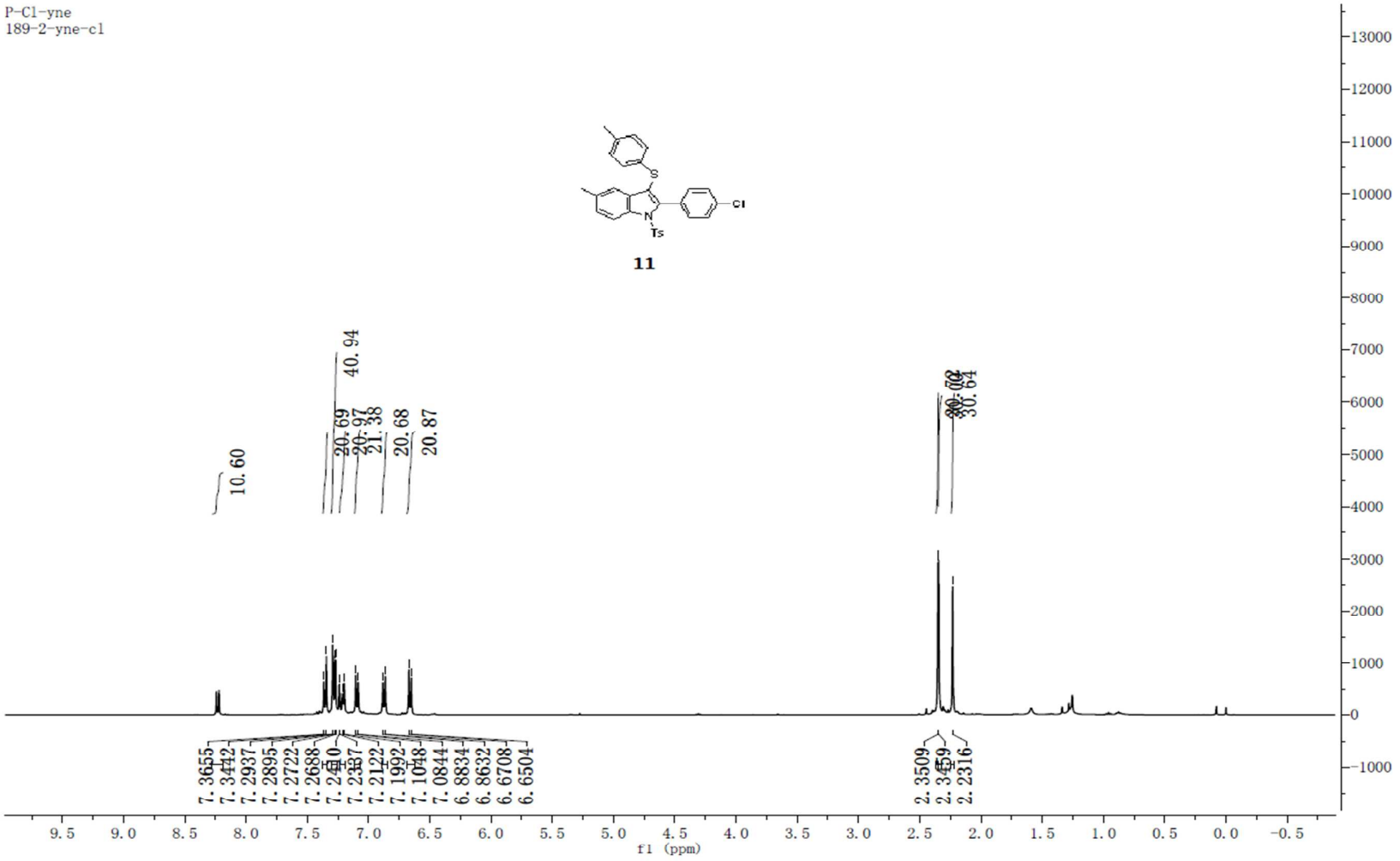

bz
196-2-bz-c
7
169.7342
144.3737
135.5683
134.9531
134.8397
134.0916
133.4973
133.2746
132.8596
131.1560
130.5692
130.4131
130.1526
130.0920
129.6705
128.2416
128.1658
127.7717
126.5175
119.9252
113.6395
21.3692
20.8752
f1 (ppm)

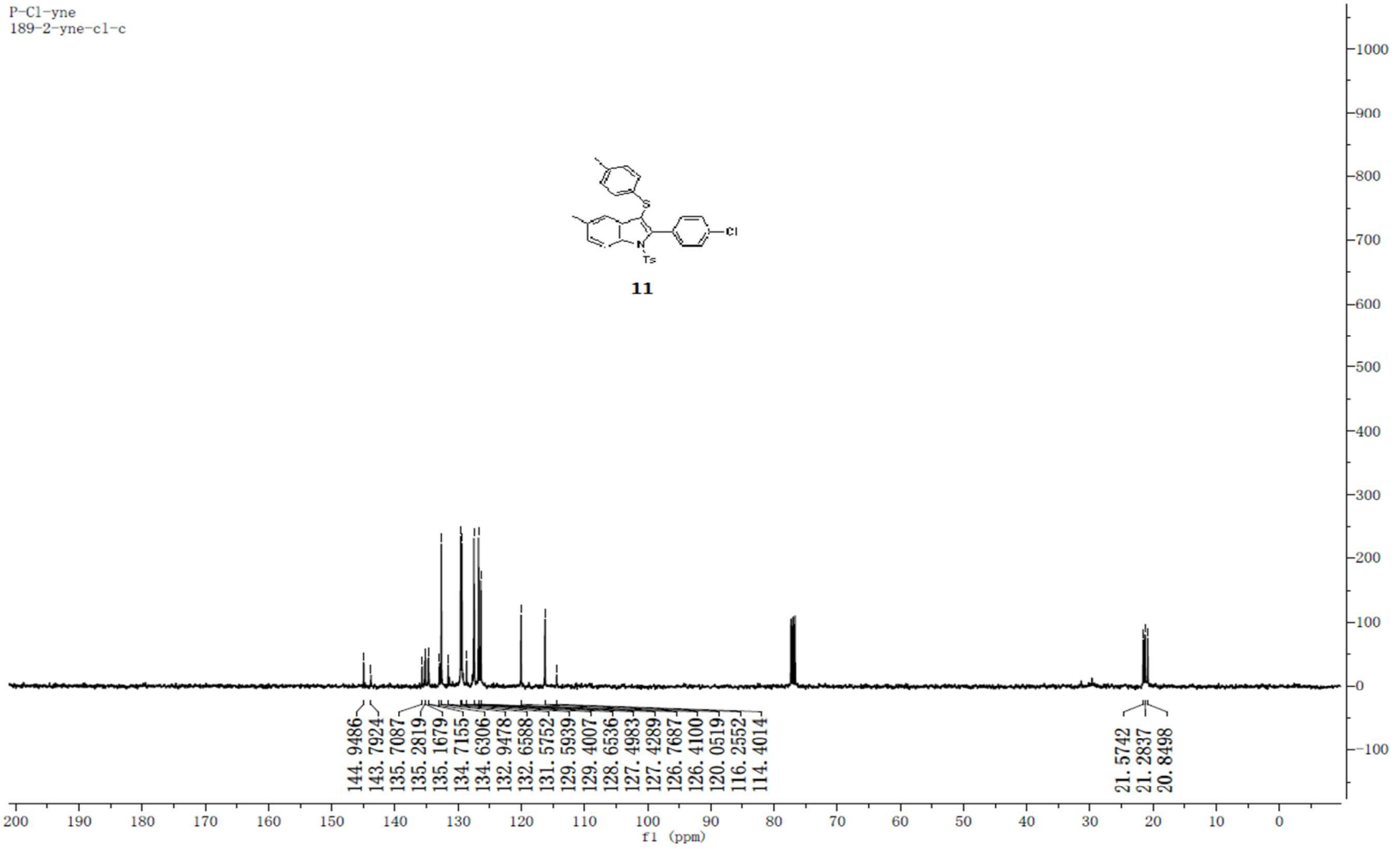

对甲基苯炔（PE）
213-1-p-ch3-yne
9
Ts
82.75
10.03
20.85
20.22
20.52
30.00
8.2389
8.2180
7.3099
7.2894
7.2682
7.2482
7.2158
7.1990
7.1778
7.0828
7.0625
6.8716
6.8516
6.6922
6.6719
2.4005
2.3285
2.3251
2.2186
f1 (ppm)

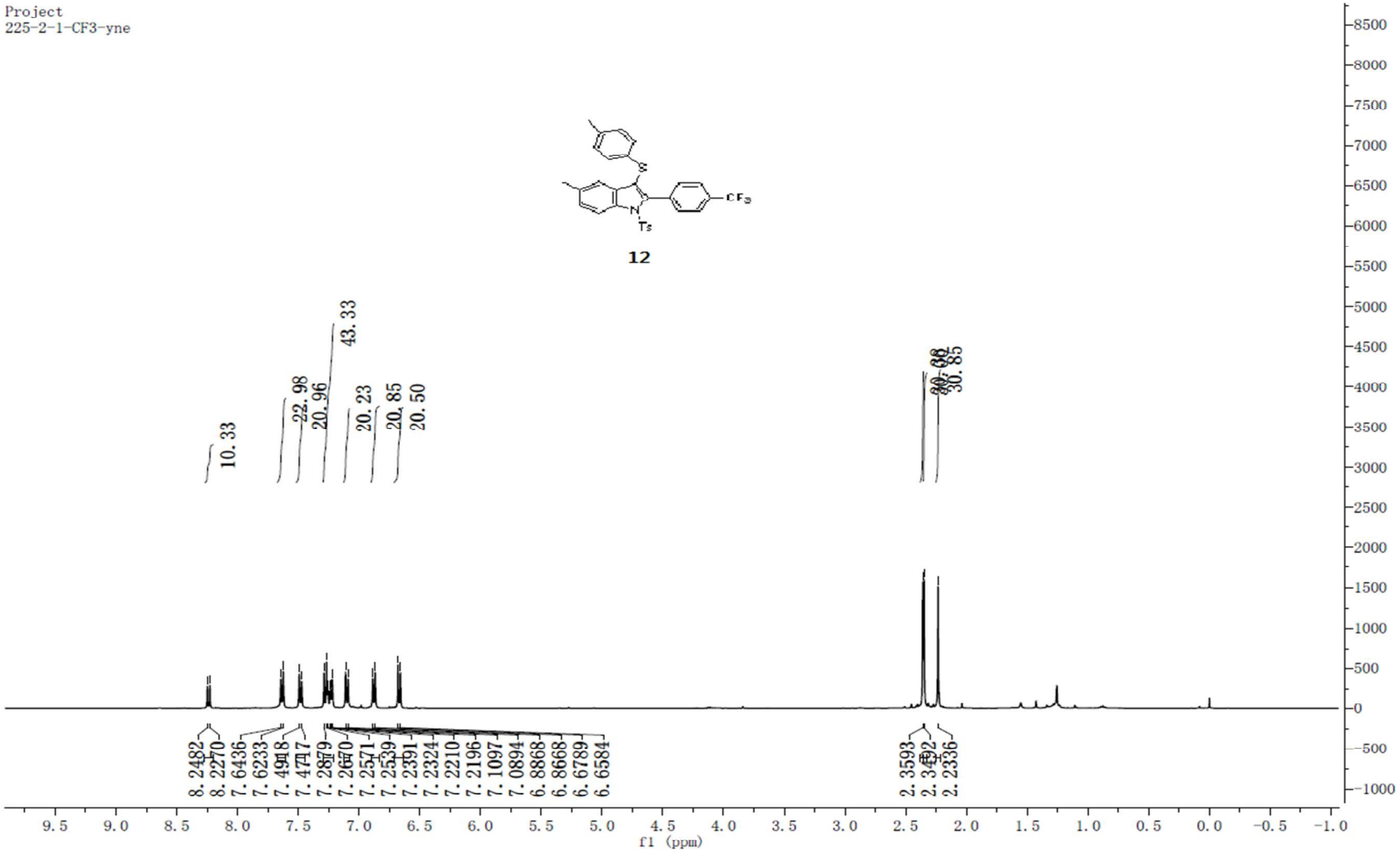

对甲基苯炔（PE）
213-1-p-ch3-yne-c
Ts
9
145.4617
144.6692
139.1017
135.6321
134.8506
134.7492
134.4592
133.3538
131.6841
131.2427
129.4705
129.2624
127.9214
127.2589
127.0020
126.8435
126.3176
119.8983
116.2300
113.4653
21.5163
21.2497
20.8181
f1 (ppm)

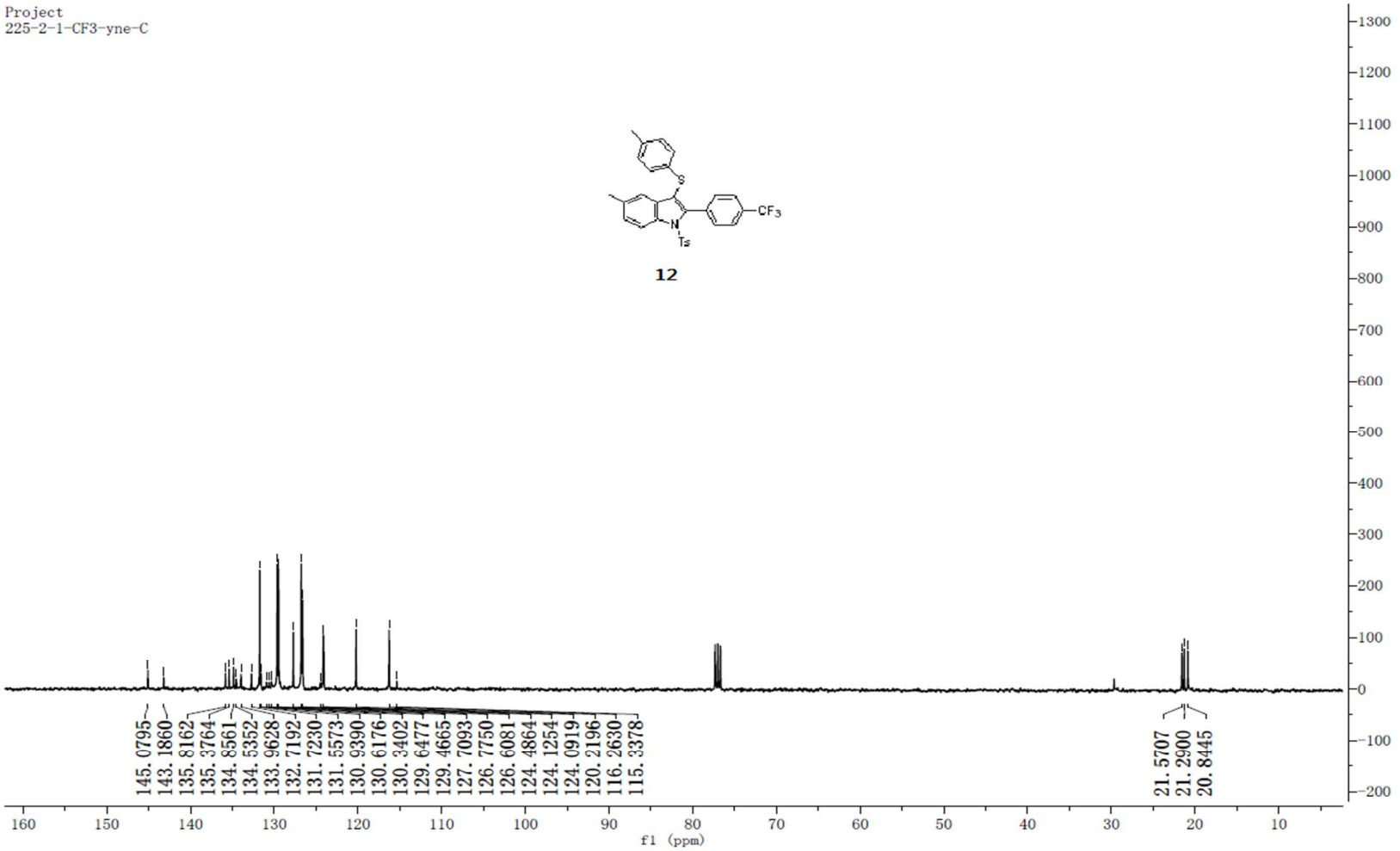

对甲氧基苯炔
177-3-1
OMe
Ts
10
40.68
40.83
21.15
20.37
20.72
10.71
30.70
30.76
8.2439
8.2229
7.2914
7.2855
7.2744
7.2694
7.2643
7.2356
7.2094
7.2065
7.1835
7.1814
7.0897
7.0695
6.9241
6.9172
6.9124
6.9000
6.8952
6.8880
6.8780
6.8580
6.6836
6.6631
3.8456
2.3457
2.3398
2.2291
f1 (ppm)

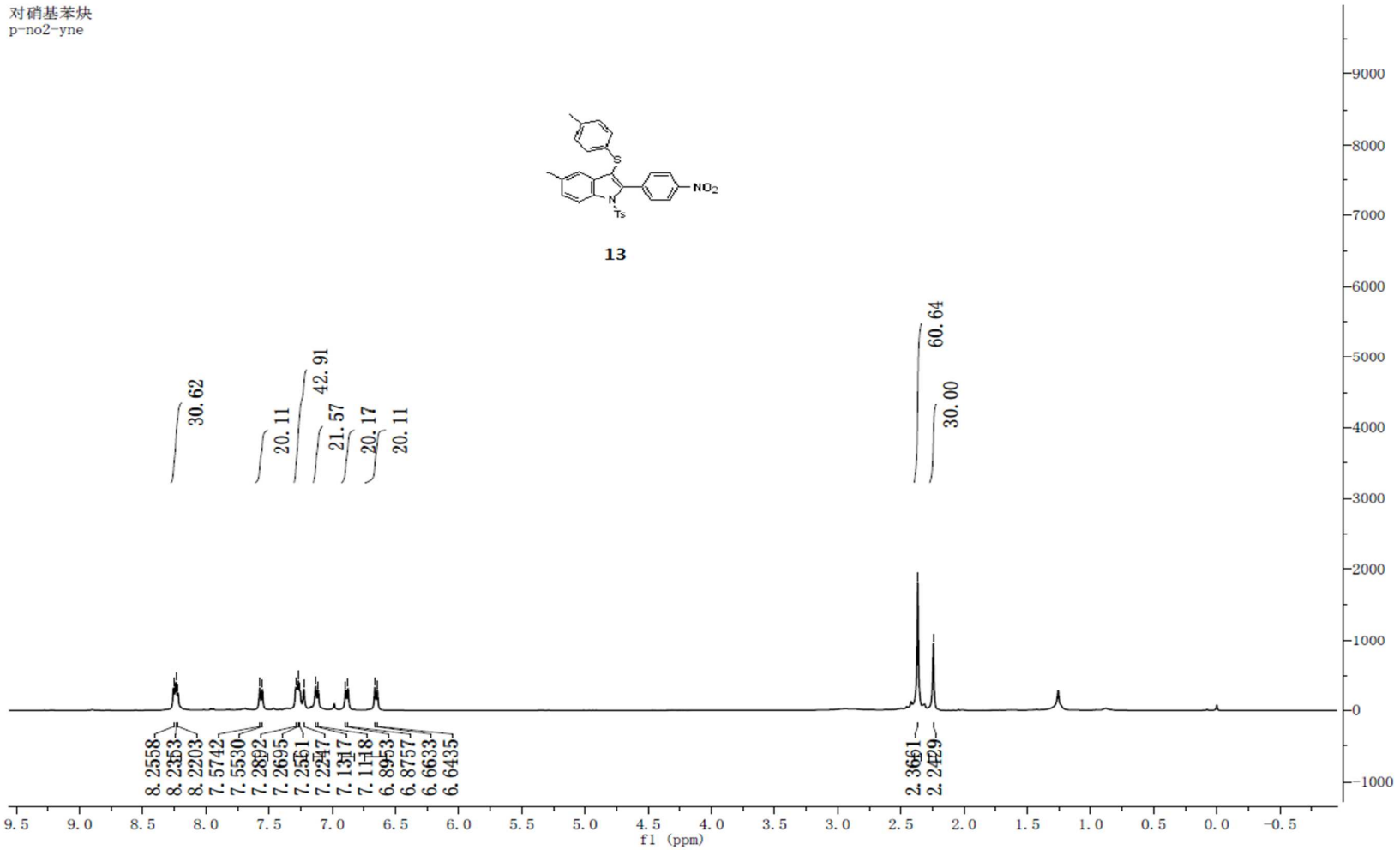

p-OMe-yne
177-3-1c
S
OMe
N
Ts
10
160.2592
145.3452
144.6685
135.6545
134.8536
134.4913
133.4434
132.8125
131.7519
129.5015
129.2763
126.9543
126.8575
126.2728
122.3266
119.8348
116.3230
113.1573
112.9240
112.6461
55.1693
21.5569
21.2796
20.8420
f1 (ppm)

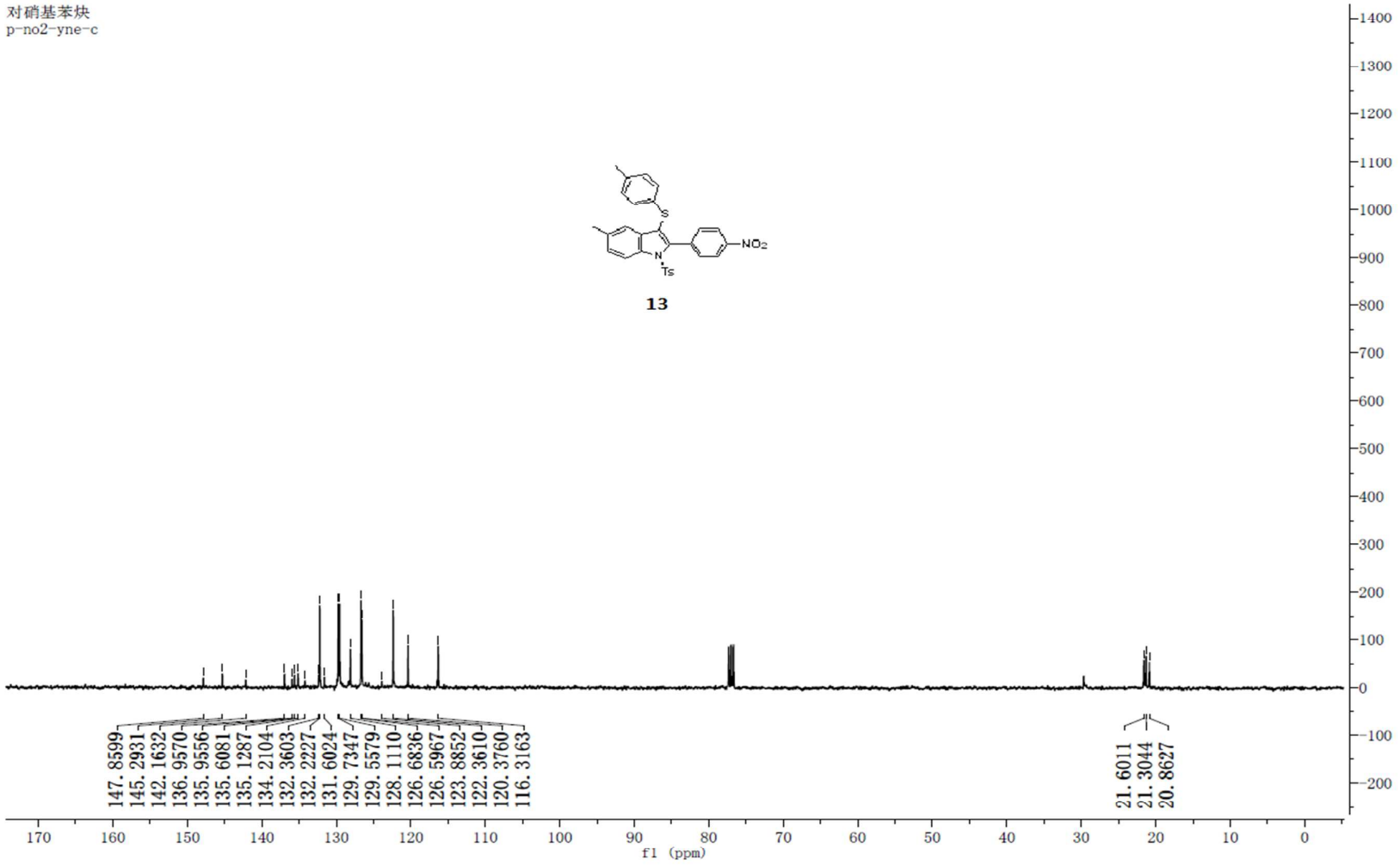

P-Cl-yne
189-2-yne-cl
11
10.60
40.94
20.69
20.97
21.38
20.68
20.87
30.64
7.3655
7.3442
7.2937
7.2895
7.2722
7.2688
7.2510
7.2337
7.2122
7.1992
7.1048
7.0844
6.8834
6.8632
6.6708
6.6504
2.3509
2.3459
2.2316
f1 (ppm)

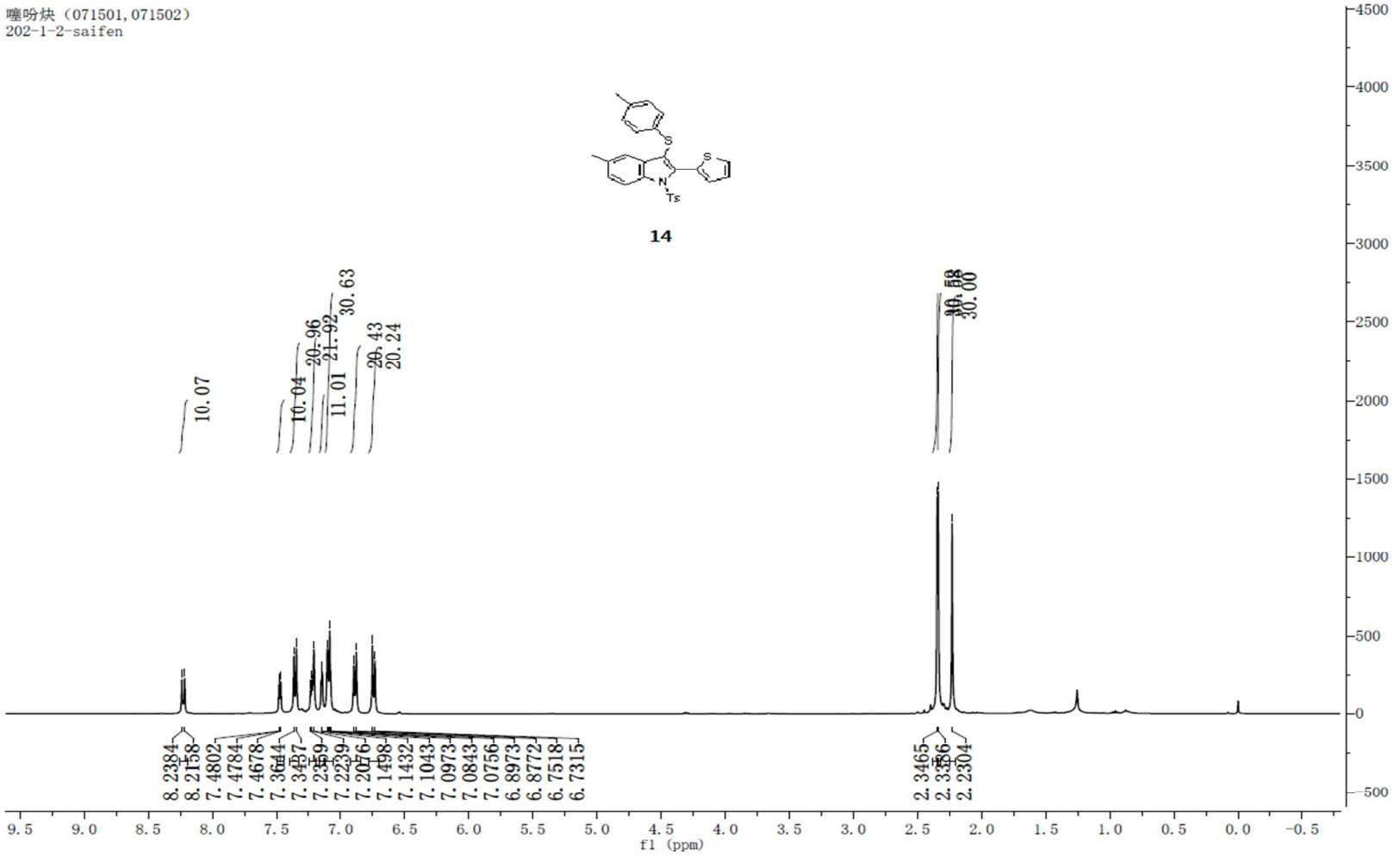

P-Cl-yne
189-2-yne-cl-c
11
144.9486
143.7924
135.7087
135.2819
135.1679
134.7155
134.6306
132.9478
132.6588
131.5752
129.5939
129.4007
128.6536
127.4983
127.4289
126.7687
126.4100
120.0519
116.2552
114.4014
21.5742
21.2837
20.8498
f1 (ppm)

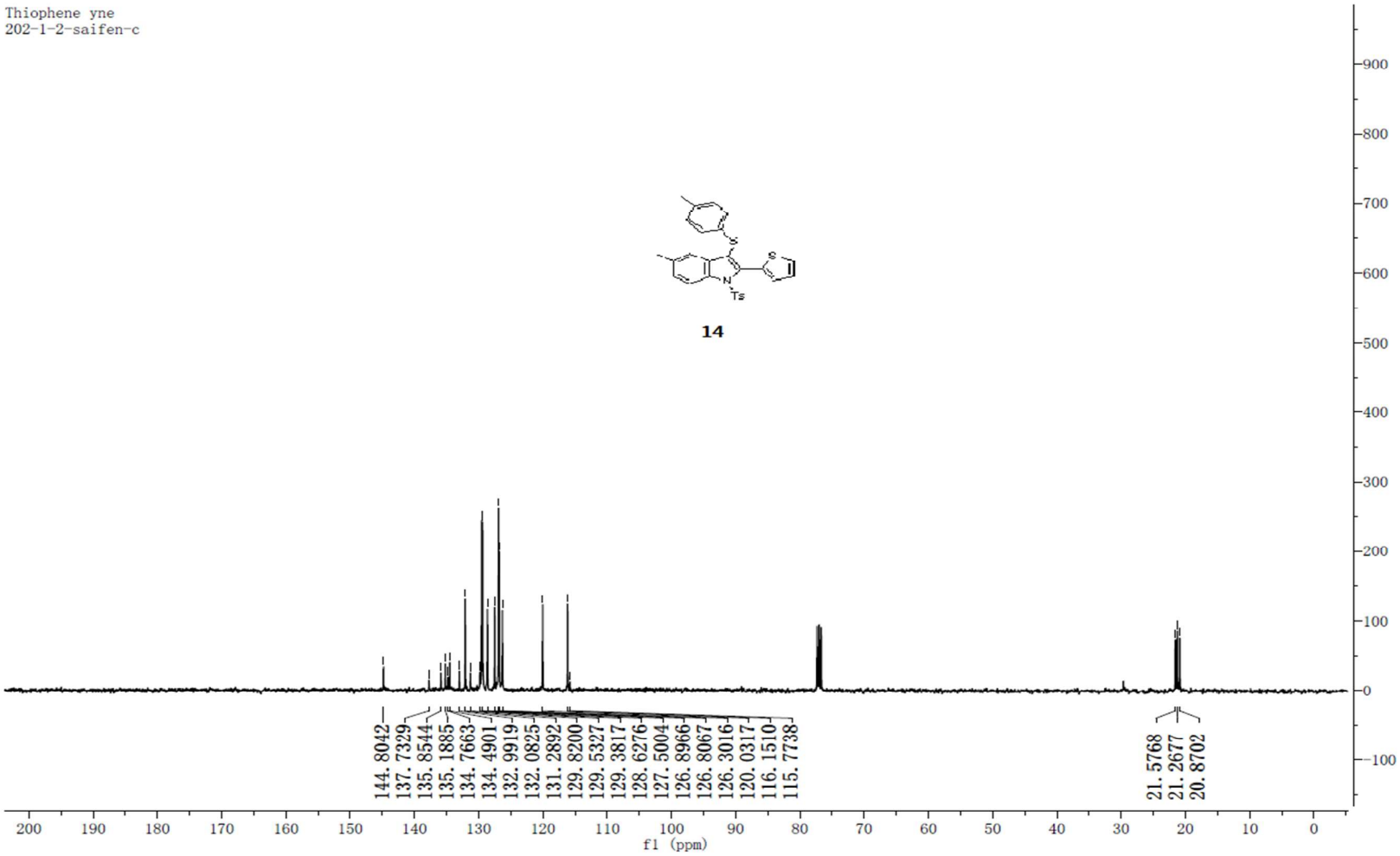

Project
225-2-1-CF3-yne
12
f1 (ppm)

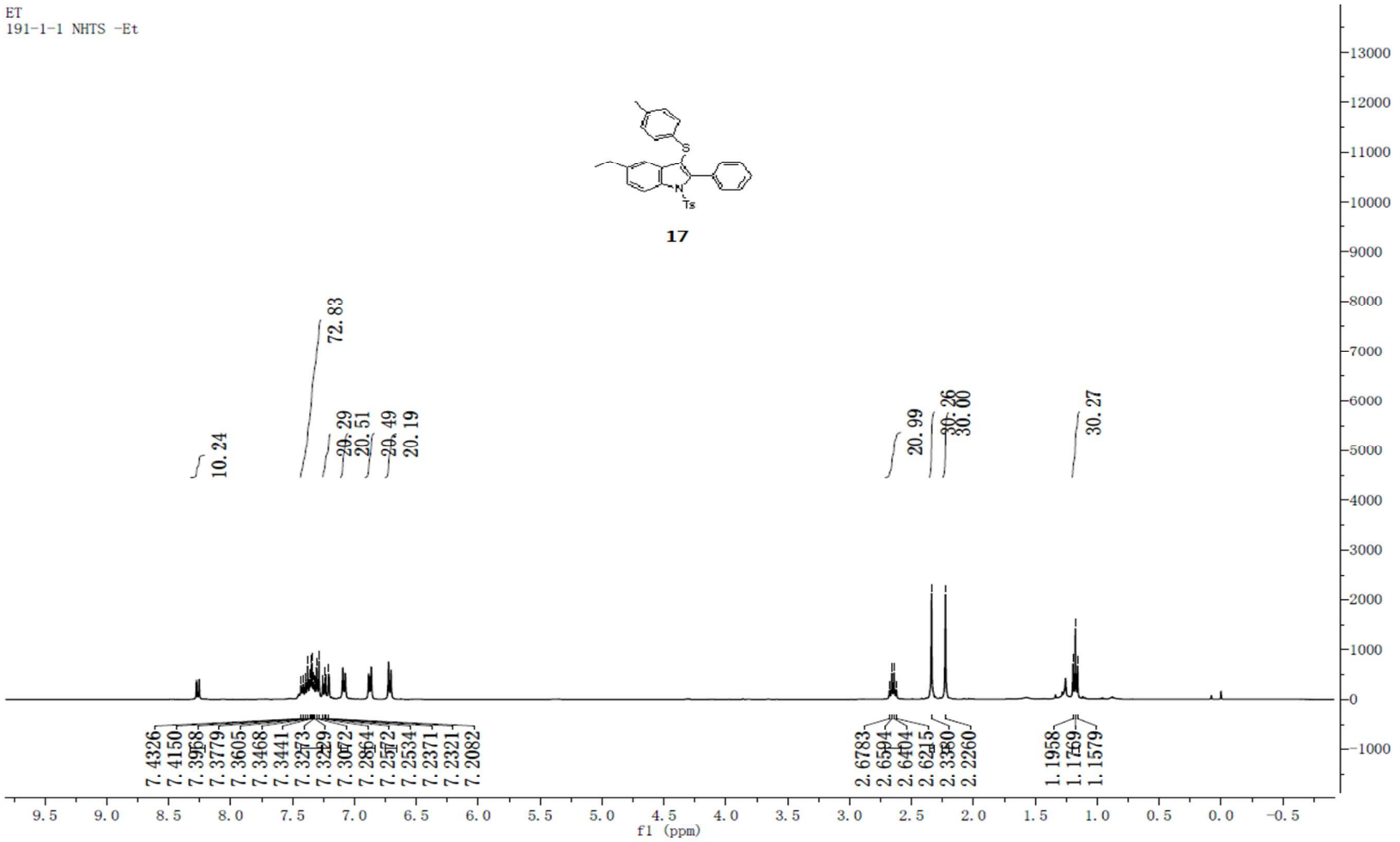

Project
225-2-1-CF3-yne-C
12
145.0795
143.1860
135.8162
135.3764
134.8561
134.5352
133.9628
132.7192
131.7230
131.5573
130.9390
130.6176
130.3402
129.6477
129.4665
127.7093
126.7750
126.6081
124.4864
124.1254
124.0919
120.2196
116.2630
115.3378
21.5707
21.2900
20.8445
f1 (ppm)

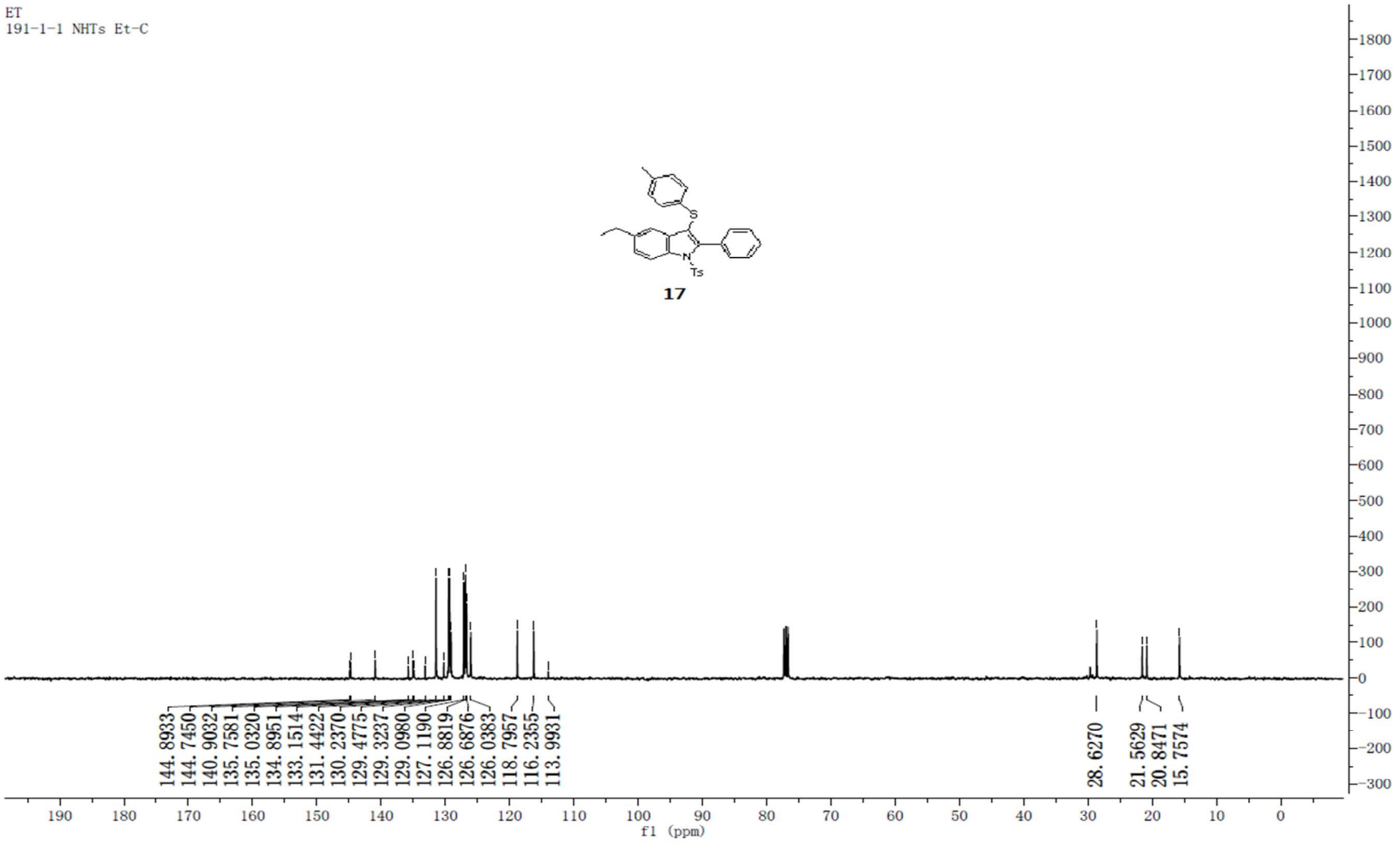

对硝基苯炔
p-no2-yne
NO2
Ts
13
30.62
20.11
42.91
21.57
20.17
20.11
60.64
30.00
8.2558
8.2353
8.2203
7.5742
7.5530
7.2892
7.2695
7.2561
7.2247
7.1317
7.1118
6.8953
6.8757
6.6633
6.6435
2.3661
2.2429
f1 (ppm)

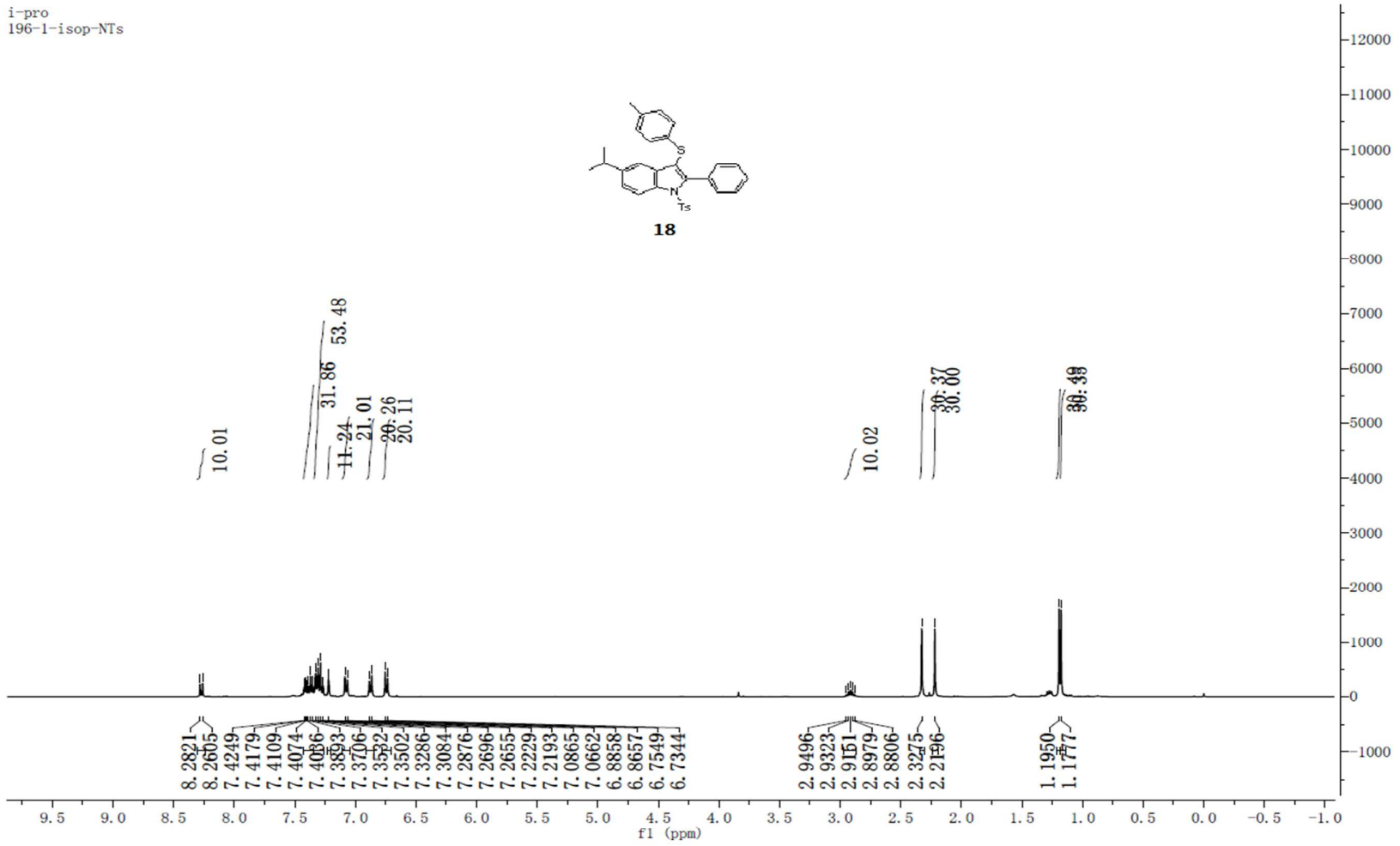

对硝基苯炔
p-no2-yne-c
13
147.8599
145.2931
142.1632
136.9570
135.9556
135.6081
135.1287
134.2104
132.3603
132.2227
131.6024
129.7347
129.5579
128.1110
126.6836
126.5967
123.8852
122.3610
120.3760
116.3163
21.6011
21.3044
20.8627
f1 (ppm)

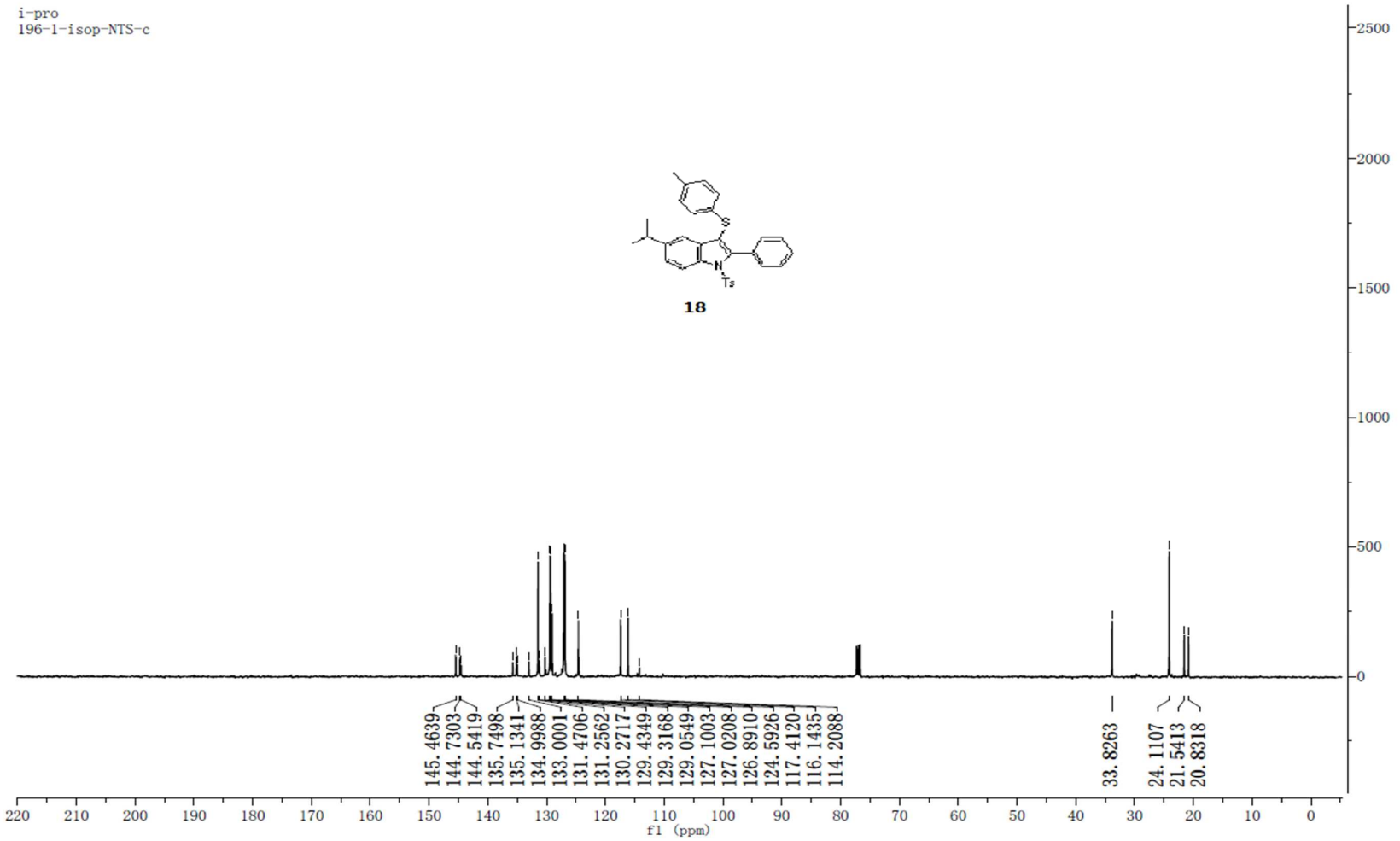

噻吩炔（071501,071502）
202-1-2-saifen
14
Ts
10.07
10.04
20.96
21.92
11.01
30.63
20.43
20.24
30.00
8.2384
8.2158
7.4802
7.4784
7.4678
7.3644
7.3457
7.2359
7.2239
7.2076
7.1498
7.1432
7.1043
7.0973
7.0843
7.0756
6.8973
6.8772
6.7518
6.7315
2.3465
2.3356
2.2304
f1 (ppm)

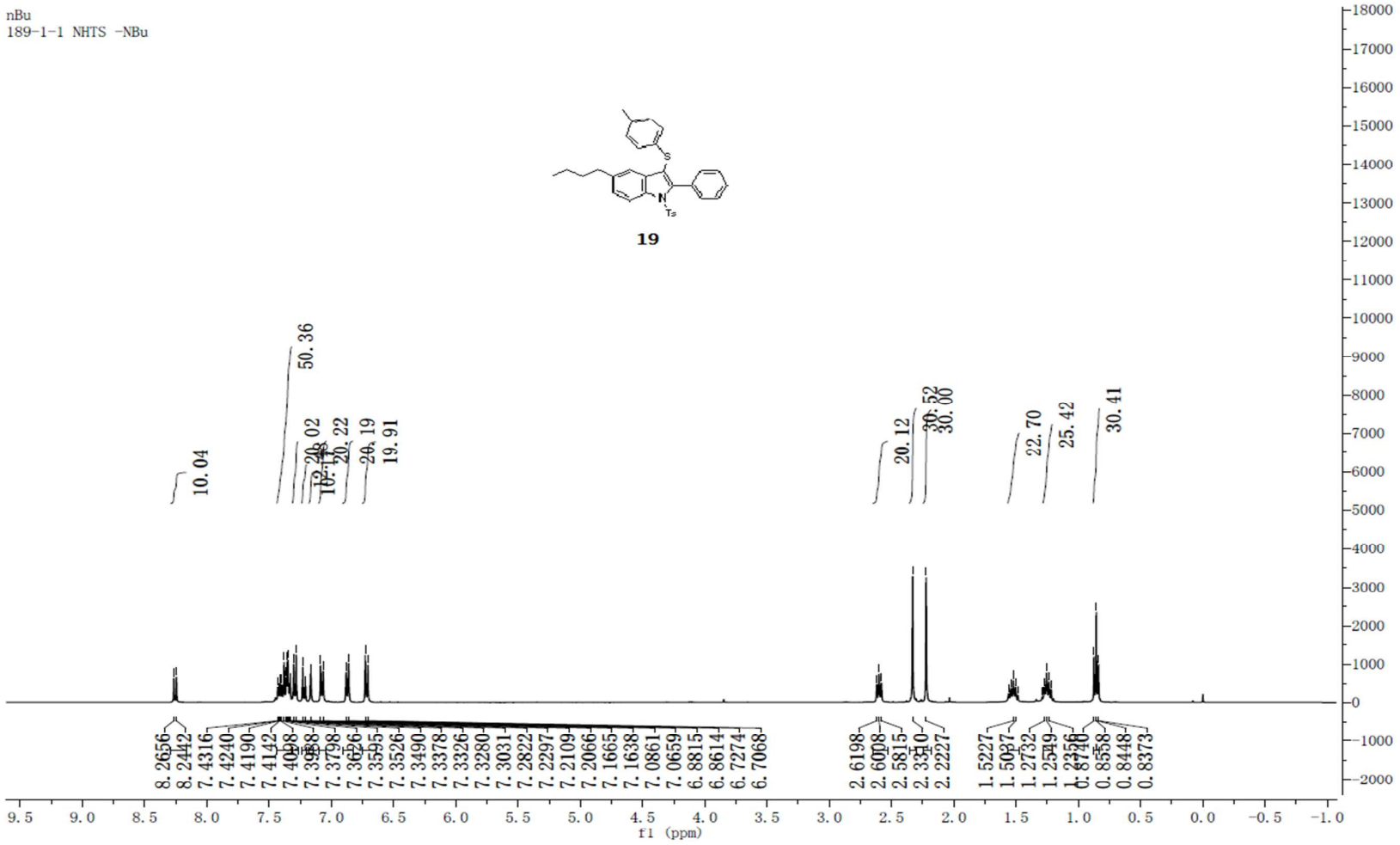

Thiophene yne
202-1-2-saifen-c
Ts
14
144.8042
137.7329
135.8544
135.1885
134.7663
134.4901
132.9919
132.0825
131.2892
129.8200
129.5327
129.3817
128.6276
127.5004
126.8966
126.8067
126.3016
120.0317
116.1510
115.7738
21.5768
21.2677
20.8702
f1 (ppm)

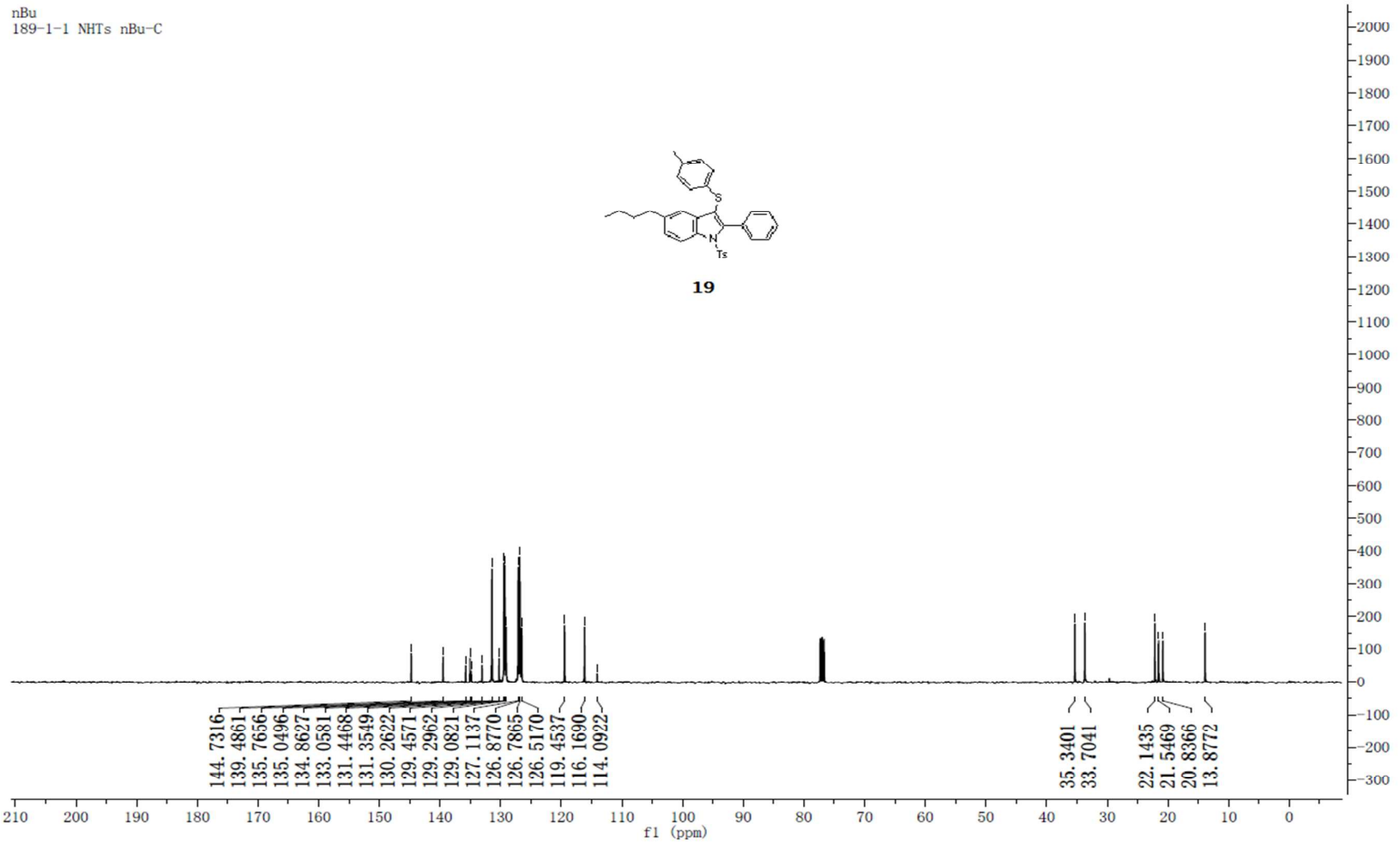

ET
191-1-1 NHTS -Et
17
Ts
10.24
72.83
20.29
20.51
20.49
20.19
20.99
30.26
30.00
30.27
7.4326
7.4150
7.3968
7.3779
7.3605
7.3468
7.3441
7.3273
7.3229
7.3072
7.2864
7.2572
7.2534
7.2371
7.2321
7.2082
2.6783
2.6594
2.6404
2.6215
2.3380
2.2260
1.1958
1.1769
1.1579
f1 (ppm)

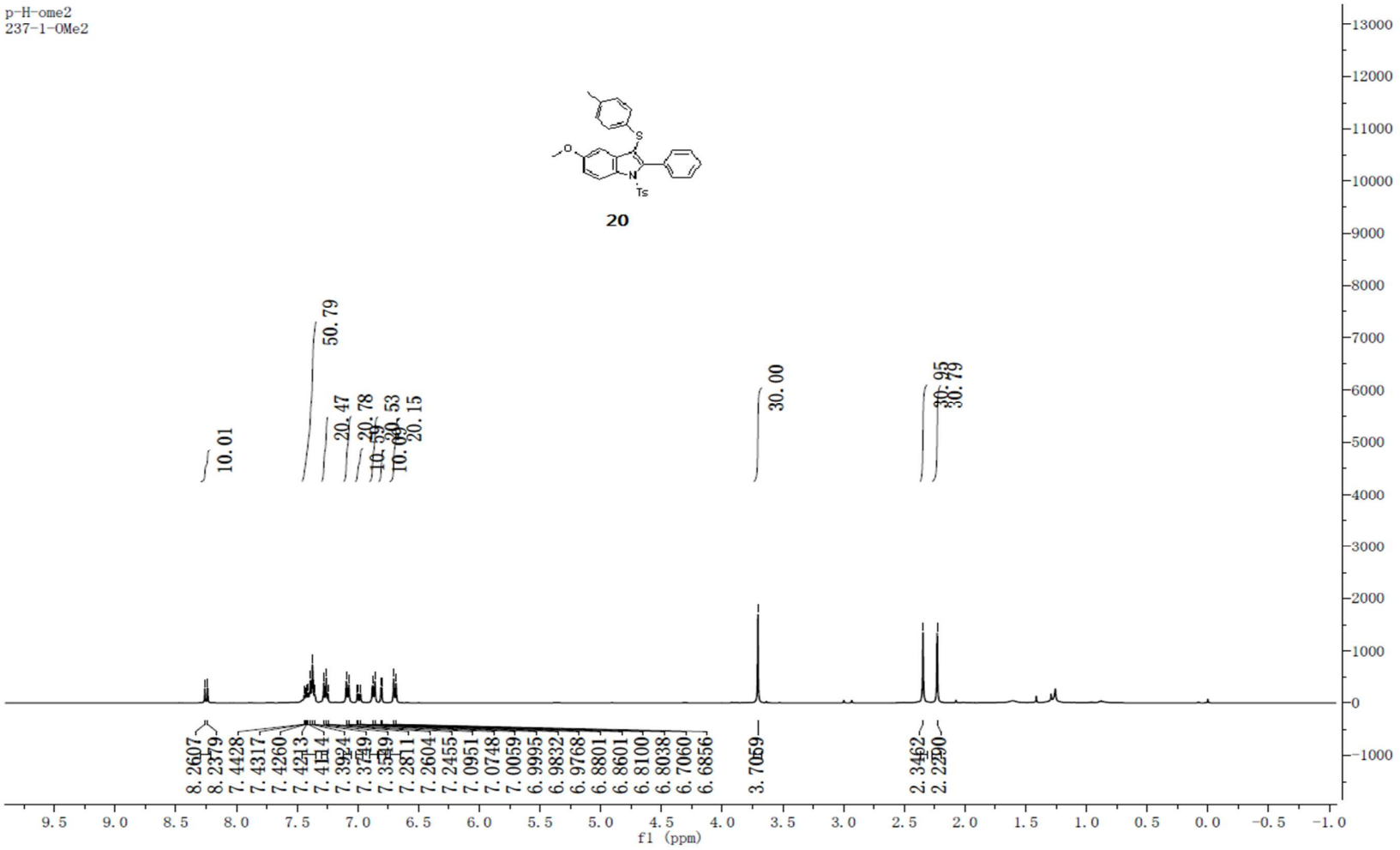

ET
191-1-1 NHTs Et-C
S
N
Ts
17
144.8933
144.7450
140.9032
135.7581
135.0320
134.8951
133.1514
131.4422
130.2370
129.4775
129.3237
129.0980
127.1190
126.8819
126.6876
126.0383
118.7957
116.2355
113.9931
28.6270
21.5629
20.8471
15.7574
f1 (ppm)

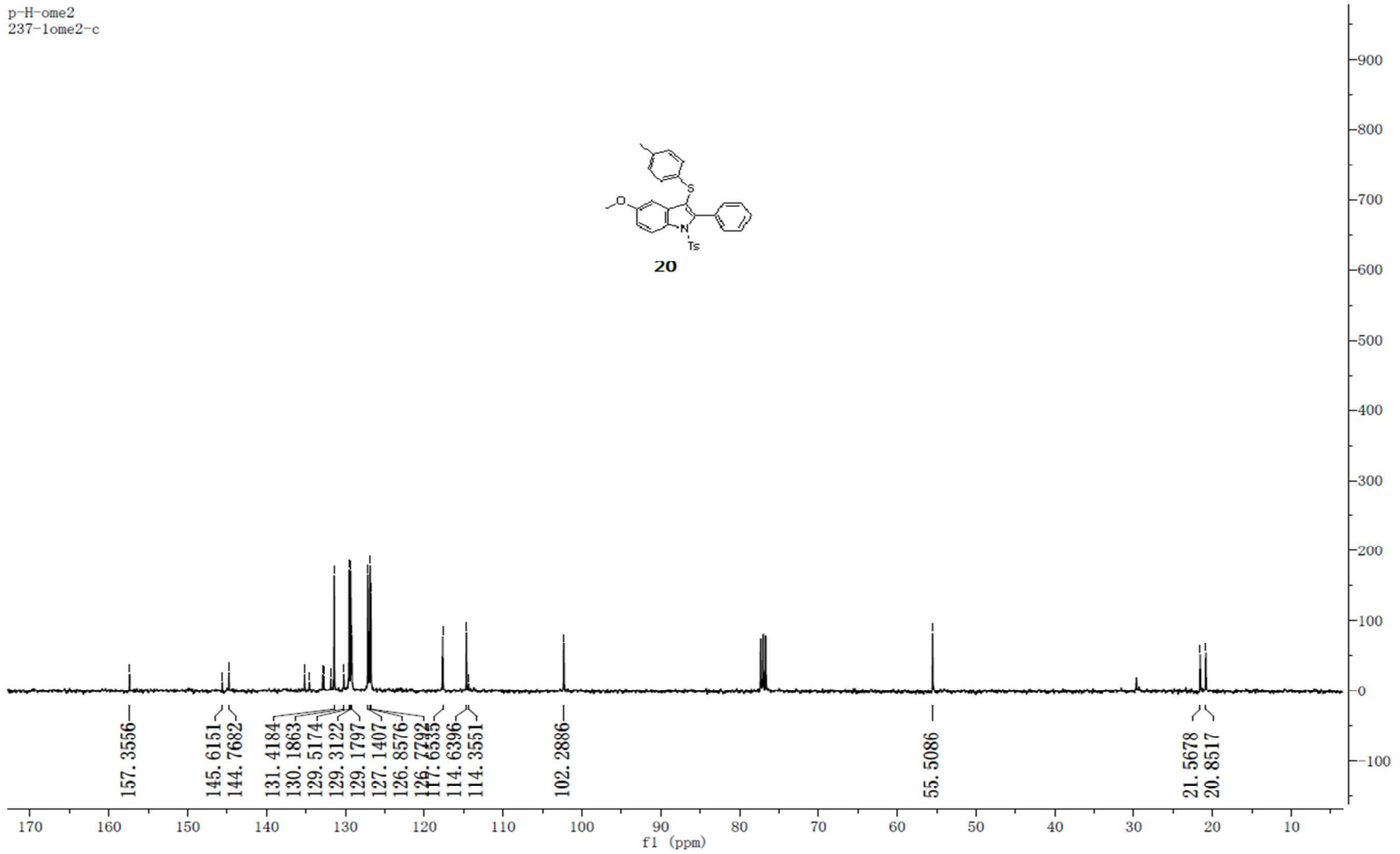

i-pro
196-1-isop-NTs
18
Ts
10.01
53.48
31.86
11.24
21.01
20.26
20.11
10.02
30.37
30.00
8.2821
8.2605
7.4249
7.4179
7.4109
7.4074
7.3853
7.3706
7.3502
7.3286
7.3084
7.2876
7.2696
7.2655
7.2229
7.2193
7.0865
7.0662
6.8858
6.8657
6.7549
6.7344
2.9496
2.9323
2.9151
2.8979
2.8806
2.3275
2.2196
1.1950
1.1777
f1 (ppm)

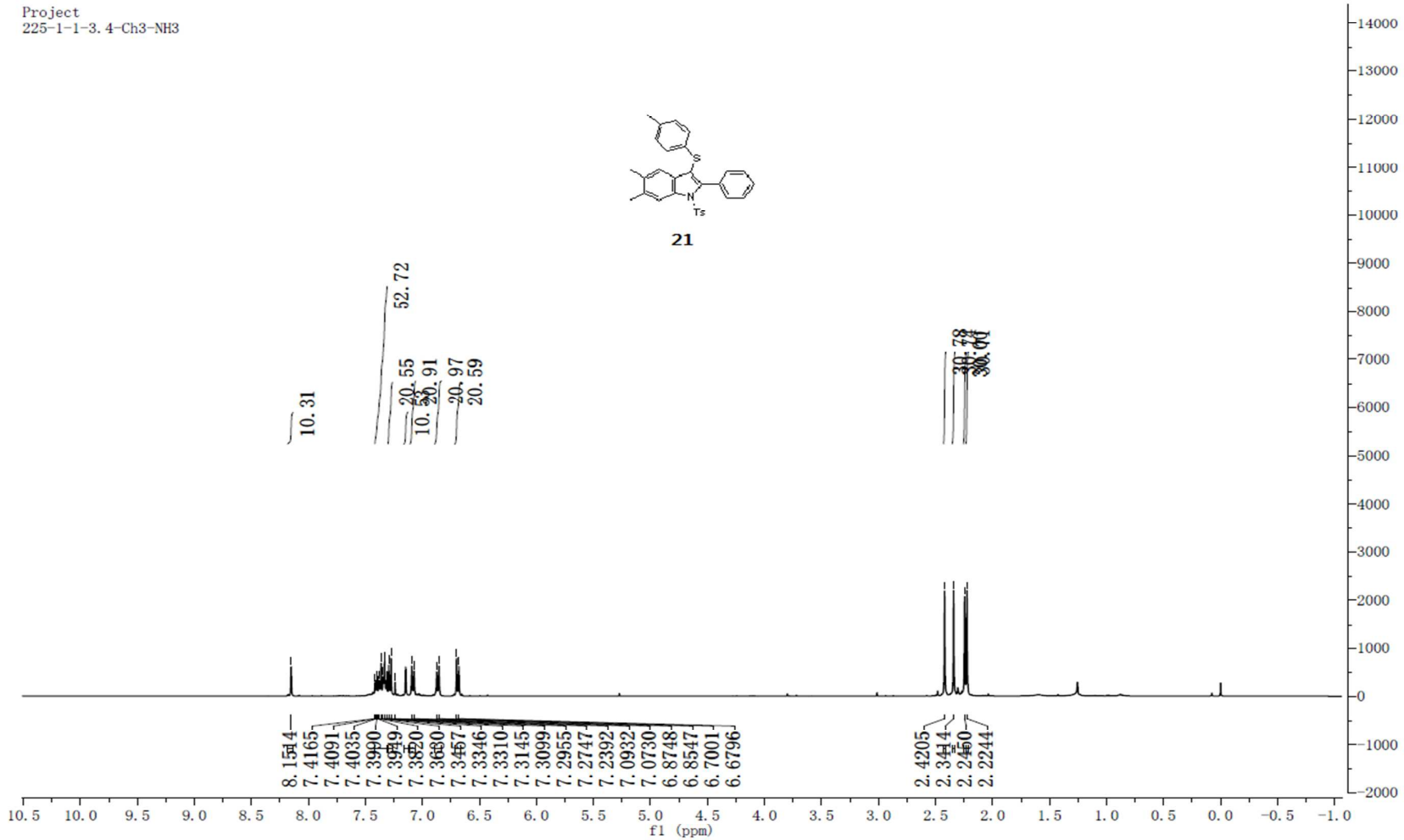

i-pro
196-1-isop-NTS-c
18
Ts
145.4639
144.7303
144.5419
135.7498
135.1341
134.9988
133.0001
131.4706
131.2562
130.2717
129.4349
129.3168
129.0549
127.1003
127.0208
126.8910
124.5926
117.4120
116.1435
114.2088
33.8263
24.1107
21.5413
20.8318
f1 (ppm)

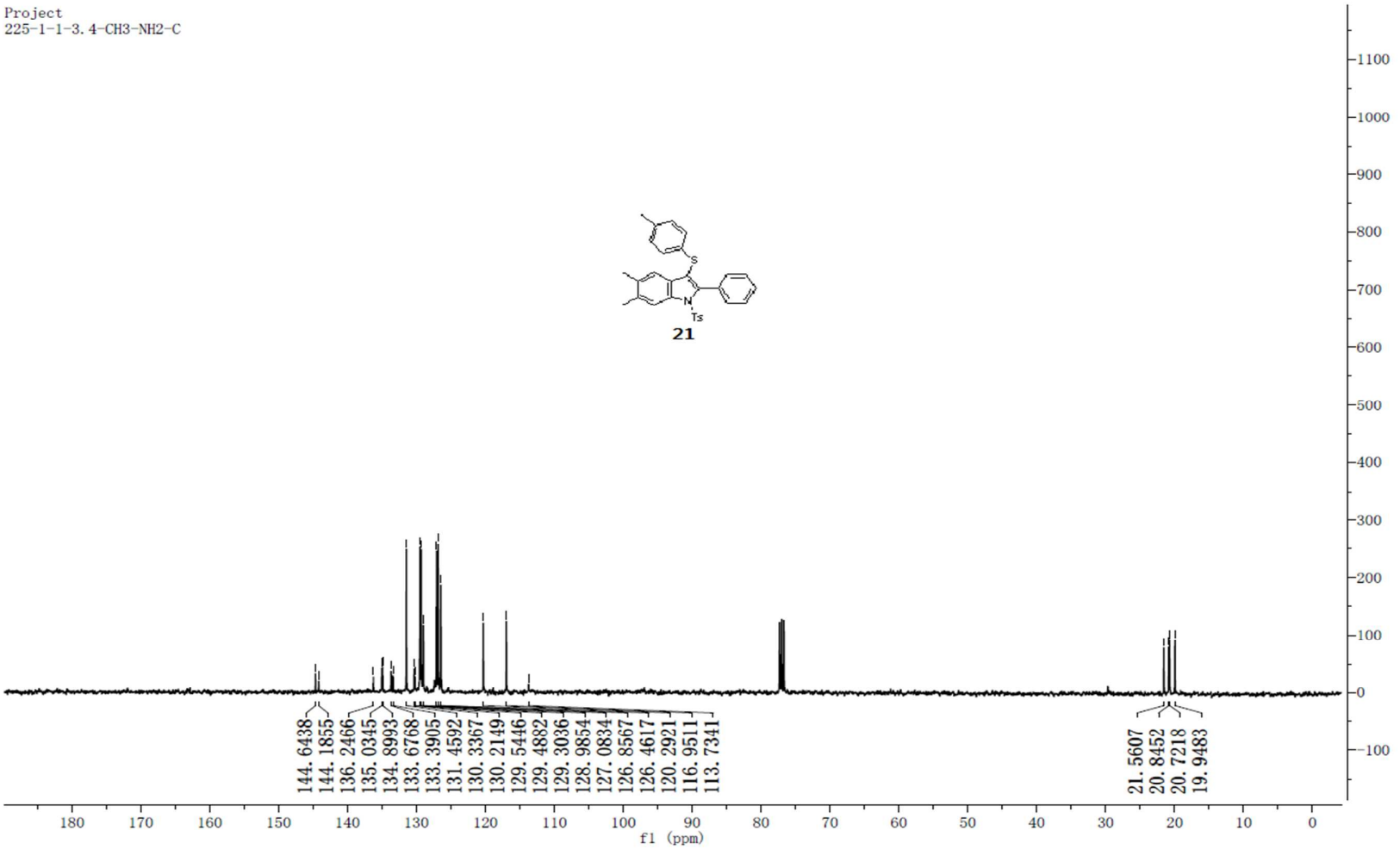

nBu
189-1-1 NHTS -NBu
19
10.04
50.36
20.02
20.22
20.19
19.91
20.12
30.52
30.00
22.70
25.42
30.41
f1 (ppm)

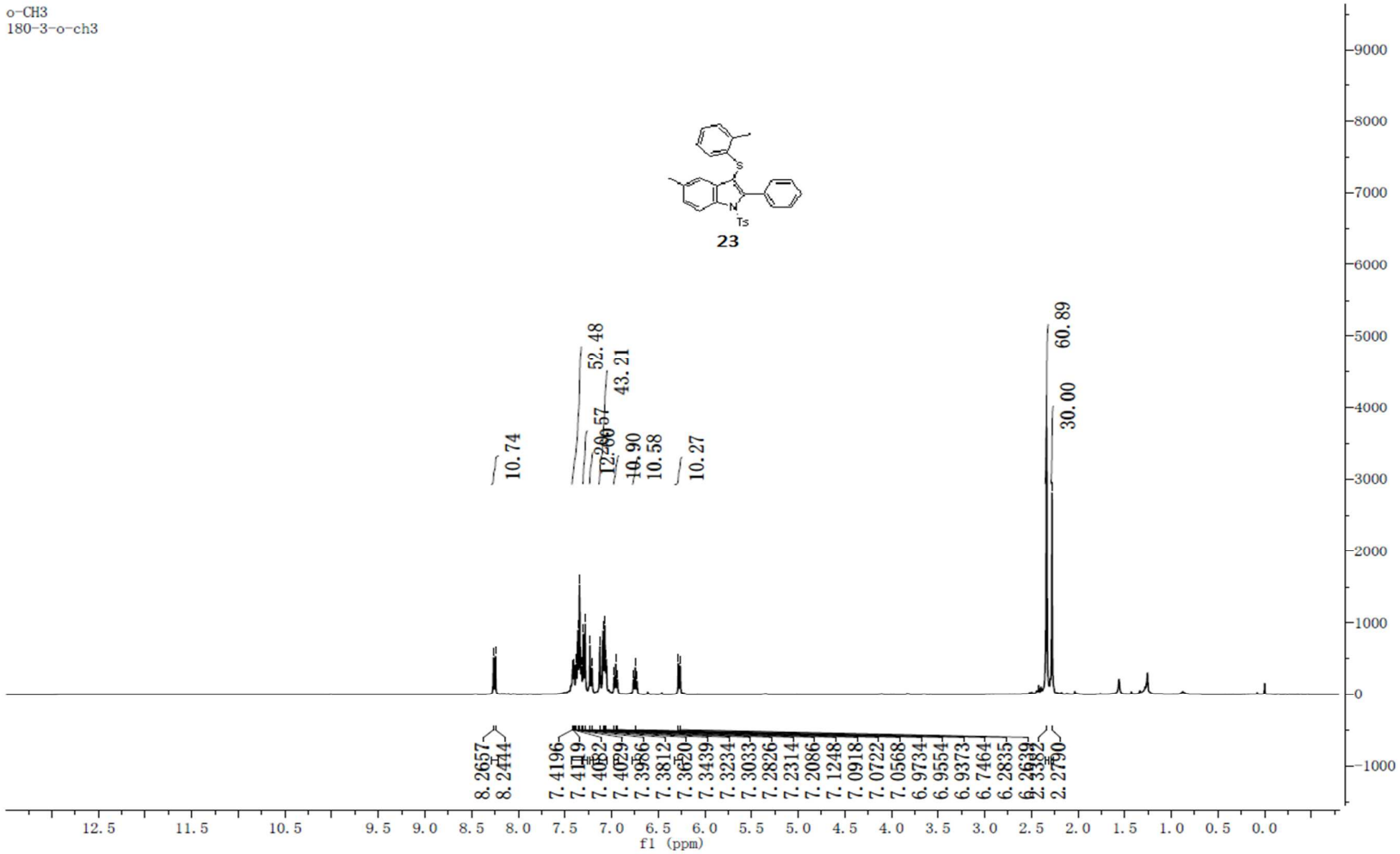

nBu
189-1-1 NHTs nBu-C
19
144.7316
139.4861
135.7656
135.0496
134.8627
133.0581
131.4468
131.3549
130.2622
129.4571
129.2962
129.0821
127.1137
126.8770
126.7865
126.5170
119.4537
116.1690
114.0922
35.3401
33.7041
22.1435
21.5469
20.8366
13.8772
f1 (ppm)

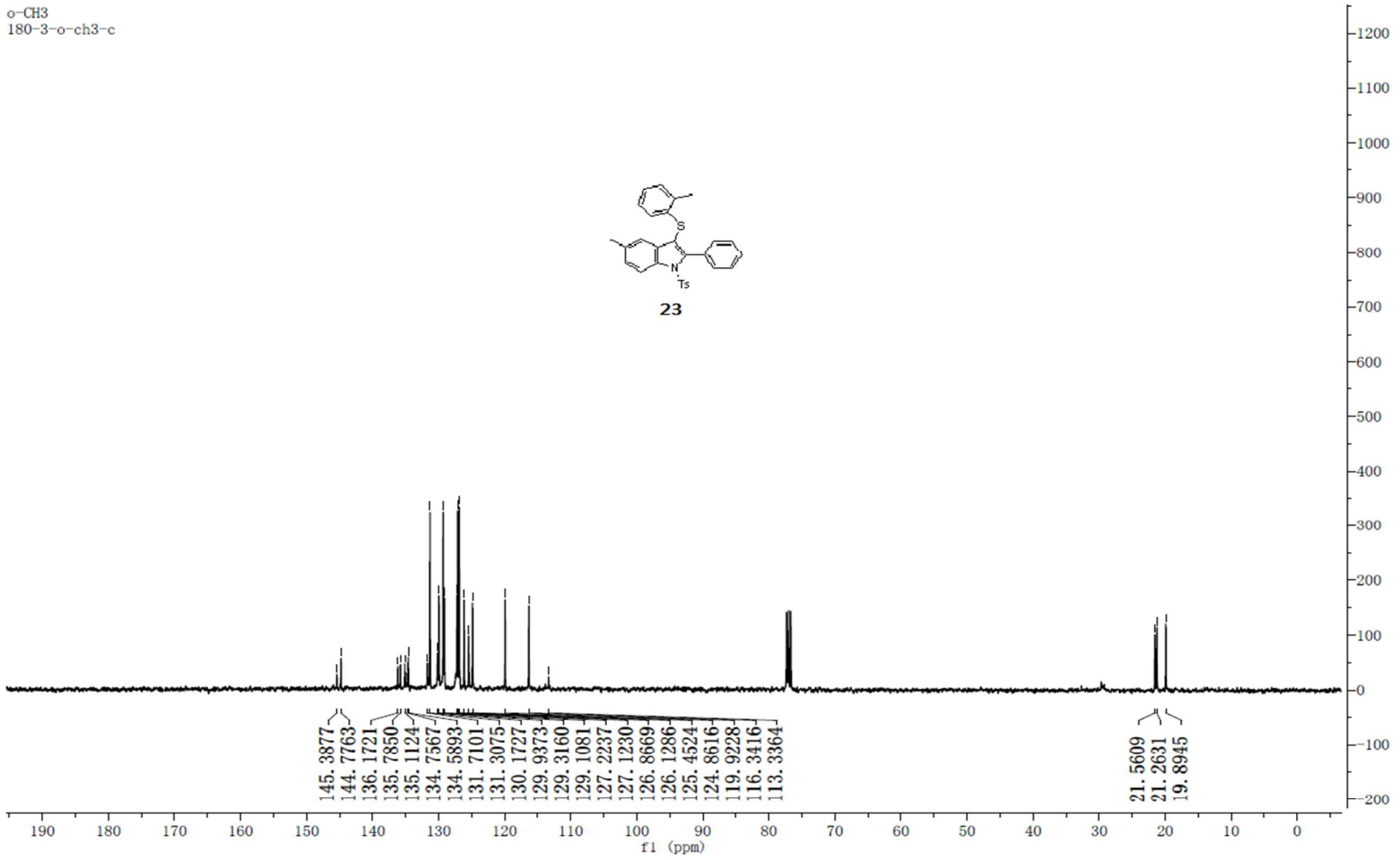

p-H-ome2
237-1-OMe2
20
10.01
50.79
20.47
20.78
10.59
10.69
20.15
30.00
30.95
30.79
8.2607
8.2379
7.4428
7.4317
7.4260
7.4213
7.4114
7.3924
7.3749
7.3589
7.2811
7.2604
7.2455
7.0951
7.0748
7.0059
6.9995
6.9832
6.9768
6.8801
6.8601
6.8100
6.8038
6.7060
6.6856
3.7059
2.3462
2.2790
f1 (ppm)

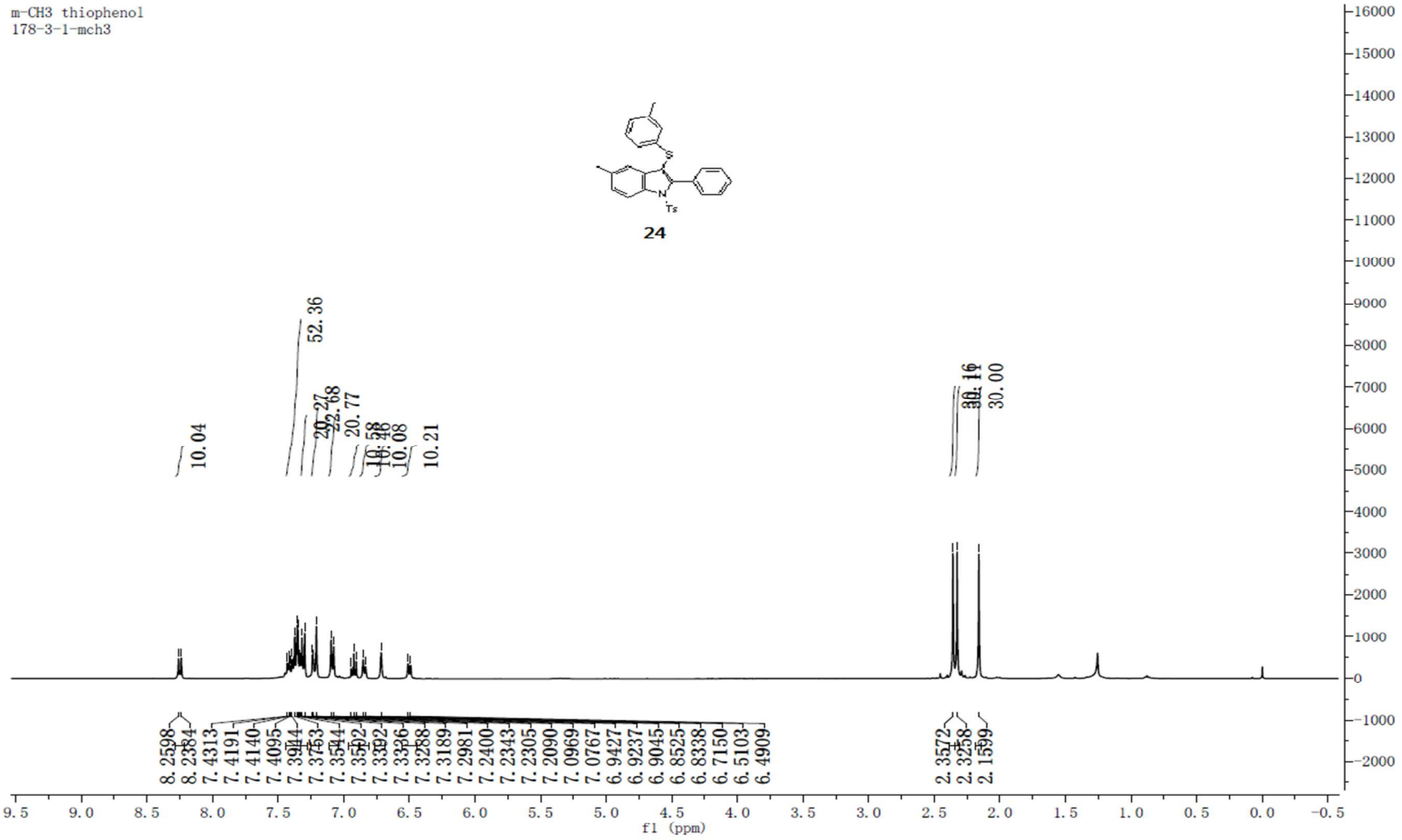

p-H-ome2
237-1ome2-c
20
157.3556
145.6151
144.7682
131.4184
130.1863
129.5174
129.3122
129.1797
127.1407
126.8576
114.6396
114.3551
102.2886
55.5086
21.5678
20.8517
f1 (ppm)

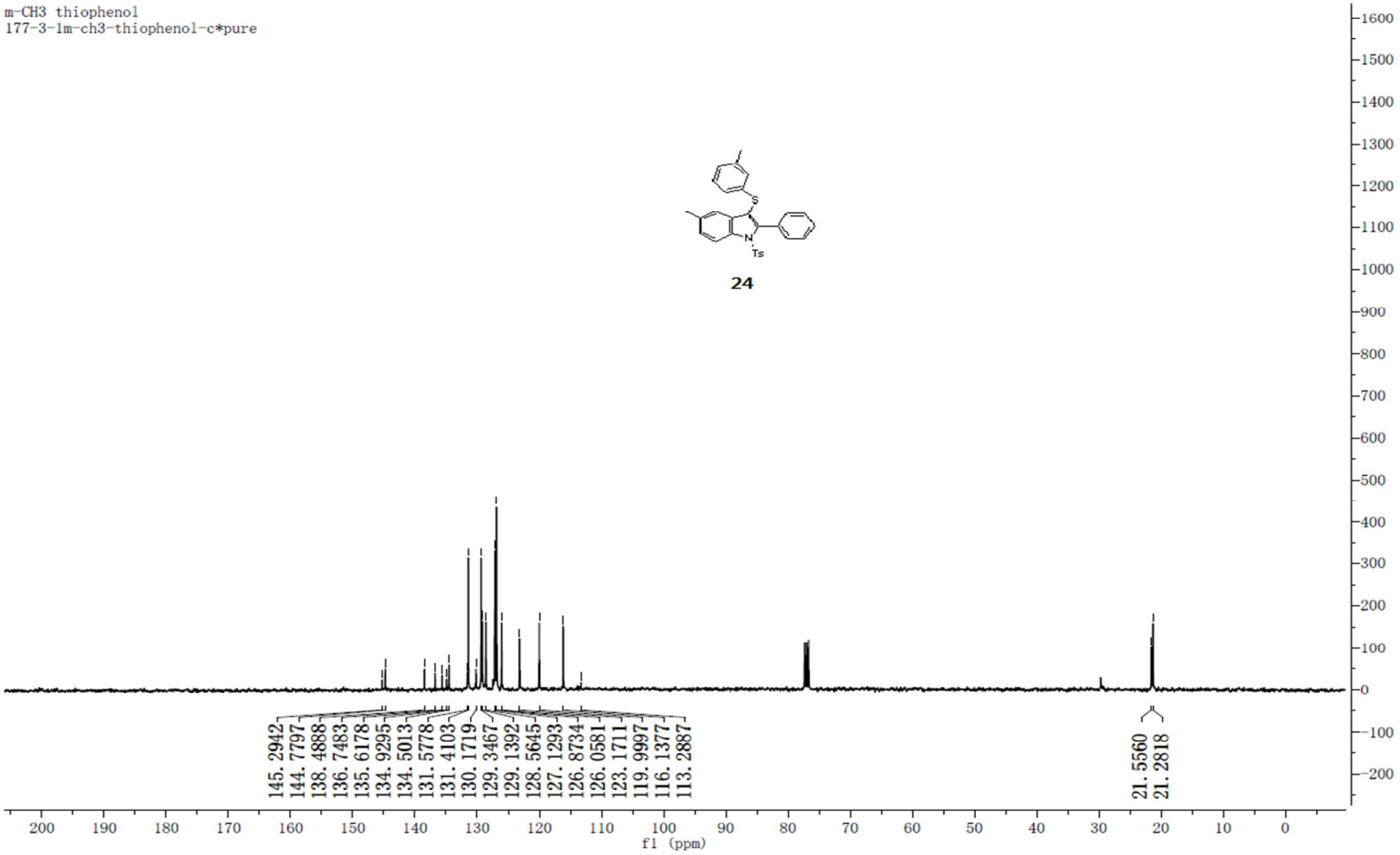

Project
225-1-1-3.4-Ch3-NH3
21
f1 (ppm)

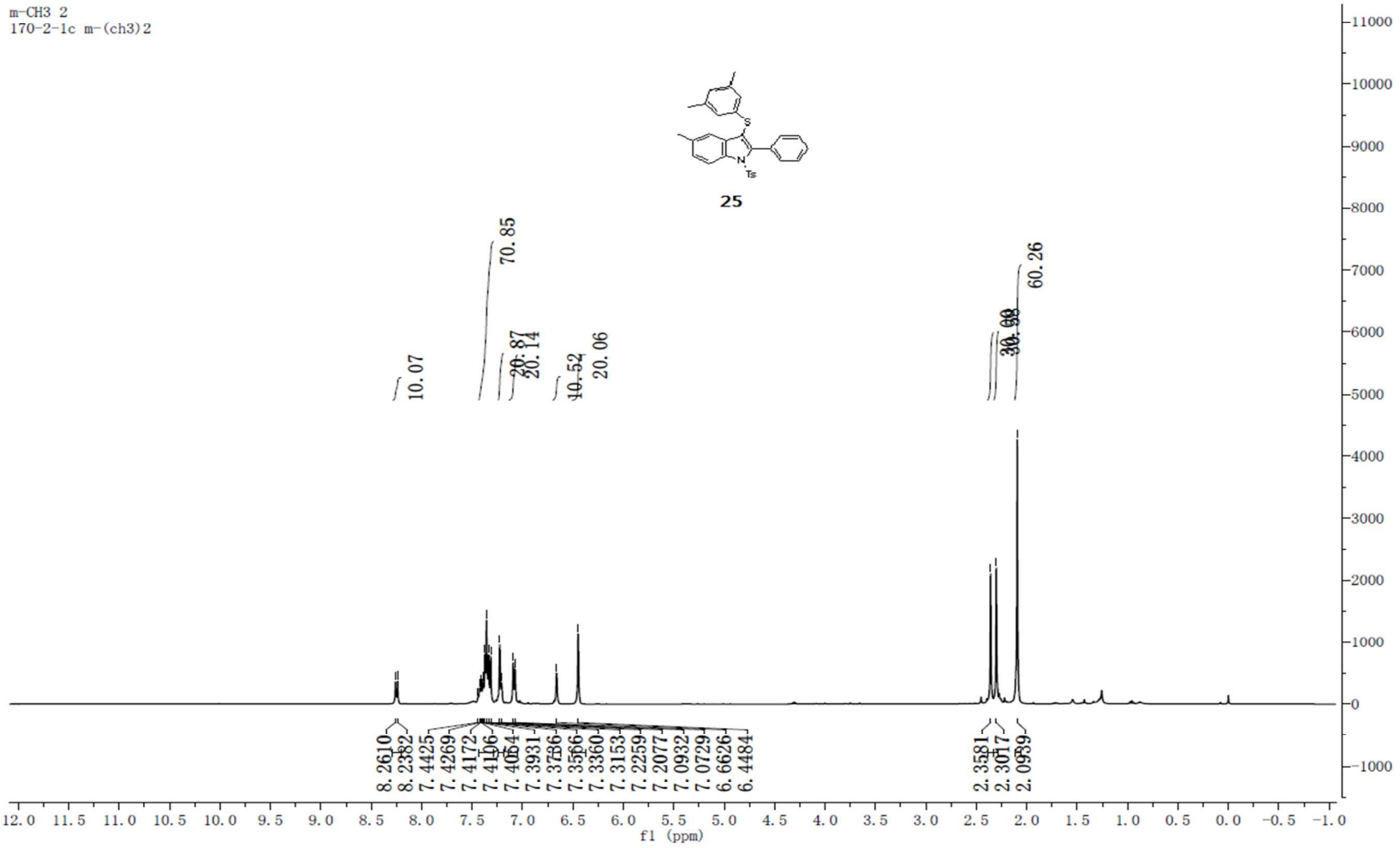

Project
225-1-1-3.4-CH3-NH2-C
S
N
Ts
21
144.6438
144.1855
136.2466
135.0345
134.8993
133.6768
133.3905
131.4592
130.3367
130.2149
129.5446
129.4882
129.3036
128.9854
127.0834
126.8567
126.4617
120.2921
116.9511
113.7341
21.5607
20.8452
20.7218
19.9483
f1 (ppm)

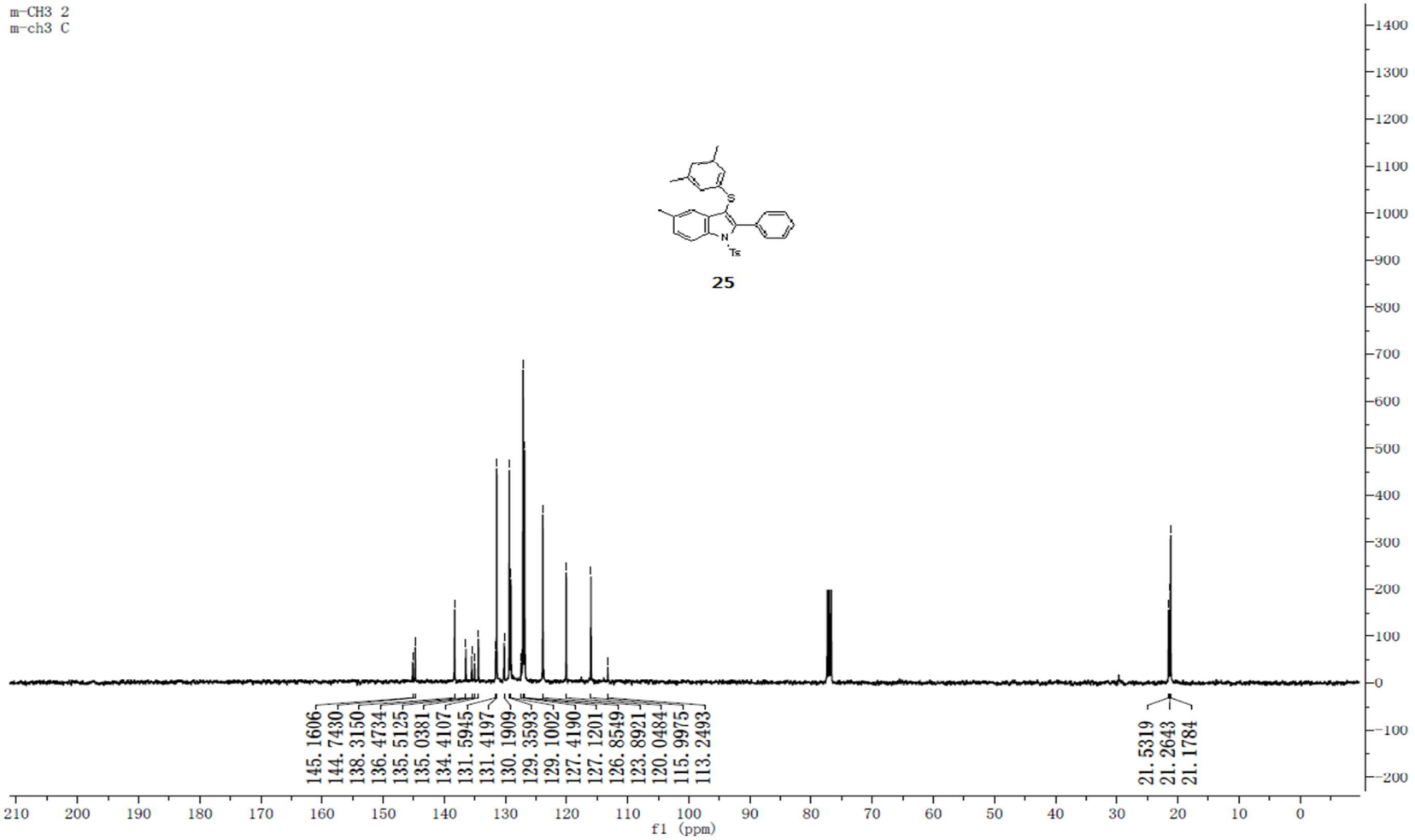

o-CH3
180-3-o-ch3
Ts
23
10.74
52.48
43.21
20.57
12.00
10.90
10.58
10.27
60.89
30.00
8.2657
8.2444
7.4196
7.4119
7.4052
7.4029
7.3986
7.3812
7.3620
7.3439
7.3234
7.3033
7.2826
7.2314
7.2086
7.1248
7.0918
7.0722
7.0568
6.9734
6.9554
6.9373
6.7464
6.2835
2.2790
f1 (ppm)

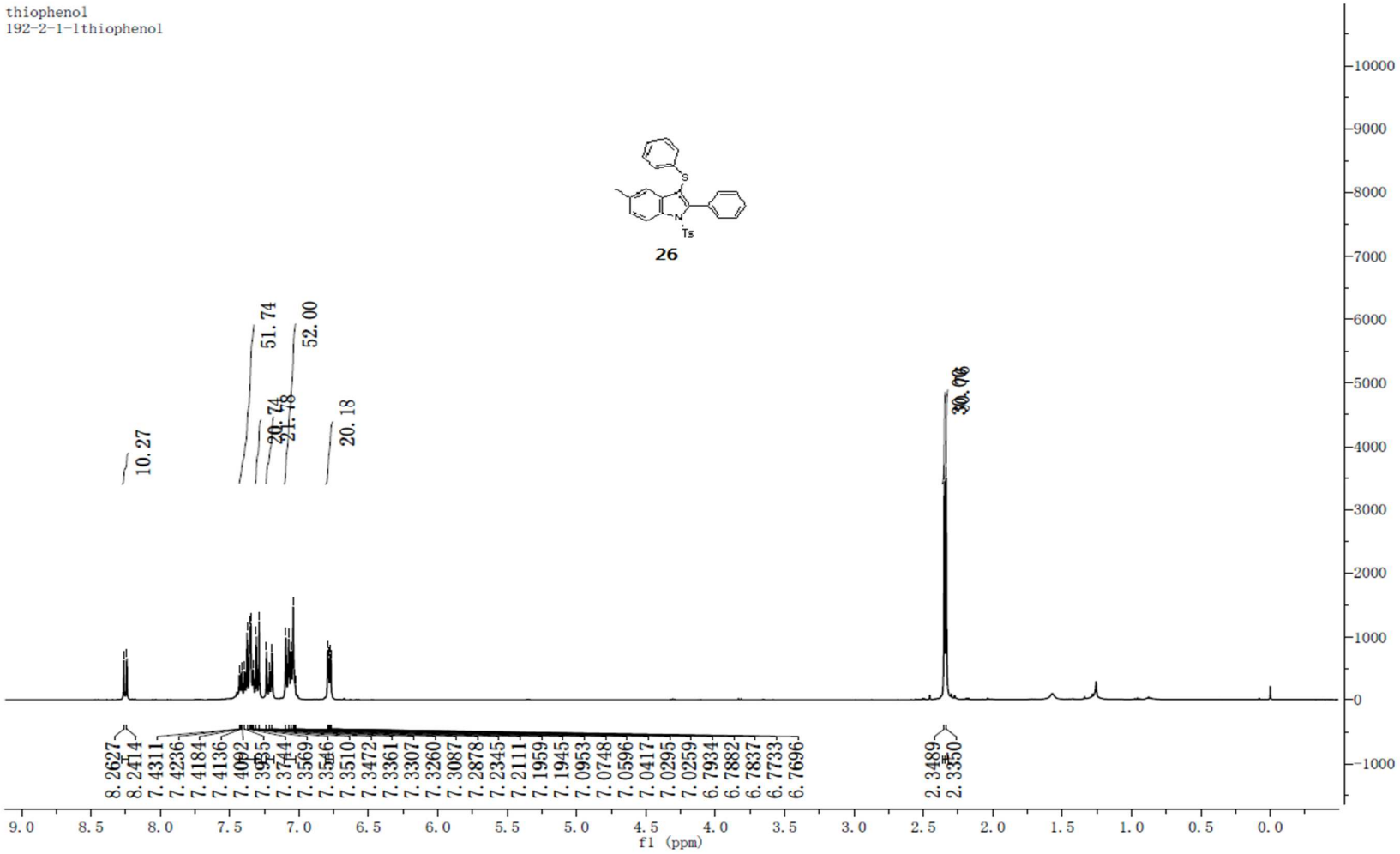

o-CH3
180-3-o-ch3-c
23
Ts
145.3877
144.7763
136.1721
135.7850
135.1124
134.7567
134.5893
131.7101
131.3075
130.1727
129.9373
129.3160
129.1081
127.2237
127.1230
126.8669
126.1286
125.4524
124.8616
119.9228
116.3416
113.3364
21.5609
21.2631
19.8945
f1 (ppm)

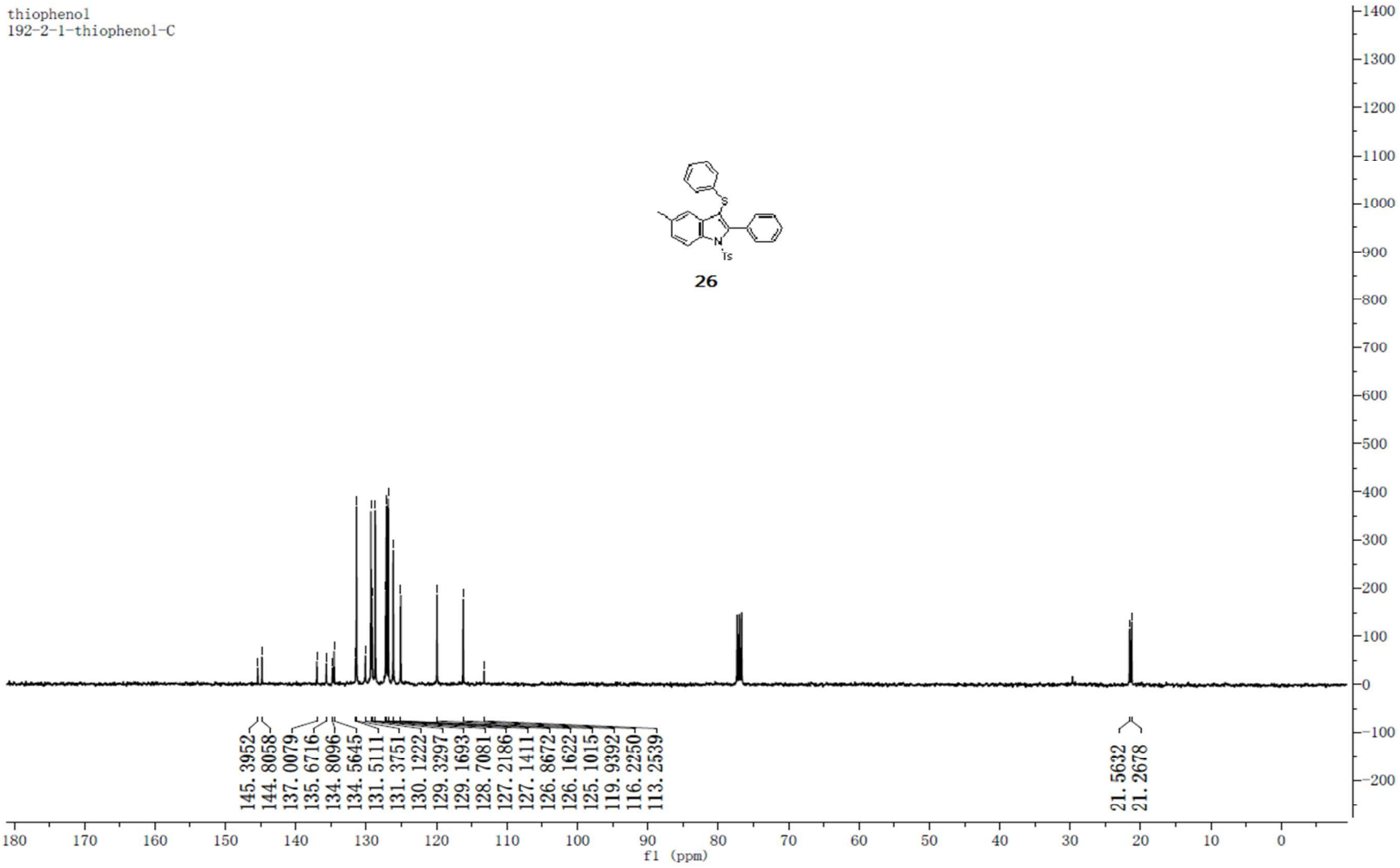

m-CH3 thiophenol
178-3-1-mch3
24
Ts
10.04
52.36
20.27
22.68
20.77
10.08
10.21
30.00
fl (ppm)

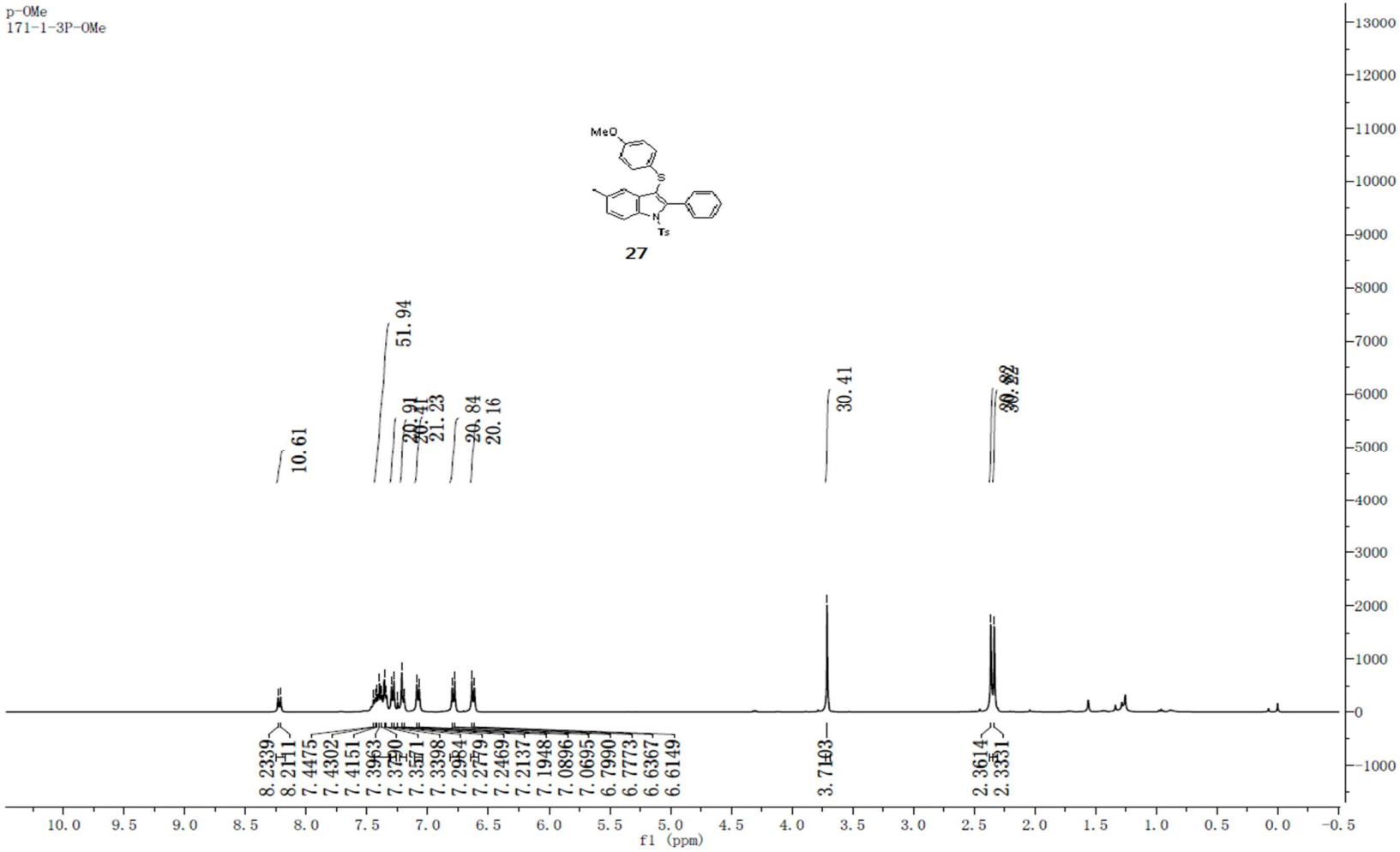

m-CH3 thiophenol
177-3-1m-ch3-thiophenol-c*pure
Ts
24
145.2942
144.7797
138.4888
136.7483
135.6178
134.9295
134.5013
131.5778
131.4103
130.1719
129.3467
129.1392
128.5645
127.1293
126.8734
126.0581
123.1711
119.9997
116.1377
113.2887
21.5560
21.2818
f1 (ppm)

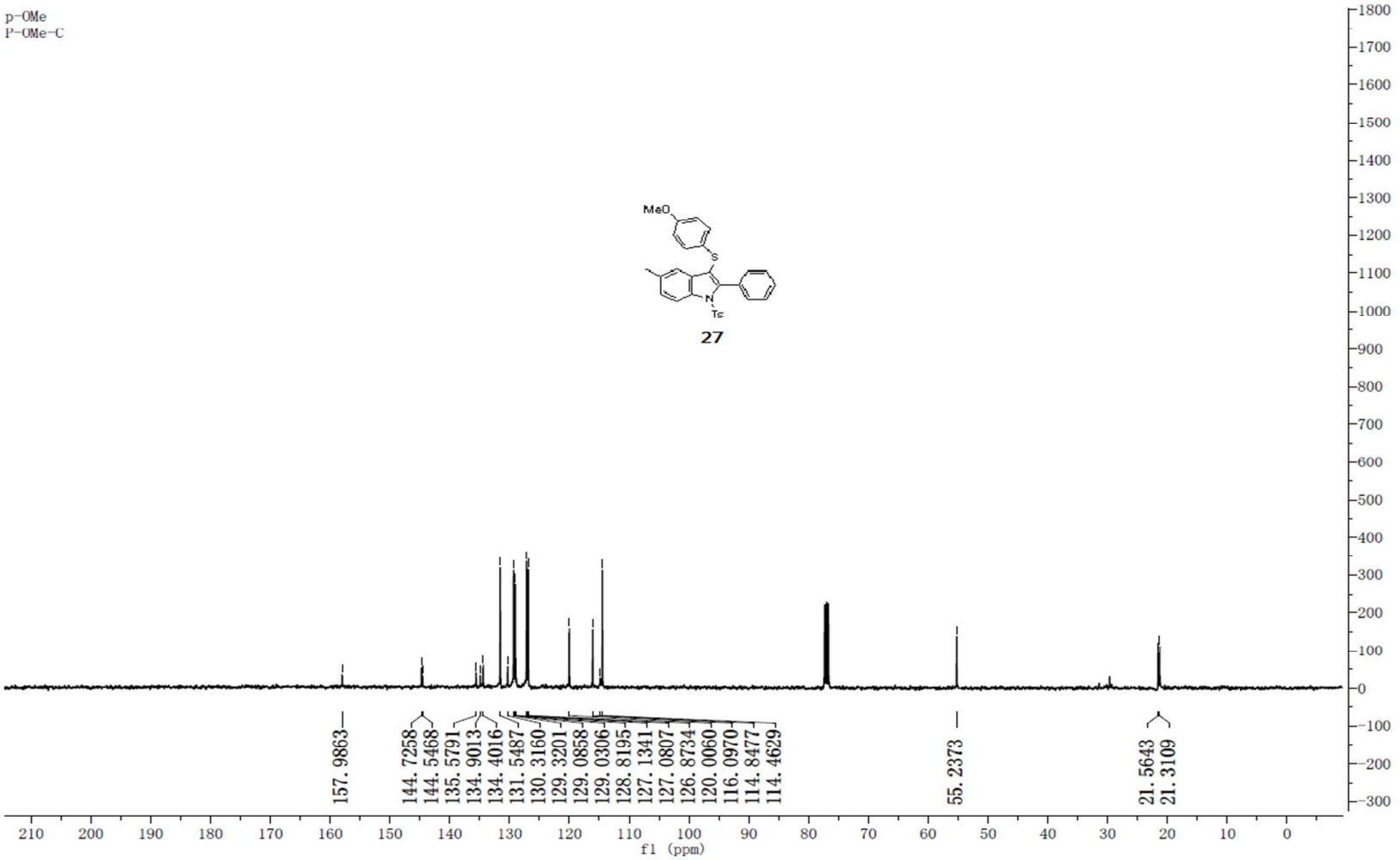

m-CH3 2
170-2-1c m-(ch3)2
25
70.85
60.26
20.87
20.14
10.52
20.06
10.07
8.2610
8.2382
7.4425
7.4269
7.4172
7.4106
7.4054
7.3931
7.3736
7.3566
7.3360
7.3153
7.2259
7.2077
7.0932
7.0729
6.6626
6.4484
2.3581
2.3017
2.0939
f1 (ppm)

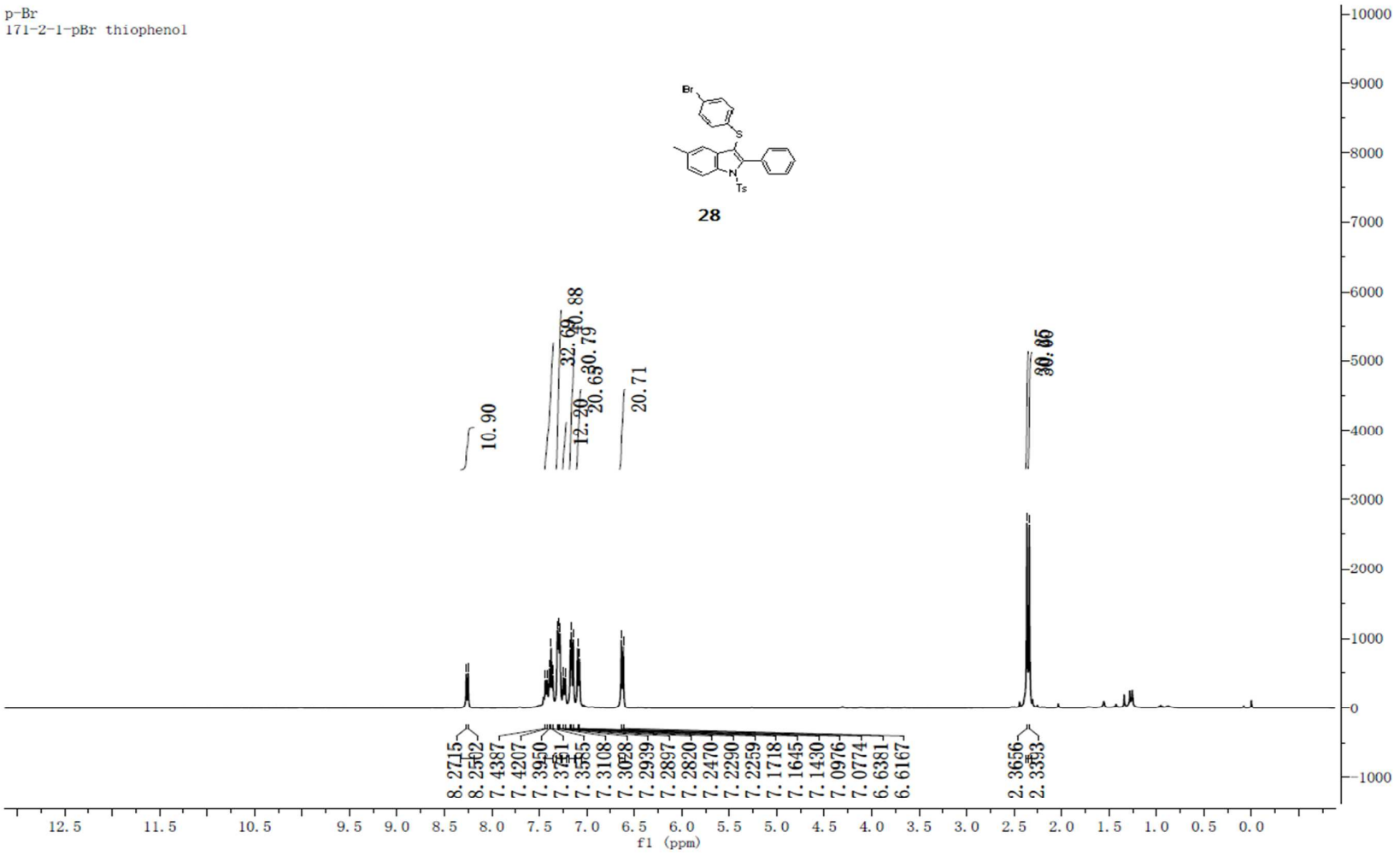

m-CH3 2
m-ch3 C
25
145.1606
144.7430
138.3150
136.4734
135.5125
135.0381
134.4107
131.5945
131.4197
130.1909
129.3593
129.1002
127.4190
127.1201
126.8549
123.8921
120.0484
115.9975
113.2493
21.5319
21.2643
21.1784
f1 (ppm)

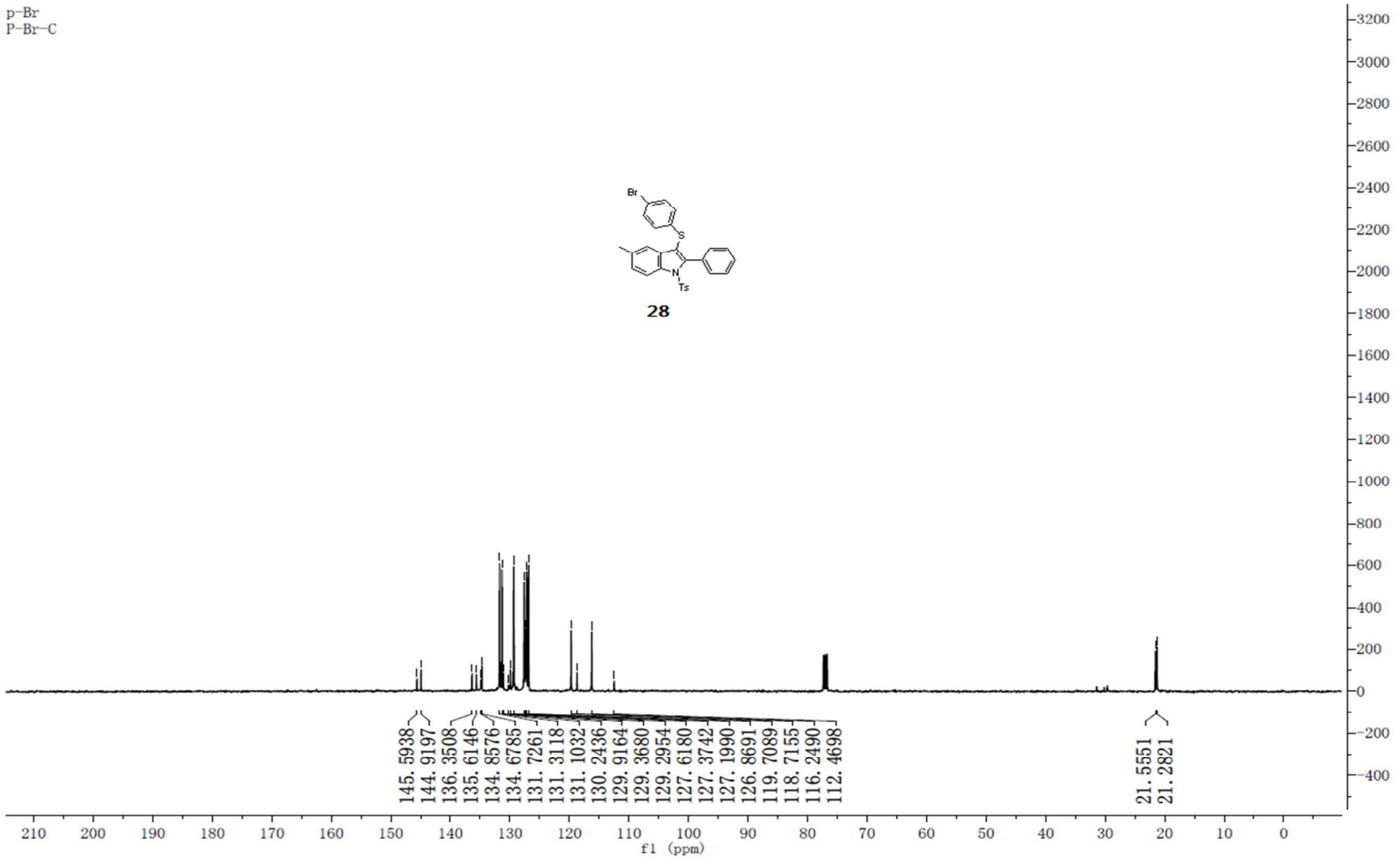

thiophenol
192-2-1-1thiophenol
26
10.27
51.74
52.00
20.74
21.48
20.18
30.00
8.2627
8.2414
7.4311
7.4236
7.4184
7.4136
7.4002
7.3965
7.3744
7.3569
7.3546
7.3510
7.3472
7.3361
7.3307
7.3260
7.3087
7.2878
7.2345
7.2111
7.1959
7.1945
7.0953
7.0748
7.0596
7.0417
7.0295
7.0259
6.7934
6.7882
6.7837
6.7733
6.7696
2.3489
2.3350
f1 (ppm)

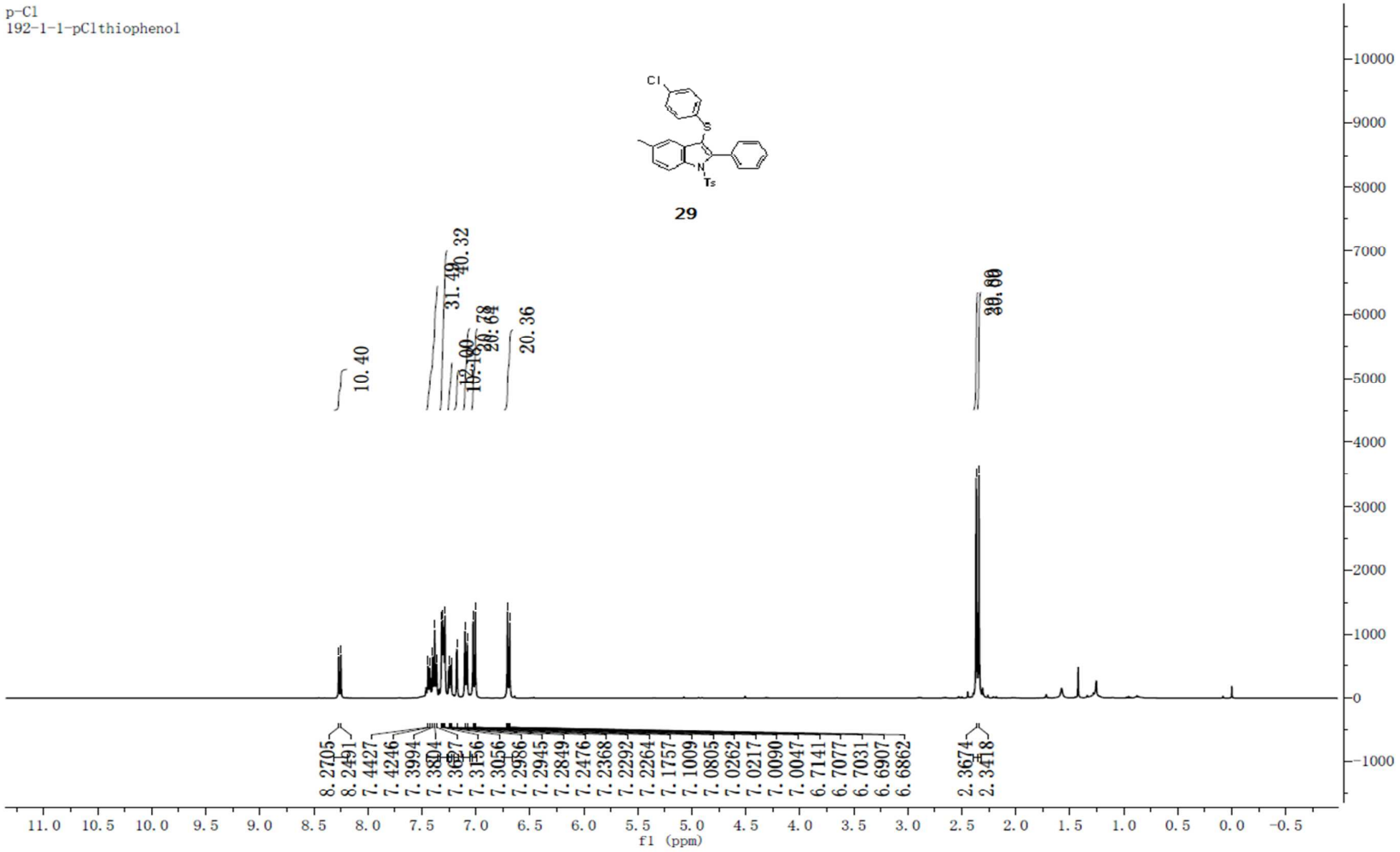

thiophenol
192-2-1-thiophenol-C
S
N
Ts
26
145.3952
144.8058
137.0079
135.6716
134.8096
134.5645
131.5111
131.3751
130.1222
129.3297
129.1693
128.7081
127.2186
127.1411
126.8672
126.1622
125.1015
119.9392
116.2250
113.2539
21.5632
21.2678
f1 (ppm)

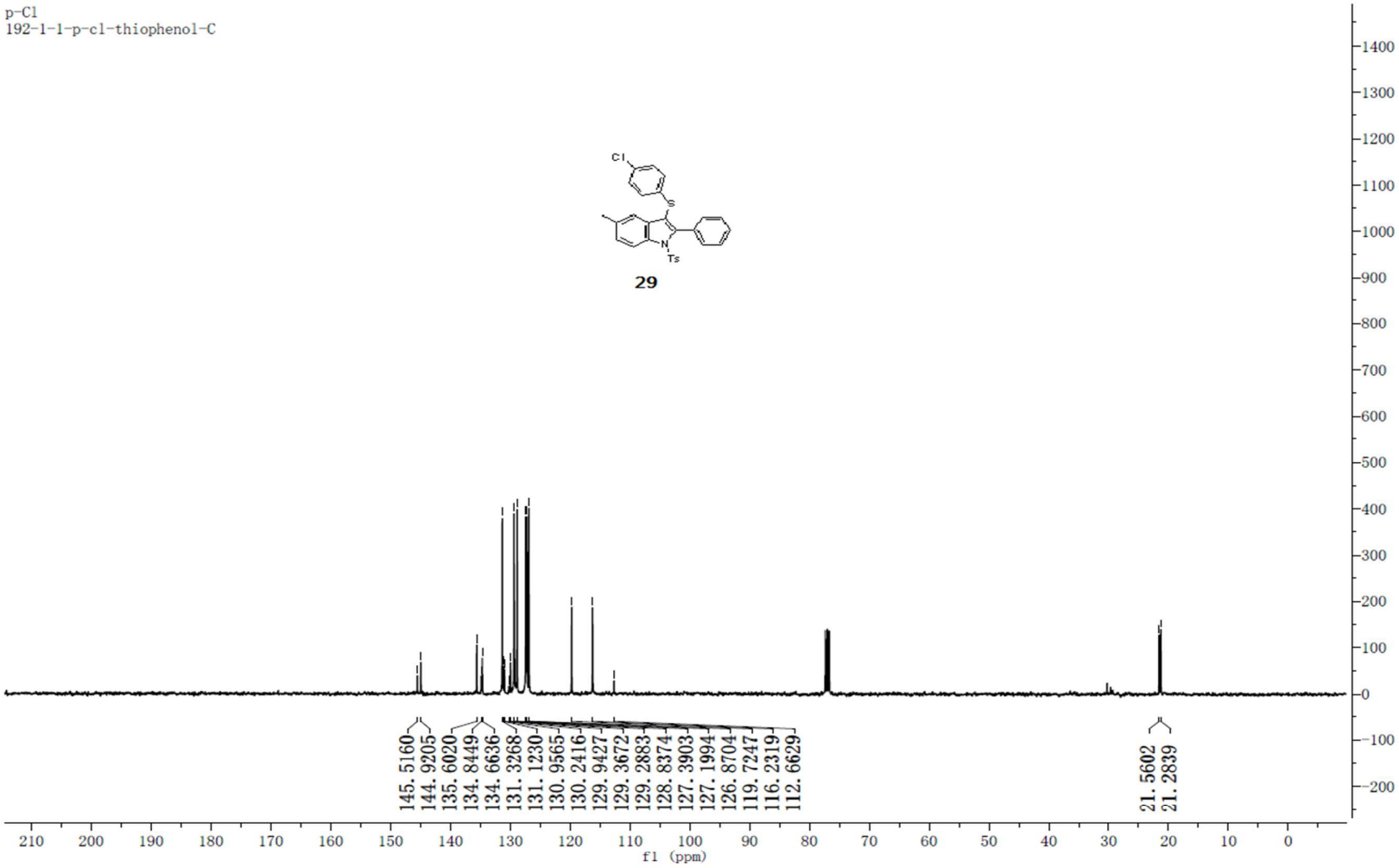

p-OMe
171-1-3P-OMe
MeO
S
N
Ts
27
51.94
30.41
10.61
20.84
20.16
21.23
8.2339
8.2111
7.4475
7.4302
7.4151
7.3963
7.3551
7.3398
7.2779
7.2469
7.2137
7.1948
7.0896
7.0695
7.7990
7.7773
6.6367
6.6149
3.7103
2.3614
2.3351
f1 (ppm)

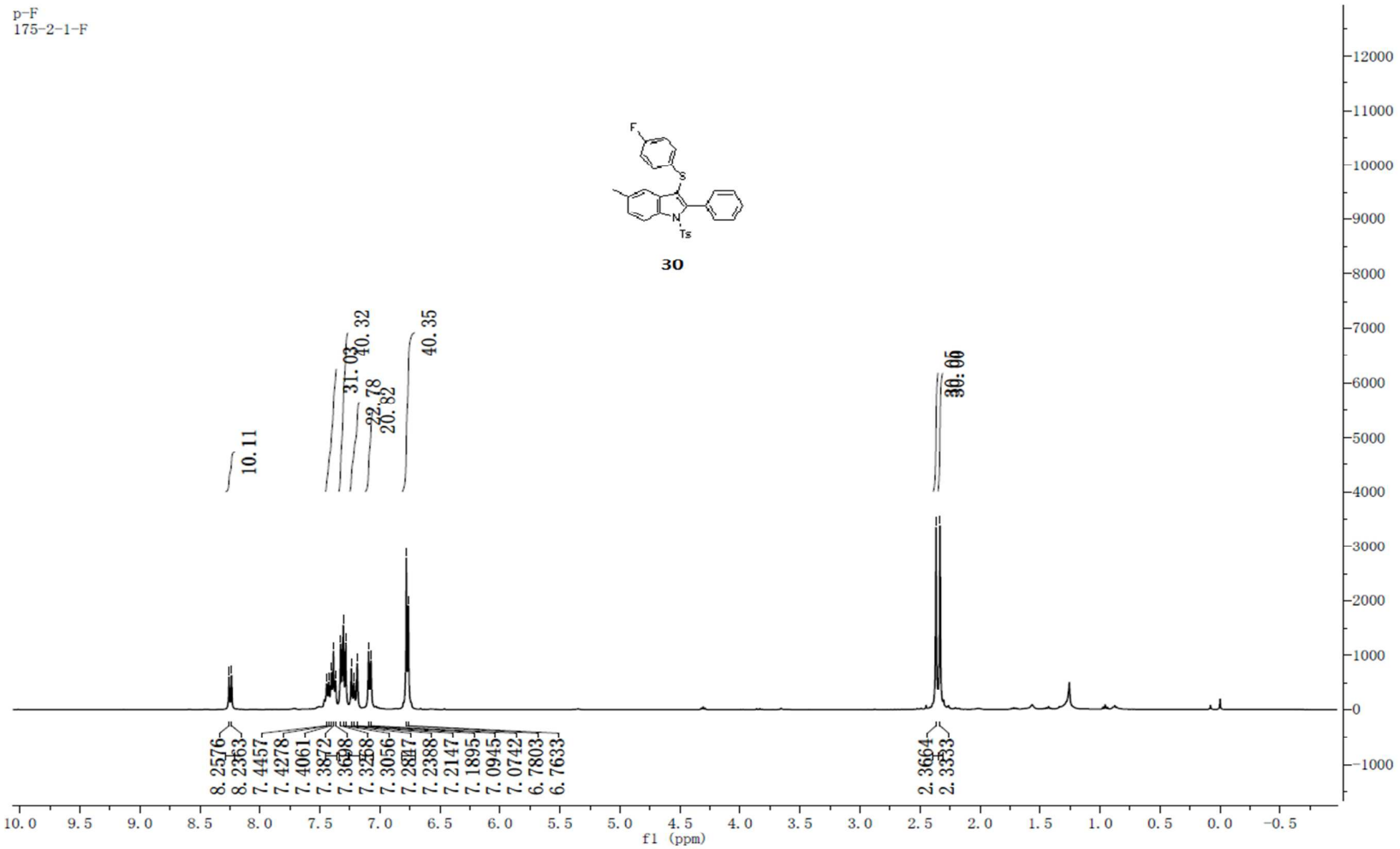

p-OMe
P-OMe-C
MeO
S
N
Ts
27
157.9863
144.7258
144.5468
135.5791
134.9013
134.4016
131.5487
130.3160
129.3201
129.0858
129.0306
128.8195
127.1341
127.0807
126.8734
120.0060
116.0970
114.8477
114.4629
55.2373
21.5643
21.3109
f1 (ppm)

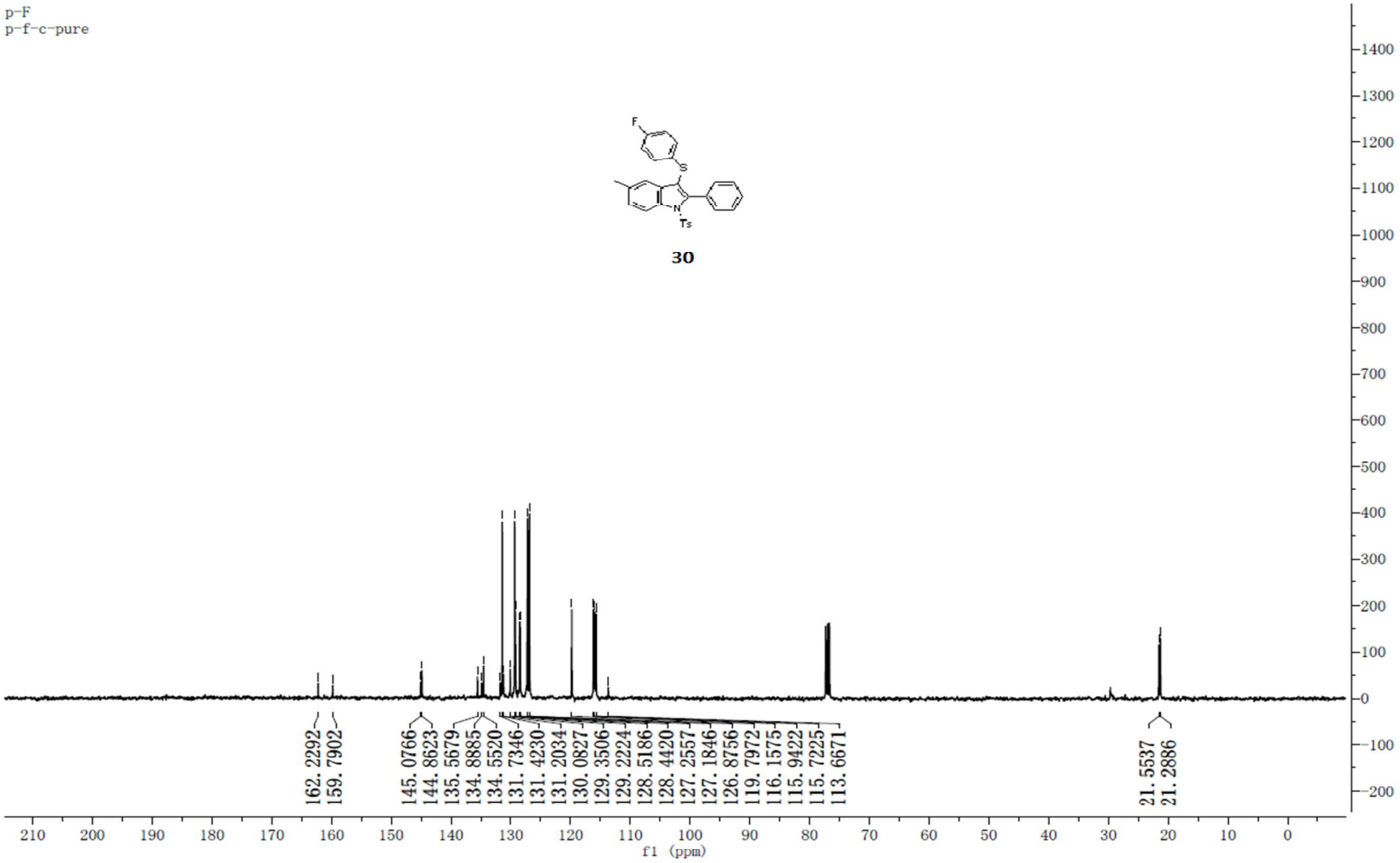

p-Br
171-2-1-pBr thiophenol
Br
S
N
Ts
28
10.90
32.69
30.88
30.79
20.63
20.71
8.2715
8.2562
7.4387
7.4207
7.3950
7.3765
7.3555
7.3108
7.3028
7.2939
7.2897
7.2820
7.2470
7.2290
7.2259
7.1718
7.1645
7.1430
7.0976
7.0774
6.6381
6.6167
2.3656
2.3393
f1 (ppm)


p-Br
P-Br-C
Br
S
N
Ts
28
145.5938
144.9197
136.3508
135.6146
134.8576
134.6785
131.7261
131.3118
131.1032
130.2436
129.9164
129.3680
129.2954
127.6180
127.3742
127.1990
126.8691
119.7089
118.7155
116.2490
112.4698
21.5551
21.2821
f1 (ppm)


p-Cl
192-1-1-pClthiophenol
Cl
S
N
Ts
29
10.40
31.48
40.32
20.36
30.00
8.2705
8.2491
7.4427
7.4246
7.3994
7.3804
7.3627
7.3156
7.3056
7.2986
7.2945
7.2849
7.2476
7.2368
7.2292
7.2264
7.1757
7.1009
7.0805
7.0262
7.0217
7.0090
7.0047
6.7141
6.7077
6.7031
6.6907
6.6862
2.3674
2.3418
f1 (ppm)


p-Cl
192-1-1-p-cl-thiophenol-C
Cl
S
N
Ts
29
145.5160
144.9205
135.6020
134.8449
134.6636
131.3268
131.1230
130.9565
130.2416
129.9427
129.3672
129.2883
128.8374
127.3903
127.1994
126.8704
119.7247
116.2319
112.6629
21.5602
21.2839
f1 (ppm)


p-F
175-2-1-F
F
S
N
Ts
30
10.11
31.03
40.32
22.78
20.82
40.35
30.00
8.2576
8.2363
7.4457
7.4278
7.4061
7.3872
7.3658
7.3258
7.3056
7.2817
7.2388
7.2147
7.1895
7.0945
7.0742
6.7803
6.7633
2.3664
2.3333
f1 (ppm)


p-F
p-f-c-pure
F
S
N
Ts
30
162.2292
159.7902
145.0766
144.8623
135.5679
134.8885
134.5520
131.7346
131.4230
131.2034
130.0827
129.3506
129.2224
128.5186
128.4420
127.2557
127.1846
126.8756
119.7972
116.1575
115.9422
115.7225
113.6671
21.5537
21.2886
f1 (ppm)