Tridentate P,N,N-ligand promoted copper-catalyzed [3+2] cycloaddition of propargylic esters with β-enamino esters: synthesis of highly functionalized pyrroles

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Supporting Information

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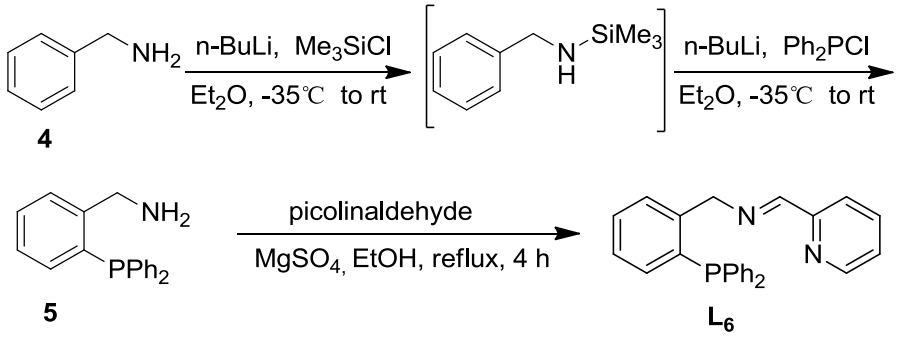
General Information

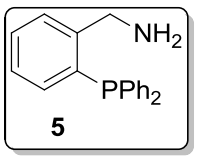
All reactions were carried out under a nitrogen atmosphere. Solvents were purified by standard procedure before use. Commercial reagents were used without further purification. Flash chromatography was performed on silica gel 60 (40-63μm, 60Å). Thin layer chromatography (TLC) was performed on glass plates coated with silica gel 60 with F254 indicator. Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded on a Bruker 400 MHz spectrometer. Chemical shifts for protons are reported in parts per million downfield from tetramethylsilane and are referenced to residual protium in the NMR solvent ($CHCl_3$ = δ 7.28). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker 100 MHz spectrometer. Chemical shifts for carbon are reported in parts per million downfield from tetramethylsilane and are referenced to the carbon resonances of the solvent ($CDCl_3$ = δ 77.07). Phosphorus nuclear magnetic resonance (^{31}P NMR) spectra were recorded on a Bruker 162 MHz spectrometer. Chemical shifts for phosphorus are reported in parts per million downfield from the external 85% H_3PO_4 signal at 0.0 ppm as a standard. Data are represented as follows: chemical shift, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants in Hertz (Hz), integration. propargylic esters **1**[1], β-enamino esters **2**[2] and (2-(diphenylphosphino)phenyl)methanamine (**5**) [3] were prepared following the method from the literature.

General Procedure for the Synthesis of P,N,N-Ligand L_6



To a solution of benzylamine **4** (1.07g, 10.0 mmol) in dry ether (10 mL) at -35℃ was added dropwise *n*-BuLi (4.0 mL, 2.5 M in hexane, 10.0 mmol). The resulting solution was stirred at -35℃ for 15 minutes, and the TMSCl (1.39 mL, 11.0 mmol) was added slowly at the same temperature. The reaction mixture was stirred for 1 hour and then *n*-BuLi (12 mL, 2.5 M in hexane, 30.0 mmol) was added dropwise. After the addition was completed, the reaction mixture was stirred at -35℃ for 3h. The reaction mixture was slowly warm to room temperature and stirred overnight. The reaction mixture was cooled at -35℃ again, and a solution of chlorodiphenylphosphine (1.8 mL, 10.0 mmol) in ether (10 mL) was added dropwise with 1 hour. The reaction mixture was stirred for another 3 hours at the same temperature, and then warmed to room temperature. After stirring for another 4 hours, a solution of 1M HCl was added slowly until the reaction mixture became clear in both phases. The aqueous phase was extracted with ether. The combined organic phase was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography to give compound **5** as white solid.

(2-(diphenylphosphino)phenyl)methanamine

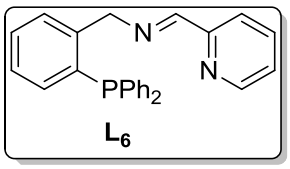


5

Mp: 105-106℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.42 (m, 1H), 7.37-7.31 (m, 7H), 7.29-7.24 (m, 4H), 7.16 (t, *J* = 7.4 Hz, 1H), 6.91-6.84 (m, 1H), 4.02 (s, 2H), 1.76 (br, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 136.4, 135.1, 134.0, 133.8, 133.5, 129.3, 128.8, 128.6, 128.5, 127.9, 127.1, 45.2; ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.90; HRMS calcd. for $C_{19}H_{19}NP$ ([M+H]+): 292.1225, found: 291.1259.

To a solution of amine **5** (291mg, 1.0 mmol) in 8 mL of EtOH was added picolinaldehyde (107 mg, 1.0 mmol) and anhydrous $MgSO_4$ (200 mg). The reaction mixture was refluxed for 4 h, and then cooled to room temperature. $MgSO_4$ were removed by the filtration. The filtrate was concentrated under reduced pressure, and the residue was purified by column chromatography to give the corresponding ligand **L_6** as a light yellow liquid.

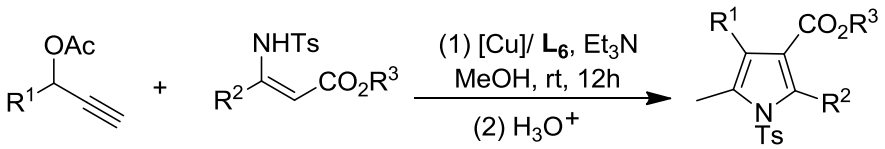
(*E*)-1-(2-(diphenylphosphino)phenyl)-N-(pyridin-2-ylmethylene)methanamine



L6

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62-8.55 (m, 1H), 8.34 (s, 1H), 7.75-7.68 (m, 1H), 7.66-7.57 (m, 1H), 7.47-7.44 (m, 1H), 7.37-7.33 (m, 1H), 7.32-7.28 (m, 8H), 7.27-7.22 (m, 3H), 7.21-7.16 (m, 1H), 6.98-6.88 (m, 1H), 5.12 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 154.6, 149.2, 143.5, 143.3, 136.7, 136.6, 136.3, 135.6, 134.1, 133.9, 133.8, 129.2, 128.8, 128.7, 128.6, 128.5, 128.4, 127.4, 124.6, 121.3, 63.0; ^{31}P NMR (162 MHz, $CDCl_3$) δ -15.51; HRMS calc. for $C_{25}H_{22}N_2P$ ($[M+H]^+$): 381.1521, found: 381.1527.

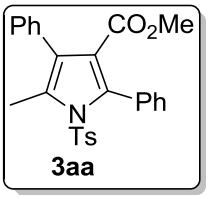
General Procedure for the Synthesis of Highly Functionalized Pyrroles



1 **2** **3**

A solution of $Cu(OTf)_2$ (5.4 mg, 0.015 mmol) and **L$_6$** (6.3 mg, 0.0165 mmol) in 1 mL of anhydrous methanol placed in an oven-dried Schlenk flask was stirred at room temperature under a nitrogen atmosphere for 1 h. A solution of propargylic esters **1** (0.36 mmol), β-enamino esters **2** (0.3 mmol) and Et_3N (50 uL, 0.36 mmol) in 2 mL of anhydrous methanol was added. The mixture was stirred at room temperature for 12 h. The reaction mixture was quenched with 1M HCl and the aqueous layer was extracted with CH_2Cl_2. The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography to afford the corresponding pyrroles products **3** as white solid..

Methyl 5-methyl-2,4-diphenyl-1-tosyl-*1H*-pyrrole-3-carboxylate

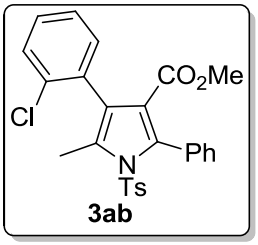


3aa

Mp: 114-116℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.27 (m, 8H), 7.23-7.19 (m, 6H), 3.29 (s, 3H), 2.45 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 145.1, 138.1, 136.5, 134.0, 131.6, 131.1, 130.1, 130.0, 129.7, 128.6, 127.9, 127.1, 127.0, 126.9, 126.0,

119.2, 51.1, 21.6, 13.6; HRMS calc. for $C_{26}H_{24}NO_4S$ ($[M+H]^+$): 446.1426, found: 446.1425.

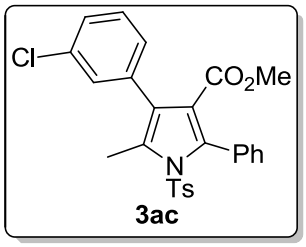
Methyl 4-(2-chlorophenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ab

Mp: 90-92℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.42 (m, 1H), 7.38-7.36 (m, 1H), 7.35-7.26 (m, 6H), 7.25-7.16 (m, 5H), 3.27 (s, 3H), 2.41 (s, 3H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.0, 145.0, 139.1, 136.7, 134.8, 133.5, 132.0, 131.6, 131.0, 129.7, 129.2, 128.8, 128.6, 126.9, 126.8, 126.3, 123.6, 51.0, 21.6, 13.7; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1040.

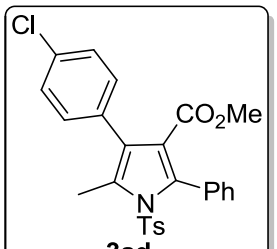
Methyl 4-(3-chlorophenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ac

Mp: 121-123℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.28 (m, 8H), 7.23-7.17 (m, 4H), 7.12-7.10 (m, 1H), 3.30 (s, 3H), 2.44 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 145.2, 138.4, 136.4, 136.0, 133.7, 131.6, 130.9, 130.2, 129.8, 129.1, 128.7, 128.5, 127.3, 127.1, 127.0, 124.7, 118.7, 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1044.

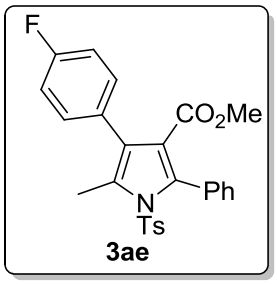
Methyl 4-(4-chlorophenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ad

Mp: 142-144℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.26 (m, 7H), 7.21-7.15 (m, 6H), 3.30 (s, 3H), 2.43 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 145.2, 138.4, 136.4, 133.1, 132.5, 131.5, 131.0, 130.1, 129.7, 128.7, 128.1, 127.1, 127.0, 124.8, 118.7, 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1036.

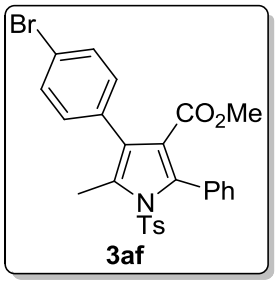
Methyl 4-(4-fluorophenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ae

Mp: 66-68℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.28 (m, 5H), 7.19 (t, *J* = 8.3 Hz, 6H), 7.06 (t, *J* = 8.7 Hz, 2H), 3.29 (s, 3H), 2.42 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 162.1(d, *J* = 245.0 Hz), 145.1, 138.3, 1365, 131.8 (d, *J* = 8.0 Hz), 131.5, 131.1, 130.1, 129.9, 129.7, 128.6, 127.1, 127.0, 125.0, 118.9, 114.9 (d, *J* = 21.0 Hz), 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SF$ ($[M+H]^+$): 464.1332, found: 464.1334.

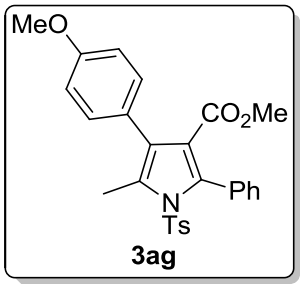
Methyl 4-(4-bromophenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3af

Mp: 166-168℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.38-7.28 (m, 5H), 7.21-7.16 (m, 4H), 7.10 (dd, *J* = 8.3, 1.7 Hz, 2H), 3.30 (s, 3H), 2.43 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 145.2, 138.4, 136.4, 133.0, 131.9, 131.5, 131.1, 131.0, 130.1, 129.8, 128.7, 127.1, 127.0, 124.8, 121.4, 118.7, 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SBr$ ($[M+H]^+$): 524.0531, found: 524.0524.

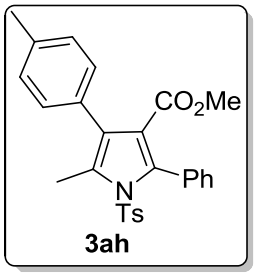
Methyl 4-(4-methoxyphenyl)-5-methyl-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ag

Mp: 94-96℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.26 (m, 5H), 7.24-7.13 (m, 6H), 6.91 (d, *J* = 7.8 Hz, 2H), 3.82 (s, 3H), 3.30 (s, 3H), 2.44 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 158.7, 145.0, 137.9, 136.6, 131.5, 131.2, 129.9, 129.7, 128.6, 127.1, 127.0, 126.1, 125.7, 119.4, 113.4, 55.2, 51.1, 21.6, 13.7; HRMS calc. for $C_{27}H_{26}NO_5S$ ($[M+H]^+$): 476.1532, found: 476.1534.

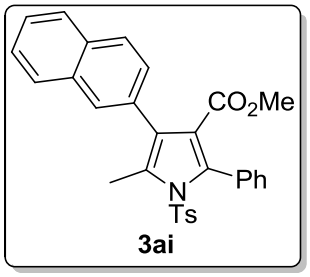
Methyl 5-methyl-2-phenyl-4-(p-tolyl)-1-tosyl-*1H*-pyrrole-3-carboxylate



3ah

Mp: 110-112℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.27 (m, 5H), 7.23-7.16 (m, 6H), 7.14-7.08 (m, 2H), 3.29 (s, 3H), 2.44 (s, 3H), 2.39 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 145.0, 137.9, 136.7, 136.6, 131.6, 131.2, 130.8, 130.0, 129.9, 129.7, 128.7, 128.6, 127.1, 127.0, 126.01, 119.4, 51.1, 21.7, 21.3, 13.7; HRMS calc. for $C_{27}H_{26}NO_4S$ ($[M+H]^+$): 460.1583, found: 460.1577.

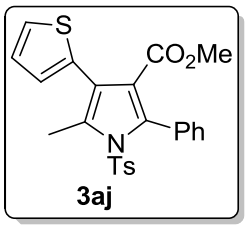
Methyl 5-methyl-4-(naphthalen-2-yl)-2-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ai

Mp: 128-130℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.79 (m, 3H), 7.70 (s, 1H), 7.48-7.45 (m, 2H), 7.40-7.28 (m, 6H), 7.21 (t, *J* = 8.3 Hz, 4H), 3.26 (s, 3H), 2.49 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 145.2, 138.3, 136.6, 133.2, 132.5, 131.6, 131.2, 130.3, 129.8, 128.8, 128.7, 128.5, 128.0, 127.7, 127.4, 127.2, 127.1, 126.1, 126.0, 125.9, 119.3, 51.1, 21.7, 13.8; HRMS calc. for $C_{30}H_{26}NO_4S$ ($[M+H]^+$): 496.1583, found: 496.1578.

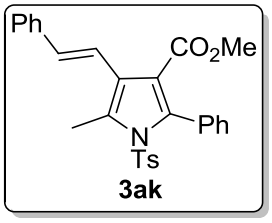
Methyl 5-methyl-2-phenyl-4-(thiophen-2-yl)-1-tosyl-*1H*-pyrrole-3-carboxylate



3aj

Mp: 114-116℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.26 (m, 6H), 7.23-7.14 (m, 4H), 7.07-7.01 (m, 1H), 6.93 (d, *J* = 2.8 Hz, 1H), 3.34 (s, 3H), 2.52 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 145.3, 137.8, 136.3, 134.4, 131.7, 131.6, 130.9, 129.8, 128.7, 128.1, 127.2, 127.0, 126.8, 126.0, 119.7, 118.3, 51.2, 21.7, 13.8; HRMS calc. for $C_{24}H_{22}NO_4S_2$ ($[M+H]^+$): 452.0990, found: 452.0983.

(*E*)-methyl 5-methyl-2-phenyl-4-styryl-1-tosyl-1H-pyrrole-3-carboxylate

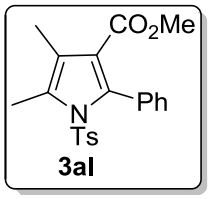


3ak

Mp: 110-112℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.39-7.24 (m, 8H), 7.21-7.12 (m, 5H), 6.61 (d, *J* = 16.5 Hz, 1H), 3.48 (s, 3H), 2.68 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 145.1, 138.8, 137.5, 136.4, 132.7, 131.4, 131.1, 130.1, 129.7, 128.6, 128.5, 127.5, 127.0, 126.9, 126.3, 122.5,

120.5, 118.1, 51.3, 21.6, 14.2; HRMS calc. for $C_{28}H_{26}NO_4S$ ($[M+H]^+$): 472.1583, found: 472.1572.

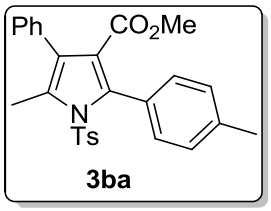
Methyl 4,5-dimethyl-2-phenyl-1-tosyl-1H-pyrrole-3-carboxylate



3al

Mp: 84-86℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (t, *J* = 7.3 Hz, 1H), 7.30-7.25 m, 4H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.6 Hz, 2H), 3.46 (s, 3H), 2.46 (s, 3H), 2.39 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 144.8, 138.8, 136.6, 131.6, 131.4, 129.6, 128.9, 128.3, 126.8, 126.7, 119.8, 118.9, 50.9, 21.6, 12.7, 10.7; HRMS calc. for $C_{21}H_{22}NO_4S$ ($[M+H]^+$): 384.1270, found: 384.1274.

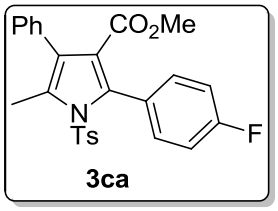
Methyl 5-methyl-4-phenyl-2-(p-tolyl)-1-tosyl-*1H*-pyrrole-3-carboxylate



3ba

Mp: 138-140℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.33 (m, 4H), 7.31-7.29 (m, 1H), 7.22-7.19 (m, 4H), 7.13-7.09 (m, 4H), 3.30 (s, 3H), 2.43 (s, 3H), 2.39 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 145.0, 138.4, 138.3, 136.6, 134.1, 131.4, 130.1, 129.8, 129.7, 128.1, 127.9, 127.8, 127.1, 126.0, 119.2, 51.1, 30.9, 21.6, 13.7; HRMS calc. for $C_{27}H_{26}NO_4S$ ($[M+H]^+$): 460.1583, found: 460.1587.

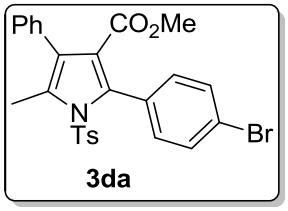
Methyl 2-(4-fluorophenyl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



3ca

Mp: 108-110℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.29 (m, 5H), 7.24-7.19 (m, 4H), 7.19-7.12 (m, 2H), 6.99 (t, *J* = 8.5 Hz, 2H), 3.31 (s, 3H), 2.45 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 163.0 (d, *J* = 247.0 Hz), 145.3, 136.8, 136.5, 133.9, 133. 5 (d, *J* = 8.3 Hz), 130.2, 130.1, 129.8, 127.9, 127.2, 127.0, 126.0, 119.4, 114.1(d, *J* = 22.0 Hz), 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SF$ ($[M+H]^+$): 464.1332, found: 464.1332.

Methyl 2-(4-bromophenyl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate

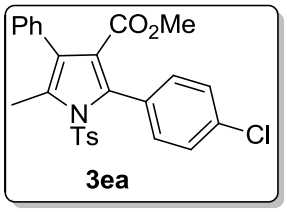


3da

Mp: 164-166℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.2 Hz, 2H), 7.40-7.28 (m, 5H), 7.25-7.17 (m, 4H), 7.07 (d, *J*

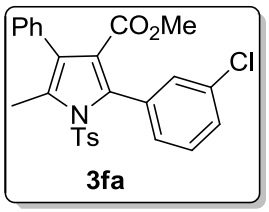
= 8.2 Hz, 2H), 3.32 (s, 3H), 2.43 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 145.3, 136.6, 136.4, 133.8, 133.1, 130.4, 130.3, 130.1, 129.8, 127.9, 127.2, 127.0, 126.2, 123.2, 119.4, 51.2, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SBr$ ($[M+H]^+$): 524.0531, found:524.0525.

Methyl 2-(4-chlorophenyl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



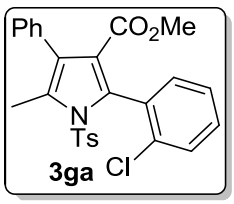
Mp: 134-136℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.32 (m, 4H), 7.30-7.19 (m, 7H), 7.13 (d, *J* = 8.2 Hz, 2H), 3.31 (s, 3H), 2.44 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 145.3, 136.7, 136.4, 134.8, 133.8, 132.9, 130.4, 130.1, 129.8, 129.6, 127.9, 127.3, 127.2, 127.0, 126.2, 119.4, 51.2, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1032.

Methyl 2-(3-chlorophenyl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



Mp: 90-92℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.31 (m, 6H), 7.28 (d, *J* = 7.8 Hz, 1H), 7.26-7.18 (m, 5H), 6.95 (s, 1H), 3.31 (s, 3H), 2.46 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 145.4, 136.4, 136.2, 133.8, 132.8, 131.4, 130.5, 130.1, 130.0, 129.83, 128.7, 128.3, 127.9, 127.2, 127.1, 126.0, 119.3, 51.1, 21.7, 13.6; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1037.

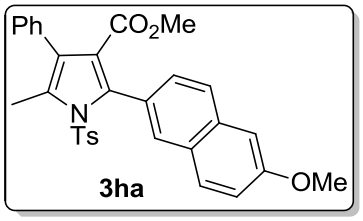
Methyl 2-(2-chlorophenyl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



Mp: 88-90℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.0 Hz, 2H), 7.38-7.34 (m, 4H), 7.32-7.28 (m, 3H), 7.26-7.22 (m, 4H), 3.32 (s, 3H), 2.42 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.1, 145.3, 136.3, 135.9, 135.1, 134.0, 133.3, 131.2, 130.3, 130.1, 129.9, 129.8, 128.7, 127.8, 127.40, 127.1, 126.1, 125.5, 118.7, 51.1, 21.7, 13.3; HRMS calc. for $C_{26}H_{23}NO_4SCl$ ($[M+H]^+$): 480.1036, found: 480.1039.

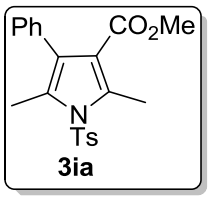
Methyl 2-(6-methoxynaphthalen-2-yl)-5-methyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-

carboxylate



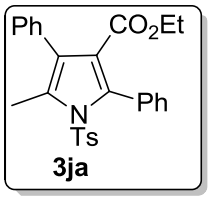
Mp: 120-122℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 1H), 7.40-7.35 (m, 4H), 7.33-7.29 (m, 1H), 7.28-7.21 (m, 4H), 7.15-7.12 (m, 2H), 7.08 (d, *J* = 8.4 Hz, 2H), 3.92 (s, 3H), 3.23 (s, 3H), 2.50 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 158.3, 145.1, 138.1, 136.6, 134.5, 134.0, 130.6, 130.2, 130.1, 129.9, 129.7, 129.6, 127.9, 127.8, 127.1, 126.2, 126.1, 125.3, 119.5, 118.9, 105.8, 55.4, 51.1, 21.6, 13.8; HRMS calc. for $C_{31}H_{28}NO_5S$ ($[M+H]^+$): 526.1688, found: 526.1689.

Methyl 2,5-dimethyl-4-phenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



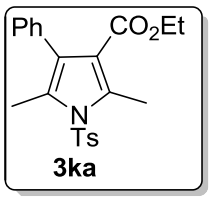
Mp: 80-82℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.37-7.24 (m, 5H), 7.18-7.08 (m, 2H), 3.52 (s, 3H), 2.73 (s, 3H), 2.43 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 145.2, 137.0, 136.9, 134.7, 130.2, 130.1, 128.9, 127.7, 126.8, 126.6, 125.7, 116.7, 51.0, 21.6, 13.5, 13.2; HRMS calc. for $C_{21}H_{22}NO_4S$ ($[M+H]^+$): 384.1270, found: 384.1263.

Ethyl 5-methyl-2,4-diphenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



Mp: 116-118℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.32 (m, 5H), 7.32-7.27 (m, 3H), 7.24-7.18 (m, 6H), 3.77 (q, *J* = 7.1 Hz, 2H), 2.44 (s, 3H), 2.39 (s, 3H), 0.67 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 145.1, 138.0, 136.6, 134.1, 131.7, 131.3, 130.2, 129.9, 129.7, 128.6, 127.9, 127.1, 127.0, 126.1, 119.5, 60.0, 21.7, 13.6, 13.3; HRMS calc. for $C_{27}H_{26}NO_4S$ ($[M+H]^+$): 460.1583, found: 460.1590.

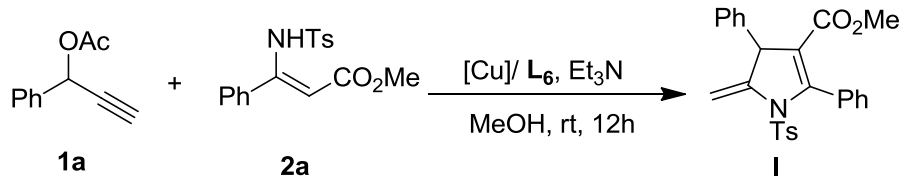
Ethyl 2,5-dimethyl-4-phenyl-1-tosyl-1H-pyrrole-3-carboxylate



Mp: 112-114℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.2 Hz, 2H), 7.29-7.17 (m, 5H), 7.04 (d, *J* = 6.9 Hz, 2H), 3.89 (q, *J* = 7.0 Hz, 2H), 2.66 (s, 3H), 2.34 (s, 3H), 2.20 (s, 3H), 0.80 (t, *J* = 7.0 Hz,

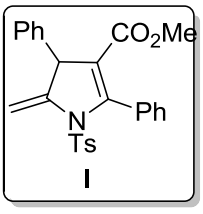
3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 145.2, 137.0, 136.9, 135.0, 130.2, 130.1, 128.7, 127.7, 126.8, 126.7, 125.8, 116.9, 59.9, 21.6, 13.6, 13.4, 13.2; HRMS calc. for $C_{22}H_{24}NO_4S$ ($[M+H]^+$): 398.1426, found: 398.1428.

Synthesis of Compound I



A solution of $Cu(OTf)_2$ (5.4 mg, 0.015 mmol) and **L_6** (6.3 mg, 0.0165 mmol) in 1 mL of anhydrous methanol placed in an oven-dried Schlenk flask was stirred at room temperature under a nitrogen atmosphere for 1 h. A solution of propargylic esters **1a** (63 mg, 0.36 mmol), β-enamino esters **2a** (99 mg, 0.3 mmol) and Et_3N (50 uL, 0.36 mmol) in 2 mL of anhydrous methanol was added. The mixture was stirred at room temperature for 12 h. The solvent was removed under reduced pressure to give the crude product which was purified by silica gel chromatography to afford the corresponding pyrroles product **I** as white solid.

Methyl 5-methyl-2,4-diphenyl-1-tosyl-*1H*-pyrrole-3-carboxylate



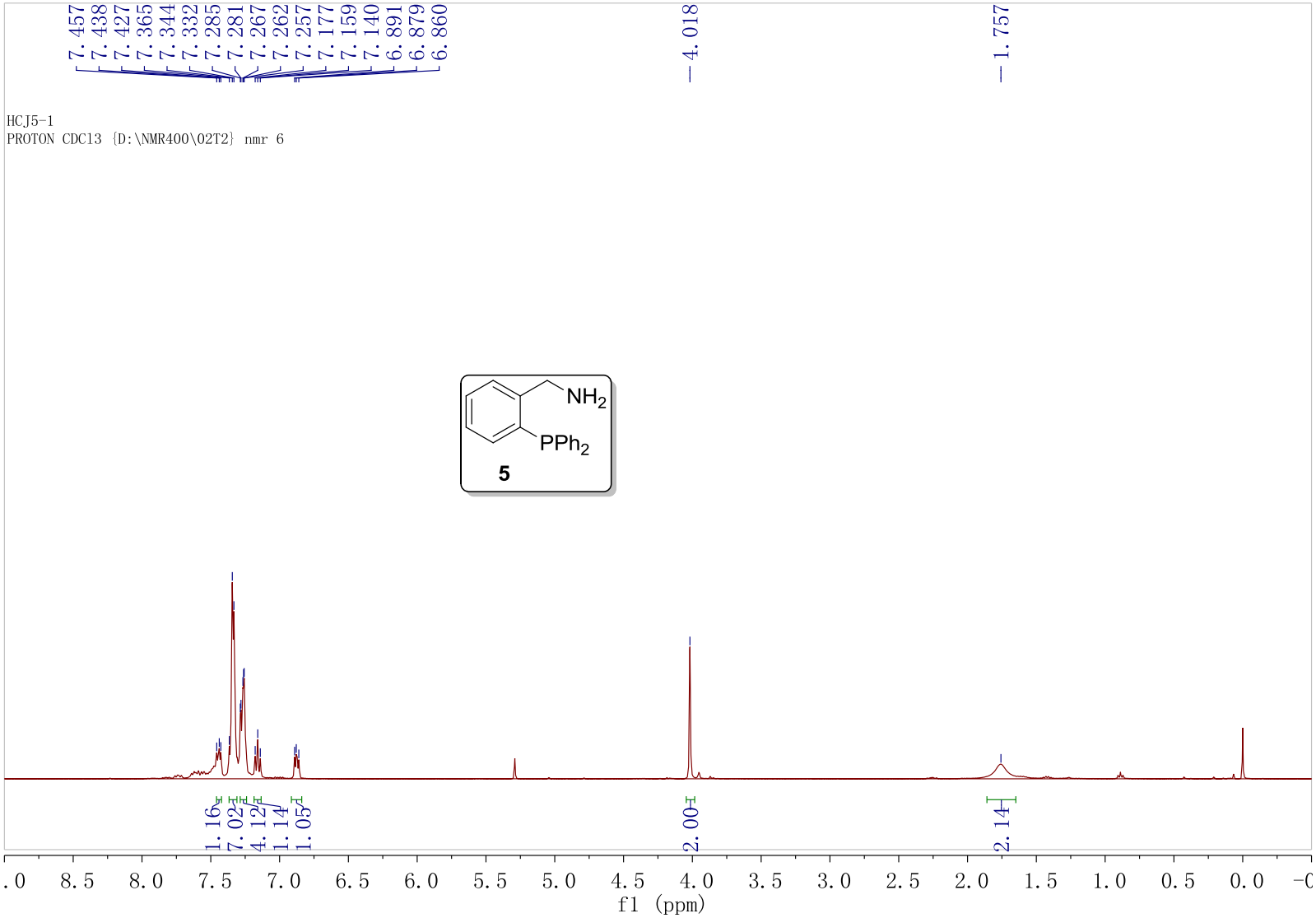
Mp: 112-114℃; ^{1}H NMR (400 MHz, DMSO) δ 7.55-7.50 (m, 2H), 7.48-7.41 (m, 5H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.17-7.12 (m, 1H), 7.08 (t, *J* = 7.3 Hz, 2H), 6.72 (d, *J* = 7.1 Hz, 2H), 5.56 (t, *J* = 2.0 Hz, 1H), 4.76 (t, *J* = 1.9 Hz, 1H), 4.69 (t, *J* = 2.1 Hz, 1H), 3.23 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 163.3, 151.9, 148.8, 145.6, 142.2, 133.6, 131.6, 130.4, 130.2, 129.9, 128.8, 128.0, 127.7, 127.3, 127.1, 117.3, 101.6, 52.3, 51.6, 21.6; HRMS calc. for $C_{26}H_{24}NO_4S$ ($[M+H]^+$): 446.1426, found: 446.1445.

Reference

[1] a) P. Fang, X.-L. Hou, *Org. Lett.* **2009**, *11*, 4612-4615; b) M. Bhanuchandra, M. R. Kuram, A. K. Sahoo, *J. Org. Chem.* **2013**, *78*, 11824-11834.

[2] a) M. Yoshida, C.Sugimura, *Tetahedron Lett.* **2013**, *54*, 2082-2084; b) M. Yoshida,K. Kinoshita, K. Namba, *Org. Biomol. Chem.* **2014**, *12*, 2394-2403.

[3] a) J.-D. Huang, X.-P. Hu, Z.-C. Duan, Q.-H. Zeng, S.-B. Yu, J. Deng, D.-Y. Wang, Z. Zheng, *Org. Lett.* **2006**, *8*, 4367; b) J.-D. Huang, X.-P. Hu, S.-B. Yu, J. Deng, D.-Y. Wang, Z.-C. Duan, Z. Zheng, *J. Mol. Catal. A: Chem.* **2007**, *270*, 127.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7.285
7.281
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7.262
7.257
7.177
7.159
7.140
6.891
6.879
6.860
4.018
1.757
HCJ5-1
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PPh2
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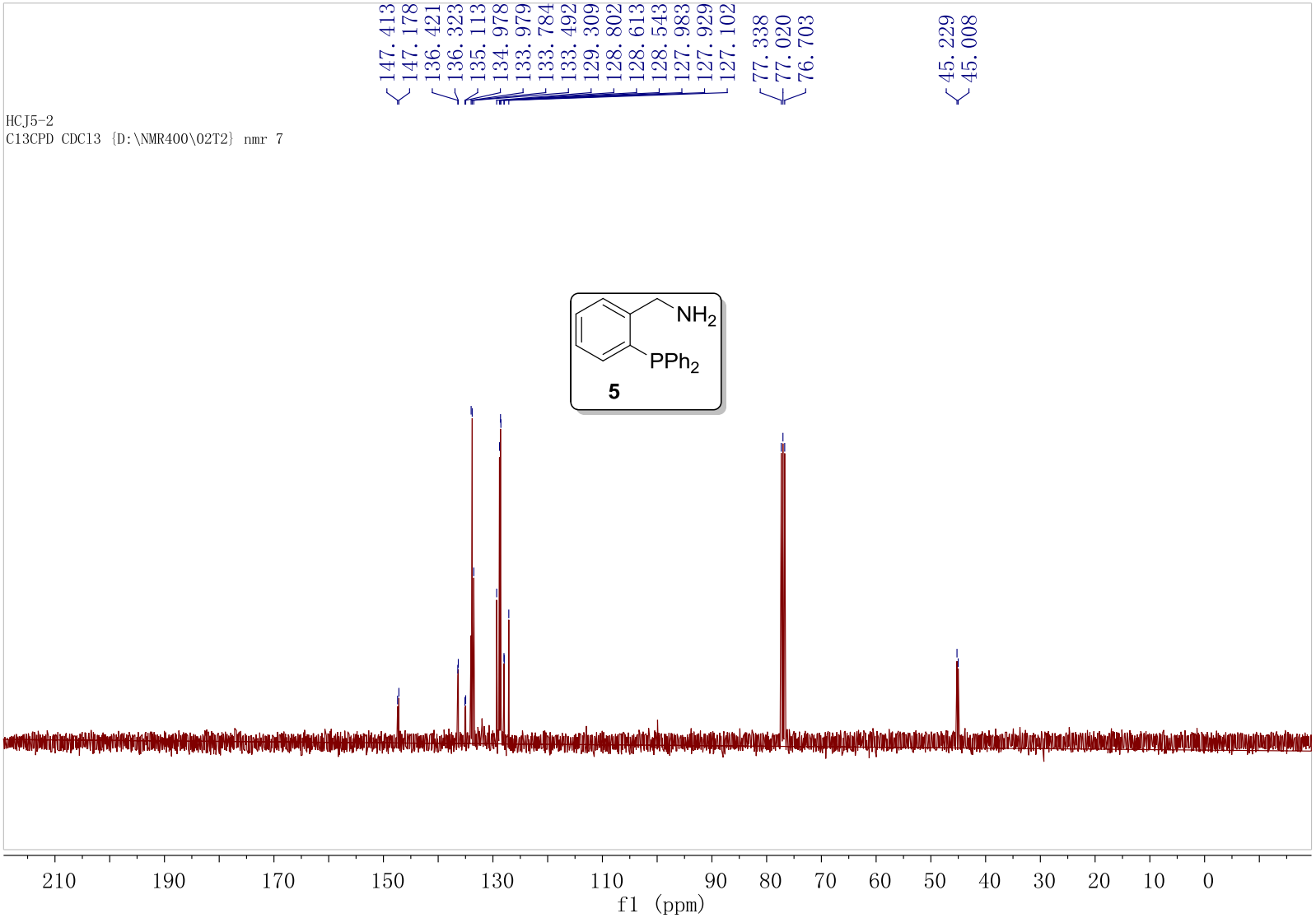
1.16
7.02
4.12
1.14
1.05
2.00
2.14
f1 (ppm)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77.020
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45.229
45.008
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PPh2
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150
130
110
90
80
70
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50
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30
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10
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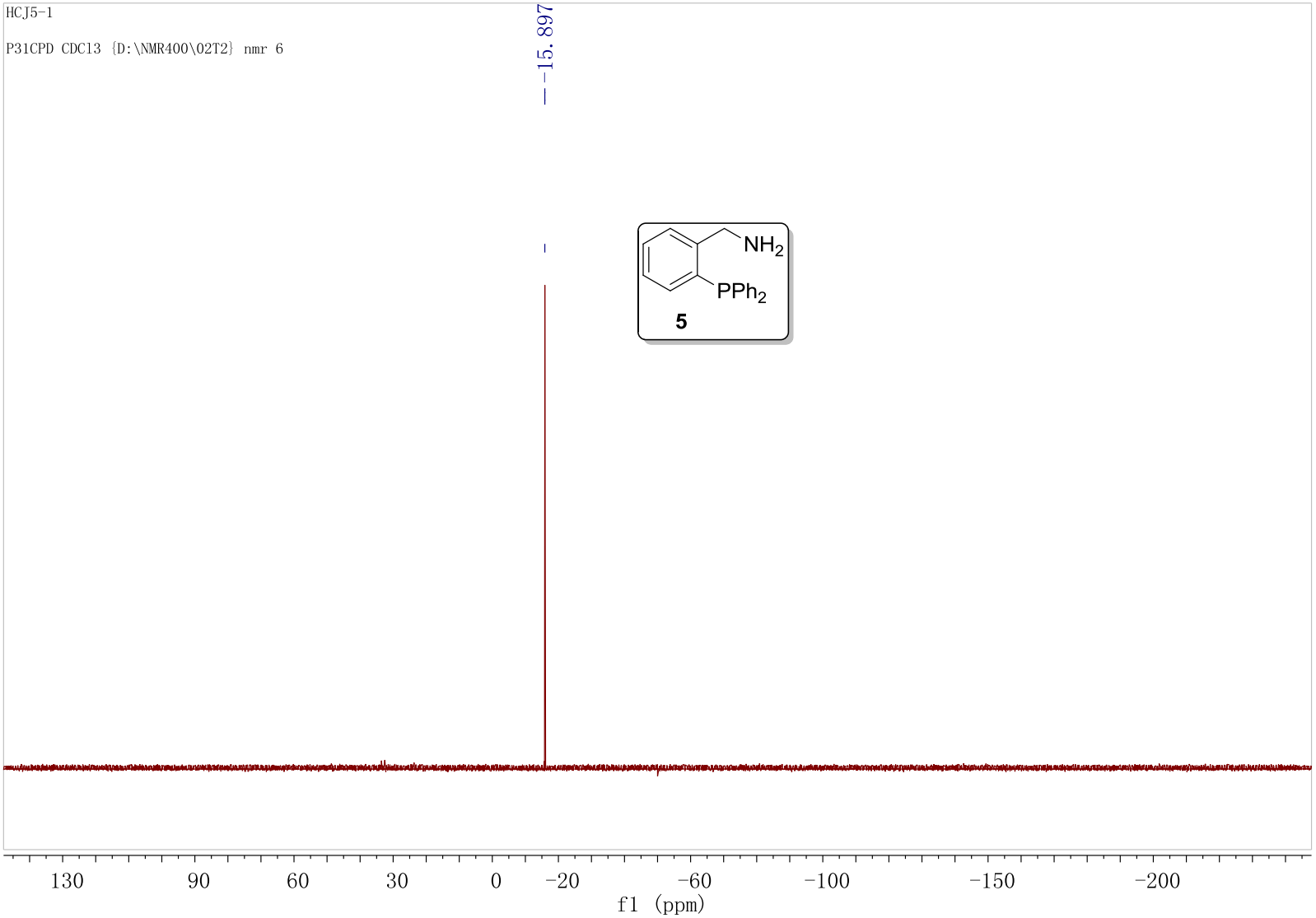
f1 (ppm)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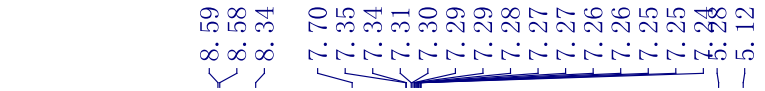
f1 (ppm)



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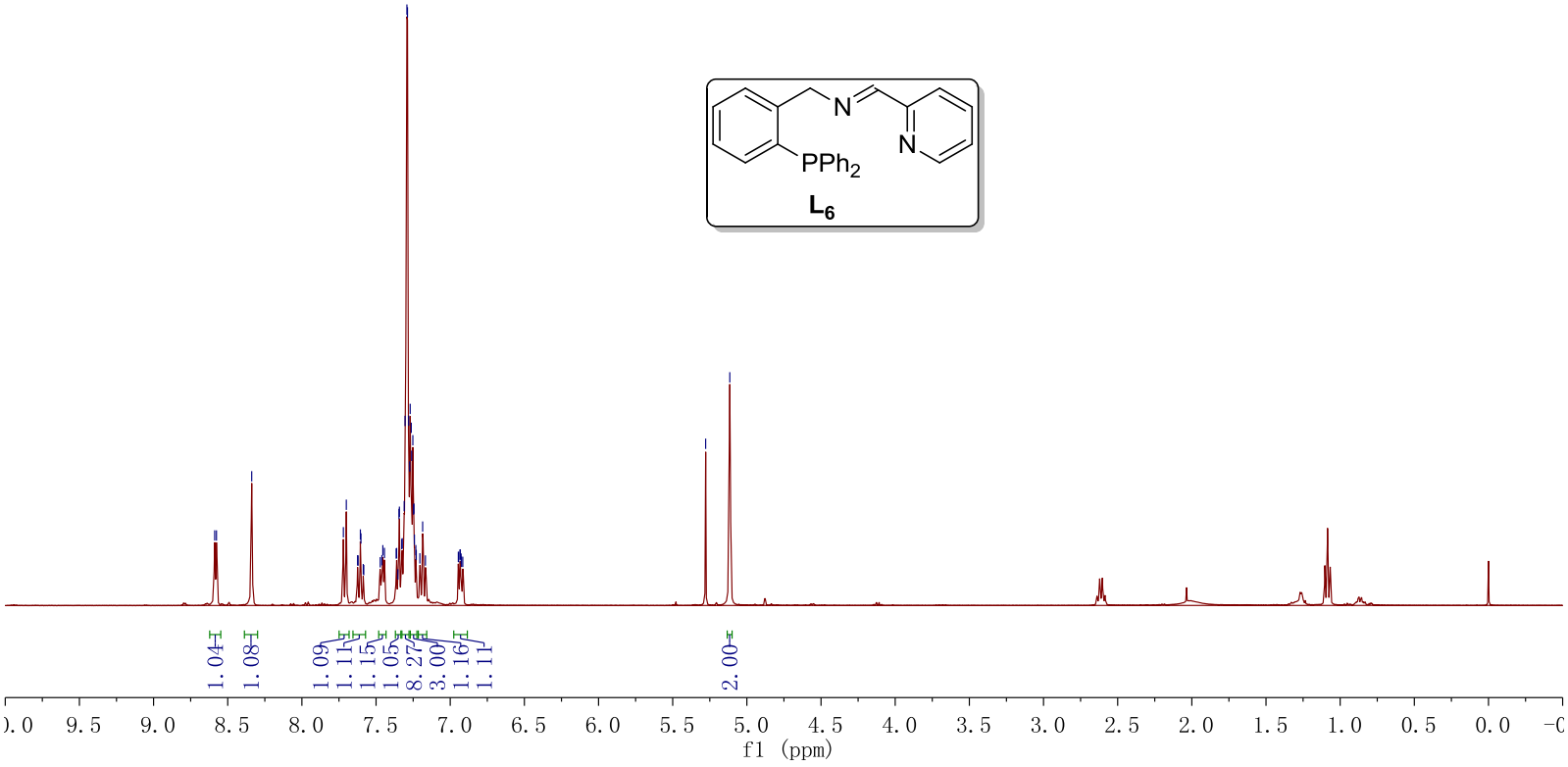

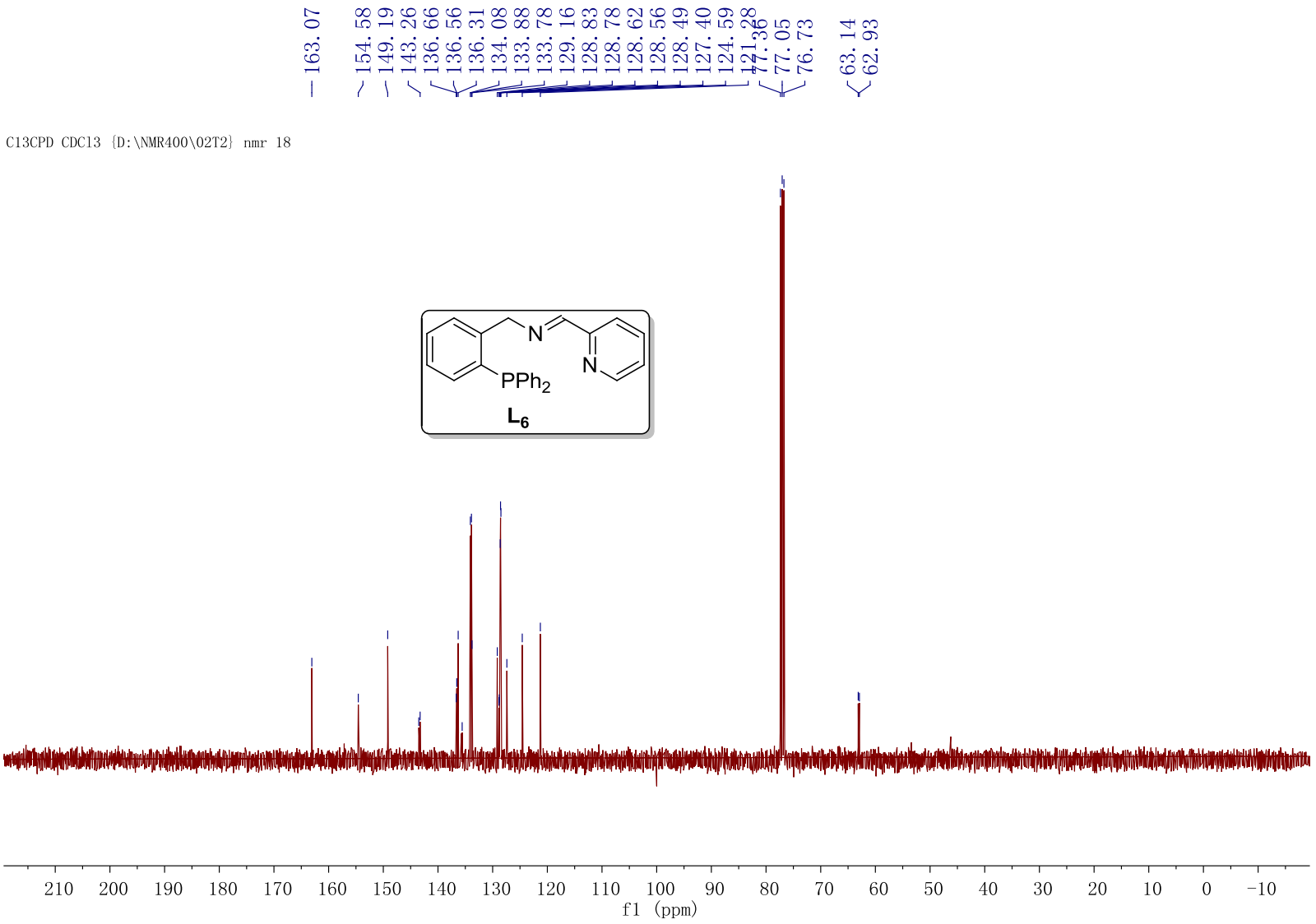
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136.56
136.31
134.08
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133.78
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124.59
121.28
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77.05
76.73
63.14
62.93
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L6
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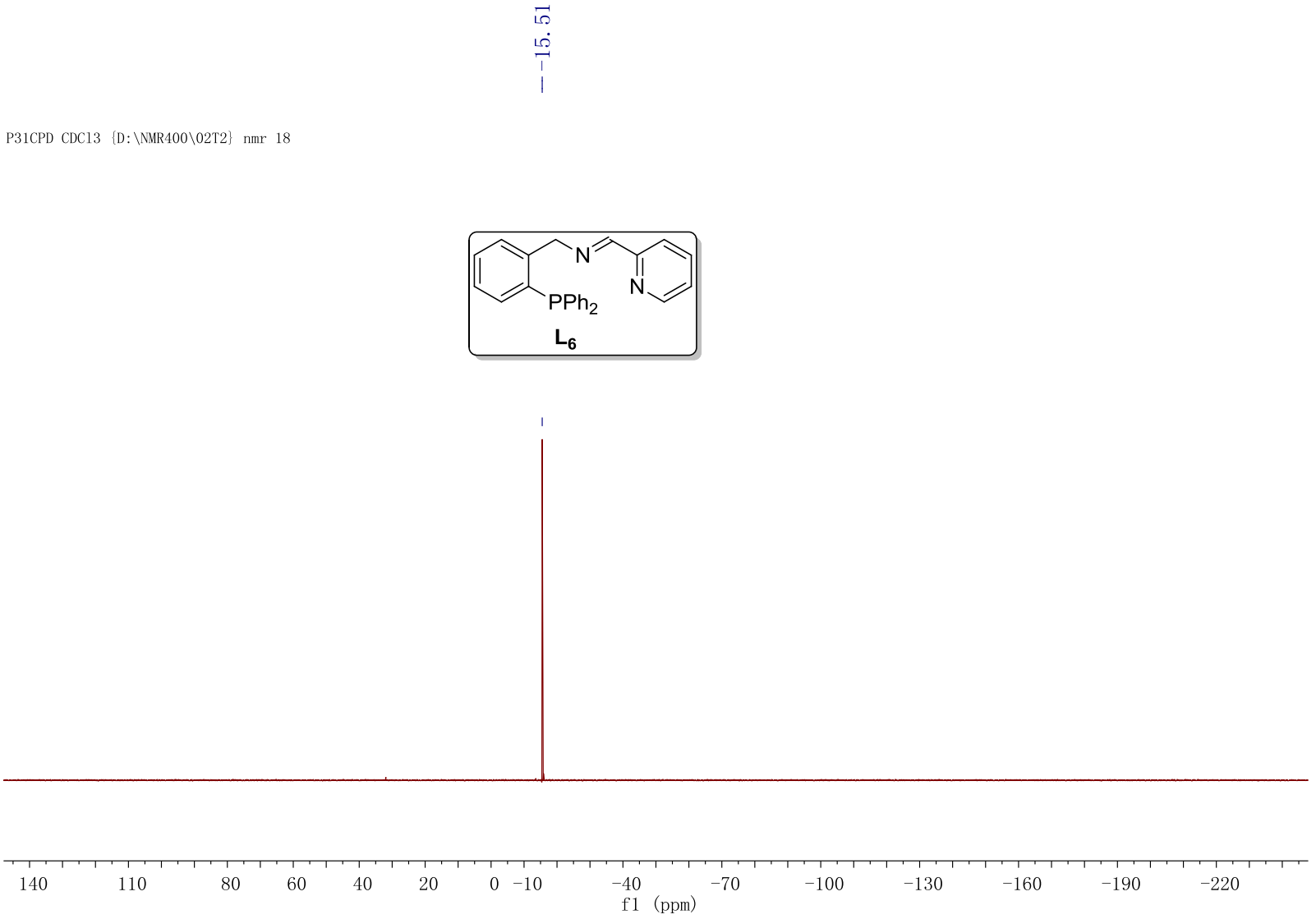
f1 (ppm)


-15.51
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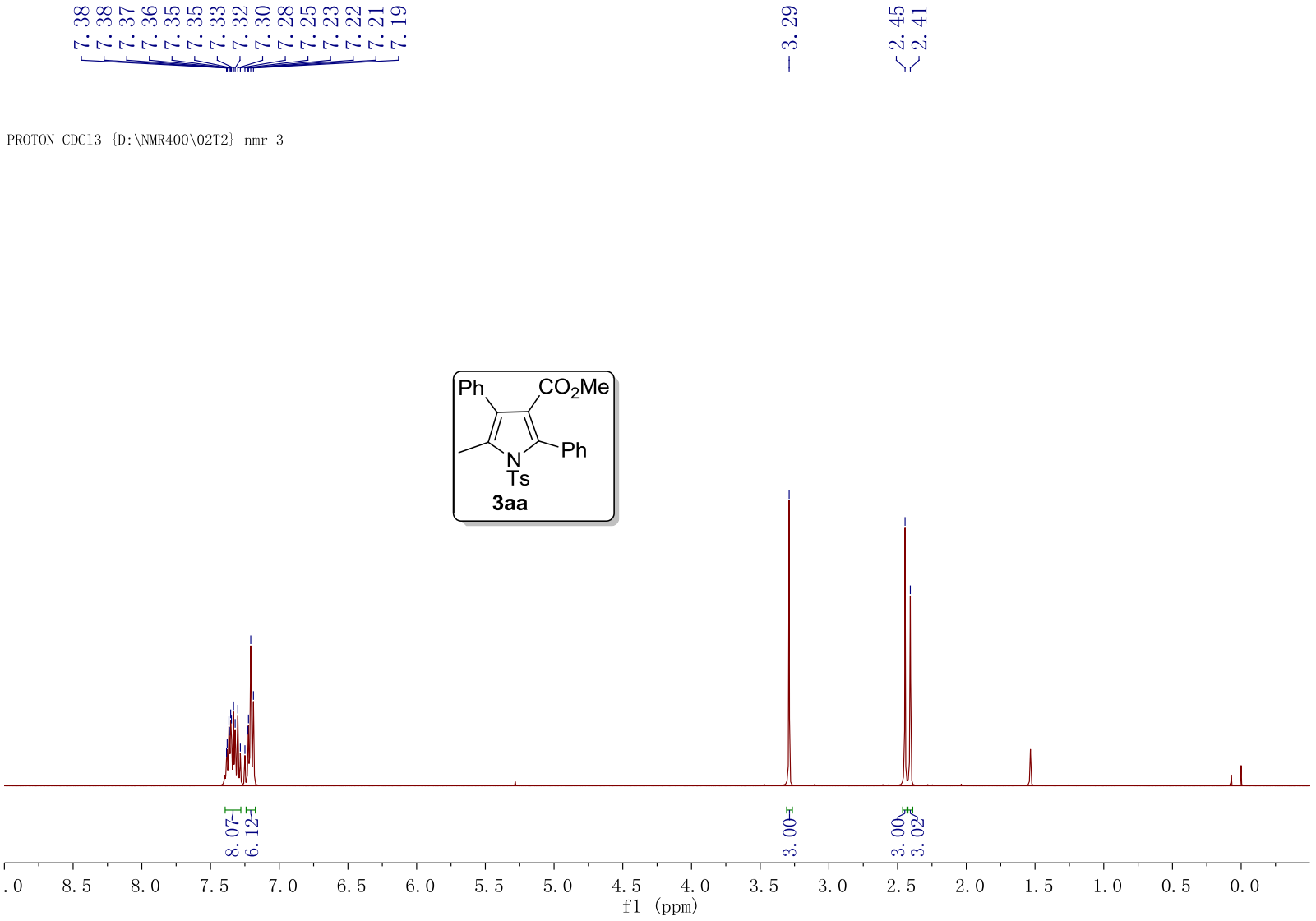
f1 (ppm)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7.37
7.36
7.35
7.35
7.33
7.32
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7.25
7.23
7.22
7.21
7.19
3.29
2.45
2.41
PROTON CDCl3 {D:\NMR400\02T2} nmr 3
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Ph
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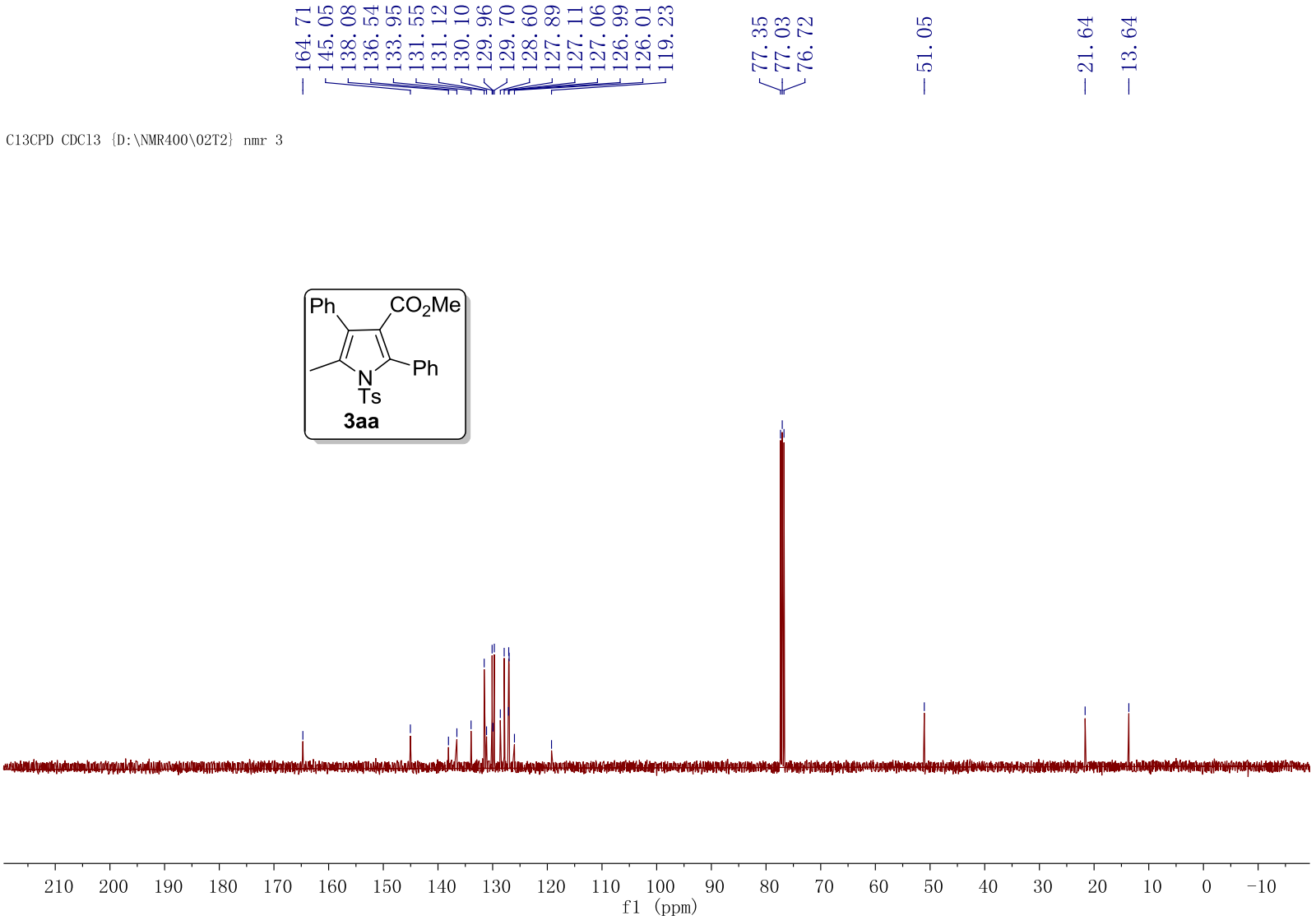
Ts
3aa
8.07
6.12
3.00
3.00
3.02
f1 (ppm)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126.01
119.23
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77.03
76.72
51.05
21.64
13.64
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Ph
N
Ts
3aa
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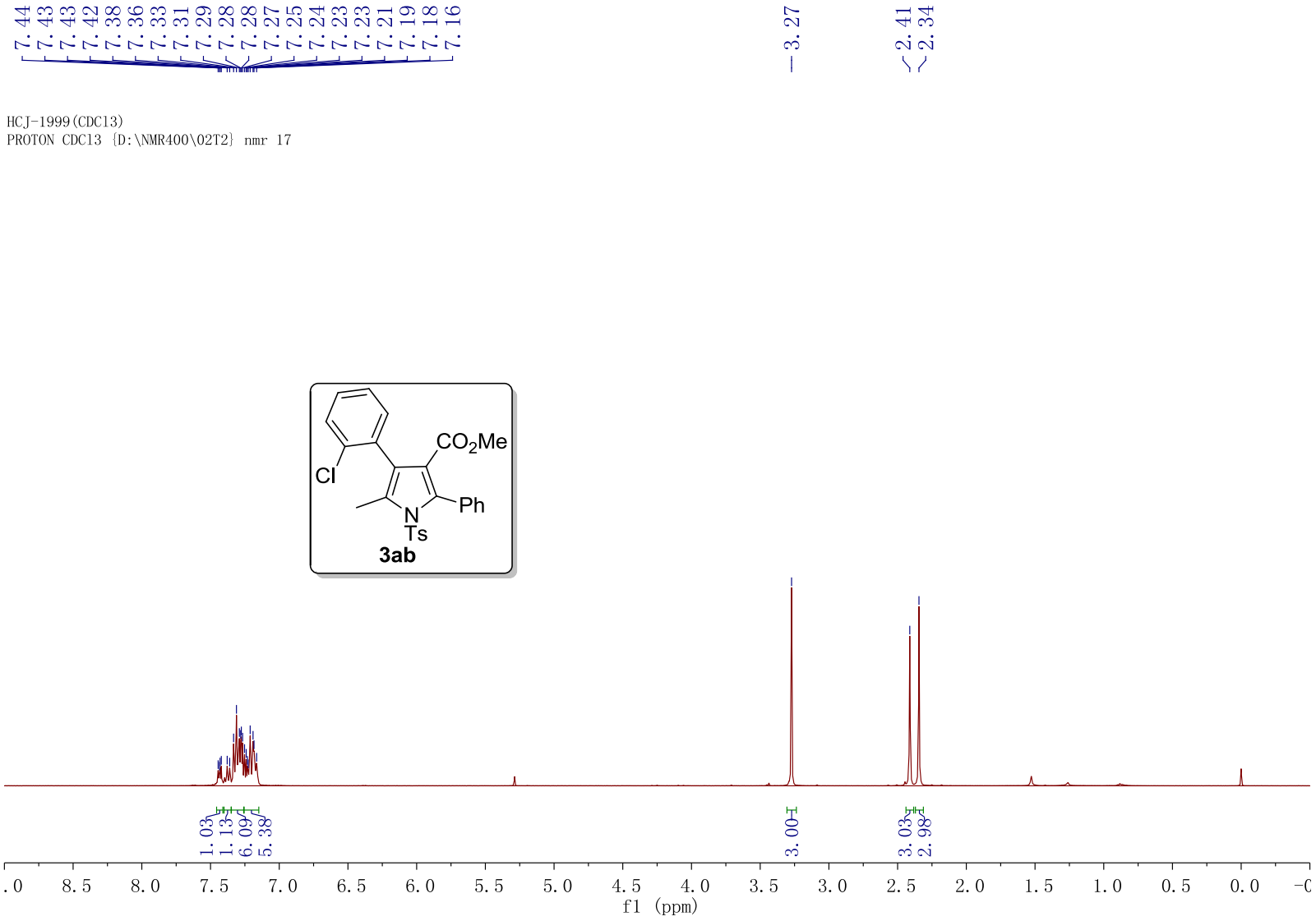
f1 (ppm)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7.38
7.36
7.33
7.31
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7.25
7.24
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7.23
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7.19
7.18
7.16
3.27
2.41
2.34
HCJ-1999(CDC13)
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CO2Me
Cl
Ph
N
Ts
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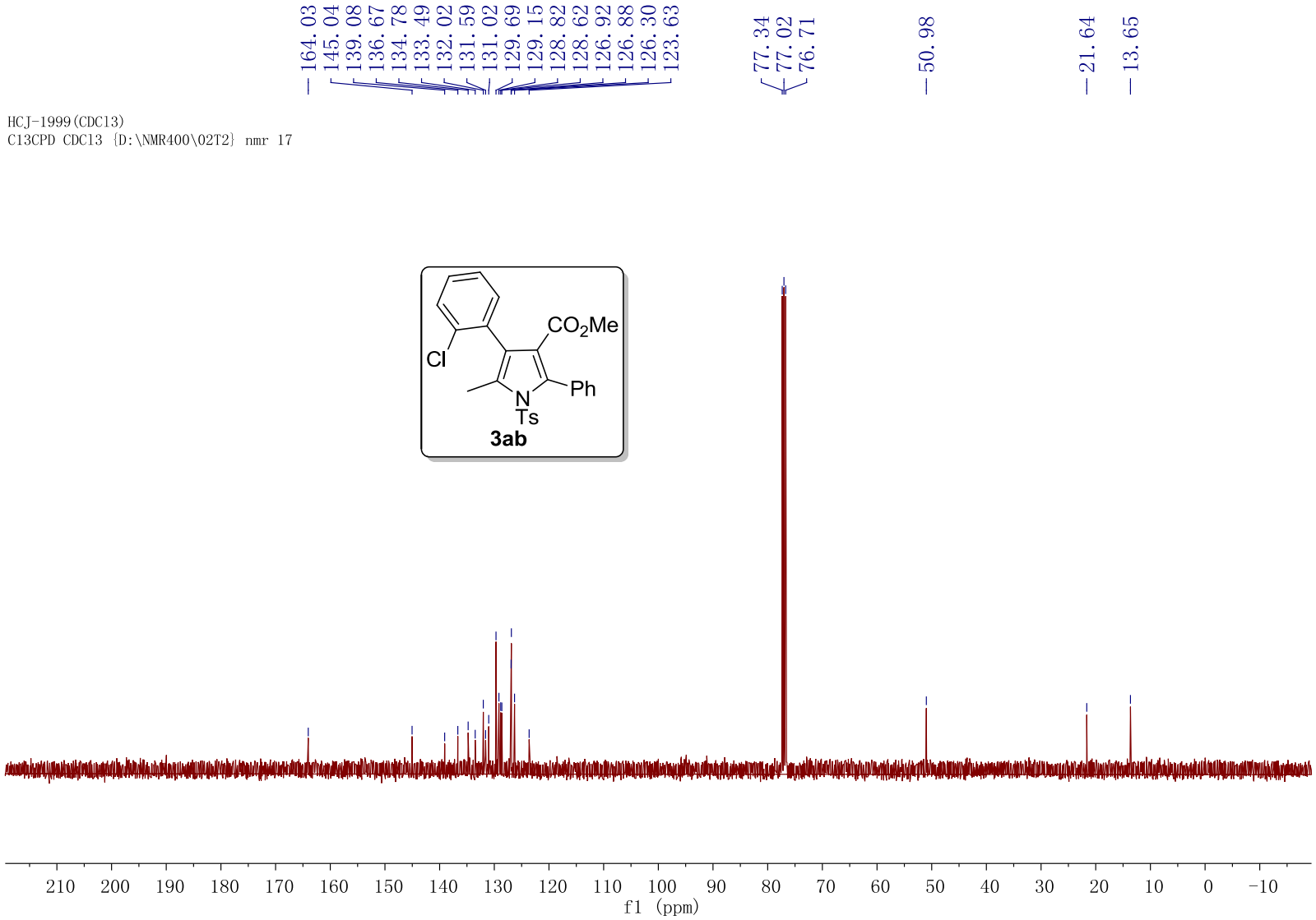
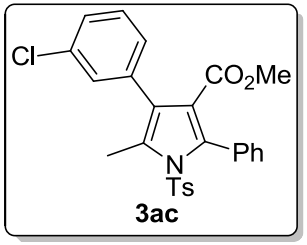
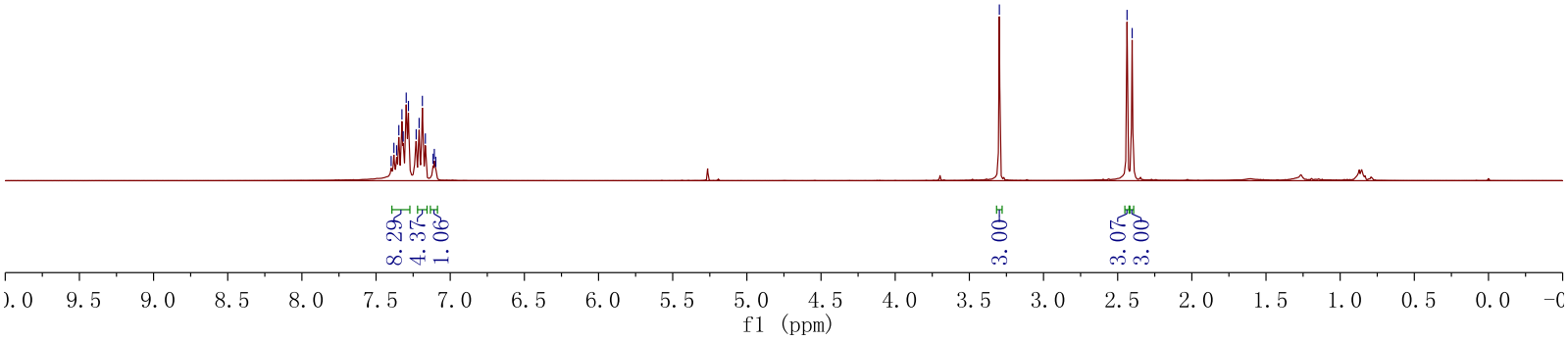
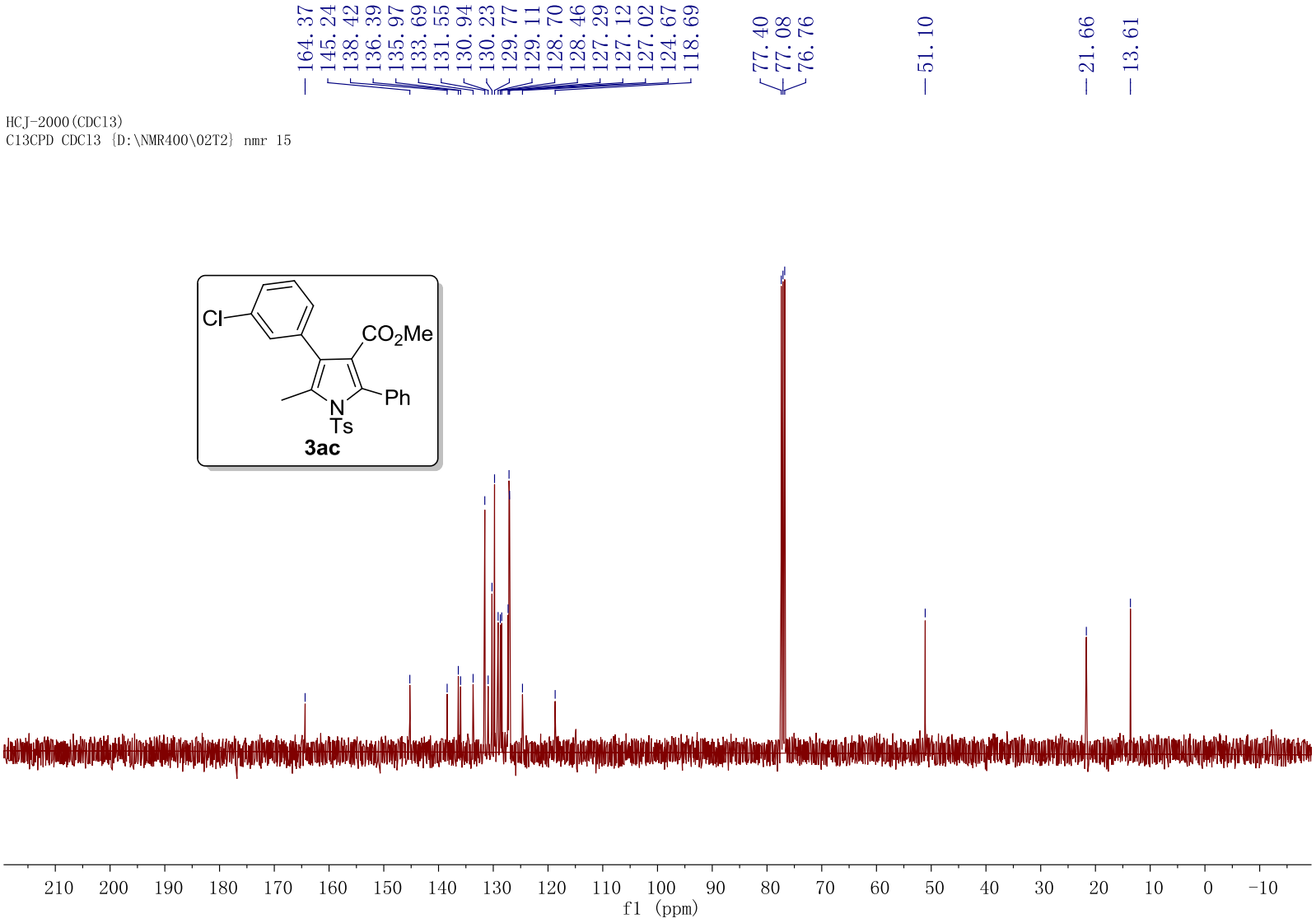
3.00
3.03
2.98
f1 (ppm)


164.03
145.04
139.08
136.67
134.78
133.49
132.02
131.59
131.02
129.69
129.15
128.82
128.62
126.92
126.88
126.30
123.63
77.34
77.02
76.71
50.98
21.64
13.65
HCJ-1999(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 17
CO2Me
Cl
Ph
N
Ts
3ab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

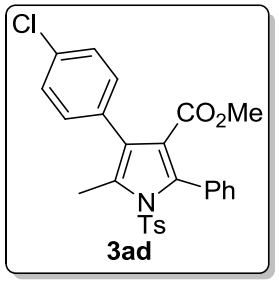
HCJ-2000-3(CDCl3)
PROTON CDCl3 {D:\NMR400\02T2} nmr 14



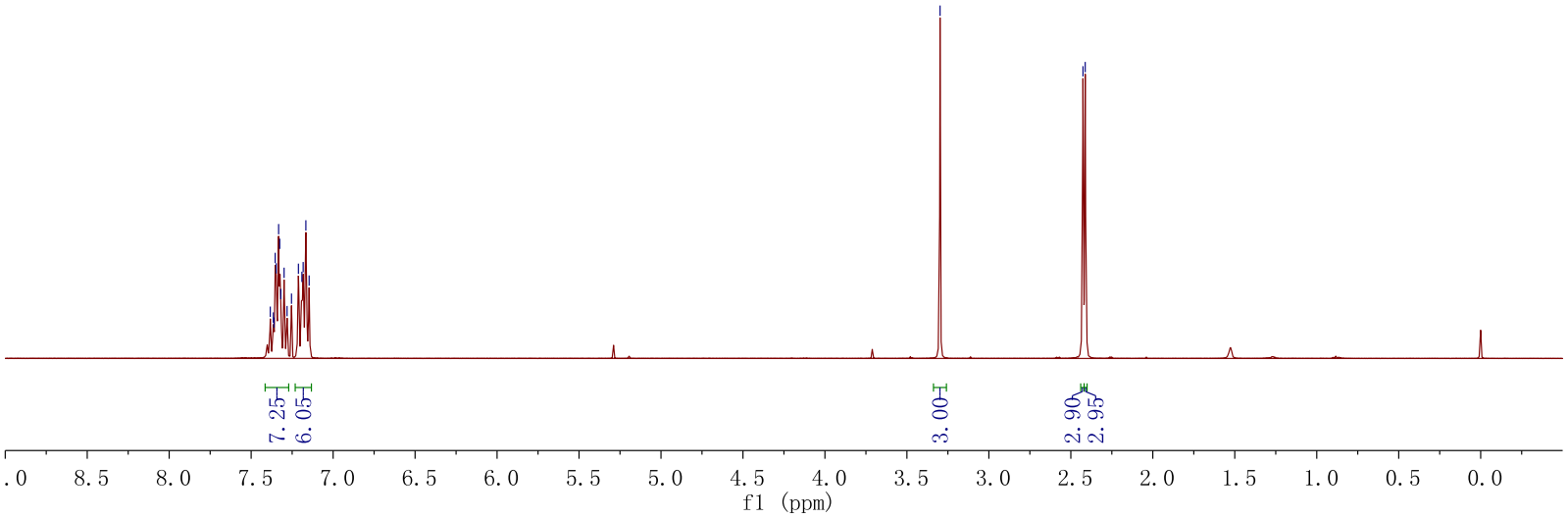


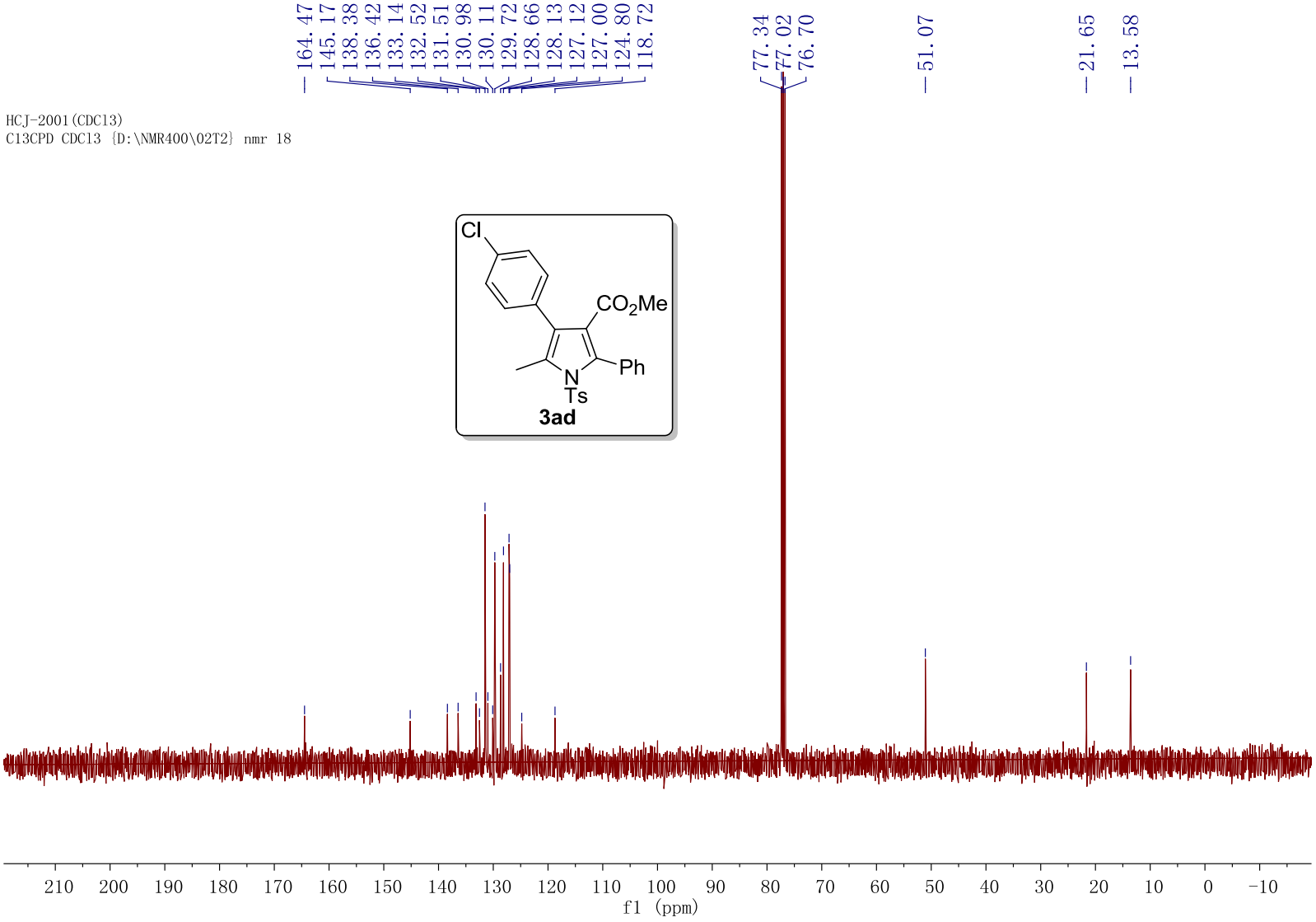

164.37
145.24
138.42
136.39
135.97
133.69
131.55
130.94
130.23
129.77
129.11
128.70
128.46
127.29
127.12
127.02
124.67
118.69
77.40
77.08
76.76
51.10
21.66
13.61
HCJ-2000(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 15
Cl
CO2Me
Ph
N
Ts
3ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

HCJ-2001(CDCl3)
PROTON CDCl3 {D:\NMR400\02T2} nmr 18

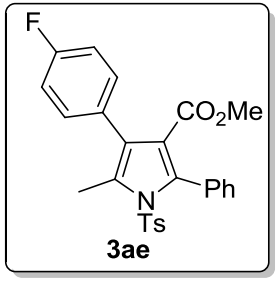


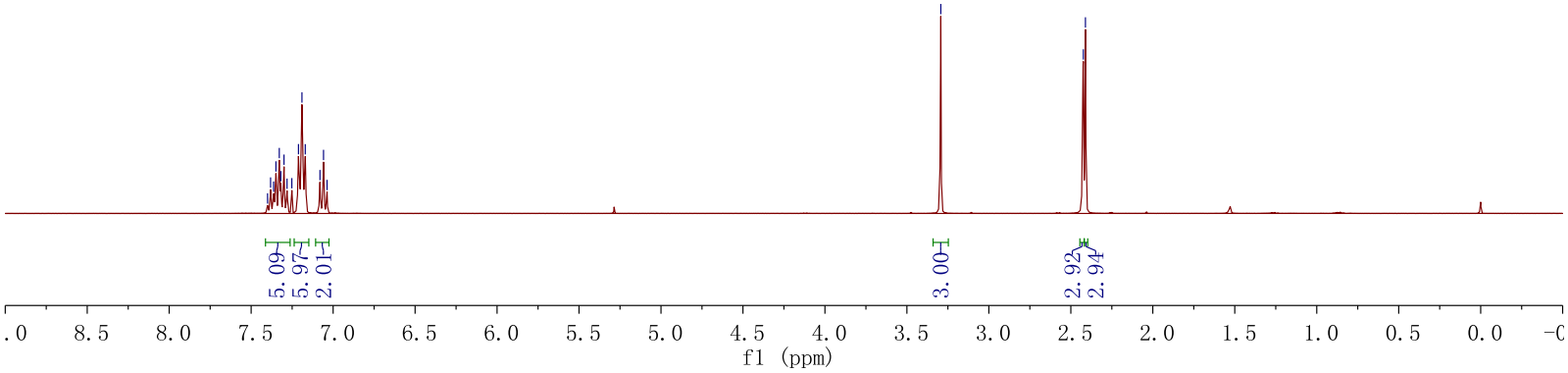
3ad

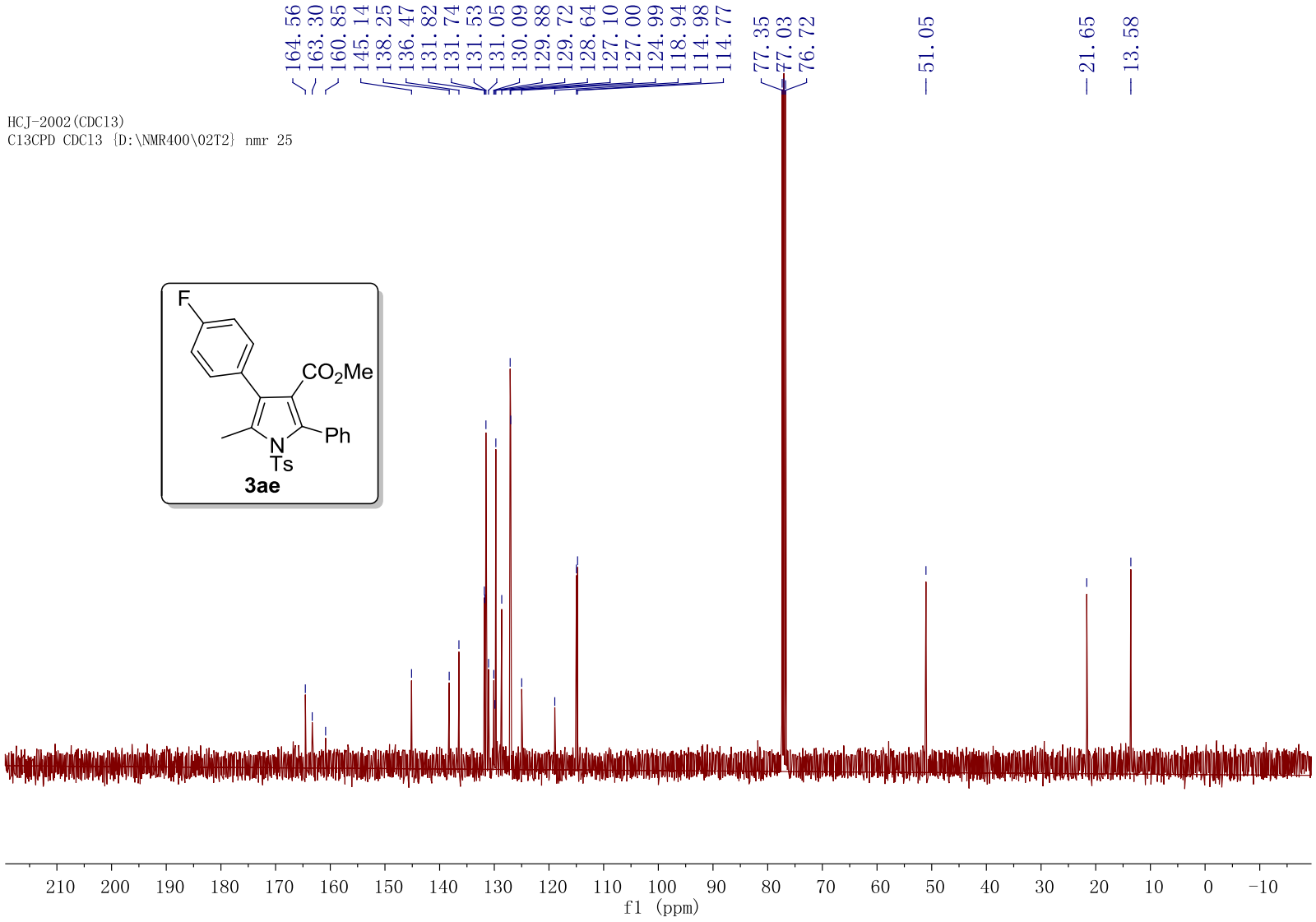


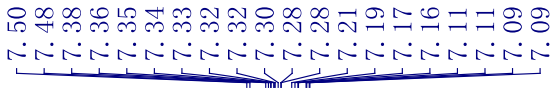

164.47
145.17
138.38
136.42
133.14
132.52
131.51
130.98
130.11
129.72
128.66
128.13
127.12
127.00
124.80
118.72
77.34
77.02
76.70
51.07
21.65
13.58
HCJ-2001(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 18
Cl
CO2Me
Ph
N
Ts
3ad
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

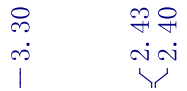
HCJ-2002(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 19



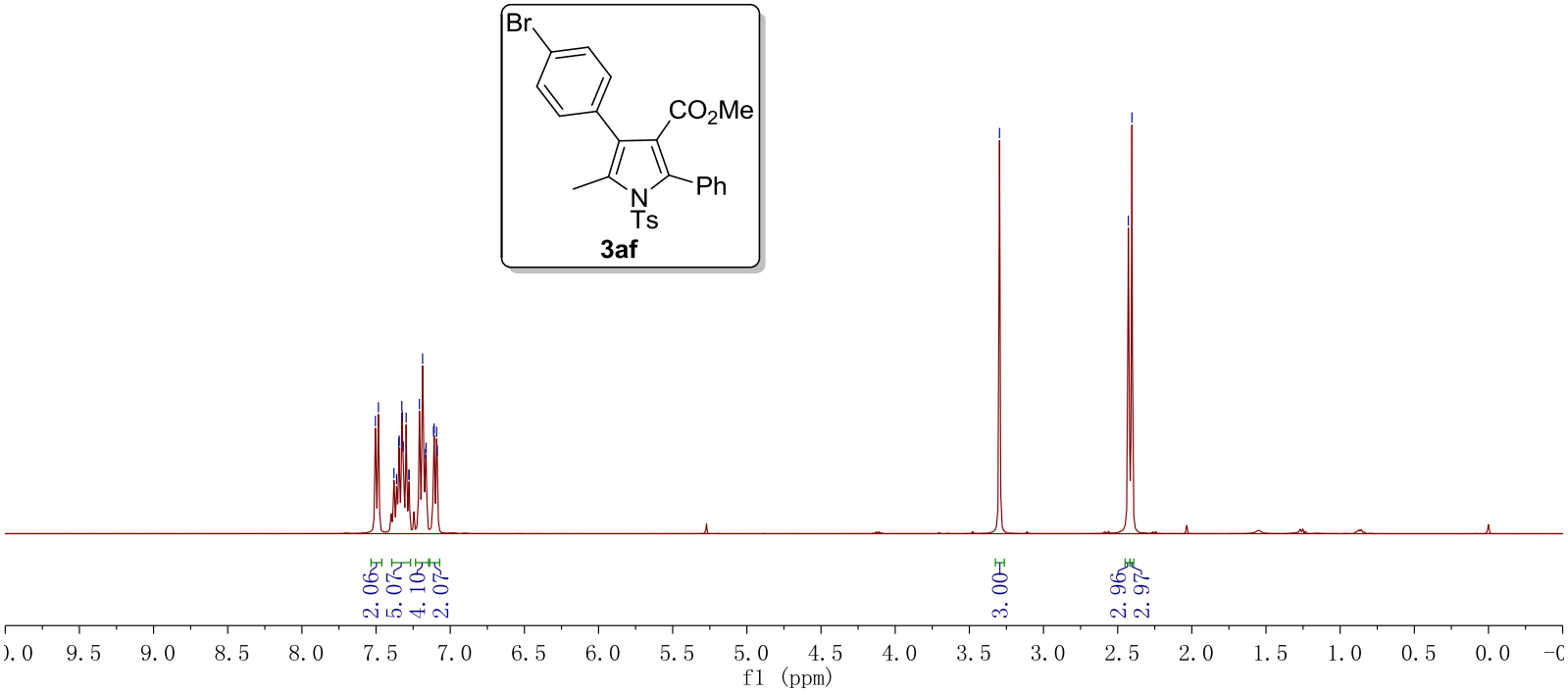


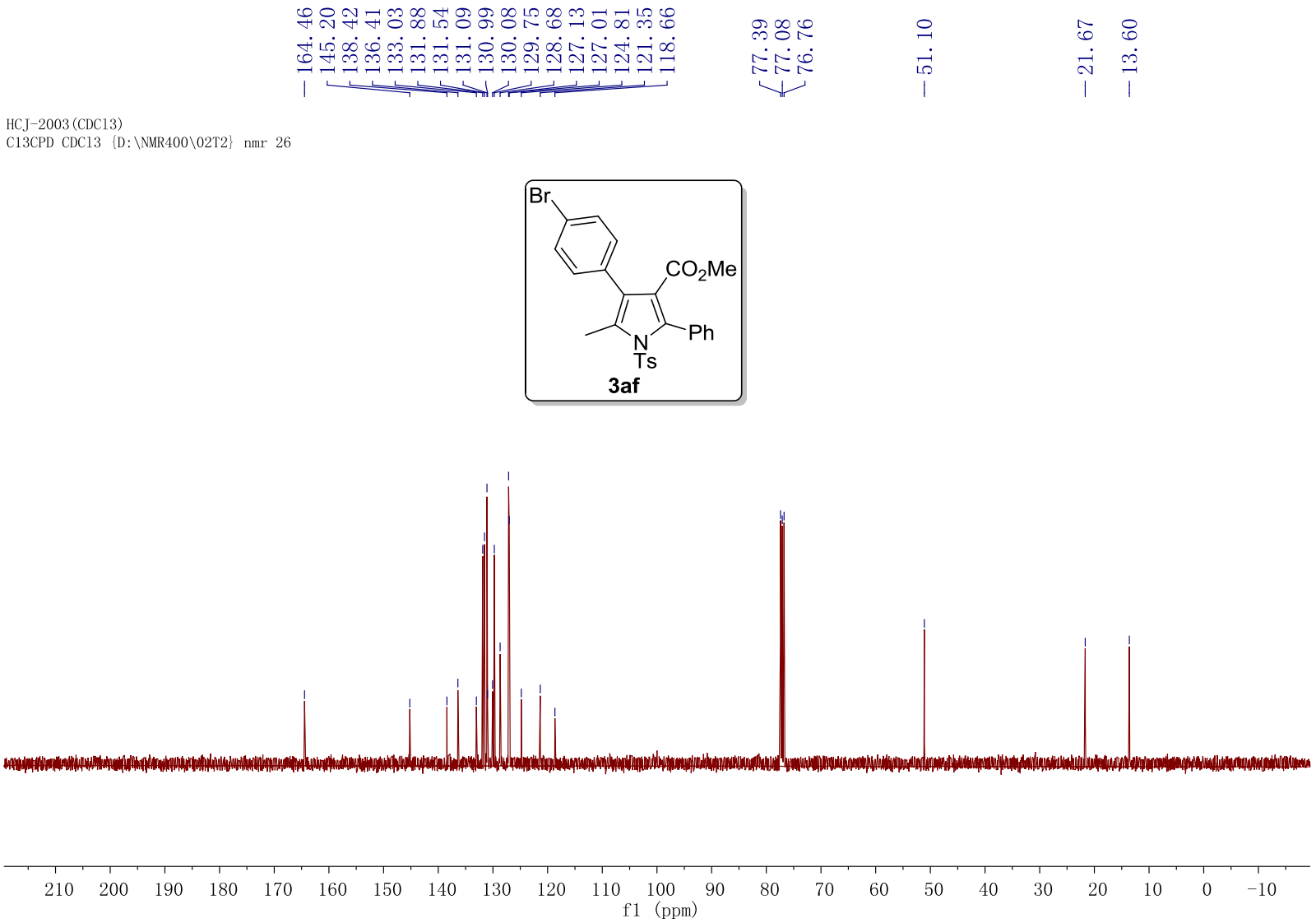

164.56
163.30
160.85
145.14
138.25
136.47
131.82
131.74
131.53
131.05
130.09
129.88
129.72
128.64
127.10
127.00
124.99
118.94
114.98
114.77
77.35
77.03
76.72
51.05
21.65
13.58
HCJ-2002(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 25
F
CO2Me
Ph
N
Ts
3ae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



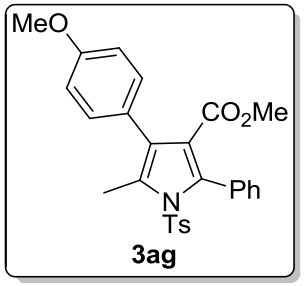


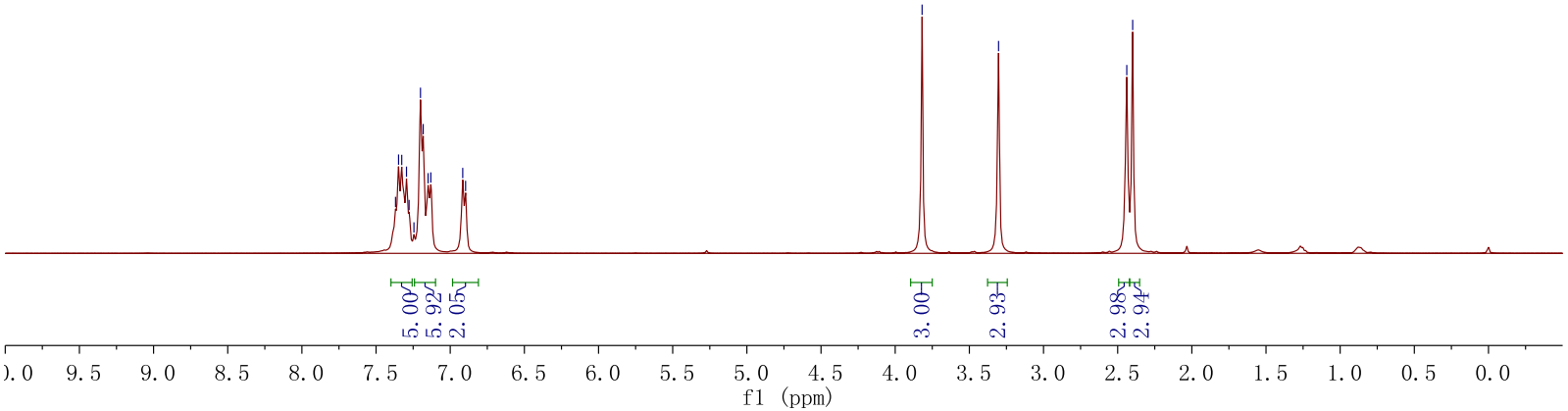
HCJ-2003(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 26

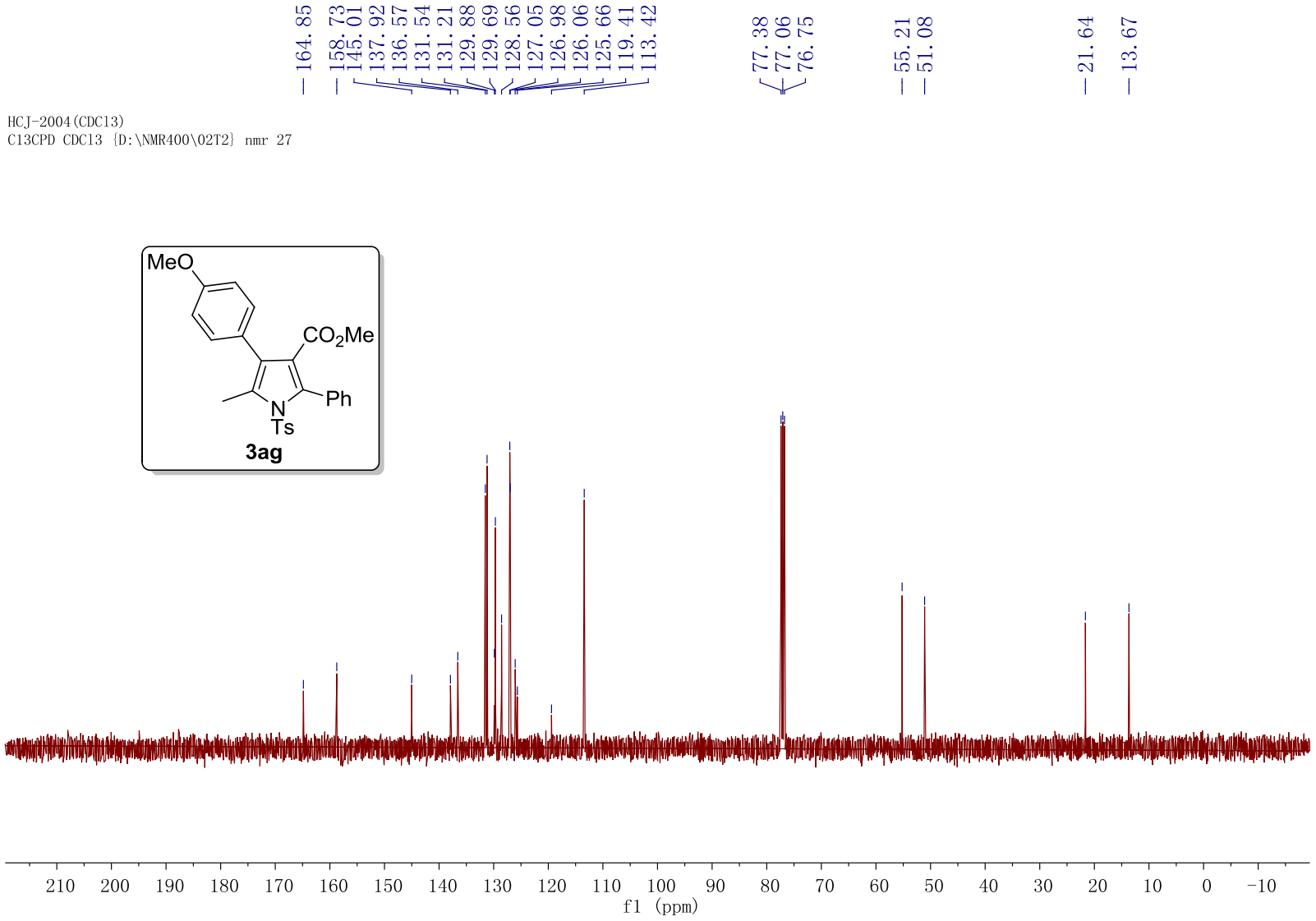


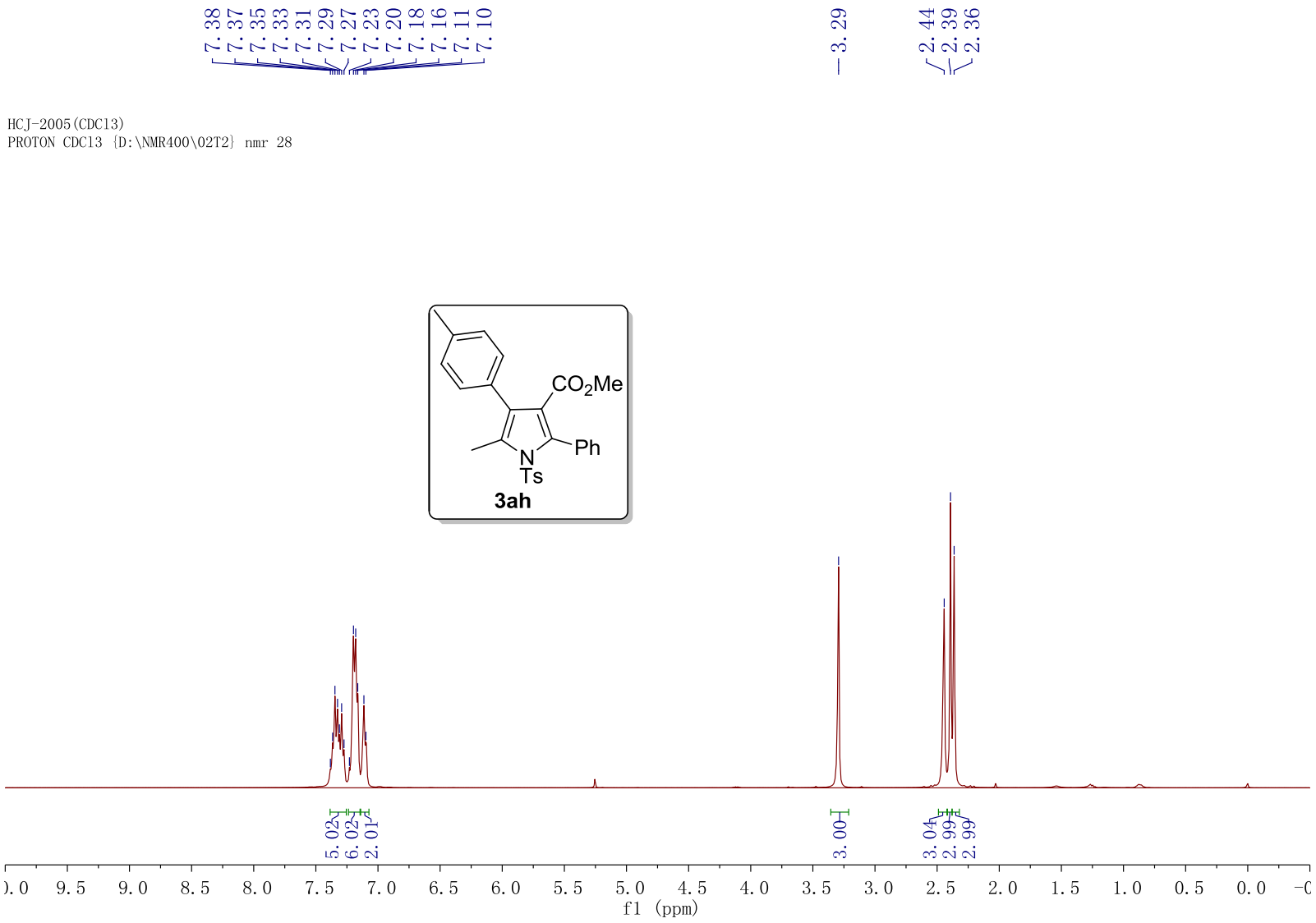

164.46
145.20
138.42
136.41
133.03
131.88
131.54
131.09
130.99
130.08
129.75
128.68
127.13
127.01
124.81
121.35
118.66
77.39
77.08
76.76
51.10
21.67
13.60
HCJ-2003(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 26
Br
CO2Me
Ph
N
Ts
3af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

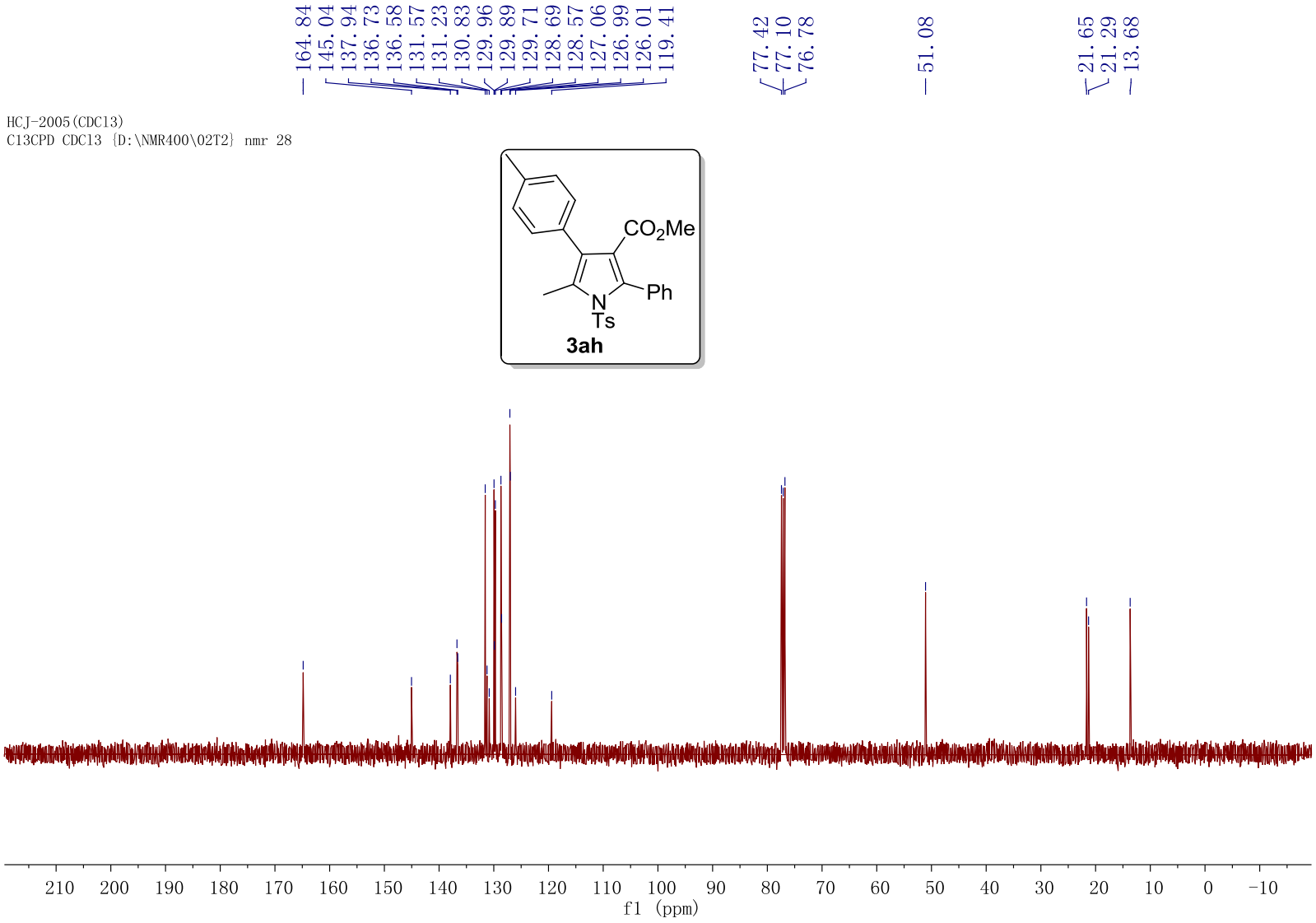
HCJ-2004(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 27

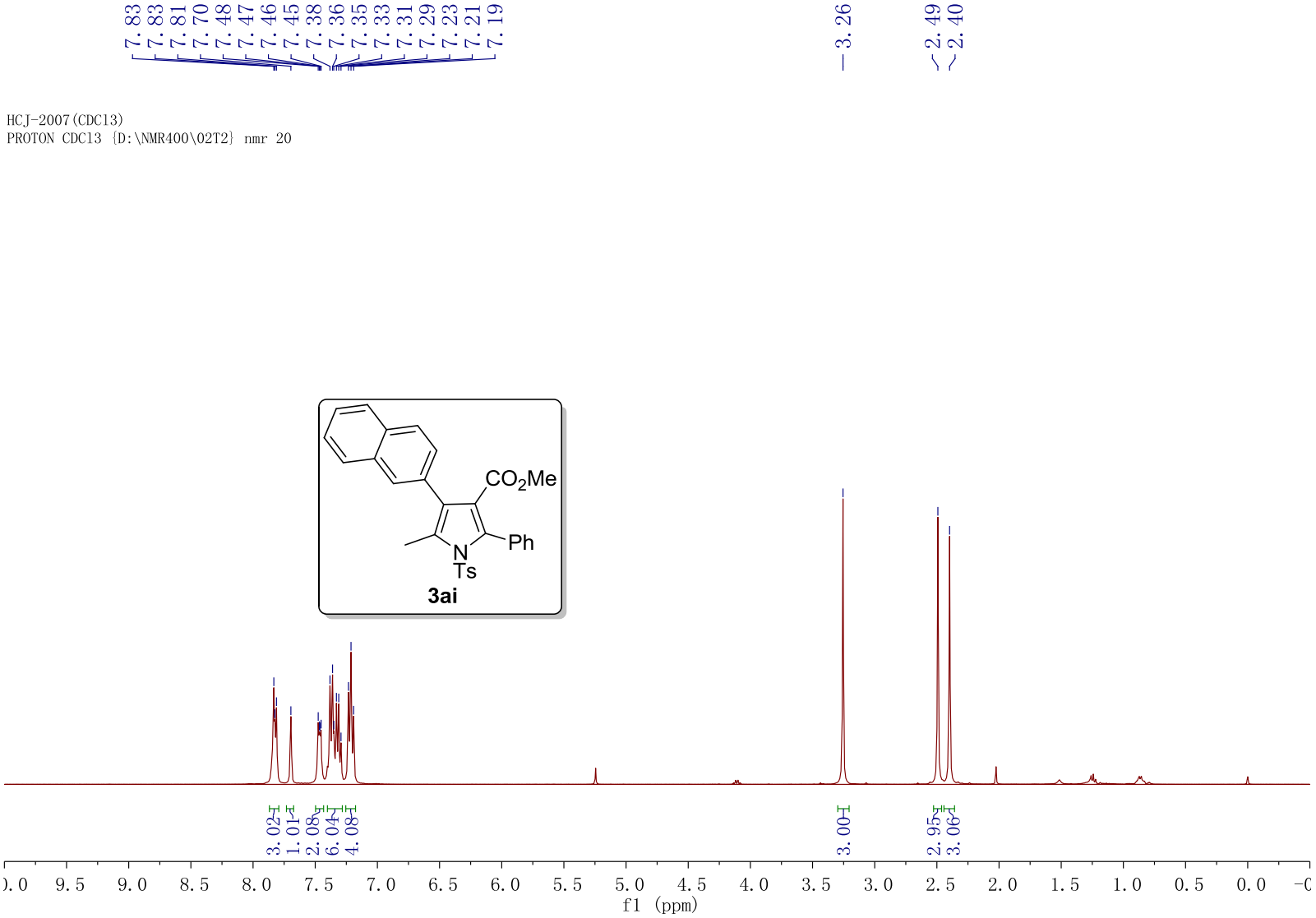


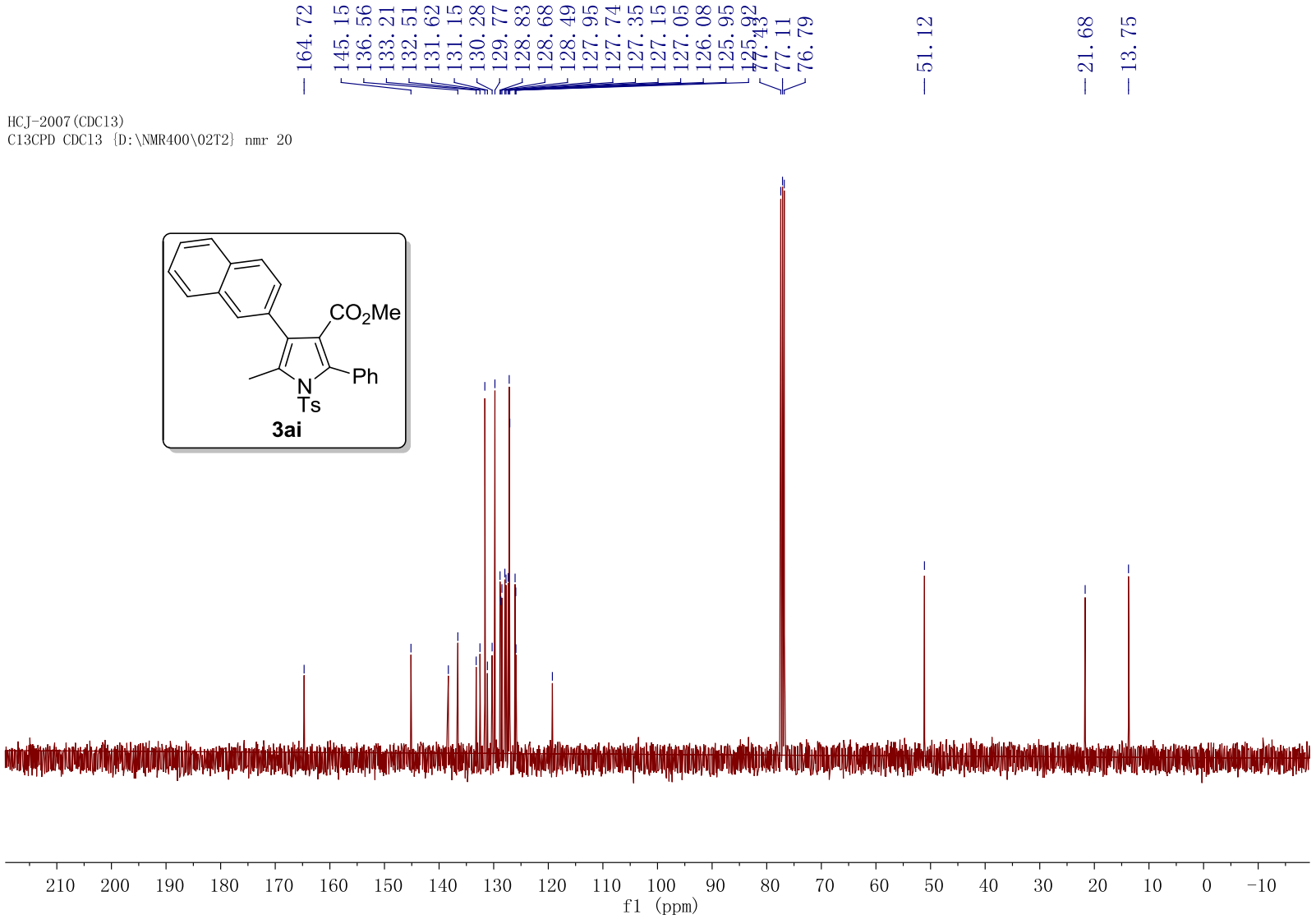


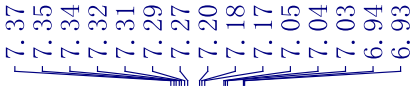

164.85
158.73
145.01
137.92
136.57
131.54
131.21
129.88
129.69
128.56
127.05
126.98
126.06
125.66
119.41
113.42
77.38
77.06
76.75
55.21
51.08
21.64
13.67
HCJ-2004(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 27
MeO
CO2Me
Ph
N
Ts
3ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.38
7.37
7.35
7.33
7.31
7.29
7.27
7.23
7.20
7.18
7.16
7.11
7.10
3.29
2.44
2.39
2.36
HCJ-2005(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 28
CO2Me
Ph
N
Ts
3ah
5.02
6.02
2.01
3.00
3.04
2.99
2.99
f1 (ppm)

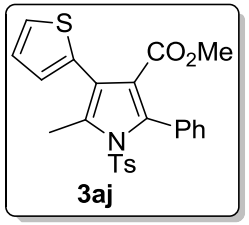

164.84
145.04
137.94
136.73
136.58
131.57
131.23
130.83
129.96
129.89
129.71
128.69
128.57
127.06
126.99
126.01
119.41
77.42
77.10
76.78
51.08
21.65
21.29
13.68
HCJ-2005(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 28
CO2Me
Ph
N
Ts
3ah
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

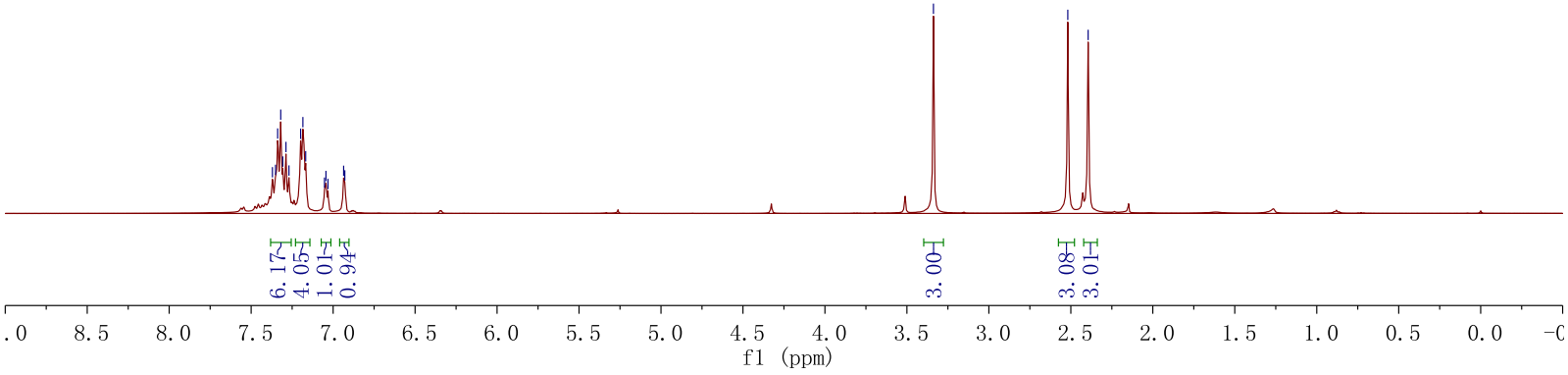

7.83
7.83
7.81
7.70
7.48
7.47
7.46
7.45
7.38
7.36
7.35
7.33
7.31
7.29
7.23
7.21
7.19
3.26
2.49
2.40
HCJ-2007(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 20
CO2Me
Ph
N
Ts
3ai
3.02
1.01
2.08
6.04
4.08
3.00
2.95
3.06
f1 (ppm)

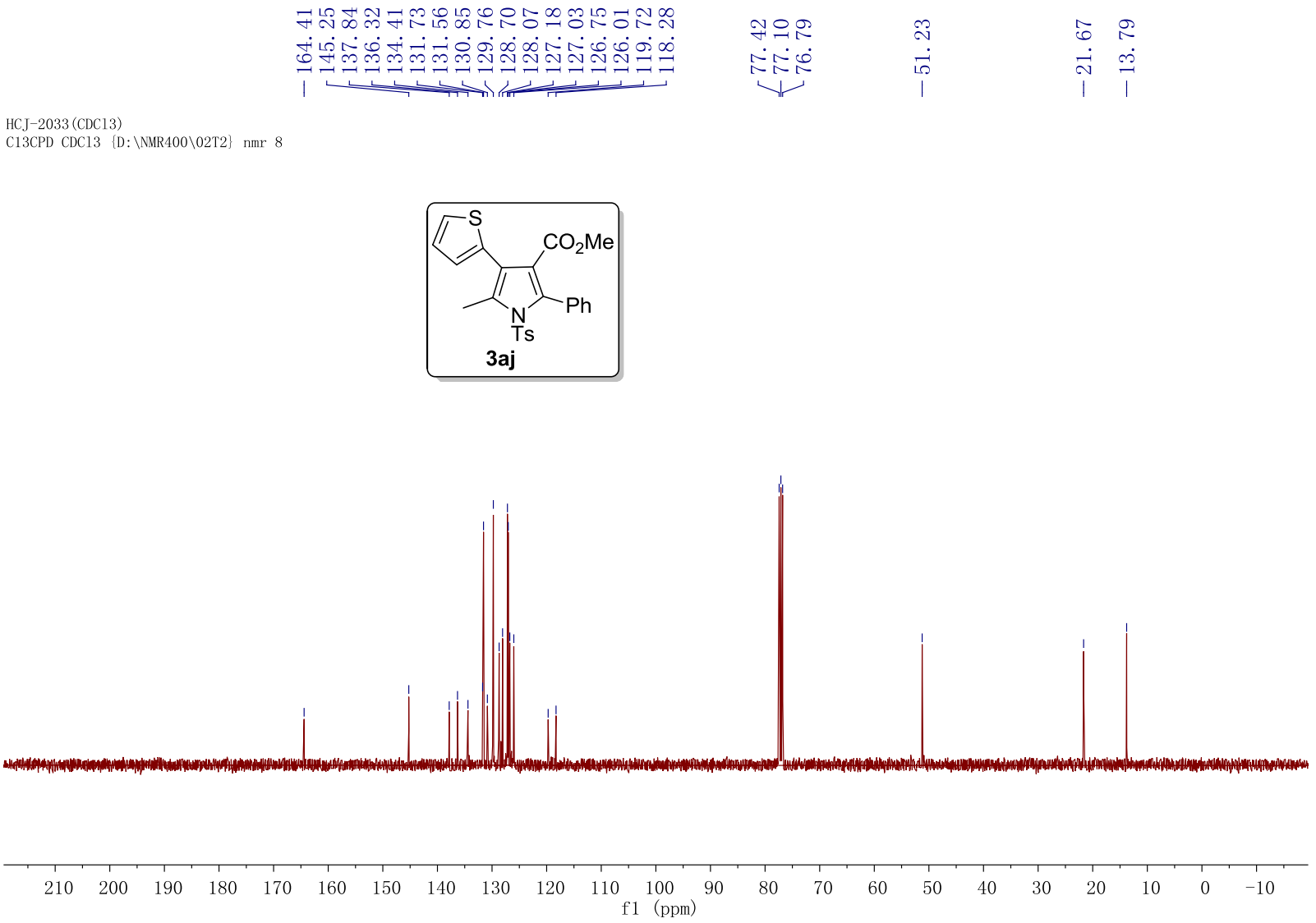

164.72
145.15
136.56
133.21
132.51
131.62
131.15
130.28
129.77
128.83
128.68
128.49
127.95
127.74
127.35
127.15
127.05
126.08
125.95
77.11
76.79
51.12
21.68
13.75
HCJ-2007(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 20
CO2Me
Ph
N
Ts
3ai
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

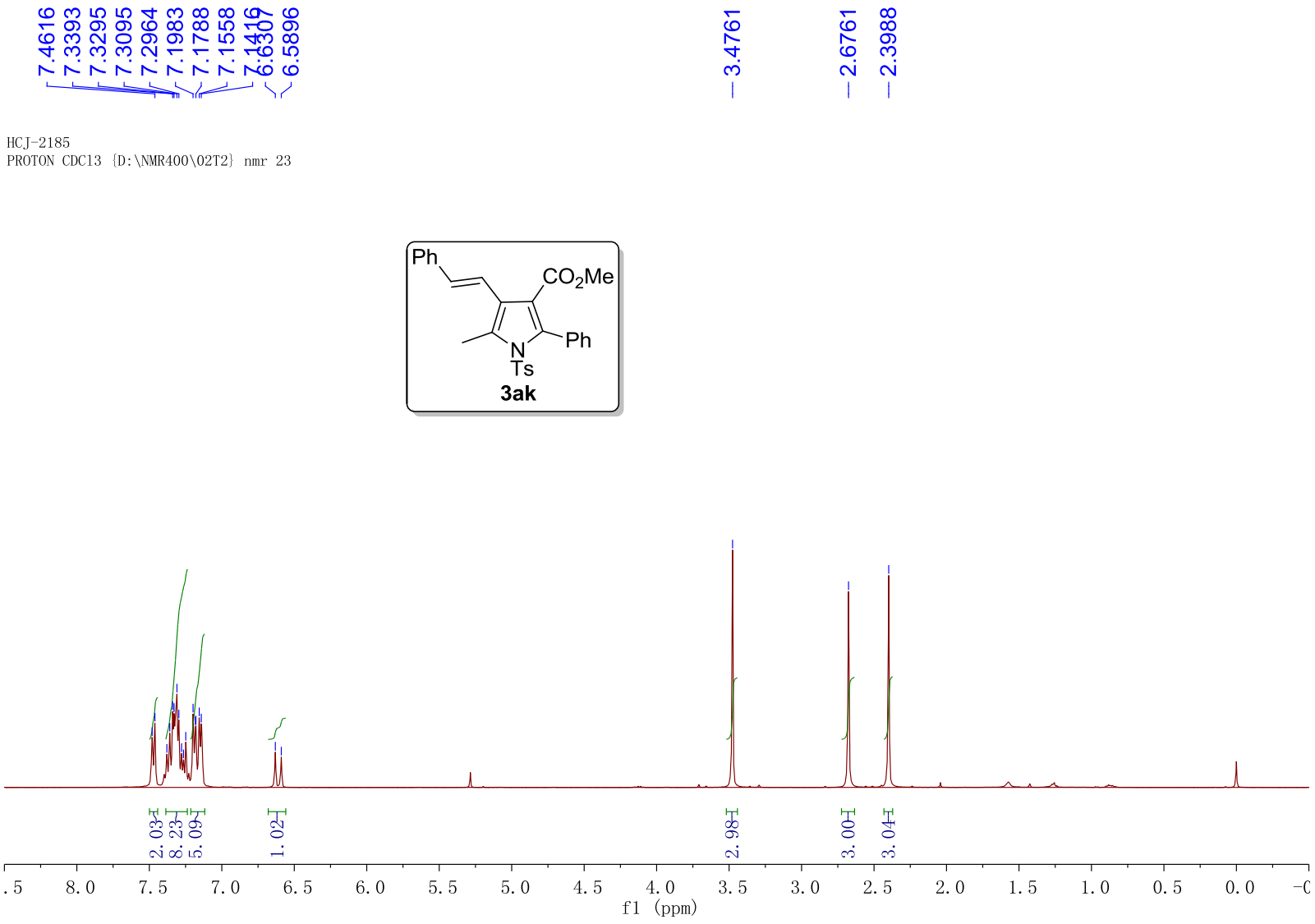


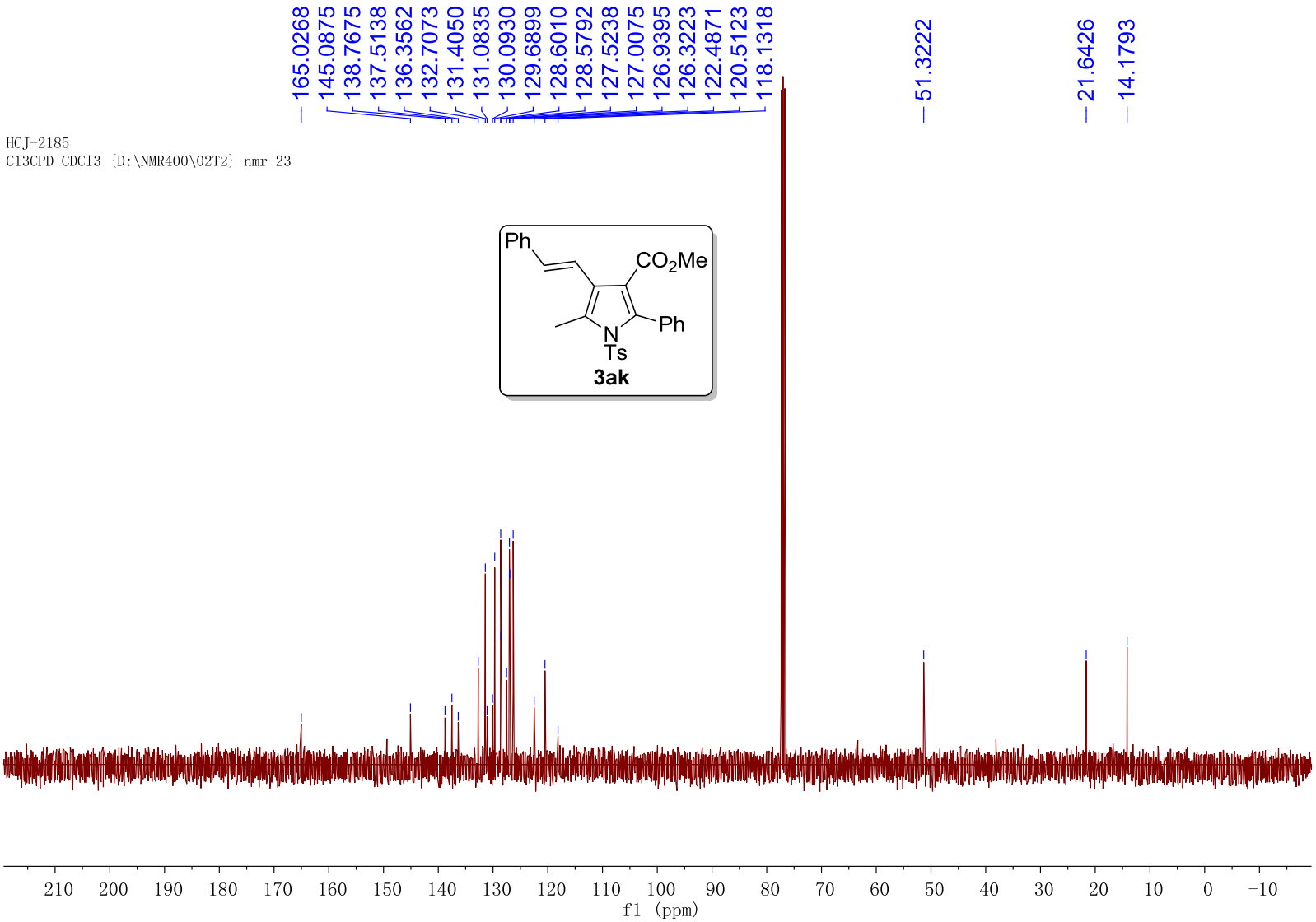
HCJ-2033(CDCl3)
PROTON CDCl3 {D:\NMR400\02T2} nmr 8

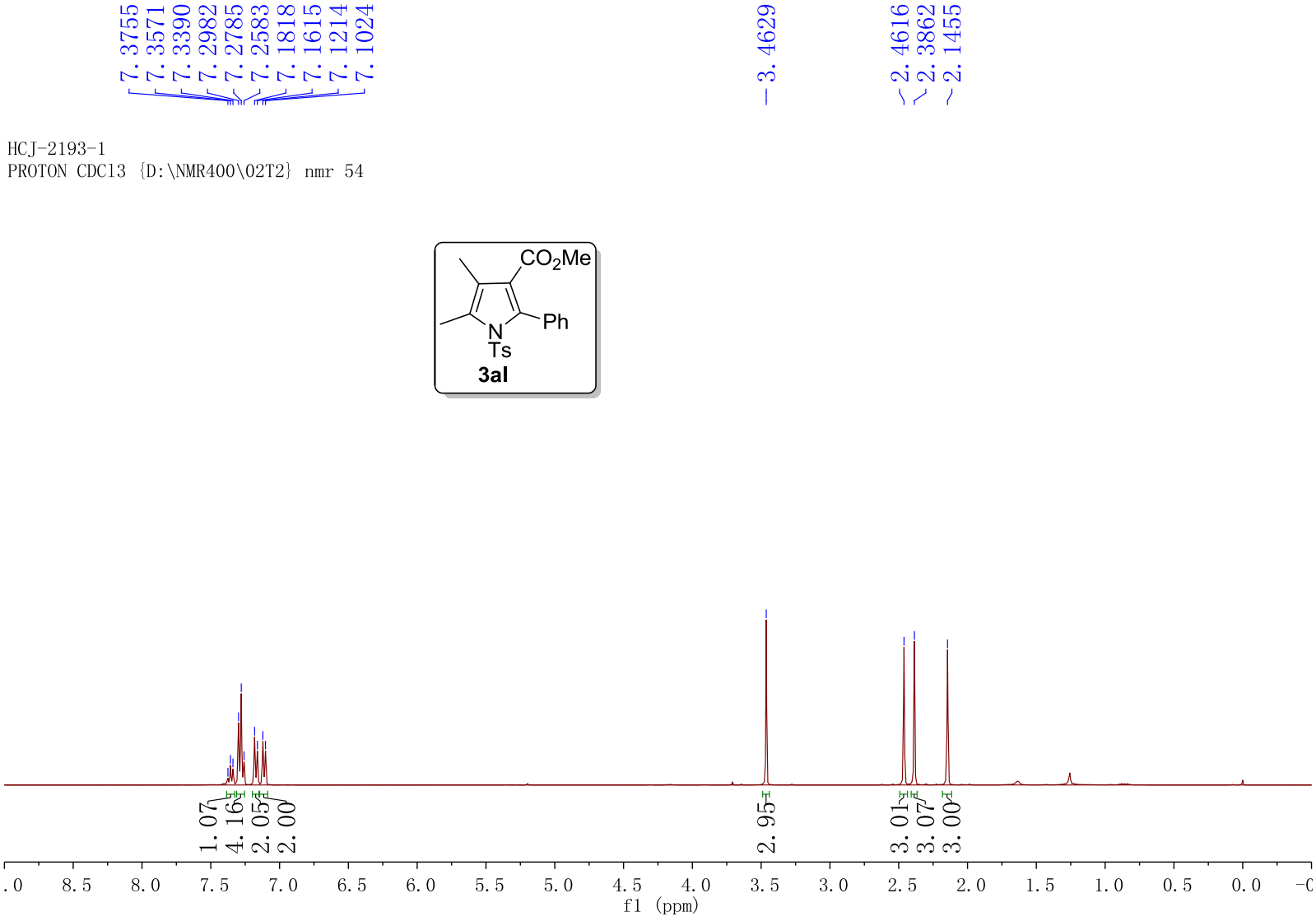





164.41
145.25
137.84
136.32
134.41
131.73
131.56
130.85
129.76
128.70
128.07
127.18
127.03
126.75
126.01
119.72
118.28
77.42
77.10
76.79
51.23
21.67
13.79
HCJ-2033(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 8
S
CO2Me
Ph
N
Ts
3aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

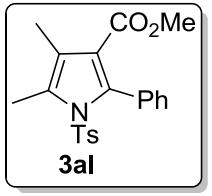

7.4616
7.3393
7.3295
7.3095
7.2964
7.1983
7.1788
7.1558
7.1416
6.6307
6.5896
3.4761
2.6761
2.3988
HCJ-2185
PROTON CDC13 {D:\NMR400\02T2} nmr 23
Ph
CO2Me
Ph
N
Ts
3ak
2.03
8.23
5.09
1.02
2.98
3.00
3.04
f1 (ppm)


165.0268
145.0875
138.7675
137.5138
136.3562
132.7073
131.4050
131.0835
130.0930
129.6899
128.6010
128.5792
127.5238
127.0075
126.9395
126.3223
122.4871
120.5123
118.1318
51.3222
21.6426
14.1793
HCJ-2185
C13CPD CDC13 {D:\NMR400\02T2} nmr 23
Ph
CO2Me
Ph
N
Ts
3ak
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

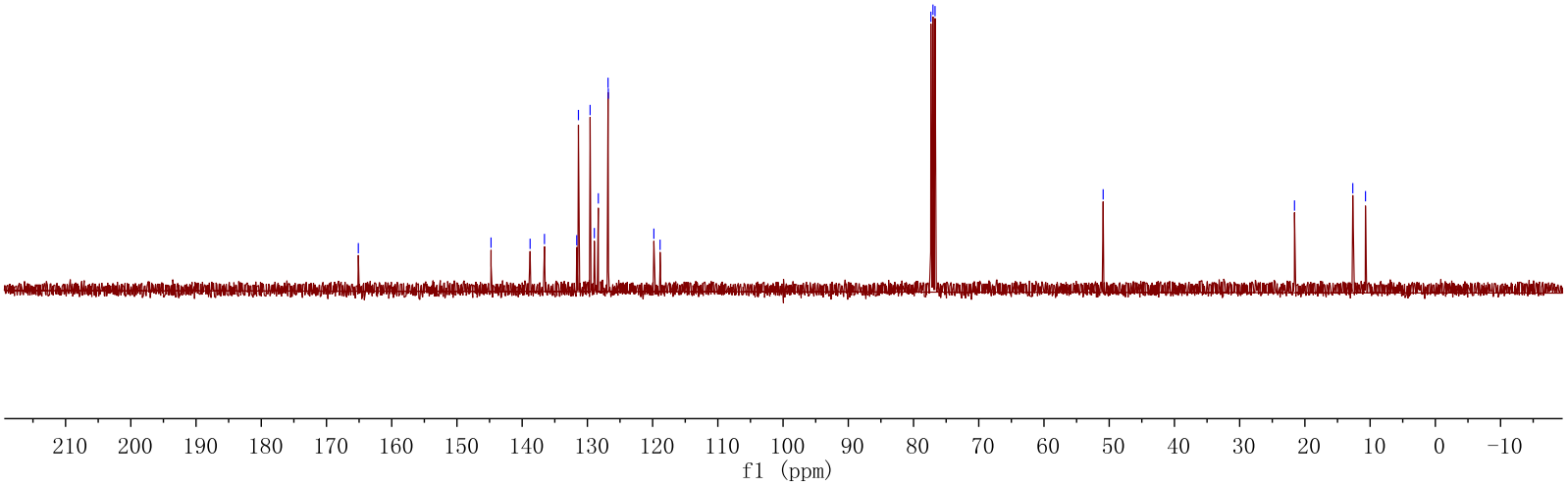

7.3755
7.3571
7.3390
7.2982
7.2785
7.2583
7.1818
7.1615
7.1214
7.1024
3.4629
2.4616
2.3862
2.1455
HCJ-2193-1
PROTON CDC13 {D:\NMR400\02T2} nmr 54
CO2Me
Ph
N
Ts
3al
1.07
4.16
2.05
2.00
2.95
3.01
3.07
3.00
f1 (ppm)

165.1167
144.7715
138.7829
136.5809
131.6346
131.3746
129.5826
128.9358
128.3265
126.8325
126.7944
119.8093
118.8541
77.3372
77.0198
76.7015
50.9282
21.5915
12.6560
10.7108

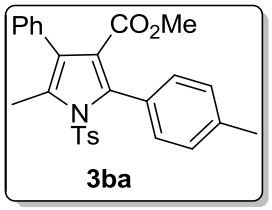
HCJ-2193-1
C13CPD CDCl3 {D:\NMR400\02T2} nmr 54



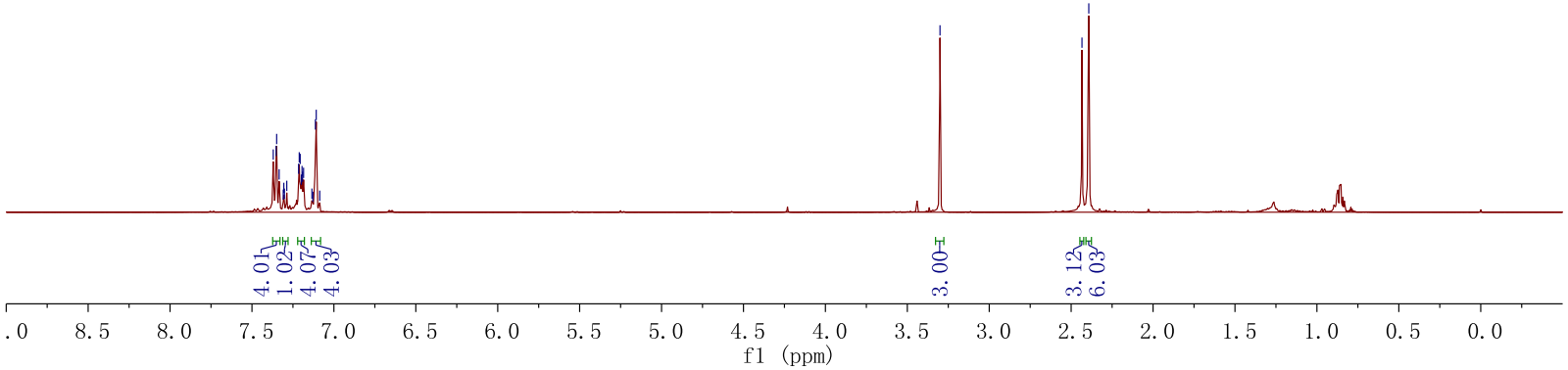
3al

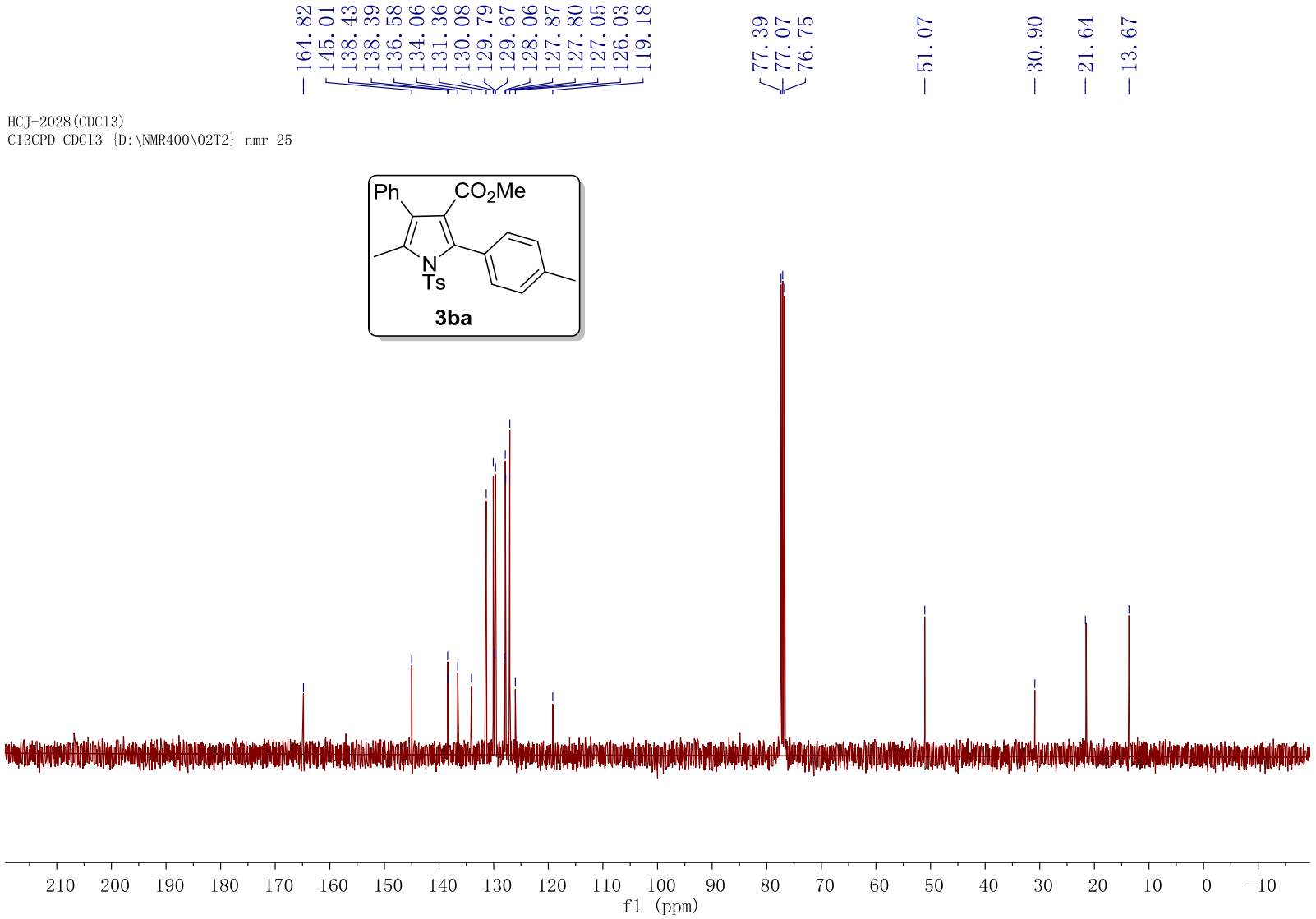


HCJ-2028(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 25



3ba




164.82
145.01
138.43
138.39
136.58
134.06
131.36
130.08
129.79
129.67
128.06
127.87
127.80
127.05
126.03
119.18
77.39
77.07
76.75
51.07
30.90
21.64
13.67
HCJ-2028(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 25
Ph
CO2Me
N
Ts
3ba
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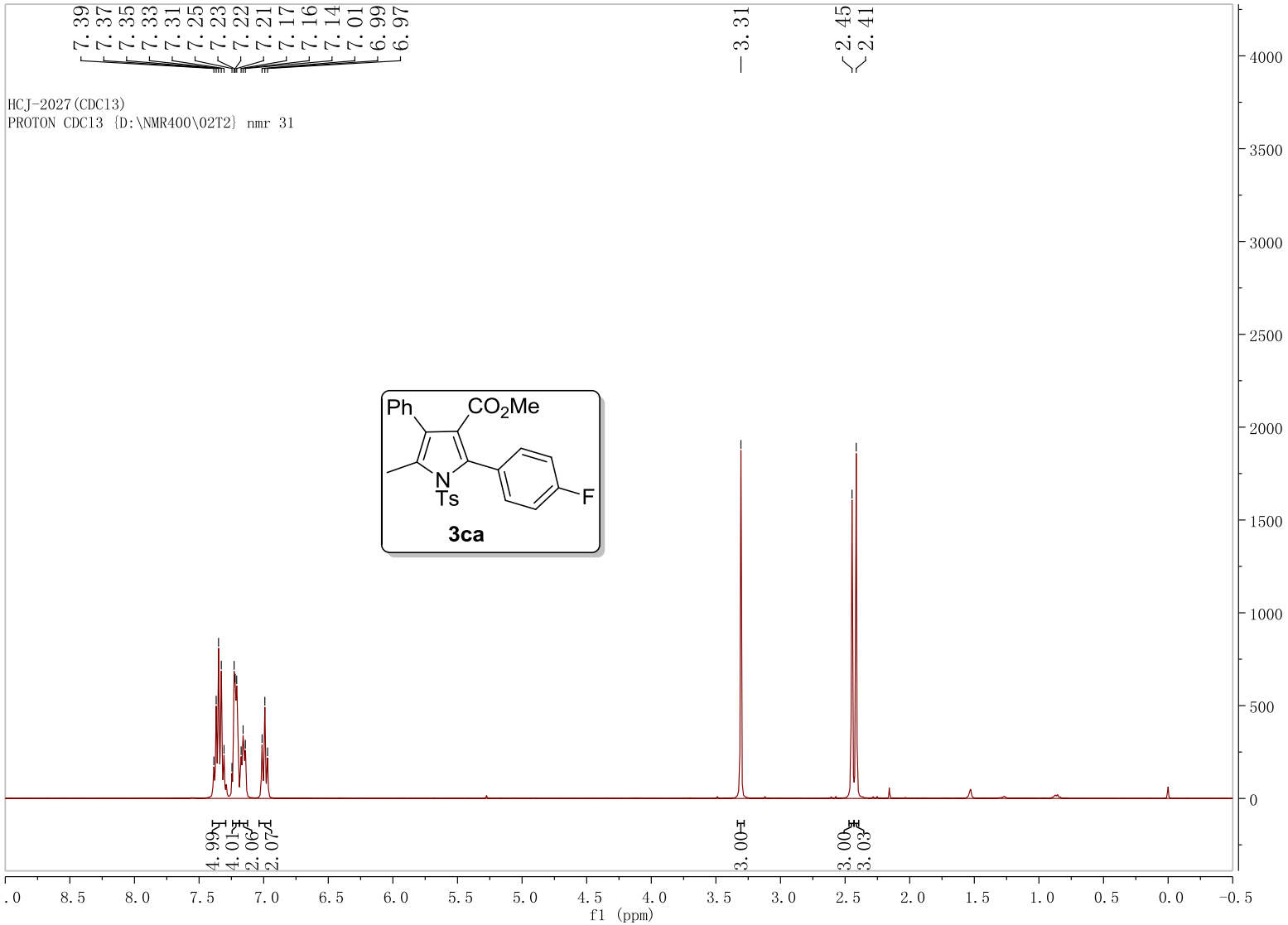
f1 (ppm)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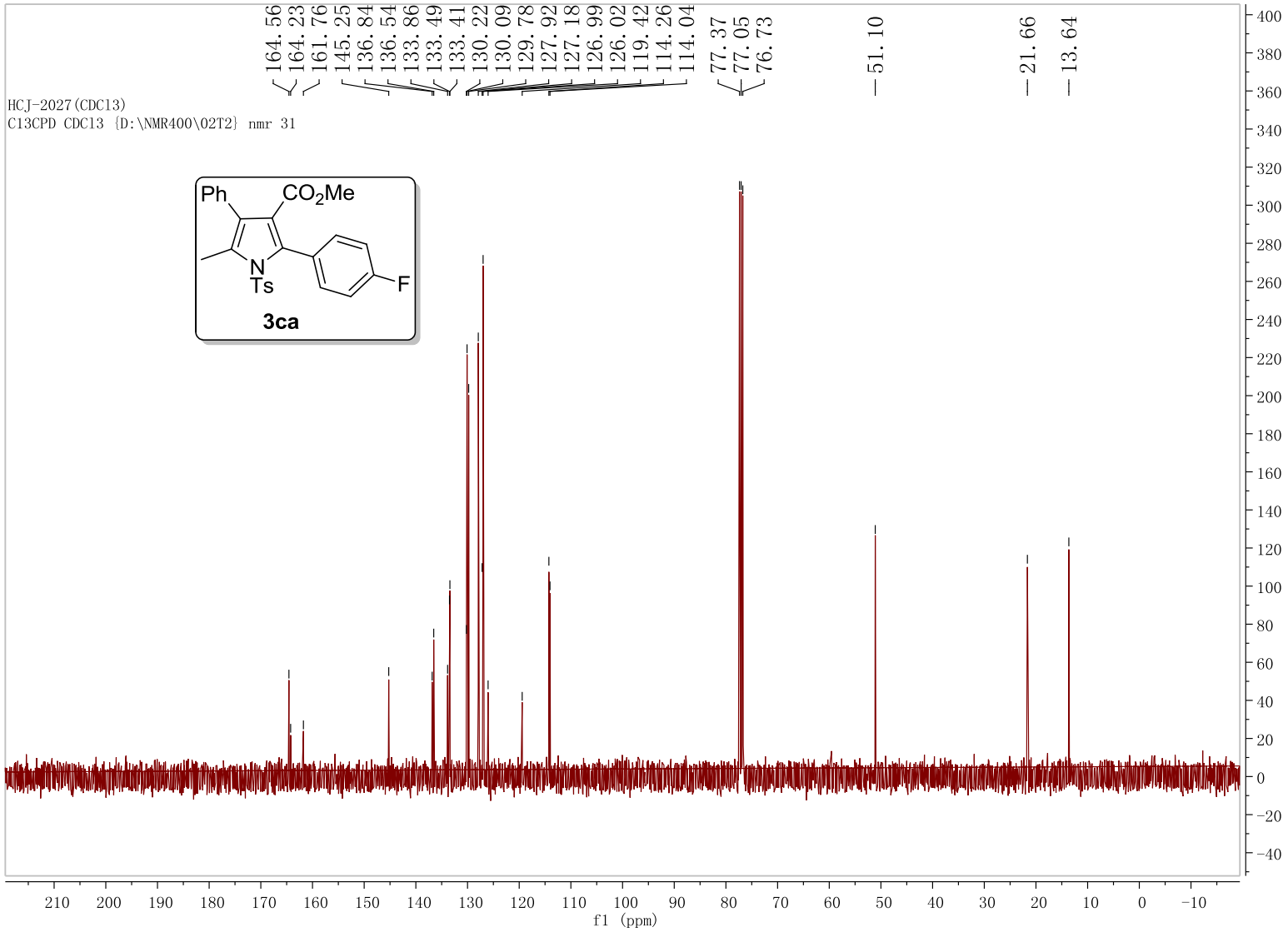
7.37
7.35
7.33
7.31
7.25
7.23
7.22
7.21
7.17
7.16
7.14
7.01
6.99
6.97
3.31
2.45
2.41
HCJ-2027(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 31
Ph
CO2Me
N
Ts
F
3ca
4.99
4.01
2.06
2.07
3.00
3.00
3.03
f1 (ppm)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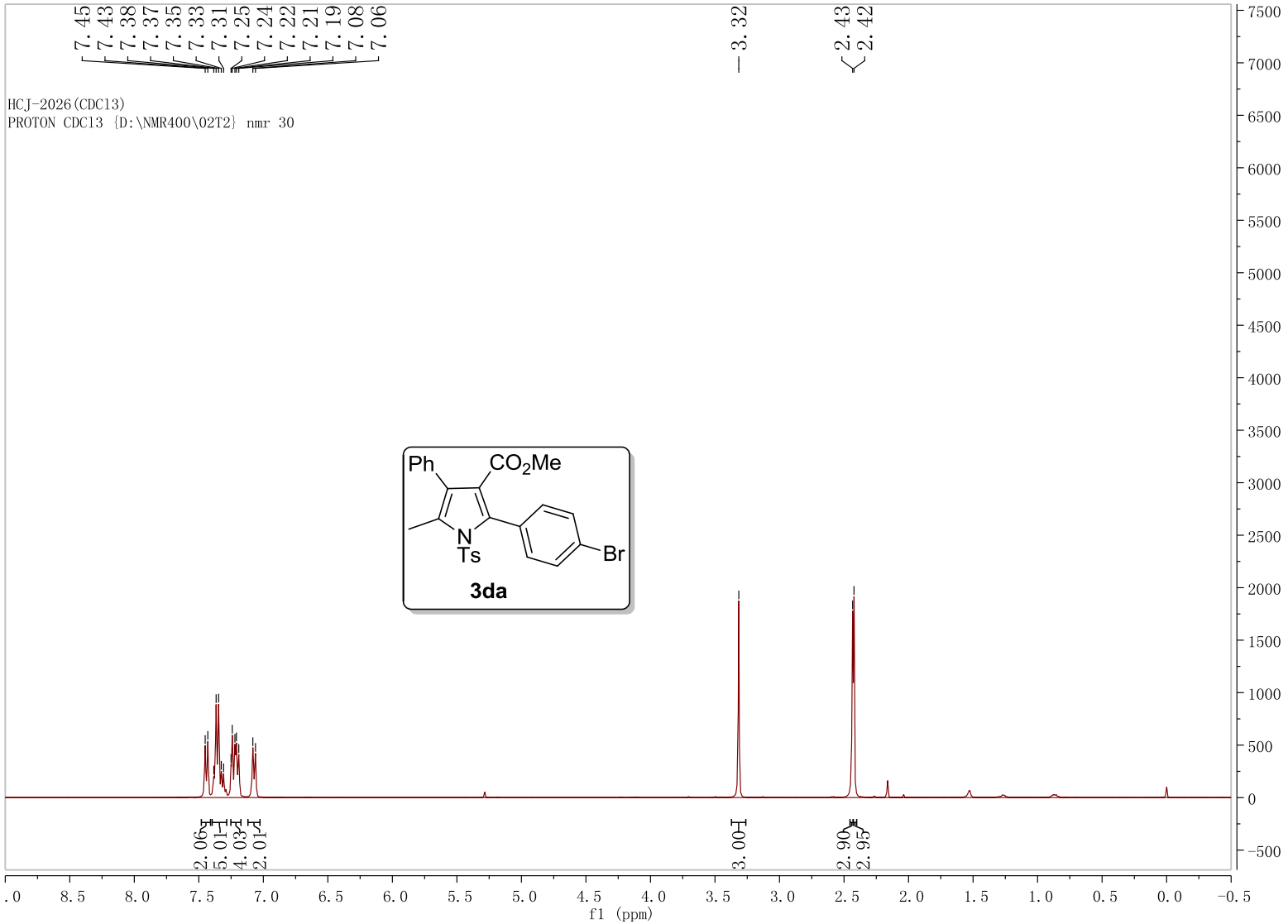
164.23
161.76
145.25
136.84
136.54
133.86
133.49
133.41
130.22
130.09
129.78
127.92
127.18
126.99
126.02
119.42
114.26
114.04
77.37
77.05
76.73
51.10
21.66
13.64
HCJ-2027(CDCl3)
C13CPD CDCl3 {D:\NMR400\02T2} nmr 31
Ph
CO2Me
N
Ts
F
3ca
f1 (ppm)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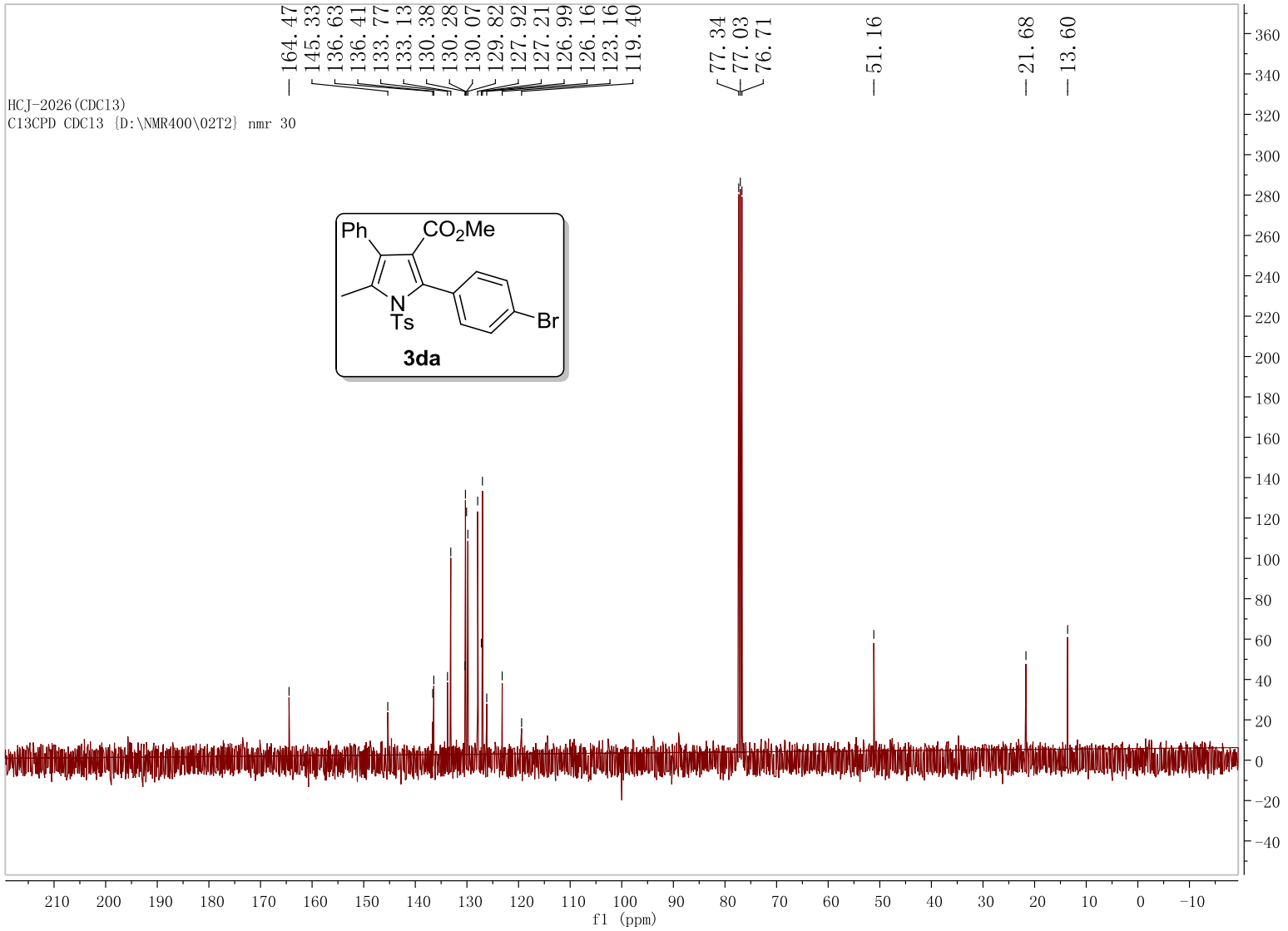
7.43
7.38
7.37
7.35
7.33
7.31
7.25
7.24
7.22
7.21
7.19
7.08
7.06
3.32
2.43
2.42
HCJ-2026(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 30
Ph
CO2Me
N
Ts
Br
3da
2.06
5.01
4.03
2.01
3.00
2.90
2.95
f1 (ppm)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145.33
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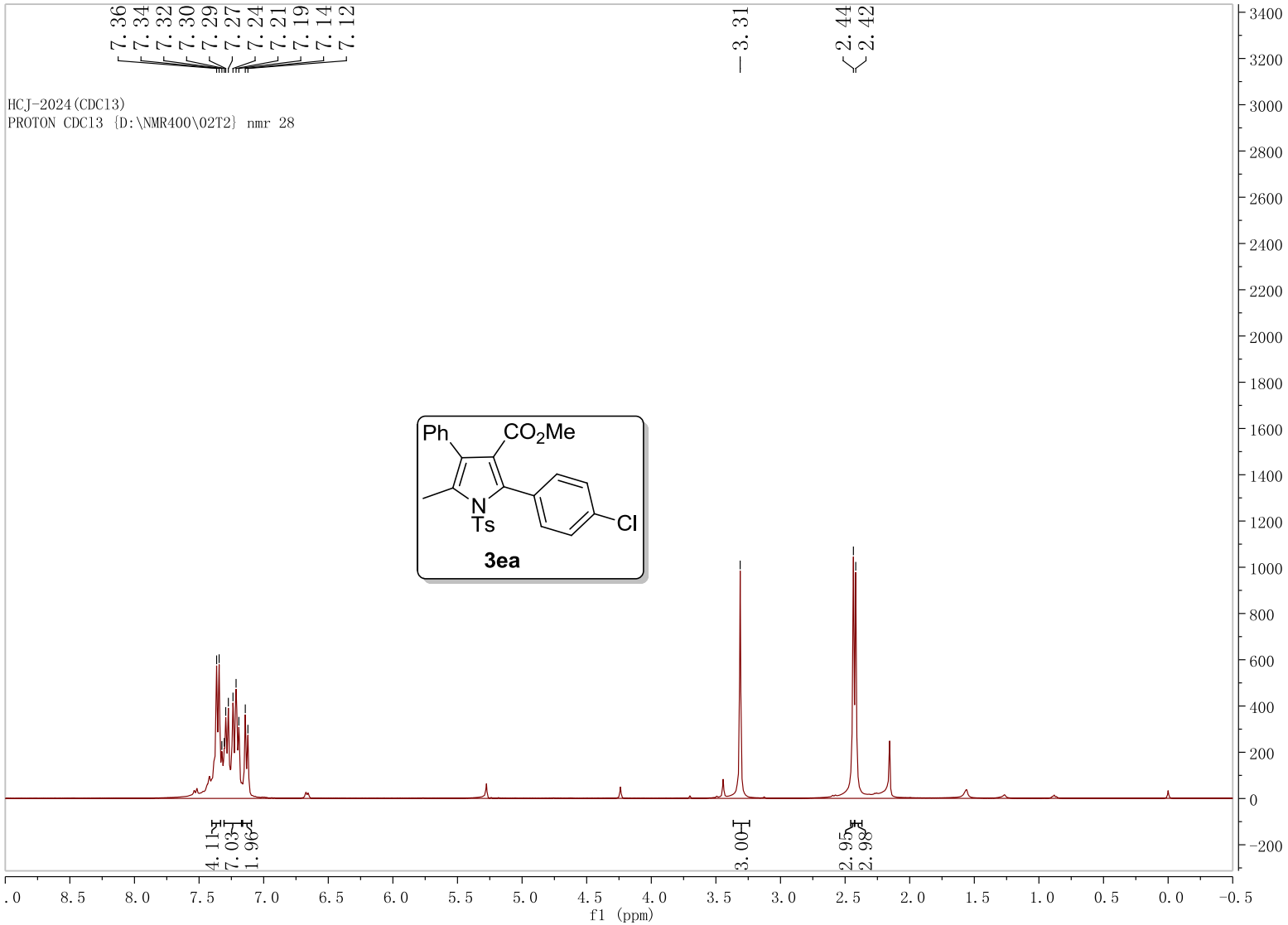
133.13
130.38
130.28
130.07
129.82
127.92
127.21
126.99
126.16
123.16
119.40
77.34
77.03
76.71
51.16
21.68
13.60
HCJ-2026(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 30
Ph
CO2Me
N
Ts
Br
3da
f1 (ppm)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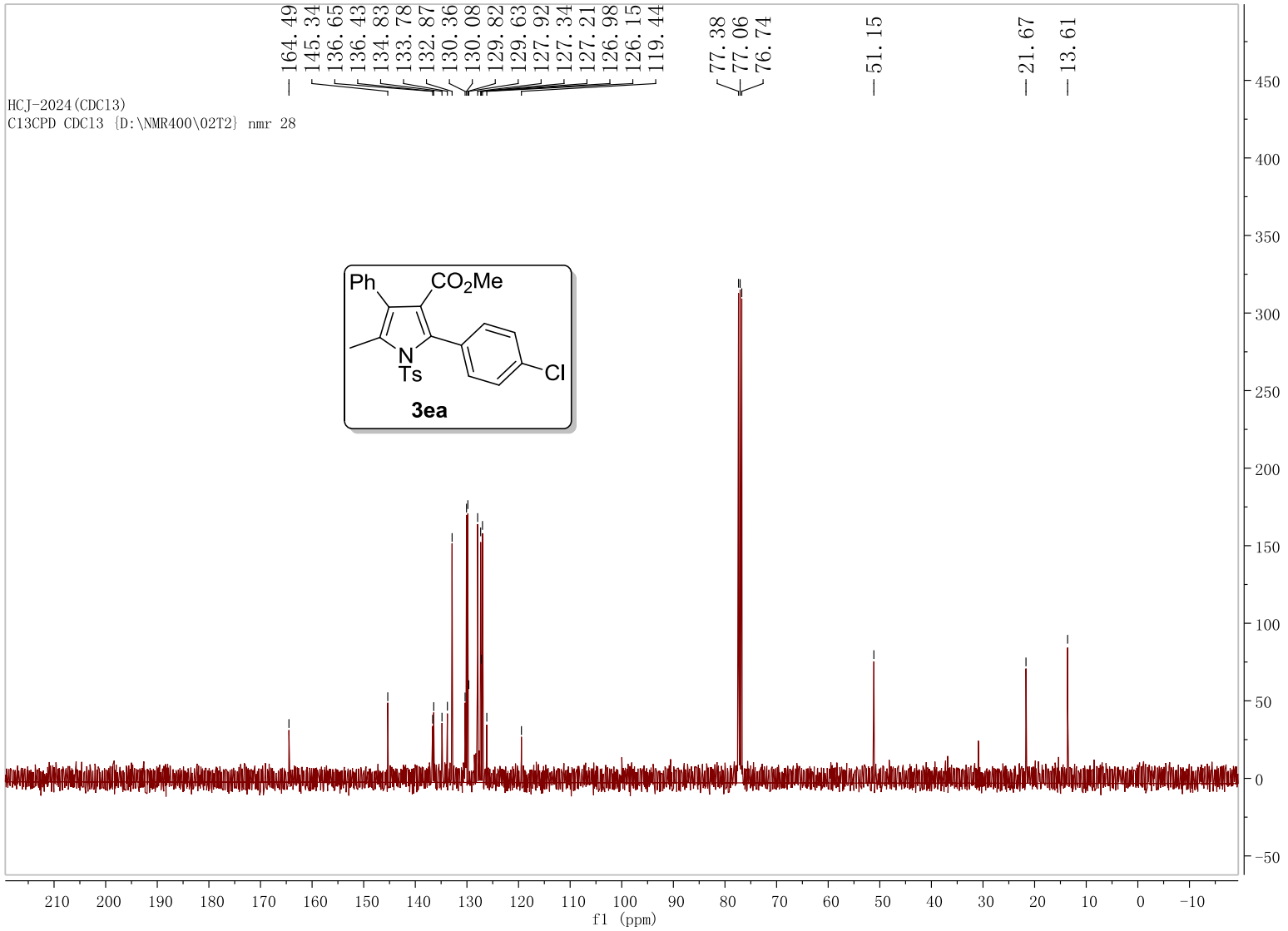
7.34
7.32
7.30
7.29
7.27
7.24
7.21
7.19
7.14
7.12
3.31
2.44
2.42
HCJ-2024(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 28
Ph
CO2Me
N
Ts
Cl
3ea
4.11H
7.03H
1.96H
3.00H
2.95H
2.98H
f1 (ppm)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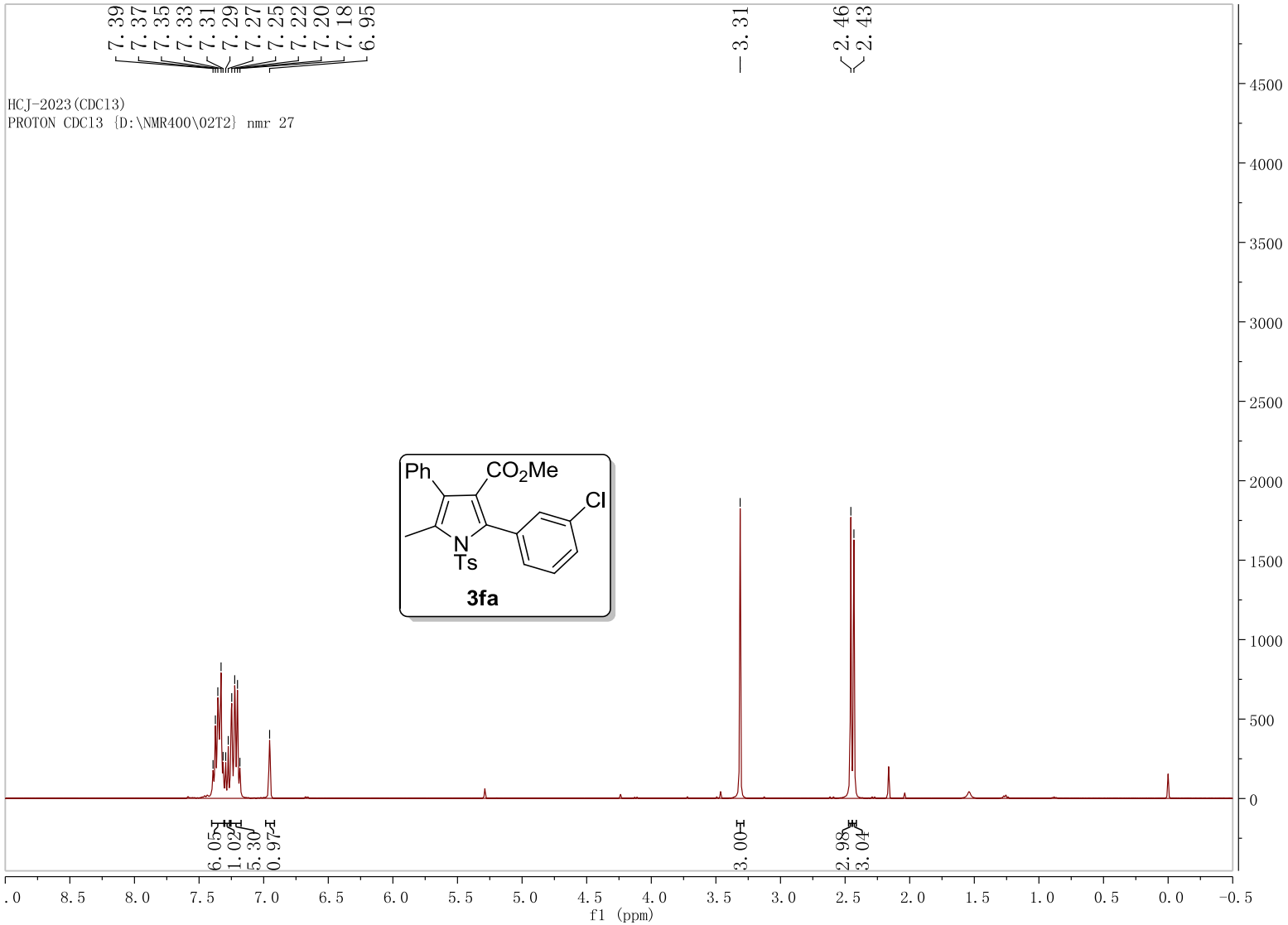
145.34
136.65
136.43
134.83
133.78
132.87
130.36
130.08
129.82
129.63
127.92
127.34
127.21
126.98
126.15
119.44
77.38
77.06
76.74
51.15
21.67
13.61
HCJ-2024(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 28
Ph
CO2Me
N
Ts
Cl
3ea
f1 (ppm)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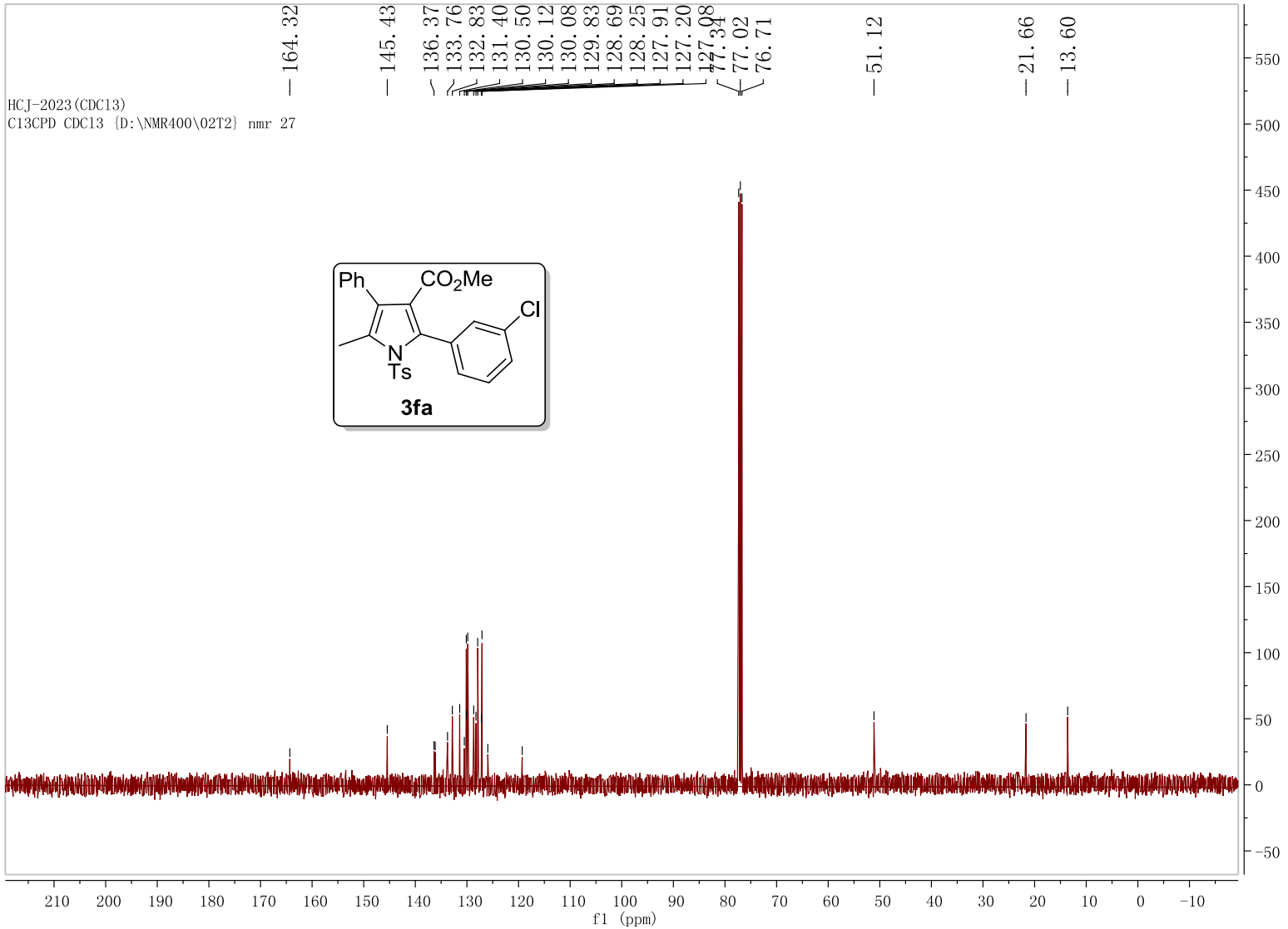
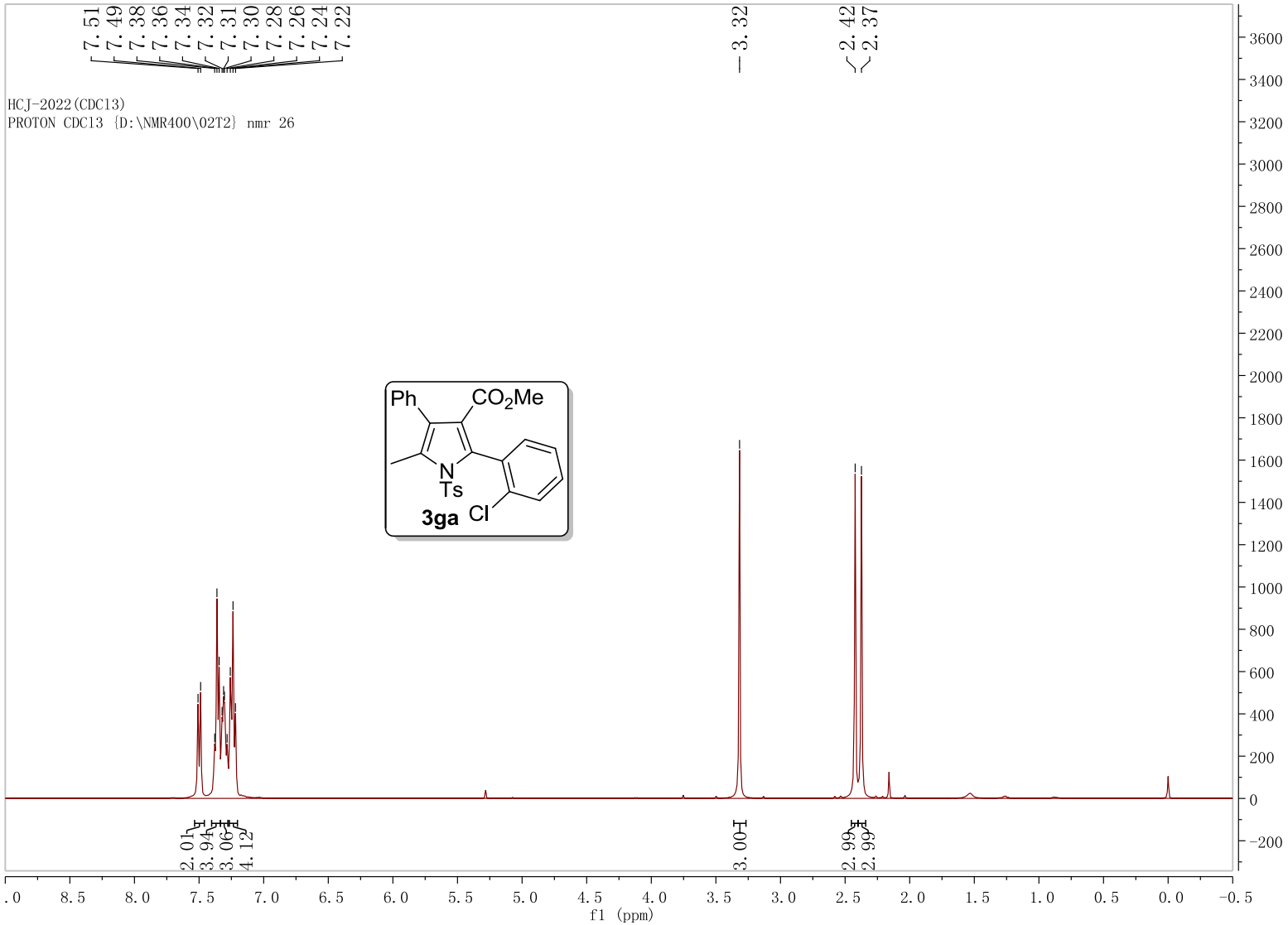
7.37
7.35
7.33
7.31
7.29
7.27
7.25
7.22
7.20
7.18
6.95
3.31
2.46
2.43
HCJ-2023(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 27
Ph
CO2Me
Cl
N
Ts
3fa
6.05
1.02
5.30
0.97
3.00
2.98
3.04
f1 (ppm)


164.32
145.43
136.37
133.76
132.83
131.40
130.50
130.12
130.08
129.83
128.69
128.25
127.91
127.20
127.08
77.34
77.02
76.71
51.12
21.66
13.60
HCJ-2023(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 27
Ph
CO2Me
Cl
N
Ts
3fa
f1 (ppm)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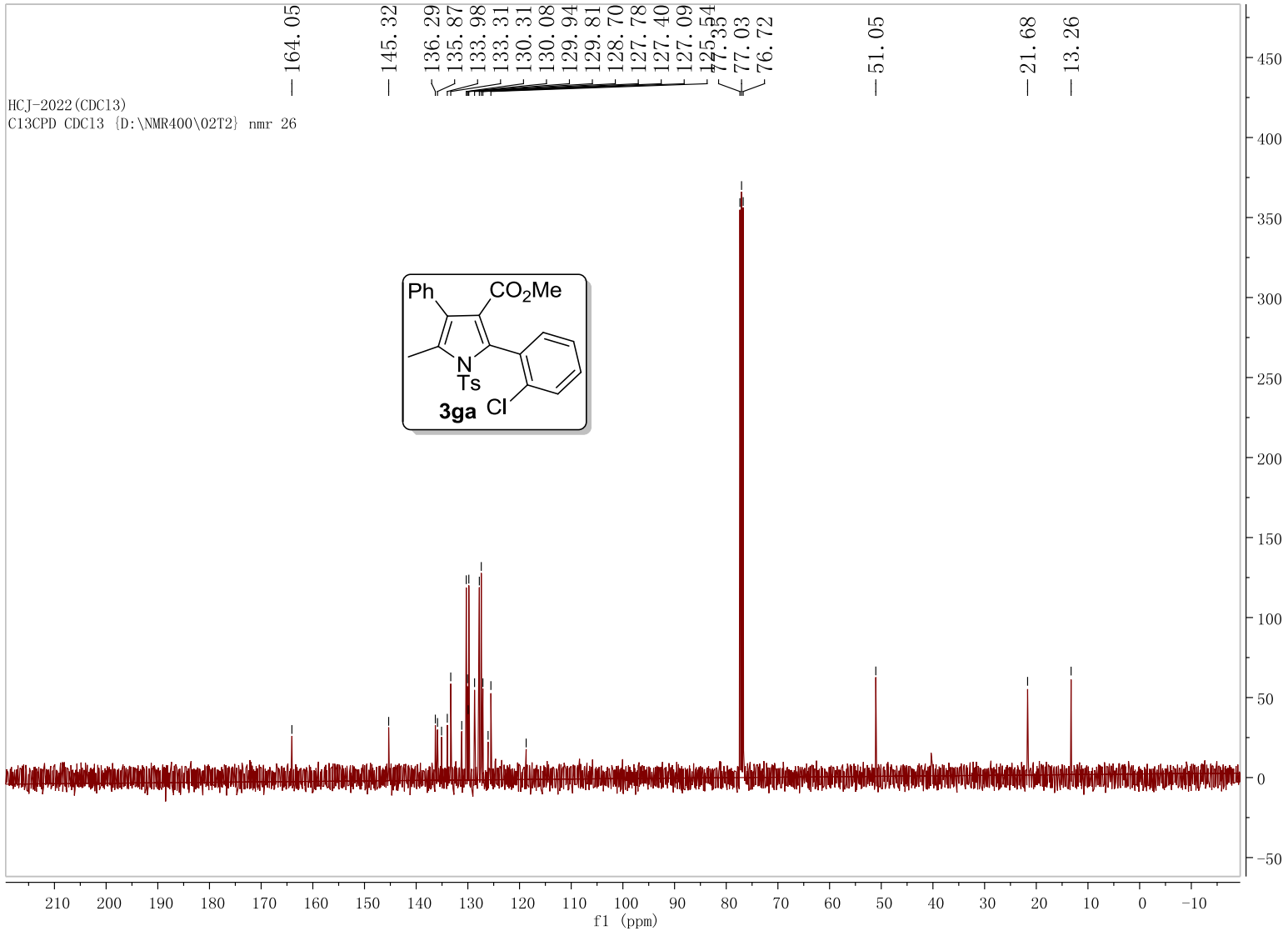
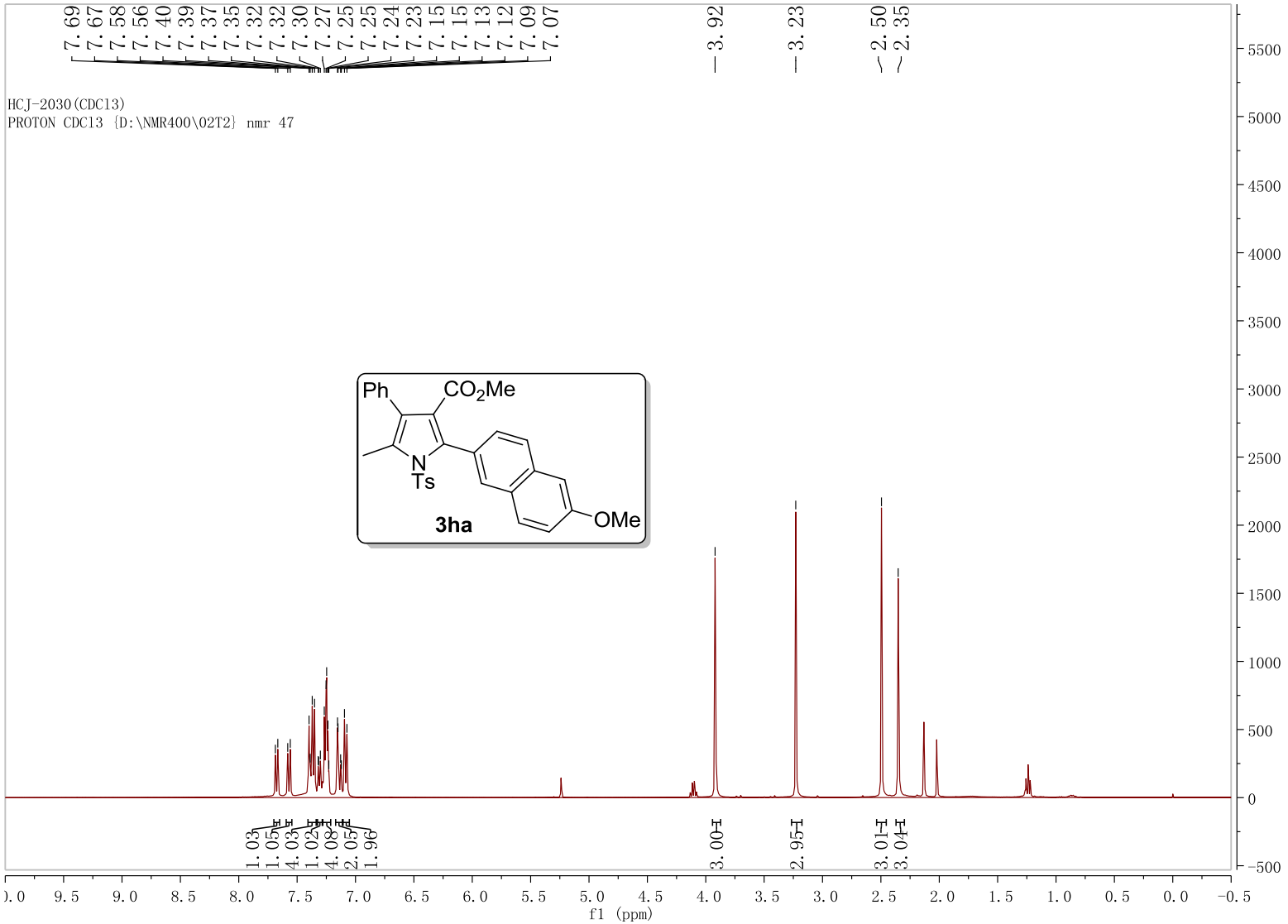
7.49
7.38
7.36
7.34
7.32
7.31
7.30
7.28
7.26
7.24
7.22
3.32
2.42
2.37
HCJ-2022(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 26
Ph
CO2Me
N
Ts
3ga
Cl
2.01
3.94
3.06
4.12
3.00
2.99
2.99
f1 (ppm)


164.05
145.32
136.29
135.87
133.98
133.31
130.31
130.08
129.94
129.81
128.70
127.78
127.40
127.09
125.54
77.35
77.03
76.72
51.05
21.68
13.26
HCJ-2022(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 26
Ph
CO2Me
N
Ts
3ga
Cl
f1 (ppm)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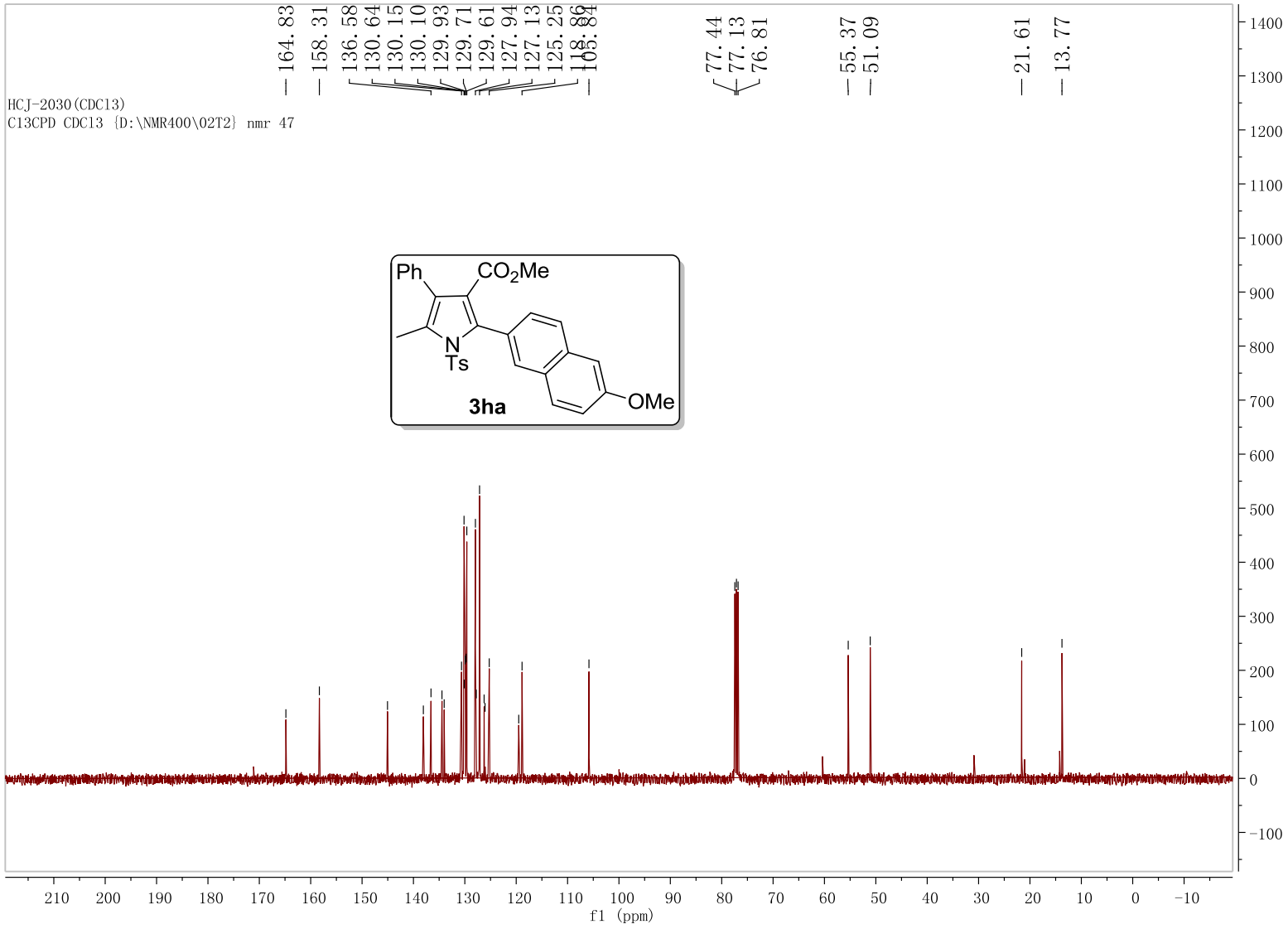
7.67
7.58
7.56
7.40
7.39
7.37
7.35
7.32
7.32
7.30
7.27
7.25
7.25
7.24
7.23
7.15
7.15
7.13
7.12
7.09
7.07
3.92
3.23
2.50
2.35
HCJ-2030(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 47
Ph
CO2Me
N
Ts
OMe
3ha
1.03
1.05
4.03
1.02
4.08
2.05
1.96
3.00
2.95
3.01
3.04
f1 (ppm)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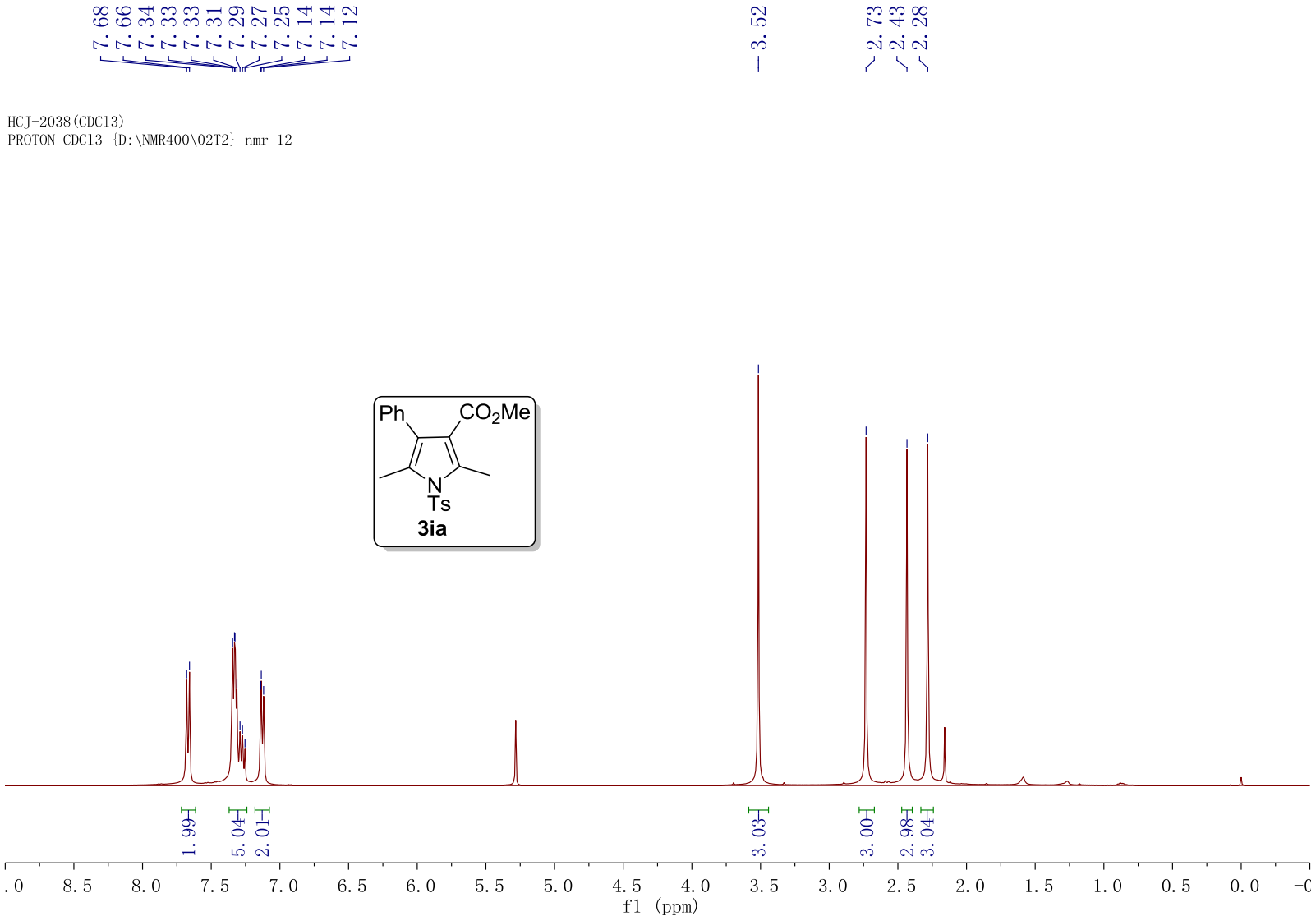
158.31
136.58
130.64
130.15
130.10
129.93
129.71
129.61
127.94
127.13
125.25
118.86
105.84
77.44
77.13
76.81
55.37
51.09
21.61
13.77
HCJ-2030(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 47
Ph
CO2Me
N
Ts
OMe
3ha
f1 (ppm)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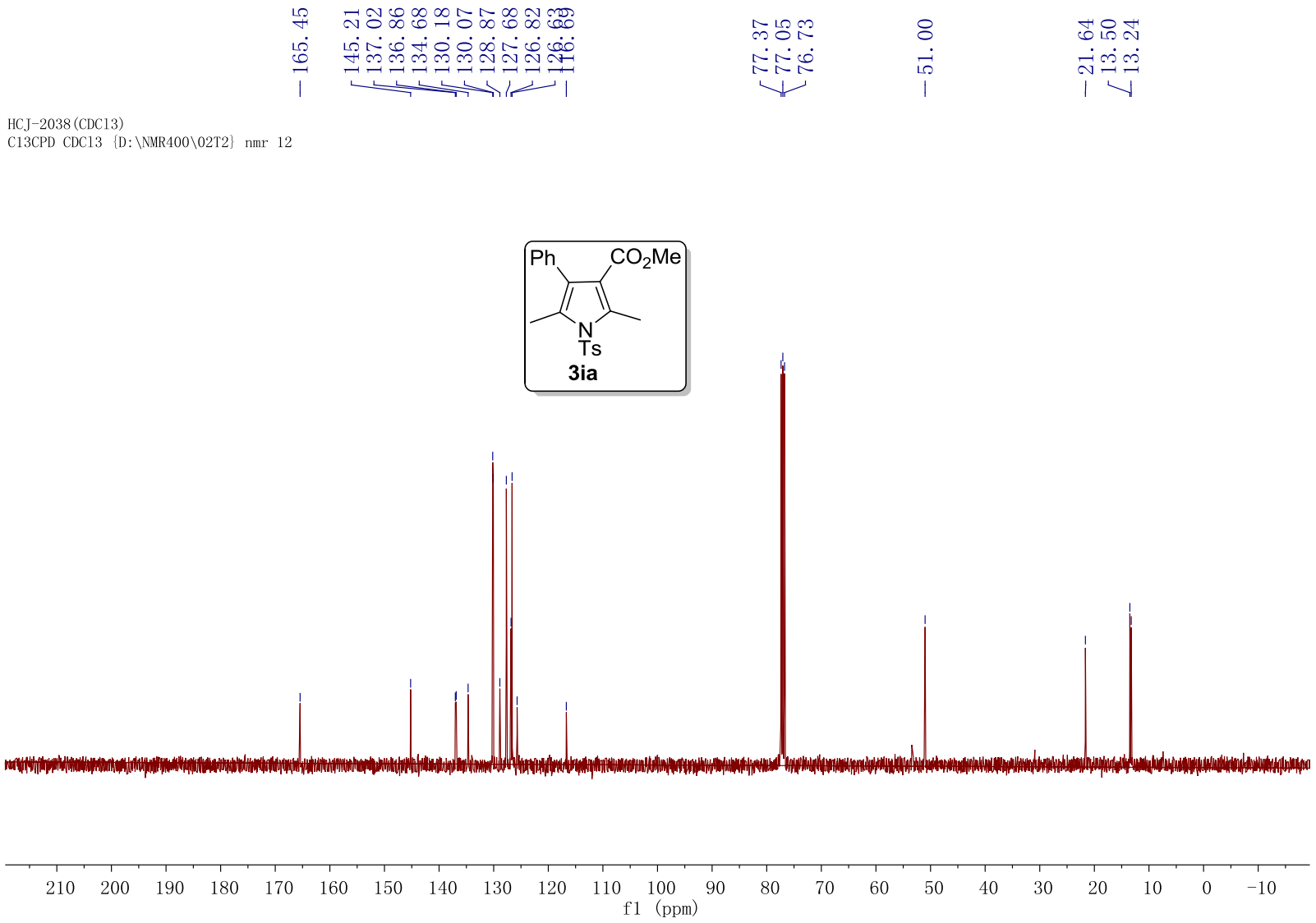
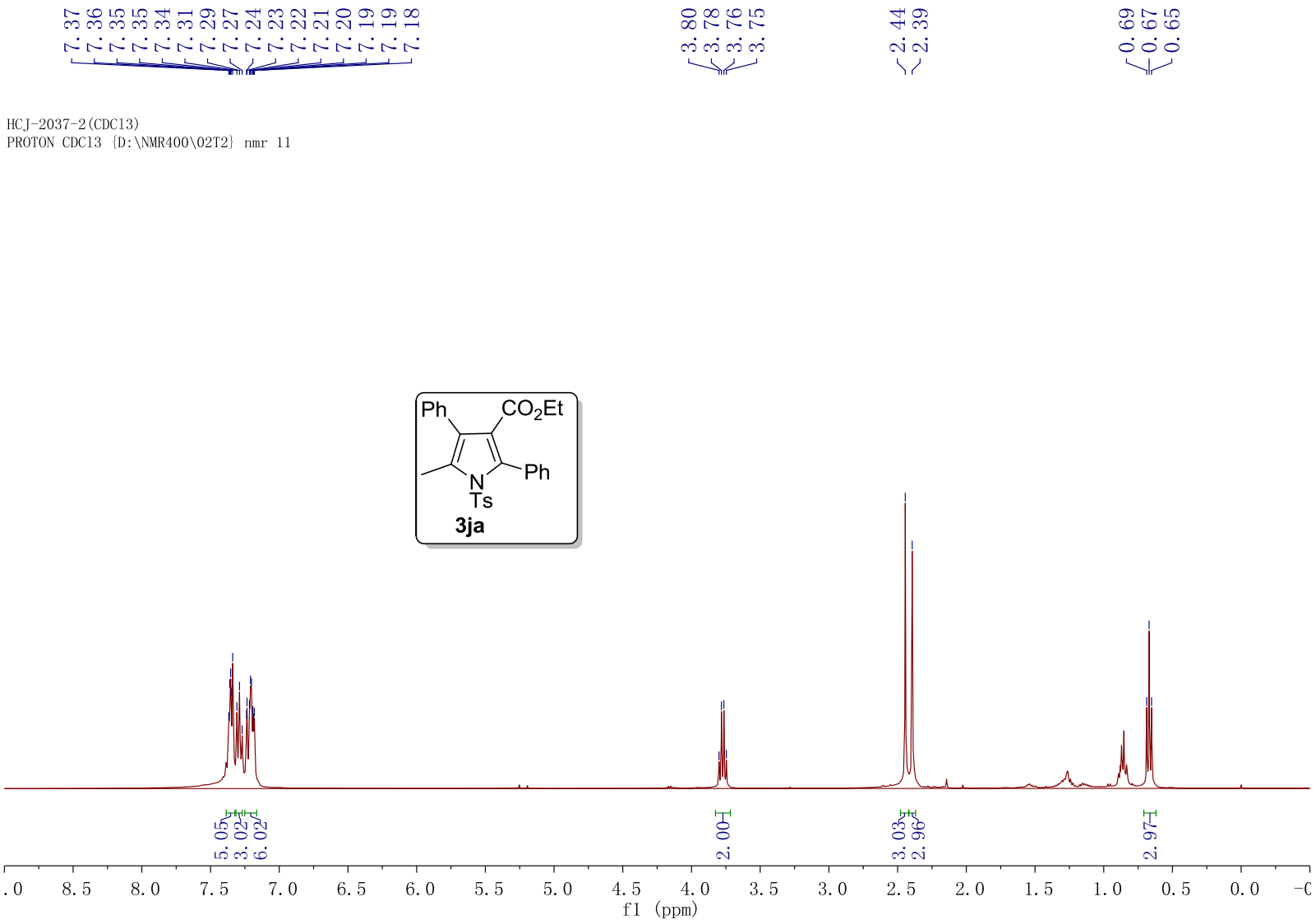
7.66
7.34
7.33
7.33
7.31
7.29
7.27
7.25
7.14
7.14
7.12
3.52
2.73
2.43
2.28
HCJ-2038(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 12
Ph
CO2Me
N
Ts
3ia
1.99
5.04
2.01
3.03
3.00
2.98
3.04
f1 (ppm)


165.45
145.21
137.02
136.86
134.68
130.18
130.07
128.87
127.68
126.82
126.63
116.69
77.37
77.05
76.73
51.00
21.64
13.50
13.24
HCJ-2038(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 12
Ph
CO2Me
N
Ts
3ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.36
7.35
7.35
7.34
7.31
7.29
7.27
7.24
7.23
7.22
7.21
7.20
7.19
7.19
7.18
3.80
3.78
3.76
3.75
2.44
2.39
0.69
0.67
0.65
HCJ-2037-2(CDCl3)
PROTON CDCl3 {D:\NMR400\02T2} nmr 11
Ph
CO2Et
Ph
N
Ts
3ja
5.05
3.02
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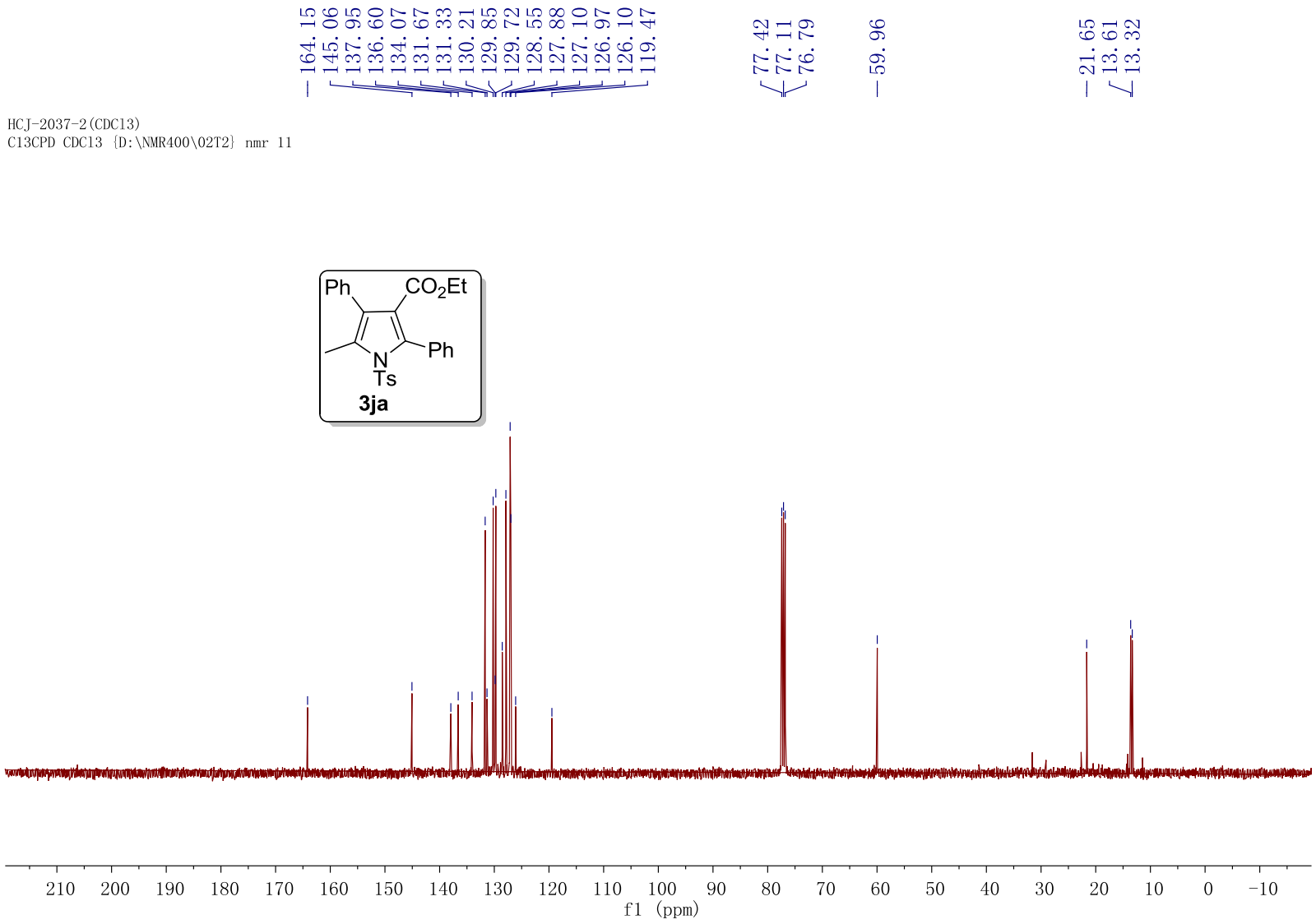
2.00
3.03
2.96
2.97
f1 (ppm)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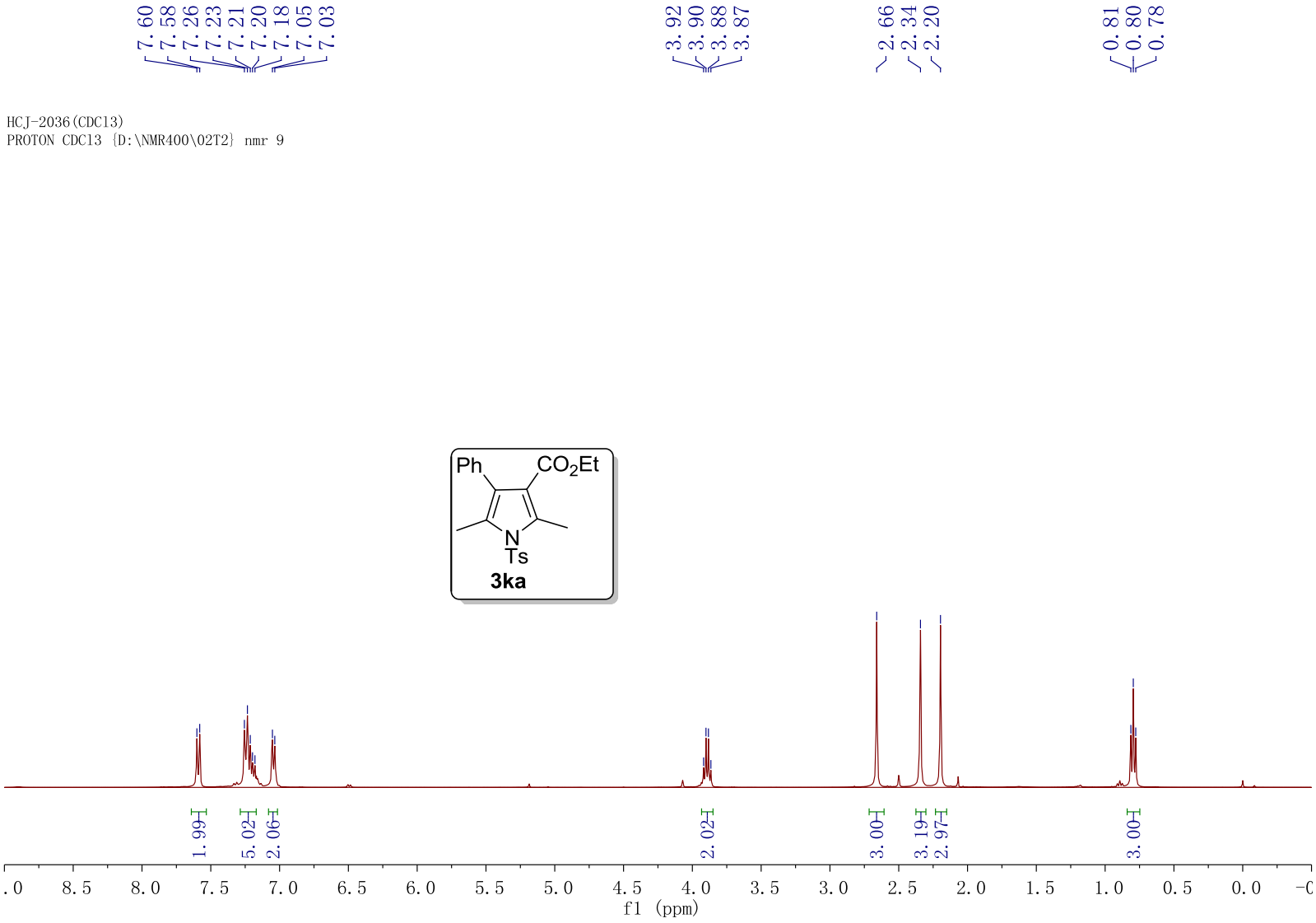
145.06
137.95
136.60
134.07
131.67
131.33
130.21
129.85
129.72
128.55
127.88
127.10
126.97
126.10
119.47
77.42
77.11
76.79
59.96
21.65
13.61
13.32
HCJ-2037-2(CDCl3)
C13CPD CDCl3 {D:\NMR400\02T2} nmr 11
Ph
CO2Et
Ph
N
Ts
3ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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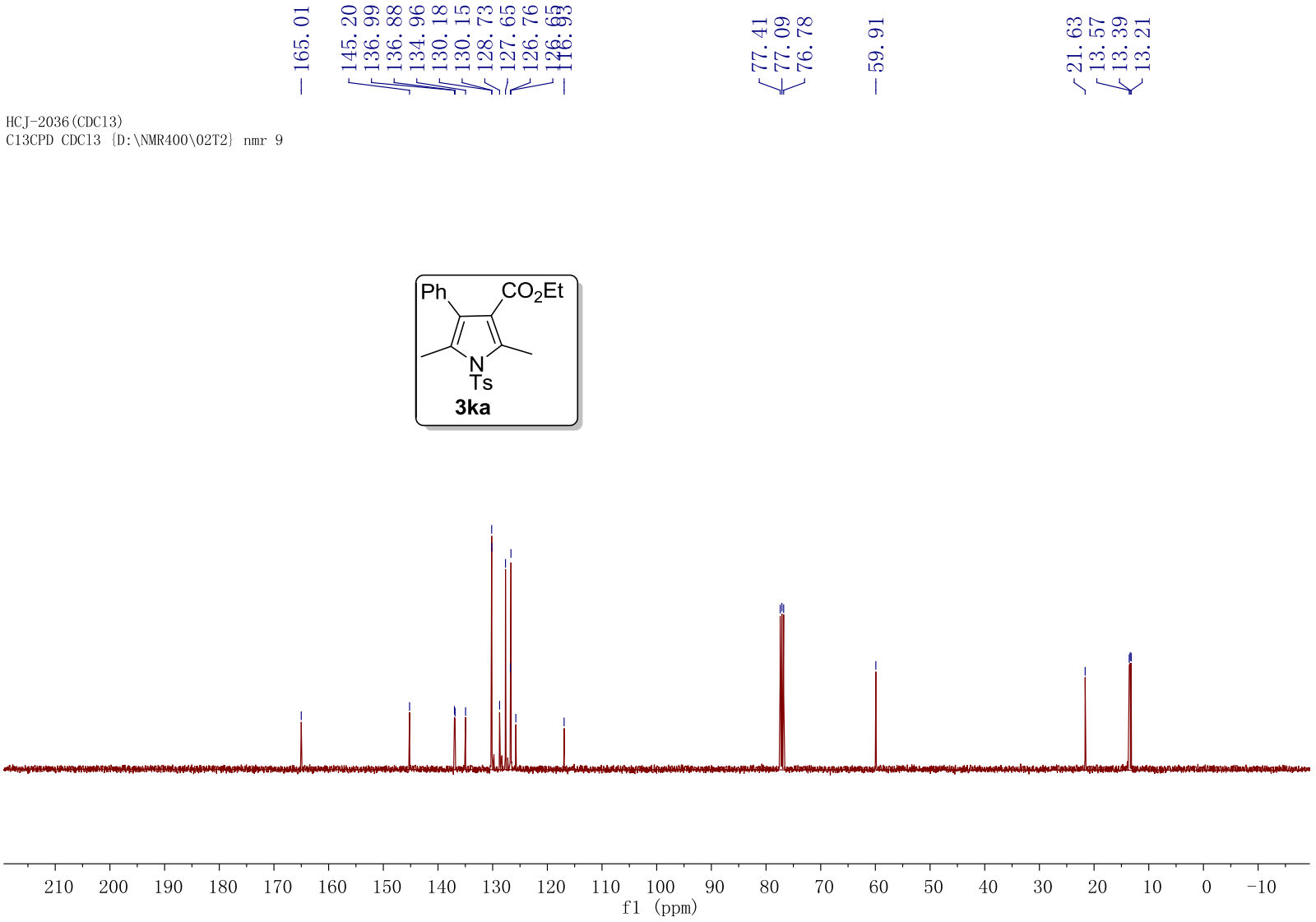
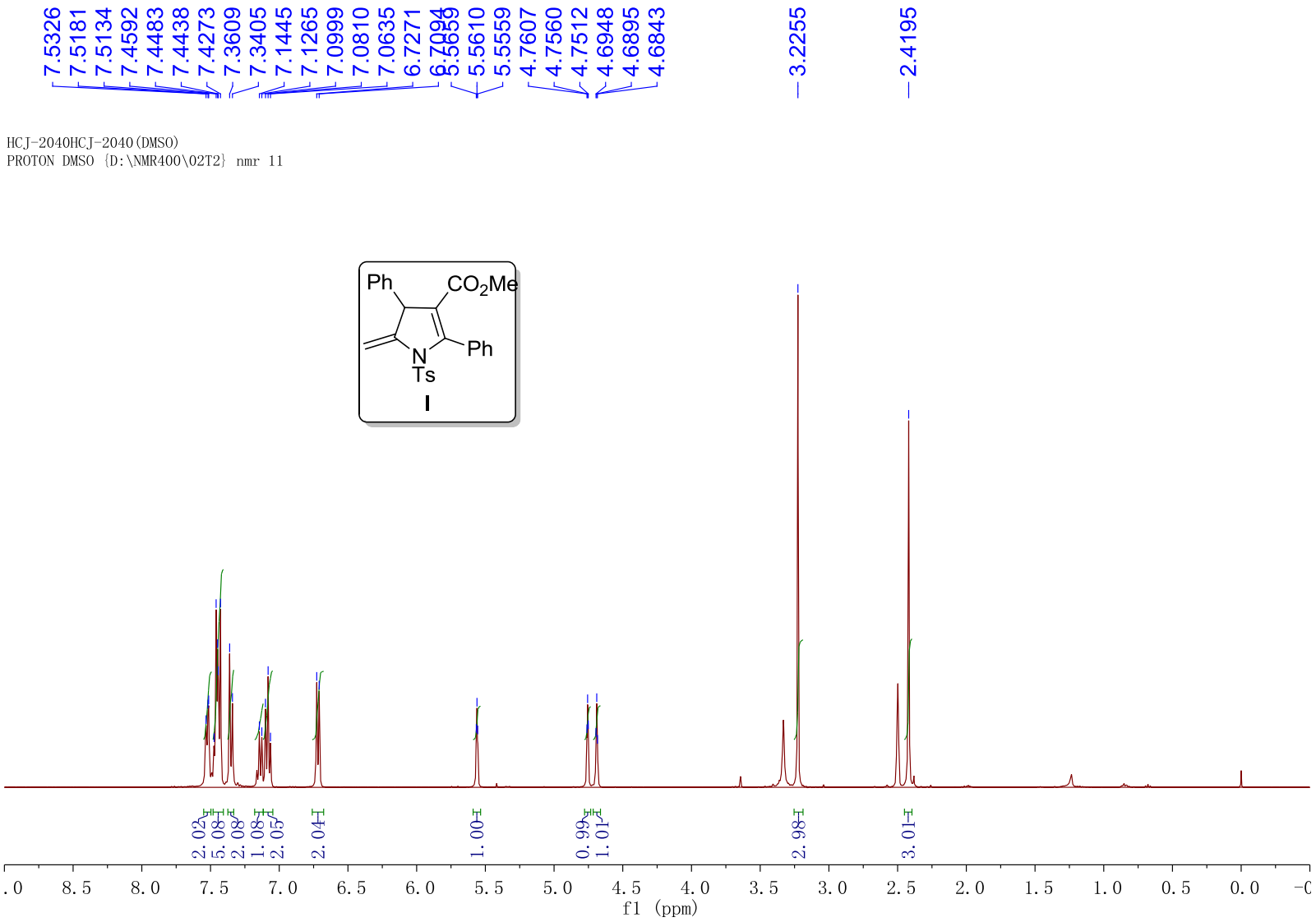
7.58
7.26
7.23
7.21
7.20
7.18
7.05
7.03
3.92
3.90
3.88
3.87
2.66
2.34
2.20
0.81
0.80
0.78
HCJ-2036(CDC13)
PROTON CDC13 {D:\NMR400\02T2} nmr 9
Ph
CO2Et
N
Ts
3ka
1.99
5.02
2.06
2.02
3.00
3.19
2.97
3.00
f1 (ppm)


165.01
145.20
136.99
136.88
134.96
130.18
130.15
128.73
127.65
126.76
126.65
116.93
77.41
77.09
76.78
59.91
21.63
13.57
13.39
13.21
HCJ-2036(CDC13)
C13CPD CDC13 {D:\NMR400\02T2} nmr 9
Ph
CO2Et
N
Ts
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.5134
7.4592
7.4483
7.4438
7.4273
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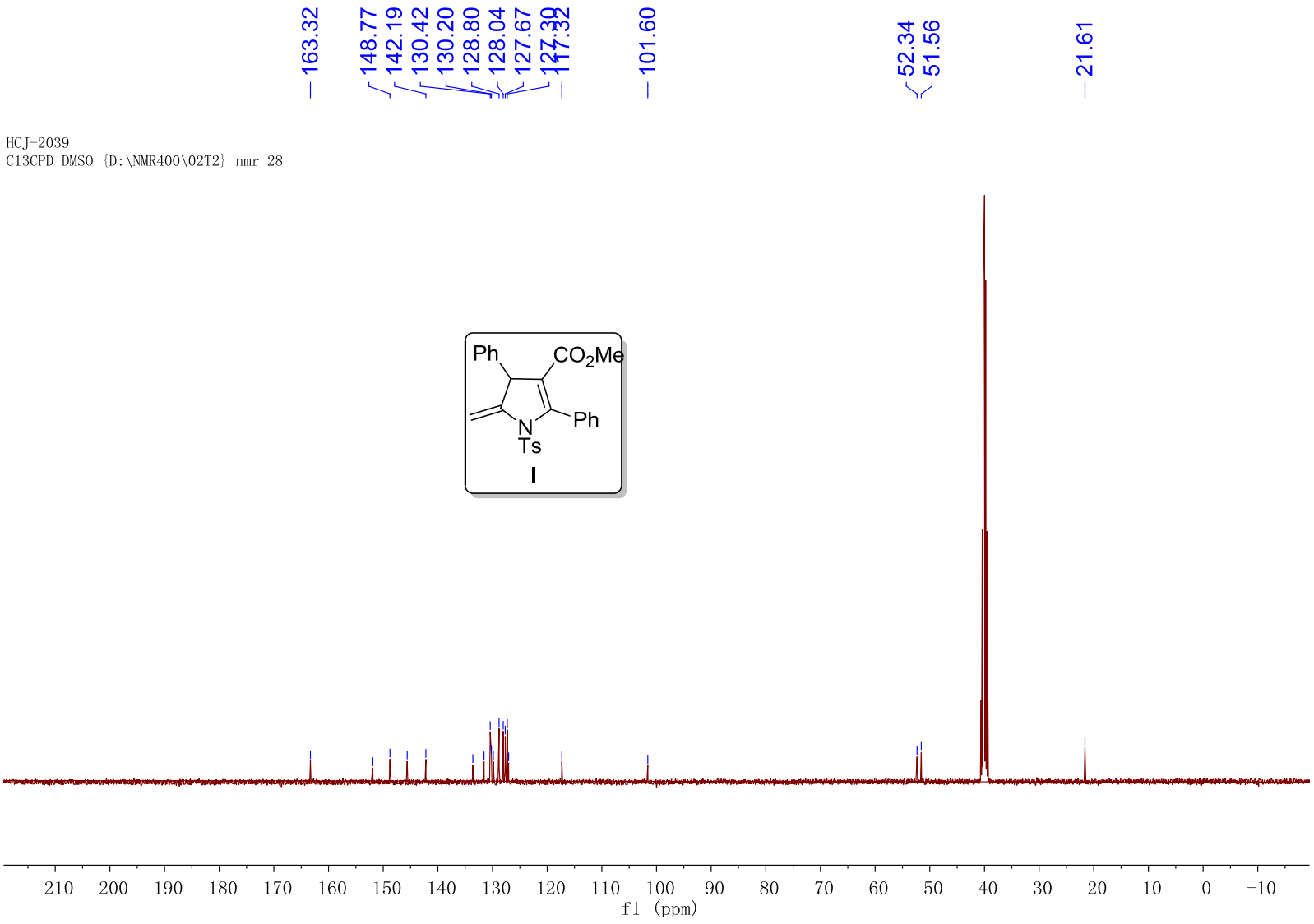
7.3405
7.1445
7.1265
7.0999
7.0810
7.0635
6.7271
6.7094
6.5659
5.5610
5.5559
4.7607
4.7560
4.7512
4.6948
4.6895
4.6843
3.2255
2.4195
HCJ-2040HCJ-2040(DMSO)
PROTON DMSO {D:\NMR400\02T2} nmr 11
Ph
CO2Me
Ph
N
Ts
I
2.02
5.08
2.08
1.08
2.05
2.04
1.00
0.99
1.01
2.98
3.01
f1 (ppm)


163.32
148.77
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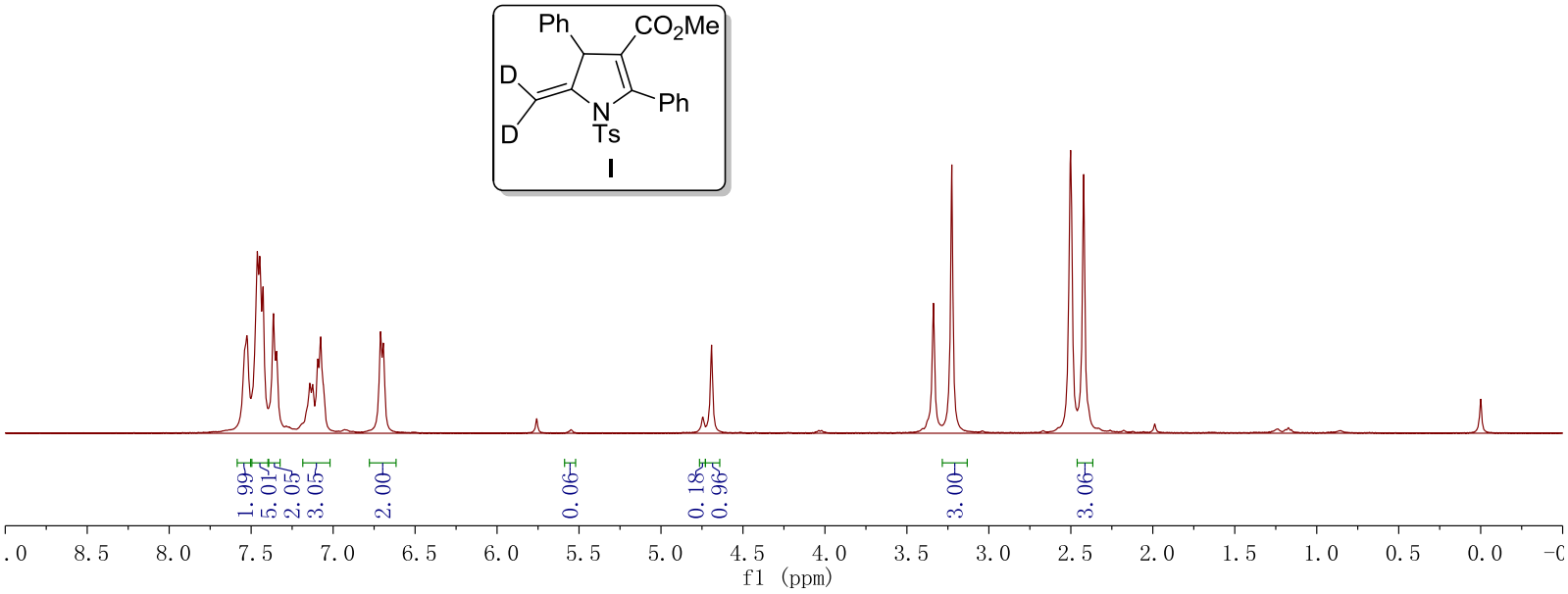
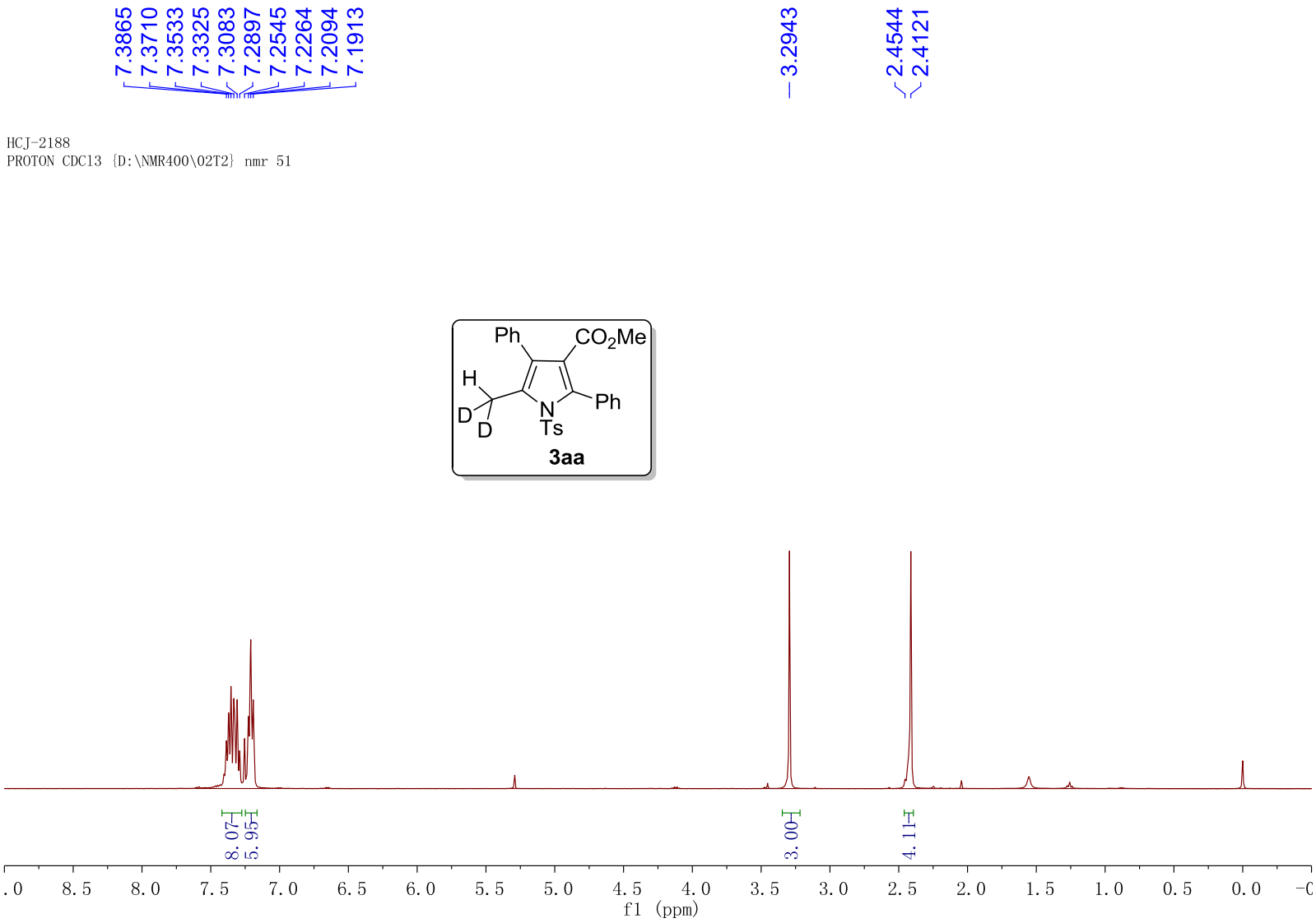
130.42
130.20
128.80
128.04
127.67
101.60
52.34
51.56
21.61
HCJ-2039
C13CPD DMSO {D:\NMR400\02T2} nmr 28
Ph
CO2Me
Ph
N
Ts
I
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

HCJ-2188
PROTON DMSO {D:\NMR400\02T2} nmr 22

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7.3325
7.3083
7.2897
7.2545
7.2264
7.2094
7.1913
3.2943
2.4544
2.4121
HCJ-2188
PROTON CDC13 {D:\NMR400\02T2} nmr 51
Ph
CO2Me
H
D
D
N
Ts
Ph
3aa
8.07
5.95
3.00
4.11
f1 (ppm)