Supporting Information

Dual Gold/Photoredox-Catalyzed Bis-Arylative Cyclization of Chiral Homopropargyl Sulfonamides with Diazonium Salts: Rapid Access to Enantioenriched 2,3-Dihydropyrroles

Ze-Shu Wang, Tong-De Tan, Cai-Ming Wang, Ding-Qiang Yuan, Te Zhang, Pengfei Zhu, Chunyin Zhu,* Jin-Mei Zhou, and Long-Wu Ye*

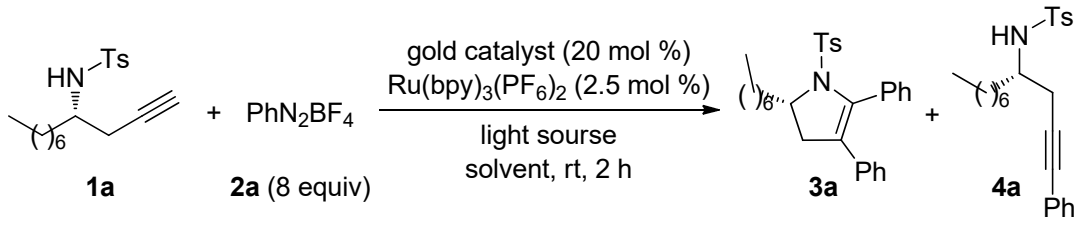
*i*ChEM, State Key Laboratory of Physical Chemistry of Solid Surfaces, Key Laboratory for Chemical Biology of Fujian Province and College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China

General Information. Ethyl acetate (ACS grade), hexanes (ACS grade), anhydrous DMF (ACS grade) and anhydrous MeOH (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Micromass $QTOF_2$ Quadrupole/Time-of-Flight Tandem mass spectrometer using electron spray ionization.

^{1}H NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

^{13}C NMR spectra were recorded on on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform-d_3. Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

More Reaction Condition Studies

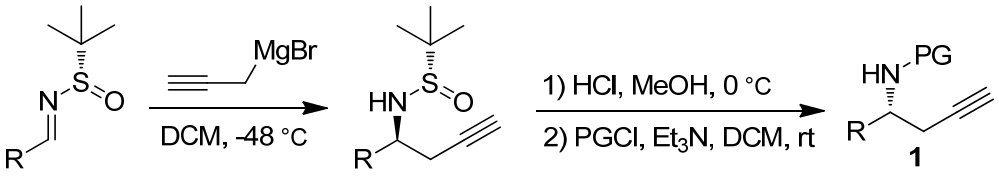


1a **2a** (8 equiv) **3a** **4a**

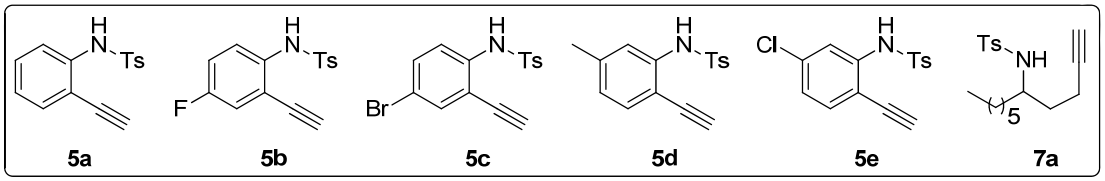
entry	gold catalyst	light sourse	solvent	yield (%)[a] 3a	4a
1[b]	IPrAuCl	13 W white LED	DMF/MeOH = 9:1	<1	<1
2	$Ph_3PAuNTf_2$	13 W white LED	DMF/MeOH = 9:1	14	<1
3	Ph_3PAuCl	3 W white LED	DMF/MeOH = 9:1	63	<1
4	Ph_3PAuCl	23 W white LED	DMF/MeOH = 9:1	53	<1
5	Ph_3PAuCl	5 W blue LED	DMF/MeOH = 9:1	60	<1
6	Ph_3PAuCl	36 W CFL	DMF/MeOH = 9:1	60	<1

[a] Measured by ^1H NMR using diethyl phthalate as the internal standard. [b] Reaction time: 12 h; >95% of **1a** remained unreacted.

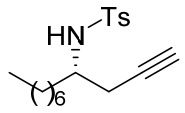
Compounds **1a-1m** were prepared according to the following procedures and their data were reported in our previous work.[1]



Compounds **5a-5e** and **7a** were reported in our previous work.[1e,1f, 2]



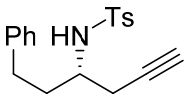
(*S*)-4-methyl-*N*-(undec-1-yn-4-yl)benzenesulfonamide (1a)



1a

98% ee (determined by HPLC: Chiralcel AS-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 200 nm, 25 ^{o}C; t_R = 42.87 min (major), 53.41 min (minor)).

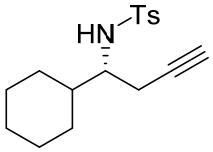
(*S*)-4-methyl-*N*-(1-phenylhex-5-yn-3-yl)benzenesulfonamide (1b)



1b

97% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 36.35 min (minor), 42.13 min (major)).

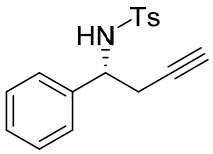
(*R*)-*N*-(1-cyclohexylbut-3-yn-1-yl)-4-methylbenzenesulfonamide (1c)



1c

98% ee (determined by HPLC: Chiralcel IC Column, 5/95 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 51.58 min (minor), 56.19 min (major)).

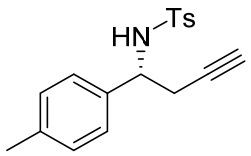
(*R*)-4-methyl-*N*-(1-phenylbut-3-yn-1-yl)benzenesulfonamide (1d)



1d

99% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 50.11 min (major), 53.24 min (minor)).

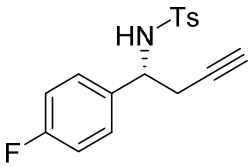
(*R*)-4-methyl-*N*-(1-(p-tolyl)but-3-yn-1-yl)benzenesulfonamide (1e)



1e

98% ee (determined by HPLC: Chiralcel AS-H Column, 20/80 *i*-PrOH/hexane, 1.0 mL/min, 200 nm, 25 ^{o}C; t_R = 24.31 min (major), 31.91 min (minor)).

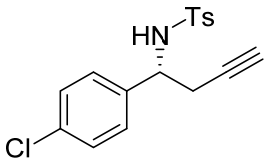
(*R*)-*N*-(1-(4-fluorophenyl)but-3-yn-1-yl)-4-methylbenzenesulfonamide (1f)



1f

98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 41.83 min (major), 45.73 min (minor)).

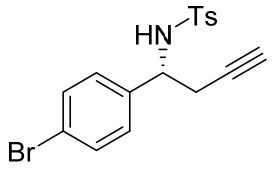
(*R*)-*N*-(1-(4-chlorophenyl)but-3-yn-1-yl)-4-methylbenzenesulfonamide (1g)



1g

98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 41.91 min (major), 47.45 min (minor)).

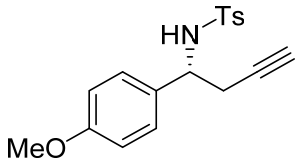
(*R*)-*N*-(1-(4-bromophenyl)but-3-yn-1-yl)-4-methylbenzenesulfonamide (1h)



1h

98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 43.18 min (major), 48.67 min (minor)).

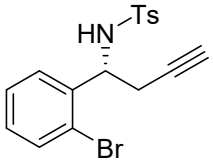
(*R*)-*N*-(1-(4-methoxyphenyl)but-3-yn-1-yl)-4-methylbenzenesulfonamide (1i)



1i

99% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 200 nm, 25 ^{o}C; t_R = 52.71 min (minor), 57.76 min (major)).

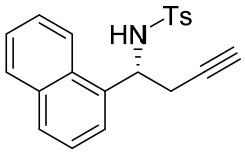
(*R*)-*N*-(1-(2-bromophenyl)but-3-yn-1-yl)-4-methylbenzenesulfonamide (1j)



1j

96% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 49.12 min (major), 76.79 min (minor)).

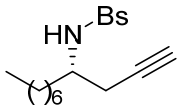
(*R*)-4-methyl-*N*-(1-(naphthalen-1-yl)but-3-yn-1-yl)benzenesulfonamide (1k)



1k

99% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 0.6 mL/min, 200 nm, 25 ^{o}C; t_R = 57.13 min (major), 77.93 min (minor)).

(*S*)-4-bromo-*N*-(undec-1-yn-4-yl)benzenesulfonamide (1l)



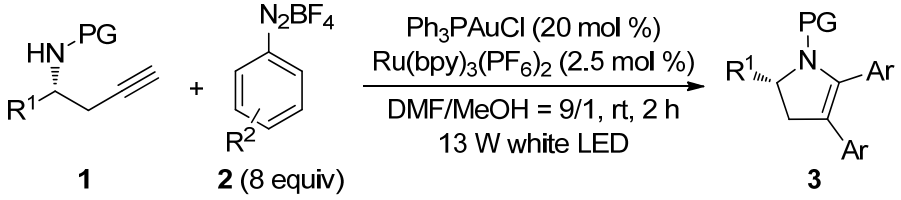
1l

97% ee (determined by HPLC: Chiralcel IB Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 200 nm, 25 ^{o}C; t_R = 16.27 min (minor), 17.81 min (major)).

(*S*)-*N*-(undec-1-yn-4-yl)benzenesulfonamide (1m)

1m

98% ee (determined by HPLC: Chiralcel AS-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 200 nm, 25 ^{o}C; t_R = 37.79 min (major), 46.33 min (minor)).

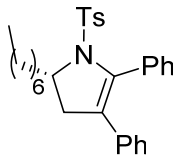


1 **2** (8 equiv) **3**

General procedure for the synthesis of dihydro-1*H*-pyrrole 3:

Chiral homopropargyl amide **1** (0.20 mmol), aryldiazonium salt **2** (1.6 mmol, 8.0 eq.), $[Ru(bpy)_3](PF_6)_2$ (4.0 mg, 2.5 mol %) and Ph_3PAuCl (20 mg, 20 mol %) were added to a flame-dried Schlenk flask containing a stirring bar and purged by evacuating the flask and backfilling with argon three times. In the absence of light, anhydrous DMF/MeOH: 9/1 (2.0 mL, 0.10 M) was added and the flask was sealed. The mixture was then stirred under irradiation from 13 W white LED. The reaction mixture was stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 2 h. Upon completion, the mixture was then concentrated and the residue was purified by chromatography on silicagel (eluent: hexanes/ethyl acetate) to afford the desired dihydro-1*H*-pyrrole **3**.

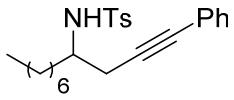
(*S*)-2-heptyl-4,5-diphenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3a)



3a

Compound **3a** was prepared in 65% yield (61.6 mg) according to the general procedure (Table 2, entry 1). Pale yellow oil. $[\alpha]_D^{20}$ = +122.2º (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 5.99 min (minor), 9.35 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 2H), 7.38 – 7.32 (m, 2H), 7.31 – 7.23 (m, 5H), 7.15 – 7.07 (m, 3H), 6.90 – 6.74 (m, 2H), 4.34 – 4.21 (m, 1H), 2.71 (dd, *J* = 15.5, 8.5 Hz, 1H), 2.45 (s, 3H), 2.02 (d, *J* = 15.5 Hz, 1H), 1.89 – 1.76 (m, 1H), 1.67 – 1.47 (m, 3H), 1.44 – 1.20 (m, 8H), 0.89 (t, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.5, 136.5, 135.9, 135.3, 132.9, 129.7, 129.3, 128.4, 128.0, 127.9, 127.6, 127.0, 126.9, 126.7, 61.1, 39.5, 36.2, 31.8, 29.5, 29.2, 25.1, 22.6, 21.6, 14.0; IR (neat): 3056, 2925 (s), 2854, 1598, 1445, 1356, 1168, 696; HRESIMS Calcd for $[C_{30}H_{35}NNaO_2S]^+$ (M + Na^+) 496.2281, found 496.2292.

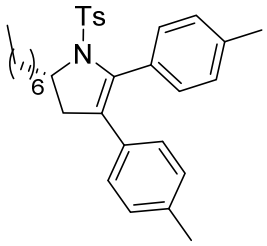
4-methyl-*N*-(1-phenylundec-1-yn-4-yl)benzenesulfonamide (4a)



4a

Yellow solid (mp 55-57 ^{o}C). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.5 Hz, 2H), 7.42 – 7.32 (m, 2H), 7.32 – 7.23 (m, 5H), 4.72 (d, *J* = 8.5 Hz, 1H), 3.45 – 3.36 (m, 1H), 2.54 – 2.48 (m, 2H), 2.40 (s, 3H), 1.63 – 1.51 (m, 2H), 1.33 – 1.10 (m, 10H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3, 138.0, 131.6, 129.6, 128.2, 128.0, 127.0, 123.1, 84.8, 83.4, 52.2, 34.3, 31.6, 29.1, 29.0, 25.9, 25.5, 22.6, 21.4, 14.0; IR (neat): 3279, 2856, 1327, 1161, 1094, 756, 666; HRESIMS Calcd for $[C_{24}H_{31}NNaO_2S]^+$ (M + Na^+) 420.1968, found 420.1967.

(*S*)-2-heptyl-4,5-di-*p*-tolyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3b)

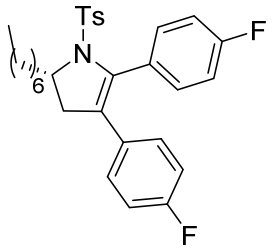


3b

Compound **3b** was prepared in 67% yield (67.2 mg) according to the general procedure (Table 2, entry 2). Pale yellow oil. $[\alpha]_D^{20}$ = +81.0º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 ^{o}C; t_R = 5.93 min (minor), 12.03 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.32 – 7.21 (m, 4H), 7.10 (d, *J* = 7.8 Hz, 2H), 6.93 (d, *J* = 8.0 Hz, 2H), 6.78 – 6.69 (m, 2H), 4.28 – 4.16 (m, 1H), 2.65 (dd, *J* = 15.6, 8.4 Hz, 1H), 2.45 (s, 3H), 2.36 (s, 3H), 2.25 (s, 3H), 1.96 (dd, *J* = 15.6, 1.2 Hz, 1H), 1.86 – 1.75 (m, 1H), 1.63 – 1.47 (m, 3H), 1.37 – 1.24 (m, 8H), 0.89 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3, 138.1, 136.4, 136.0, 135.4, 133.1, 130.1, 129.6,

129.2, 128.7, 128.6, 127.6, 126.9, 126.3, 61.0, 39.4, 36.1, 31.8, 29.5, 29.2, 25.1, 22.6, 21.6, 21.4, 21.1, 14.1; IR (neat): 3025, 2925 (s), 2855, 1356, 1168, 1090, 814; HRESIMS Calcd for $[C_{32}H_{39}NNaO_2S]^+$ (M + Na^+) 524.2594, found 524.2610.

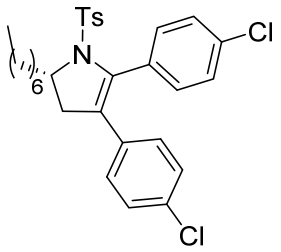
(*S*)-4,5-bis(4-fluorophenyl)-2-heptyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3c)



3c

Compound **3c** was prepared in 72% yield (73.4 mg) according to the general procedure (Table 2, entry 3). Pale yellow oil. $[\alpha]_D^{20}$ = +118.8º (c = 1.0, $CHCl_3$). 97% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 ºC; t_R = 6.79 min (minor), 10.51 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 8.0 Hz, 2H), 7.30 – 7.20 (m, 4H), 6.99 – 6.91 (m, 2H), 6.83 – 6.71 (m, 4H), 4.31 – 4.20 (m, 1H), 2.68 (dd, *J* = 15.5, 8.5 Hz, 1H), 2.42 (s, 3H), 1.97 (dd, *J* = 15.5, 1.0 Hz, 1H), 1.82 – 1.72 (m, 1H), 1.63 – 1.43 (m, 3H), 1.40 – 1.20 (m, 8H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6 (d, *J* = 246.2 Hz), 161.4 (d, *J* = 245.0 Hz), 143.7, 135.6, 135.3, 131.7 (d, *J* = 2.5 Hz), 131.5 (d, *J* = 8.7 Hz), 129.4, 128.8 (d, *J* = 8.8 Hz), 128.7 (d, *J* = 3.7 Hz), 127.6, 125.9, 115.2 (d, *J* = 21.2 Hz), 115.1 (d, *J* = 21.2 Hz), 61.0, 39.4, 36.2, 31.8, 29.5, 29.2, 25.1, 22.6, 21.6, 14.0; IR (neat): 2927 (s), 2855, 1505, 1512, 1357, 1232, 1169, 835; HRESIMS Calcd for $[C_{30}H_{33}F_2NNaO_2S]^+$ (M + Na^+) 532.2092, found 532.2109.

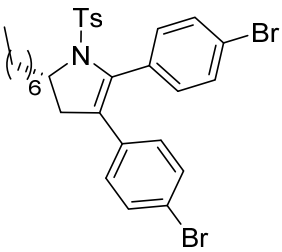
(*S*)-4,5-bis(4-chlorophenyl)-2-heptyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3d)



3d

Compound **3d** was prepared in 54% yield (58.6 mg) according to the general procedure (Table 2, entry 4). Pale yellow oil. $[\alpha]_D^{20}$ = +127.0º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 6.55 min (minor), 10.66 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.18 (m, 6H), 7.10 – 7.04 (m, 2H), 6.74 – 6.66 (m, 2H), 4.32 – 4.19 (m, 1H), 2.68 (dd, *J* = 15.5, 8.5 Hz, 1H), 2.43 (s, 3H), 1.97 (dd, *J* = 15.5, 1.0 Hz, 1H), 1.82 – 1.73 (m, 1H), 1.61 – 1.45 (m, 3H), 1.39 – 1.21 (m, 8H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.8, 136.0, 135.2, 134.5, 134.0, 132.7, 131.1, 131.0, 129.4, 128.5, 128.4, 128.3, 127.6, 126.3, 61.1, 39.4, 36.2, 31.8, 29.4, 29.2, 25.1, 22.6, 21.6, 14.0; IR (neat): 2925 (s), 2854, 1494, 1357, 1167, 1091, 1013, 829; HRESIMS Calcd for $[C_{30}H_{33}Cl_2NNaO_2S]^+$ (M + Na^+) 564.1501, found 564.1522.

(*S*)-4,5-bis(4-bromophenyl)-2-heptyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3e)

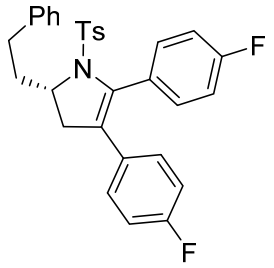


3e

Compound **3e** was prepared in 55% yield (69.5 mg) according to the general procedure (Table 2, entry 5). Pale yellow oil. $[\alpha]_D^{20}$ = +74.9º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min,

254 nm, 25 °C; t_R = 7.14 min (minor), 11.77 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.33 – 7.15 (m, 6H), 6.67 (d, *J* = 8.4 Hz, 2H), 4.35 – 4.18 (m, 1H), 2.70 (dd, *J* = 15.6, 8.8 Hz, 1H), 2.45 (s, 3H), 1.99 (d, *J* = 15.6 Hz, 1H), 1.87 – 1.71 (m, 1H), 1.67 – 1.46 (m, 3H), 1.42 – 1.21 (m, 8H), 0.89 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.8, 136.1, 135.2, 134.5, 131.5, 131.4, 131.3, 131.3, 129.4, 128.6, 127.6, 126.4, 122.8, 120.8, 61.1, 39.4, 36.2, 31.8, 29.4, 29.2, 25.0, 22.6, 21.6, 14.1; IR (neat): 2924 (s), 2853, 1358, 1167, 1089, 1009, 580; HRESIMS Calcd for $[C_{30}H_{33}Br_2NNaO_2S]^+$ (M + Na^+) 652.0491, found 652.0531.

(*S*)-4,5-bis(4-fluorophenyl)-2-phenethyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3g)

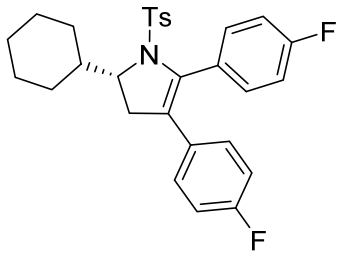


3g

Compound **3g** was prepared in 56% yield (57.7 mg) according to the general procedure (Table 2, entry 7). Pale yellow oil. $[\alpha]_D^{20}$ = +90.3° (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel AD-H Column, 8/92 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 10.88 min (minor), 16.87 min (major)). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.37 – 7.25 (m, 8H), 7.24 – 7.18 (m, 1H), 7.03 – 6.94 (m, 2H), 6.88 – 6.74 (m, 4H), 4.40 – 4.30 (m, 1H), 3.02 – 2.83 (m, 2H), 2.74 (dd, *J* = 15.6, 8.8 Hz, 1H), 2.47 (s, 3H), 2.25 – 2.11 (m, 1H), 2.04 (dd, *J* = 15.6, 1.2 Hz, 1H), 1.98 – 1.86 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6 (d, *J* = 246.2 Hz), 161.5 (d, *J* = 246.2 Hz), 143.8, 141.6, 135.6, 135.0, 131.5 (d, *J* = 8.2 Hz), 129.4, 128.7 (d, *J* = 7.9 Hz), 128.6 (d, *J* = 3.5 Hz), 128.4, 127.6, 126.0, 125.9, 115.3 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 21.2 Hz), 60.6, 39.6, 37.9, 31.5, 21.6; IR (neat): 2925, 2853,

1601, 1512, 1504, 1355, 1168, 835; HRESIMS Calcd for $[C_{31}H_{27}F_2NNaO_2S]^+$ (M + Na^+) 538.1623, found 538.1617.

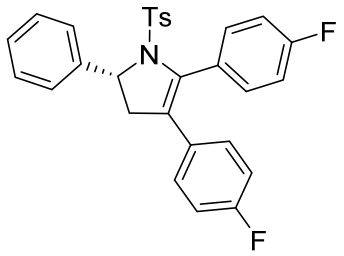
(*R*)-2-cyclohexyl-4,5-bis(4-fluorophenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3h)



3h

Compound **3h** was prepared in 74% yield (73.1 mg) according to the general procedure (Table 2, entry 8). Pale yellow oil. $[\alpha]_D^{20}$ = +112.5º (c = 1.0, $CHCl_3$). 97% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 9.27 min (minor), 15.05 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.34 – 7.27 (m, 4H), 6.97 (t, *J* = 8.5 Hz, 2H), 6.83 (t, *J* = 8.5 Hz, 2H), 6.78 – 6.72 (m, 2H), 4.12 – 4.01 (m, 1H), 2.60 (dd, *J* = 16.0, 9.0 Hz, 1H), 2.46 (s, 3H), 2.12 (d, *J* = 16.0 Hz, 1H), 1.90 – 1.75 (m, 4H), 1.74 – 1.61 (m, 2H), 1.30 – 1.12 (m, 5H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.6 (d, *J* = 247.5 Hz), 161.5 (d, *J* = 246.2 Hz), 143.7, 136.3, 135.1, 131.6 (d, *J* = 3.5 Hz), 131.4 (d, *J* = 8.1 Hz), 129.3, 128.7 (d, *J* = 7.9 Hz), 128.5 (d, *J* = 3.4 Hz), 127.6, 126.6, 115.2 (d, *J* = 21.2 Hz), 115.1 (d, *J* = 21.2 Hz), 65.4, 43.2, 36.8, 28.5, 28.1, 26.4, 26.1, 26.0, 21.6; IR (neat): 2926 (s), 2853, 1600, 1512, 1504, 1357, 1232, 1169, 834; MS (ESI, m/z) 516 (M + Na^+); HRESIMS Calcd for $[C_{29}H_{29}F_2NNaO_2S]^+$ (M + Na^+) 516.1779, found 516.1793.

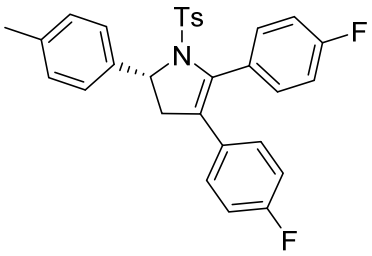
(*R*)-4,5-bis(4-fluorophenyl)-2-phenyl-1-tosyl-2,3-dihydro-1*H*-pyrrole (3i)



3i

Compound **3i** was prepared in 69% yield (67.3 mg) according to the general procedure (Table 2, entry 9). Yellow solid (mp 169-172 ^{o}C). $[\alpha]_D^{20}$ = +206.3º (c = 1.0, $CHCl_3$). 99% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 ^{o}C; t_R = 13.71 min (minor), 17.38 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.48 (m, 4H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.23 (m, 5H), 6.97 (t, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 7.0 Hz, 4H), 5.44 (d, *J* = 2.0 Hz, 1H), 3.26 (dd, *J* = 16.0, 10.0 Hz, 1H), 2.54 (dd, *J* = 16.0, 1.5 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.5 Hz), 161.5 (d, *J* = 246.2 Hz), 143.9, 142.5, 136.1, 135.5, 131.8 (d, *J* = 8.2 Hz), 131.1 (d, *J* = 3.5 Hz), 129.5, 128.8, 128.7 (d, *J* = 7.9 Hz), 128.1 (d, *J* = 3.4 Hz), 127.7, 127.6, 125.8, 124.4, 115.3 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 22.5 Hz), 62.6, 41.6, 21.6; IR (neat): 2961, 2924, 1512, 1504, 1356, 1168, 1090, 835; HRESIMS Calcd for $[C_{29}H_{23}F_2NNaO_2S]^+$ (M + Na^+) 510.1310, found 510.1324.

(*R*)-4,5-bis(4-fluorophenyl)-2-(*p*-tolyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3j)

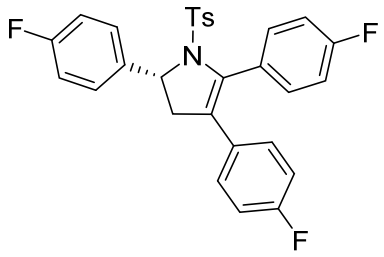


3j

Compound **3j** was prepared in 65% yield (65.2 mg) according to the general procedure (Table 2, entry 10). Pale yellow oil. $[\alpha]_D^{20}$ = +300.6º (c = 1.0, $CHCl_3$). 97%

ee (determined by HPLC: Chiralcel AD-H Column, 2/98 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 ^{o}C; t_R = 36.93 min (minor), 45.18 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.34 – 7.27 (m, 4H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.02 – 6.94 (m, 2H), 6.81 (d, *J* = 7.0 Hz, 4H), 5.41 (d, *J* = 8.5 Hz, 1H), 3.23 (dd, *J* = 15.5, 9.5 Hz, 1H), 2.53 (dd, *J* = 15.5, 2.0 Hz, 1H), 2.46 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.7 (d, *J* = 245.0 Hz), 161.5 (d, *J* = 246.2 Hz), 143.8, 139.6, 137.4, 136.0, 135.5, 131.7 (d, *J* = 8.2 Hz), 131.1 (d, *J* = 3.4 Hz), 129.4, 129.3, 128.7 (d, *J* = 7.9 Hz), 128.2 (d, *J* = 3.4 Hz), 127.6, 125.7, 124.6, 115.3 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 21.2 Hz), 62.5, 41.5, 21.6, 21.0; IR (neat): 2924, 2853, 1600, 1512, 1504, 1357, 1232, 1167, 1090, 836; HRESIMS Calcd for $[C_{30}H_{25}F_2NNaO_2S]^+$ (M + Na^+) 524.1466, found 524.1485.

(*R*)-2,4,5-tris(4-fluorophenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3k)

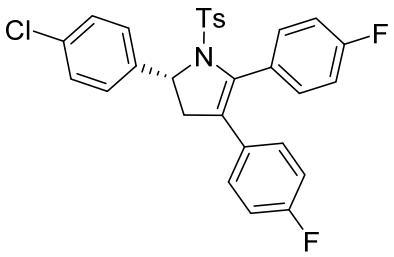


3k

Compound **3k** was prepared in 88% yield (89.0 mg) according to the general procedure (Table 2, entry 11). Pale yellow oil. $[\alpha]_D^{20}$ = +161.8º (c = 1.0, $CHCl_3$). 99% ee (determined by HPLC: Chiralcel AD-H Column, 2/98 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 ^{o}C; t_R = 15.67 min (minor), 17.37 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.40 (m, 2H), 7.31 – 7.20 (m, 4H), 7.04 (t, *J* = 8.5 Hz, 2H), 6.95 (t, *J* = 8.5 Hz, 2H), 6.83 – 6.74 (m, 4H), 5.38 (d, *J* = 9.0 Hz, 1H), 3.21 (dd, *J* = 16.0, 9.5 Hz, 1H), 2.48 (dd, *J* = 16.0, 1.5 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.5 Hz), 162.2 (d, *J* = 243.7 Hz), 161.5 (d, *J* = 246.2 Hz), 144.0, 138.3 (d, *J* = 3.2 Hz), 135.9, 135.3, 134.1, 131.7 (d, *J* = 8.2 Hz), 130.9 (d, *J* = 3.4 Hz), 129.5, 128.7 (d, *J* = 7.9 Hz), 127.9 (d, *J* = 3.4 Hz), 127.6 (d, *J* =

7.5 Hz), 127.5, 124.3, 115.6 (d, J = 21.5 Hz), 115.3 (d, J = 22.5 Hz), 115.2 (d, J = 21.2 Hz), 62.0, 41.4, 21.5; IR (neat): 2961, 2924, 1512, 1504, 1356, 1168, 1090, 835; HRESIMS Calcd for $[C_{29}H_{22}F_3NNaO_2S]^+$ (M + Na^+) 528.1216, found 528.1228.

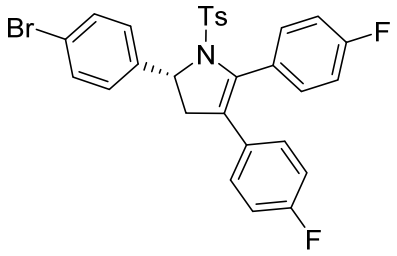
(*R*)-2-(4-chlorophenyl)-4,5-bis(4-fluorophenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3l)



3l

Compound **3l** was prepared in 89% yield (92.9 mg) according to the general procedure (Table 2, entry 12). Pale yellow oil. $[\alpha]_D^{20}$ = +146.1° (c = 1.0, $CHCl_3$). 97% ee (determined by HPLC: Chiralcel AD-H Column, 2/98 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 41.99 min (minor), 51.21 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 7.36 (d, J = 8.5 Hz, 2H), 7.31 – 7.25 (m, 4H), 6.98 (t, J = 8.5 Hz, 2H), 6.86 – 6.77 (m, 4H), 5.41 (d, J = 8.5 Hz, 1H), 3.25 (dd, J = 16.0, 9.5 Hz, 1H), 2.50 (dd, J = 16.0, 1.5 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, J = 247.5 Hz), 161.5 (d, J = 246.2 Hz), 144.0, 141.0, 136.0, 135.3, 133.5, 131.8 (d, J = 8.3 Hz), 130.8 (d, J = 3.4 Hz), 129.5, 128.9, 128.7 (d, J = 7.9 Hz), 127.9 (d, J = 3.5 Hz), 127.6, 127.3, 124.2, 115.3 (d, J = 22.5 Hz), 115.2 (d, J = 21.2 Hz), 62.0, 41.4, 21.6; IR (neat): 2925, 2853, 1600, 1512, 1505, 1357, 1232, 1168, 1089, 835; HRESIMS Calcd for $[C_{29}H_{22}ClF_2NNaO_2S]^+$ (M + Na^+) 544.0920, found 544.0940.

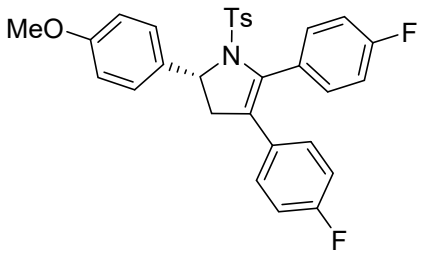
(*R*)-2-(4-bromophenyl)-4,5-bis(4-fluorophenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3m)



3m

Compound **3m** was prepared in 87% yield (98.6 mg) according to the general procedure (Table 2, entry 13). Pale yellow oil. $[\alpha]_D^{20}$ = +123.0º (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel IB Column, 8/92 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 18.76 min (major)), 21.28 min (minor). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.47 (m, 4H), 7.38 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.22 (m, 4H), 6.97 (t, *J* = 8.5 Hz, 2H), 6.86 – 6.74 (m, 4H), 5.38 (d, *J* = 8.5 Hz, 1H), 3.24 (dd, *J* = 16.0, 9.5 Hz, 1H), 2.48 (dd, *J* = 16.0, 1.5 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 247.5 Hz), 161.5 (d, *J* = 246.2 Hz), 144.1, 141.5, 135.9, 135.3, 131.8, 131.7 (d, *J* = 8.2 Hz), 130.8 (d, *J* = 3.5 Hz), 129.5, 128.7 (d, *J* = 7.9 Hz), 127.8 (d, *J* = 3.5 Hz), 127.6, 127.5, 124.2, 121.6, 115.3 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 22.5 Hz), 62.0, 41.3, 21.6; IR (neat): 2925, 2854, 1512, 1505, 1357, 1232, 1168, 1089, 836; HRESIMS Calcd for $[C_{29}H_{22}BrF_2NNaO_2S]^+$ (M + Na^+) 588.0415, found 588.0441.

(*R*)-4,5-bis(4-fluorophenyl)-2-(4-methoxyphenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3n)

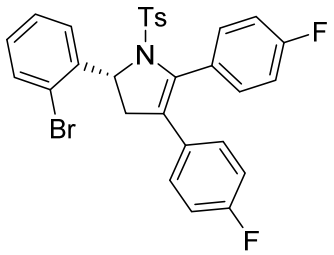


3n

Compound **3n** was prepared in 63% yield (65.2 mg) according to the general procedure (Table 2, entry 14). Pale yellow oil. $[\alpha]_D^{20}$ = +157.8º (c = 1.0, $CHCl_3$). 97%

ee (determined by HPLC: Chiralcel IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 21.43 min (minor), 24.13 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.32 – 7.23 (m, 4H), 7.01 – 6.89 (m, 4H), 6.80 (d, *J* = 7.0 Hz, 4H), 5.38 (d, *J* = 8.5 Hz, 1H), 3.80 (s, 3H), 3.20 (dd, *J* = 16.0, 9.5 Hz, 1H), 2.51 (dd, *J* = 16.0, 1.5 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.7 (d, *J* = 247.5 Hz), 161.5 (d, *J* = 247.5 Hz), 159.1, 143.8, 135.9, 135.5, 134.6, 131.7 (d, *J* = 8.2 Hz), 131.1 (d, *J* = 3.4 Hz), 129.4, 128.7 (d, *J* = 7.9 Hz), 128.2 (d, *J* = 3.5 Hz), 127.5, 127.1, 124.6, 115.3 (d, *J* = 21.2 Hz), 115.2 (d, *J* = 21.2 Hz), 114.1, 62.2, 55.2, 41.4, 21.5; IR (neat): 2925, 2853, 1600, 1512, 1356, 1248, 1233, 1167, 1089, 836; HRESIMS Calcd for $[C_{30}H_{25}F_2NNaO_3S]^+$ (M + Na^+) 540.1415, found 540.1426.

(*R*)-2-(2-bromophenyl)-4,5-bis(4-fluorophenyl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3o)

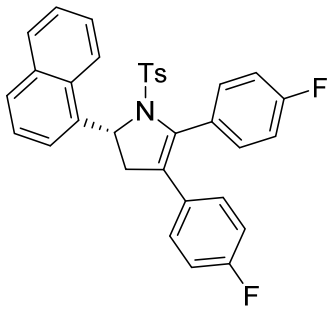


3o

Compound **3o** was prepared in 88% yield (99.7 mg) according to the general procedure (Table 2, entry 15). Pale yellow oil. $[\alpha]_D^{20}$ = +260.0º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel IC Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 31.51 min (minor), 34.48 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 – 7.76 (m, 1H), 7.59 (d, *J* = 8.0 Hz, 3H), 7.48 – 7.38 (m, 3H), 7.32 (d, *J* = 8.0 Hz, 2H), 7.22 – 7.15 (m, 1H), 7.05 (t, *J* = 8.5 Hz, 2H), 6.83 – 6.73 (m, 4H), 5.69 (dd, *J* = 10.0, 2.5 Hz, 1H), 3.40 (dd, *J* = 16.0, 10.5 Hz, 1H), 2.48 (s, 3H), 2.33 (dd, *J* = 16.0, 2.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9 (d, *J* = 247.5 Hz), 161.5 (d, *J* = 246.2 Hz), 144.1, 141.9, 136.3, 134.9, 133.0, 131.9 (d, *J* = 8.2 Hz),

130.9 (d, J = 3.4 Hz), 129.6, 129.0, 128.8 (d, J = 7.9 Hz), 128.0 (d, J = 3.5 Hz), 127.8, 127.7, 126.8, 123.6, 121.6, 115.4 (d, J = 21.7 Hz), 115.2 (d, J = 21.5 Hz), 62.2, 42.3, 21.6; IR (neat): 2924, 2853, 1600, 1512, 1504, 1360, 1232, 1170, 1089, 836; HRESIMS Calcd for $[C_{29}H_{22}BrF_2NNaO_2S]^+$ (M + Na^+) 588.0415, found 588.0436.

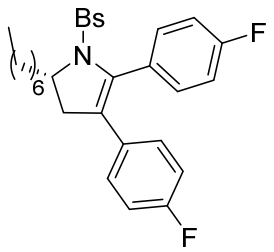
(*R*)-4,5-bis(4-fluorophenyl)-2-(naphthalen-1-yl)-1-tosyl-2,3-dihydro-1*H*-pyrrole (3p)



3p

Compound **3p** was prepared in 55% yield (59.1 mg) according to the general procedure (Table 2, entry 16). Pale yellow oil. $[\alpha]_D^{20}$ = +280.0º (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 24.33 min (minor), 29.11 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, J = 7.0 Hz, 1H), 7.93 – 7.86 (m, 2H), 7.82 (d, J = 8.0 Hz, 1H), 7.63 – 7.45 (m, 7H), 7.31 (d, J = 8.0 Hz, 2H), 7.04 (t, J = 8.5 Hz, 2H), 6.81 – 6.69 (m, 4H), 6.18 (dd, J = 10.0, 1.5 Hz, 1H), 3.57 (dd, J = 16.0, 10.5 Hz, 1H), 2.50 (dd, J = 16.0, 2.5 Hz, 1H), 2.48 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9 (d, J = 247.5 Hz), 161.5 (d, J = 246.2 Hz), 144.0, 137.8, 136.4, 135.5, 134.2, 132.0 (d, J = 8.2 Hz), 131.0 (d, J = 3.4 Hz), 129.6, 129.5, 129.2, 128.7 (d, J = 7.9 Hz), 128.1, 127.7, 126.2, 125.6, 125.5, 124.5, 122.7, 122.4, 115.4 (d, J = 21.7 Hz), 115.1 (d, J = 21.5 Hz), 60.1, 42.8, 21.6; IR (neat): 3059, 2926, 2853, 1600, 1512, 1505, 1358, 1233, 1169, 1090, 835; HRESIMS Calcd for $[C_{33}H_{25}F_2NNaO_2S]^+$ (M + Na^+) 560.1466, found 560.1488.

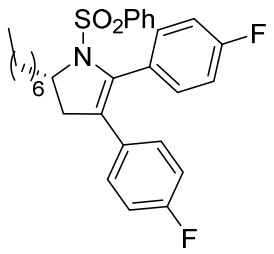
(*S*)-1-((4-bromophenyl)sulfonyl)-4,5-bis(4-fluorophenyl)-2-heptyl-2,3-dihydro-1*H*-pyrrole (3q)



3q

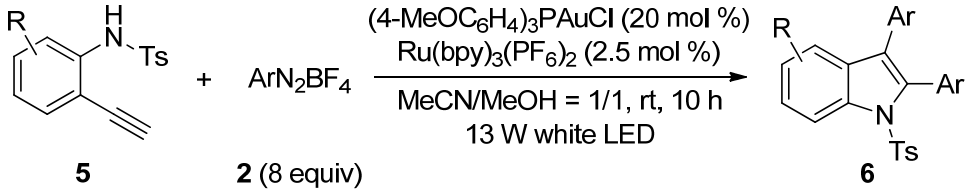
Compound **3q** was prepared in 54% yield (62.0 mg) according to the general procedure (Table 2, entry 17). Pale yellow oil. $[\alpha]_D^{20}$ = +51.0º (c = 1.0, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel AD-H Column, 2/98 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 8.92 min (minor), 12.19 min (major)). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.5 Hz, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.26 (t, *J* = 7.0 Hz, 2H), 6.98 (t, *J* = 8.5 Hz, 2H), 6.88 – 6.73 (m, 4H), 4.31 – 4.24 (m 1H), 2.78 (dd, *J* = 16.0, 8.5 Hz, 1H), 2.06 (d, *J* = 16.0 Hz, 1H), 1.87 – 1.75 (m, 1H), 1.68 – 1.58 (m, 1H), 1.57 – 1.47 (m, 2H), 1.40 – 1.25 (m, 8H), 0.89 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8 (d, *J* = 248.7 Hz), 161.6 (d, *J* = 246.2 Hz), 137.4, 135.2, 132.1, 131.6 (d, *J* = 8.2 Hz), 131.3 (d, *J* = 3.5 Hz), 129.1, 128.7 (d, *J* = 7.9 Hz), 128.3 (d, *J* = 3.5 Hz), 128.0, 126.2, 115.4 (d, *J* = 21.2 Hz), 115.3 (d, *J* = 21.2 Hz), 61.2, 39.4, 36.2, 31.8, 29.5, 29.2, 25.1, 22.6, 14.1; IR (neat): 2925, 2854, 1512, 1504, 1233, 1172, 1157, 1087, 1069, 835; HRESIMS Calcd for $[C_{29}H_{30}BrF_2NNaO_2S]^+$ (M + Na^+) 596.1041, found 596.1071.

(*S*)-4-(3-fluorophenyl)-5-(4-fluorophenyl)-2-heptyl-1-(phenylsulfonyl)-2,3-dihydro-1*H*-pyrrole (3r)



3r

Compound **3r** was prepared in 74% yield (73.4 mg) according to the general procedure (Table 2, entry 18). Pale yellow oil. $[\alpha]_D^{20}$ = +51.0º (c = 1.0, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 5.79 min (minor), 7.43 min (major)). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 7.5 Hz, 2H), 7.62 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 2H), 7.33 – 7.25 (m, 2H), 6.98 (t, *J* = 8.4 Hz, 2H), 6.82 (t, *J* = 8.4 Hz, 2H), 6.78 – 6.72 (m, 2H), 4.32 – 4.25 (q, *J* = 7.2 Hz, 1H), 2.65 (dd, *J* = 15.6, 8.4 Hz, 1H), 1.99 (d, *J* = 15.6 Hz, 1H), 1.89 – 1.74 (m, 1H), 1.68 – 1.47 (m, 3H), 1.39 – 1.26 (m, 8H), 0.90 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.6 (d, *J* = 246.0 Hz), 161.5 (d, *J* = 246.0 Hz), 138.0, 135.4, 132.9, 131.6 (d, *J* = 4.5 Hz), 131.5 (d, *J* = 8.2 Hz), 128.8, 128.6 (d, *J* = 7.8 Hz), 128.5 (d, *J* = 3.4 Hz), 127.5, 126.2, 115.3 (d, *J* = 22.5 Hz), 115.2 (d, *J* = 21.0 Hz), 61.1, 39.4, 36.1, 31.8, 29.5, 29.2, 25.1, 22.6, 14.1; IR (neat): 2925 (s), 2853, 1601, 1512, 1504, 1357, 1171, 835; HRESIMS Calcd for $[C_{29}H_{31}F_2NNaO_2S]^+$ (M + Na^+) 518.1936, found 518.1953.

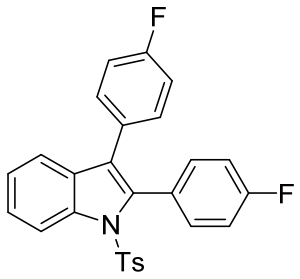


General procedure for the synthesis of 2,3-arylindole 6:

o-Ethynylaniline **5** (0.20 mmol), aryldiazonium salt **2** (1.6 mmol, 8.0 eq.), $[Ru(bpy)_3](PF_6)_2$ (4.0 mg, 2.5 mol %) and $(4\text{-}MeOC_6H_4)_3PAuCl$ (23.4 mg, 20 mol %) were added to a flame-dried Schlenk flask containing a stirring bar and purged by evacuating the flask and backfilling with argon three times. In the absence of light,

anhydrous MeCN/MeOH: 1/1 (2.0 mL, 0.10 M) was added and the flask was sealed. The mixture was then stirred under irradiation from 13 W white LED. The reaction mixture was stirred at room temperature and the progress of the reaction was monitored by TLC. The reaction typically took 10 h. Upon completion, the mixture was then concentrated and the residue was purified by chromatography on silicagel (eluent: hexanes/ethyl acetate) to afford the desired 2,3-arylindole **6**.

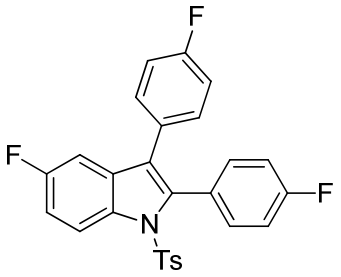
2,3-bis(4-fluorophenyl)-1-tosyl-1*H*-indole (6a)



6a

Compound **6a** was prepared in 71% yield (65.1 mg) according to the general procedure (eq 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 2H), 7.37 – 7.28 (m, 3H), 7.23 – 7.17 (m, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 7.08 – 7.02 (m, 2H), 7.02 – 6.89 (m, 4H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.6 (d, *J* = 248.0 Hz), 161.8 (d, *J* = 246.0 Hz), 144.7, 137.1, 135.7, 135.4, 133.8 (d, *J* = 8.4 Hz), 131.4 (d, *J* = 8.0 Hz), 130.1, 129.3, 128.3 (d, *J* = 3.4 Hz), 126.8, 126.7 (d, *J* = 3.5 Hz), 125.4, 124.2, 123.9, 119.7, 116.2, 115.4 (d, *J* = 21.0 Hz), 114.4 (d, *J* = 21.0 Hz), 21.5; IR (neat): 2924, 1596, 1499, 1380, 1224, 1188, 1177, 840, 578; HRESIMS Calcd for $[C_{27}H_{19}F_2NNaO_2S]^+$ (M + Na^+) 482.0997, found 482.0999.

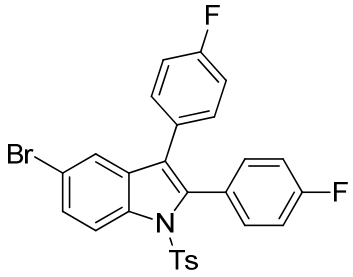
5-fluoro-2,3-bis(4-fluorophenyl)-1-tosyl-1*H*-indole (6b)



6b

Compound **6b** was prepared in 85% yield (81.1 mg) according to the general procedure (eq 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 – 8.31 (m, 1H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.22 – 7.13 (m, 3H), 7.12 – 7.06 (m, 3H), 7.04 – 6.90 (m, 6H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 248.0 Hz), 162.0 (d, *J* = 246.0 Hz), 160.4 (d, *J* = 240.0 Hz), 145.0, 137.5, 135.1, 133.8 (d, *J* = 9.0 Hz), 133.4, 131.3 (d, *J* = 8.0 Hz), 129.4, 127.9 (d, *J* = 3.0 Hz), 126.8, 126.3 (d, *J* = 3.0 Hz), 123.8 (d, *J* = 4.0 Hz), 117.6 (d, *J* = 8.0 Hz), 115.6 (d, *J* = 21.0 Hz), 114.7 (d, *J* = 22.0 Hz), 113.3 (d, *J* = 25.0 Hz), 105.5, 105.3, 21.6; IR (neat): 2925, 1606, 1595, 1500, 1464, 1228, 1188, 1176, 808, 566; HRESIMS Calcd for $[C_{27}H_{18}F_3NNaO_2S]^+$ (M + Na^+) 500.0903, found 500.0913.

5-bromo-2,3-bis(4-fluorophenyl)-1-tosyl-1*H*-indole (6c)

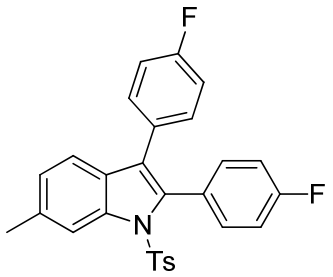


6c

Compound **6c** was prepared in 78% yield (84.2 mg) according to the general procedure (eq 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (d, *J* = 9.2 Hz, 1H), 7.58 – 7.47 (m, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.21 – 7.14 (m, 2H), 7.11 (d, *J* = 8.4 Hz, 2H), 7.05 – 6.88 (m, 6H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 249.0 Hz), 162.0 (d, *J* = 246.0 Hz), 145.1, 136.9, 135.8, 135.1, 133.8 (d, *J* =

8.0 Hz), 131.8, 131.3 (d, J = 8.0 Hz), 129.5, 128.2, 127.7 (d, J = 3.0 Hz), 126.8, 126.1 (d, J = 3.0 Hz), 123.1, 122.4, 117.9, 117.7, 115.6 (d, J = 21.0 Hz), 114.7 (d, J = 22.0 Hz), 21.6; IR (neat): 2925, 1606, 1596, 1515, 1464, 1228, 1188, 1176, 1154, 808, 566; HRESIMS Calcd for $[C_{27}H_{18}BrF_2NNaO_2S]^+$ (M + Na^+) 560.0102, found 560.0116.

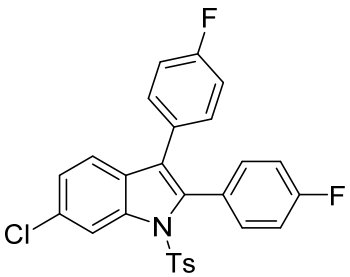
2,3-bis(4-fluorophenyl)-6-methyl-1-tosyl-1*H*-indole (6d)



6d

Compound **6d** was prepared in 64% yield (60.5 mg) according to the general procedure (eq 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.32 – 7.29 (m, 3H), 7.22 – 7.07 (m, 5H), 7.06 – 6.86 (m, 6H), 2.56 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, J = 248.0 Hz), 161.8 (d, J = 245.0 Hz), 144.7, 137.6, 135.6, 135.5, 135.0, 133.9 (d, J = 8.0 Hz), 131.4 (d, J = 8.0 Hz), 129.4, 128.6 (d, J = 4.0 Hz), 127.9, 126.8 (d, J = 5.0 Hz), 125.7, 123.9, 119.3, 116.3, 115.3 (d, J = 21.0 Hz), 114.5 (d, J = 21.0 Hz), 22.1, 21.5; IR (neat): 2925, 1606, 1596, 1500, 1464, 1381, 1228, 1188, 1176, 808, 566; HRESIMS Calcd for $[C_{28}H_{21}F_2NNaO_2S]^+$ (M + Na^+) 496.1153, found 496.1158.

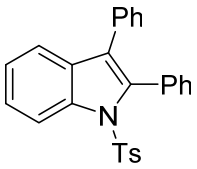
6-chloro-2,3-bis(4-fluorophenyl)-1-tosyl-1*H*-indole (6e)



6e

Compound **6e** was prepared in 62% yield (61.2 mg) according to the general procedure (eq 1). Pale yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 1.6 Hz, 1H), 7.39 – 7.24 (m, 4H), 7.18 – 7.10 (m, 4H), 7.07 – 6.87 (m, 6H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.0 (d, *J* = 248 Hz), 161.9 (d, *J* = 248 Hz), 145.1, 137.4, 136.1, 135.3, 133.9 (d, *J* = 8.4 Hz), 131.3(4) (d, *J* = 8 Hz), 131.3(3), 129.5, 128.4, 127.9 (d, *J* = 3.4 Hz), 126.9, 126.2 (d, *J* = 3.4 Hz), 124.8, 123.4, 120.5, 116.2, 115.4 (d, *J* = 21.5 Hz), 114.6 (d, *J* = 21.8 Hz), 21.6; IR (neat): 2925, 1606, 1596, 1500, 1464, 1381, 1228, 1188, 1176, 808, 566; HRESIMS Calcd for $[C_{27}H_{18}ClF_2NNaO_2S]^+$ (M + Na^+) 516.0607, found 516.0616.

2,3-diphenyl-1-tosyl-1*H*-indole (6f)



6f

Compound **6f** was prepared in 79% yield (67.4 mg) according to the general procedure (eq 1). Pale yellow oil. This compound is known and the spectroscopic data match those reported.[3] ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.45 – 7.38 (m, 1H), 7.36 – 7.17 (m, 11H), 7.14 – 7.03 (m, 4H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.5, 137.2, 136.8, 135.3, 132.6, 132.0, 130.8, 130.4, 129.8, 129.2, 128.4, 128.1, 127.2, 126.9, 125.1, 124.7, 124.1, 119.9, 116.2, 21.5.

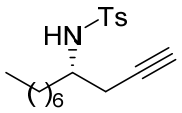
References:

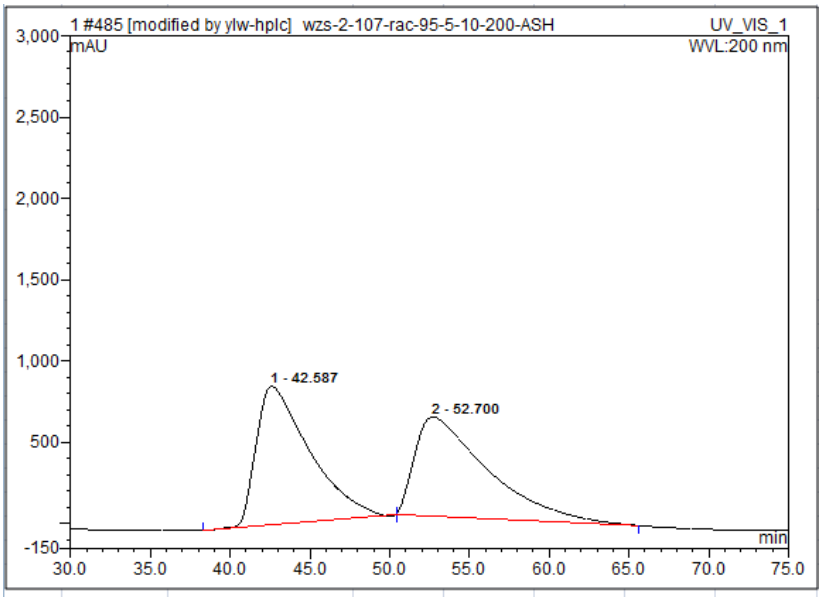
1. (a) Shu, C.; Liu, M.-Q.; Wang, S.-S.; Li, L.; Ye, L.-W. *J. Org. Chem.* **2013**, *78*, 3292. (b) Yu, Y.-F.; Shu, C.; Shen, C.-H.; Li, T.-Y.; Ye, L.-W. *Chem. Asian J.* **2013**, *8*, 2920. (c) Shu, C.; Li, L.; Yu, Y.-F.; Jiang, S.; Ye, L.-W. *Chem. Commun.*

2014, *50*, 2522. (d) Yu, Y.-F.; Shu, C.; Zhou, B.; Li, J.-Q.; Zhou, J.-M.; Ye, L.-W. *Chem. Commun.* **2015**, *51*, 2126. (e) Shu, C.; Li, L.; Shen, C.-H.; Ruan, P.-P.; Liu, C.-Y.; Ye, L.-W. *Chem. Eur. J.* **2016**, *22*, 2282. (f) Shu, C.; Li, L.; Xiao, X.-Y.; Yu, Y.-F.; Ping, Y.-F.; Zhou, J.-M.; Ye, L.-W. *Chem. Commun.* **2014**, *50*, 8689.

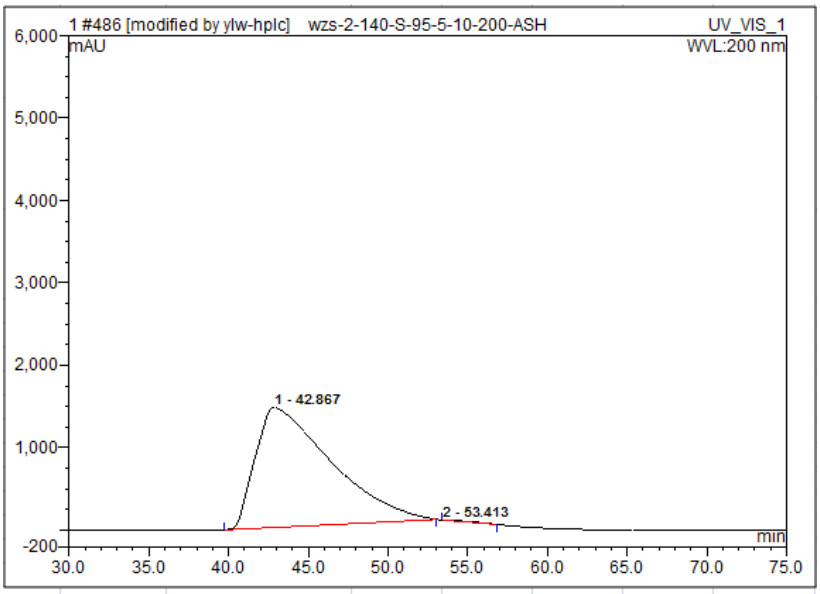
2. Shu, C.; Li, L.; Xiao, X.-Y.; Yu, Y.-F.; Ping, Y.-F.; Zhou, J.-M.; Ye, L.-W. *Chem. Commun.* **2014**, *50*, 8689.
3. Qu, C.; Zhang, S.; Du, H.; Zhu, C. *Chem. Commun.* **2016**, *52*, 14400.

Compound **1a**



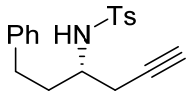


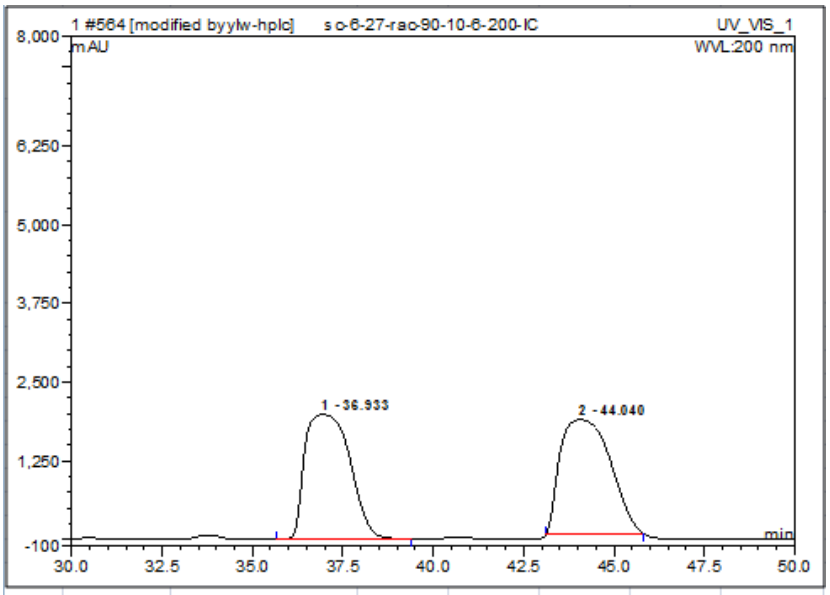
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	42.59	n.a.	851.377	3267.962	50.44	n.a.	BMb*
2	52.70	n.a.	610.391	3210.768	49.56	n.a.	bMB*
Total:			1461.769	6478.729	100.00	0.000	



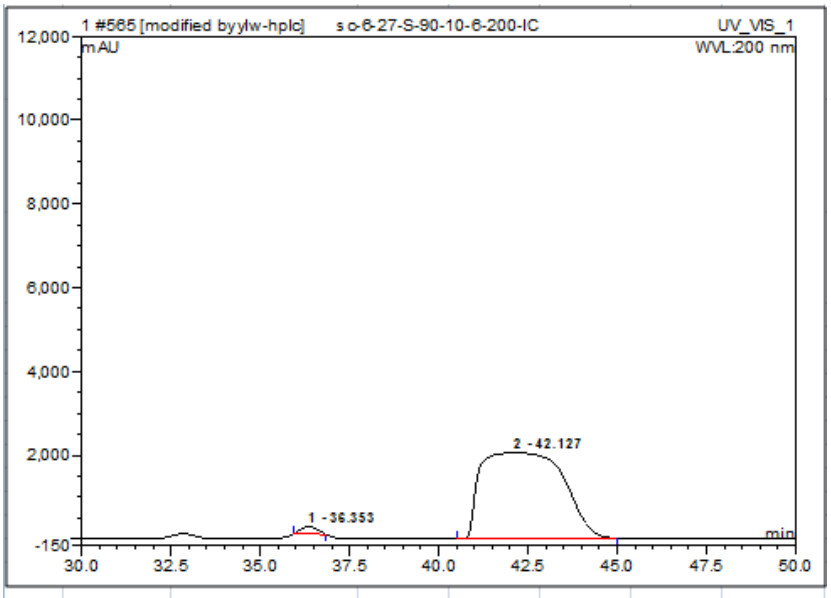
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	42.87	n.a.	1456.016	7964.824	99.78	n.a.	BMB*
2	53.41	n.a.	0.002	17.813	0.22	n.a.	BMB*
Total:			1456.018	7982.637	100.00	0.000	

Compound **1b**



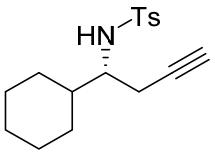


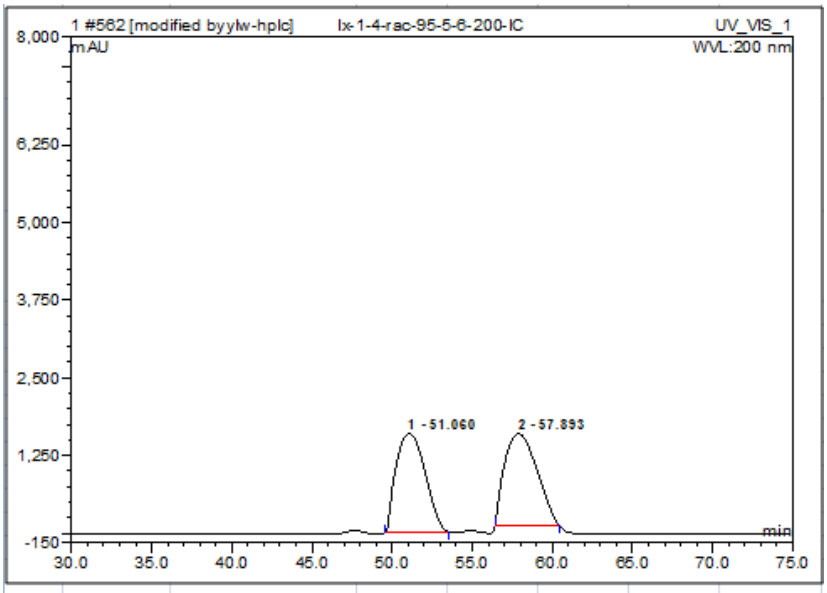
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	36.93	n.a.	1972.618	2851.567	49.35	n.a.	BMB*
2	44.04	n.a.	1817.498	2926.317	50.65	n.a.	BMB*
Total:			3790.117	5777.884	100.00	0.000	



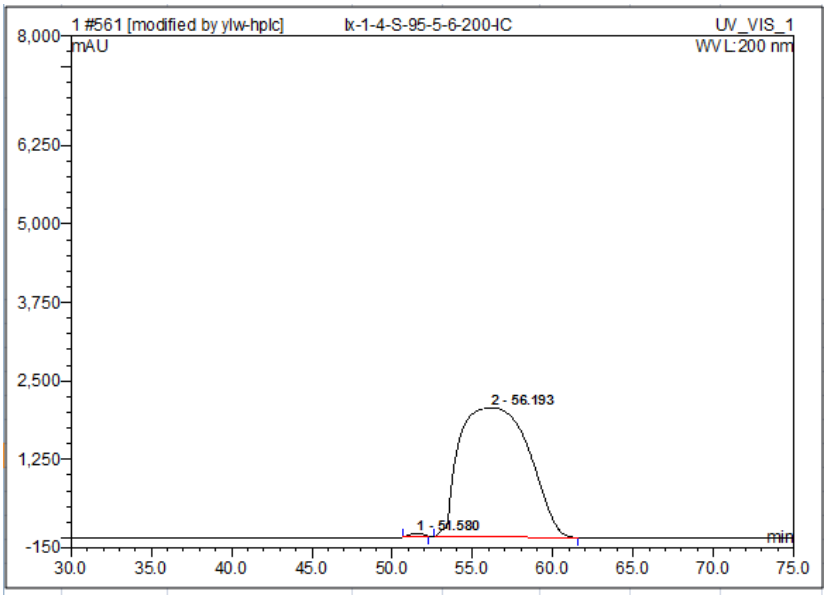
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	36.35	n.a.	172.031	93.303	1.68	n.a.	BMB*
2	42.13	n.a.	2042.468	5464.641	98.32	n.a.	BMB*
Total:			2214.499	5557.945	100.00	0.000	

Compound **1c**



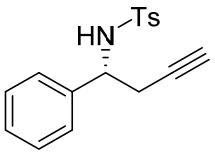


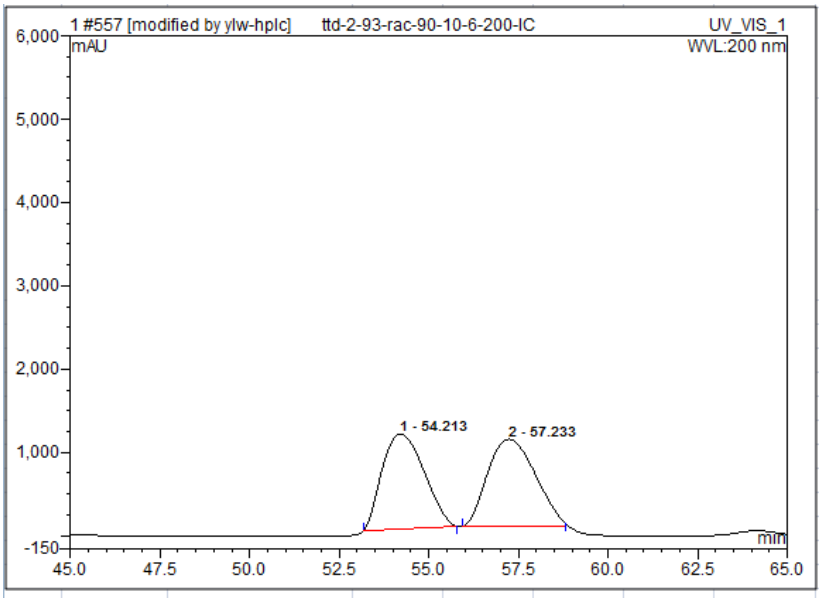
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	51.06	n.a.	1588.998	3364.568	49.12	n.a.	BMB*
2	57.89	n.a.	1481.951	3484.805	50.88	n.a.	BMB*
Total:			3070.948	6849.373	100.00	0.000	



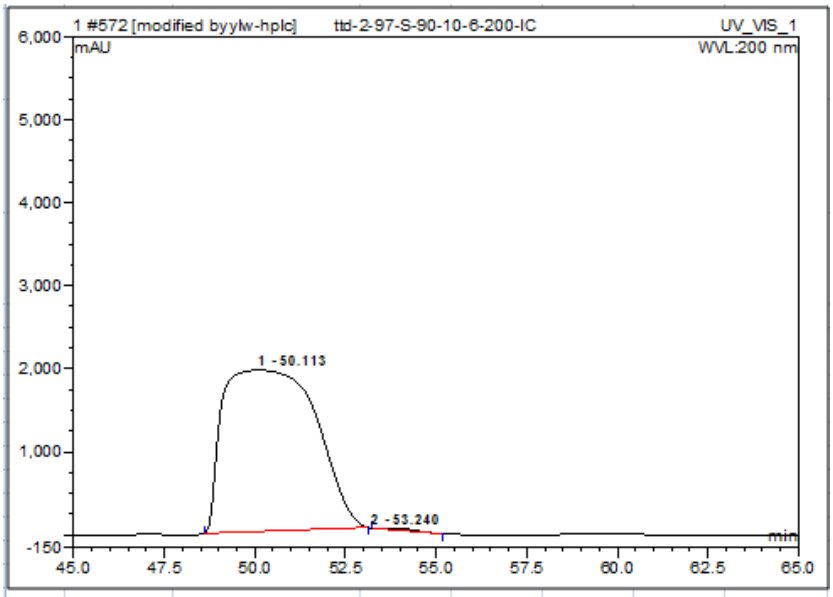
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	51.58	n.a.	47.516	47.697	0.46	n.a.	BMB*
2	56.19	n.a.	2055.196	10333.812	99.54	n.a.	BMB*
Total:			2102.711	10381.508	100.00	0.000	

Compound **1d**



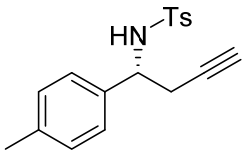


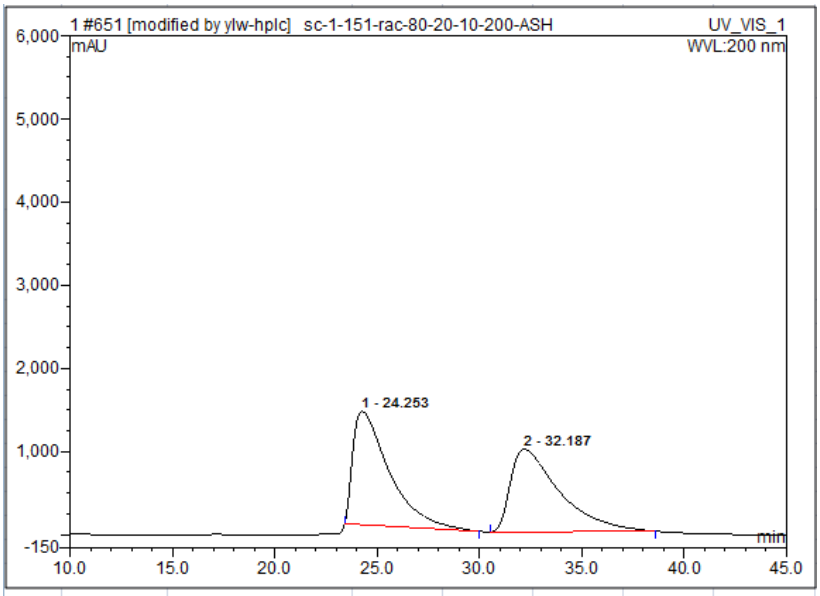
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	54.21	n.a.	1138.843	1551.667	49.09	n.a.	BMB*
2	57.23	n.a.	1042.997	1609.286	50.91	n.a.	BM *
Total:			2181.840	3160.954	100.00	0.000	



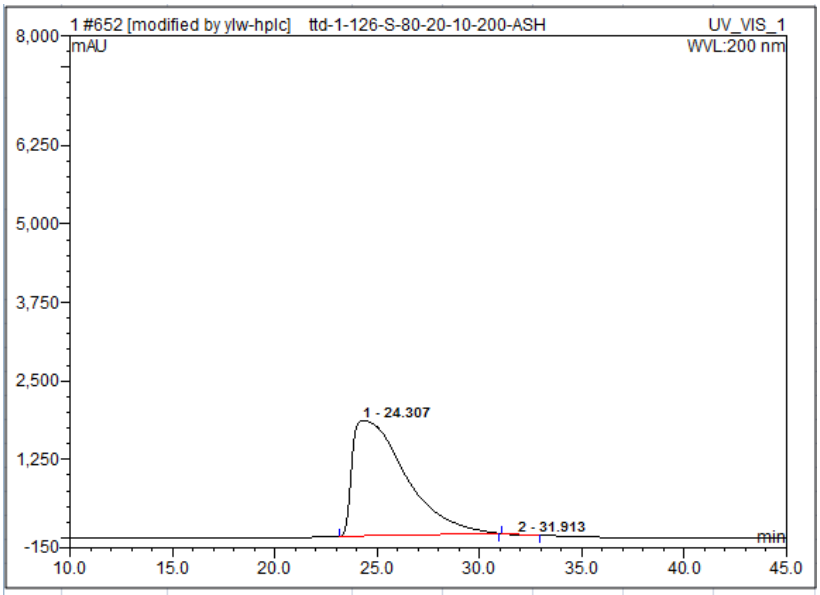
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	50.11	n.a.	1940.012	5761.979	99.66	n.a.	BMB*
2	53.24	n.a.	0.160	19.497	0.34	n.a.	BMB*
Total:			1940.172	5781.476	100.00	0.000	

Compound **1e**



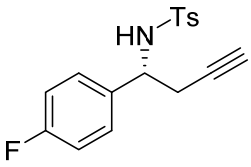


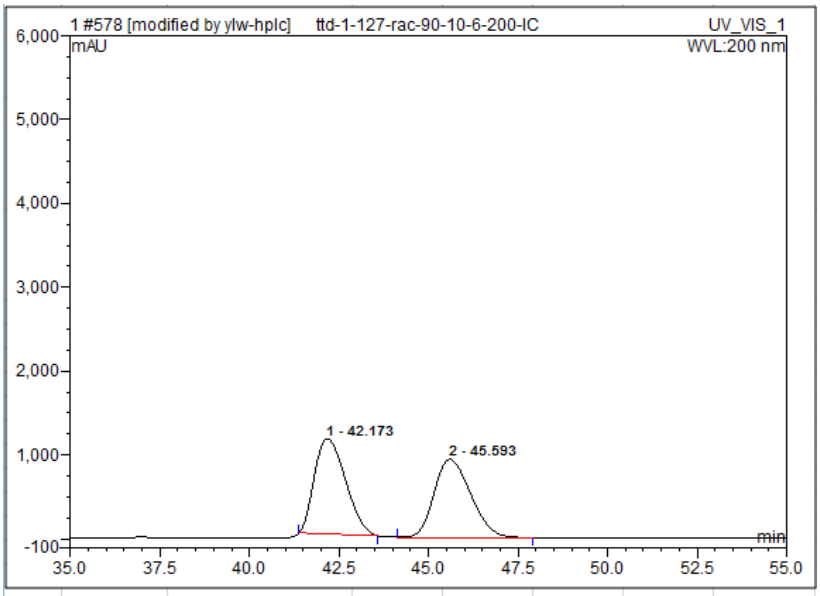
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	24.25	n.a.	1362.284	2814.547	50.56	n.a.	BMB*
2	32.19	n.a.	992.878	2752.634	49.44	n.a.	BMB*
Total:			2355.162	5567.182	100.00	0.000	



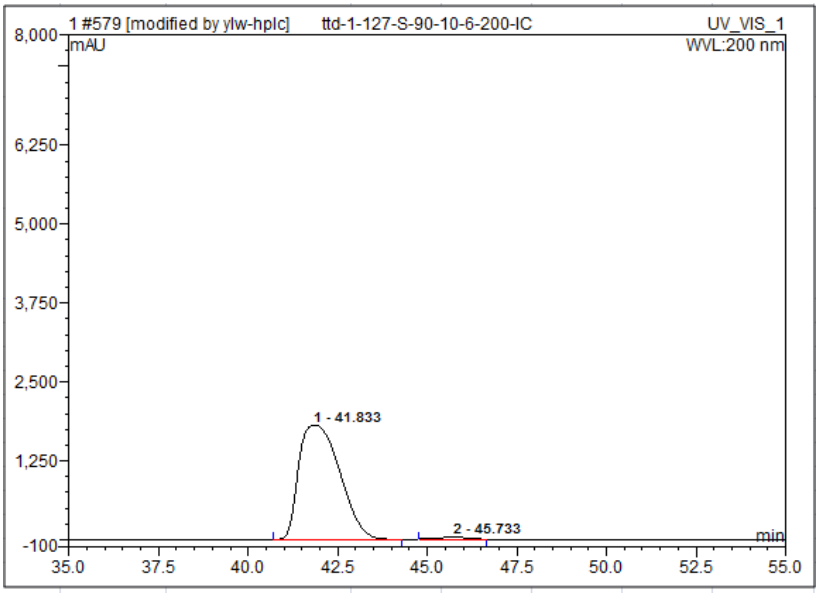
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	24.31	n.a.	1836.663	5548.010	99.79	n.a.	BMB*
2	31.91	n.a.	10.469	11.934	0.21	n.a.	BMB*
Total:			1847.132	5559.944	100.00	0.000	

Compound **1f**



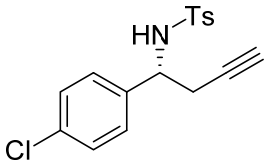


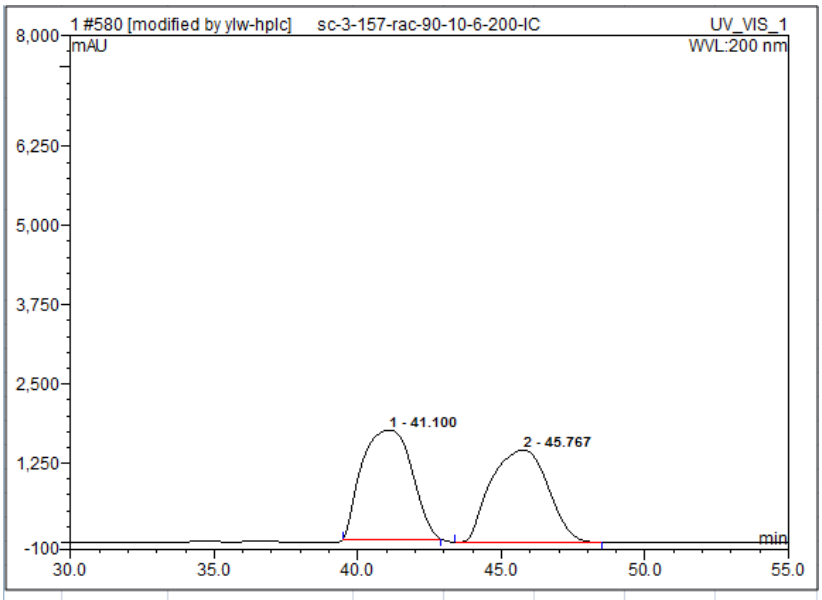
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	42.17	n.a.	1131.708	1143.087	50.96	n.a.	BMB*
2	45.59	n.a.	930.350	1099.911	49.04	n.a.	BMB*
Total:			2062.058	2242.998	100.00	0.000	



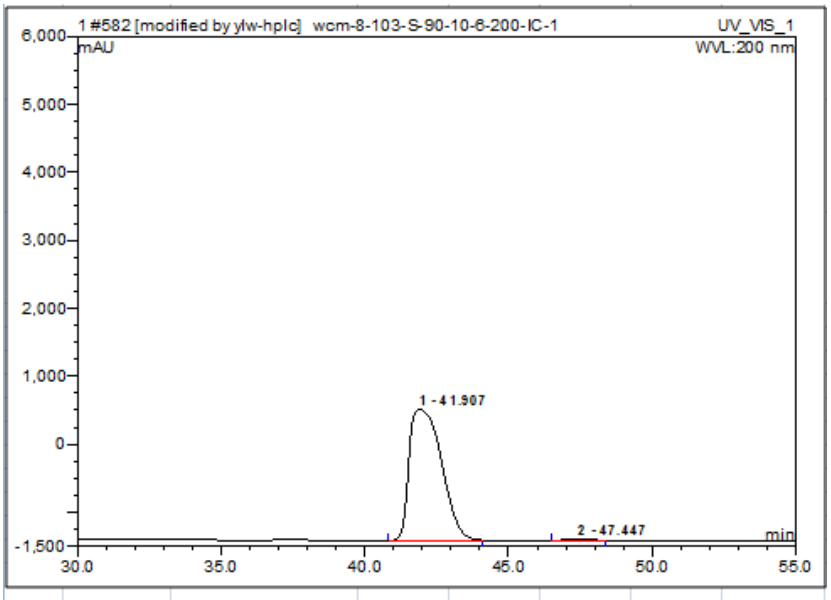
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	41.83	n.a.	1816.306	2403.692	98.81	n.a.	BMB*
2	45.73	n.a.	29.685	29.008	1.19	n.a.	BMB*
Total:			1845.991	2432.700	100.00	0.000	

Compound **1g**



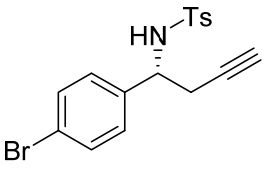


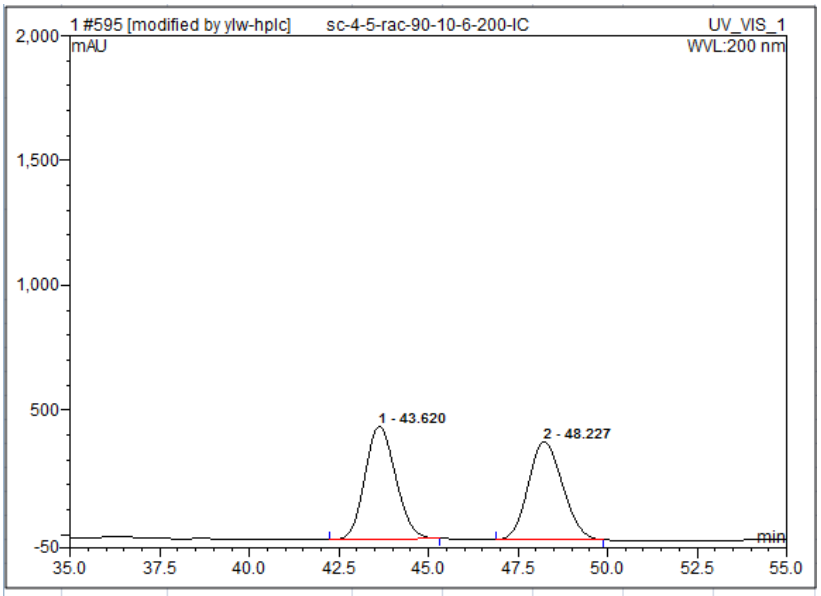
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	41.10	n.a.	1721.497	3473.465	50.93	n.a.	BMB*
2	45.77	n.a.	1455.693	3346.636	49.07	n.a.	BMB*
Total:			3177.191	6820.101	100.00	0.000	



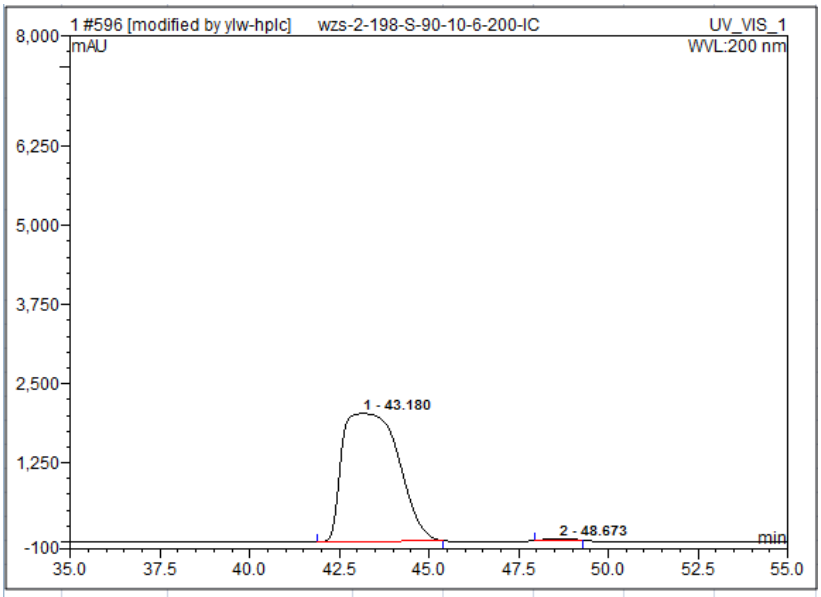
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	41.91	n.a.	1918.690	2507.385	99.30	n.a.	BMB*
2	47.45	n.a.	18.698	17.730	0.70	n.a.	BMB*
Total:			1937.388	2525.115	100.00	0.000	

Compound **1h**



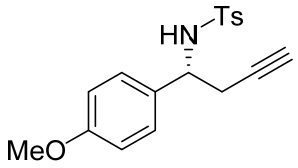


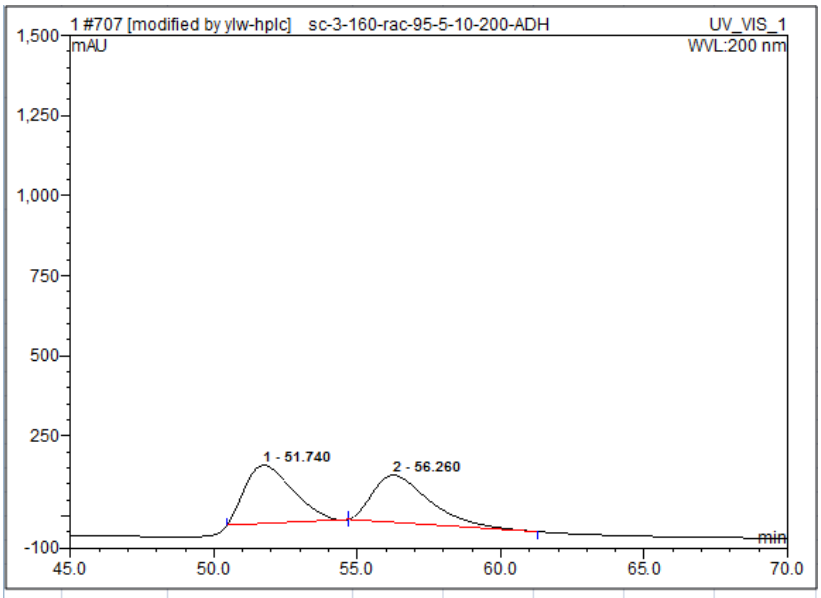
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	43.62	n.a.	451.491	449.381	50.82	n.a.	BMB*
2	48.23	n.a.	391.767	434.902	49.18	n.a.	BMB*
Total:			843.259	884.282	100.00	0.000	



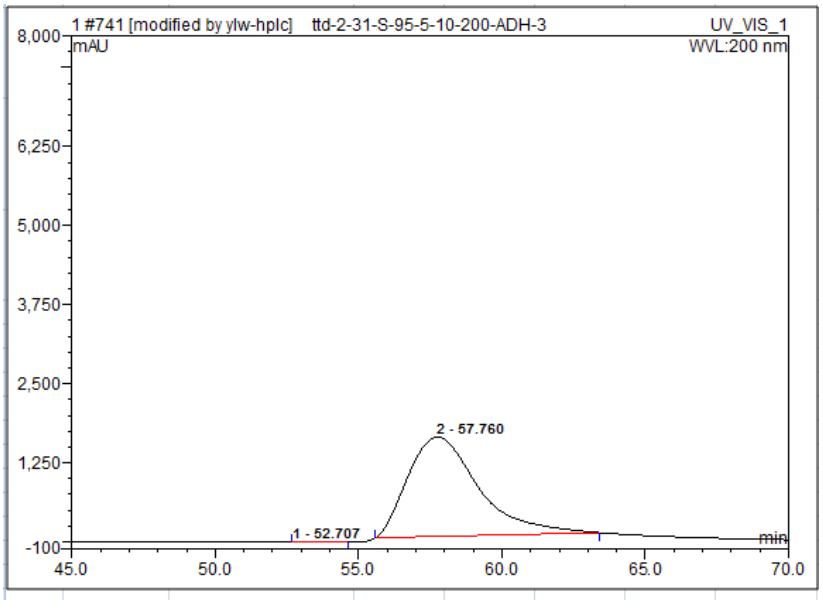
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	43.18	n.a.	2020.315	3668.656	99.27	n.a.	BMB*
2	48.67	n.a.	33.290	27.078	0.73	n.a.	BMB*
Total:			2053.605	3695.734	100.00	0.000	

Compound **1i**



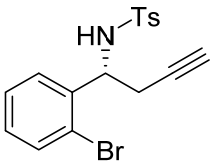


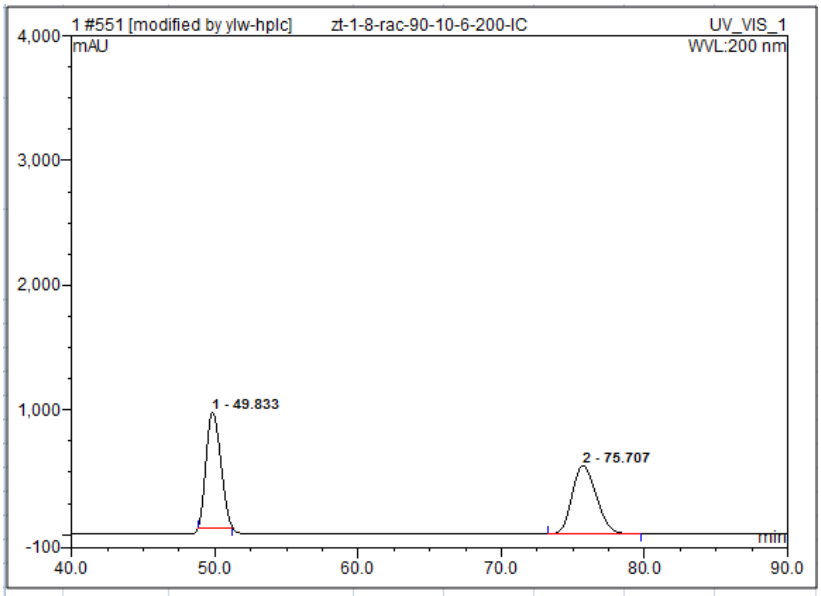
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	51.74	n.a.	181.283	348.079	50.73	n.a.	BMb*
2	56.26	n.a.	147.130	338.104	49.27	n.a.	bMB*
Total:			328.413	686.183	100.00	0.000	



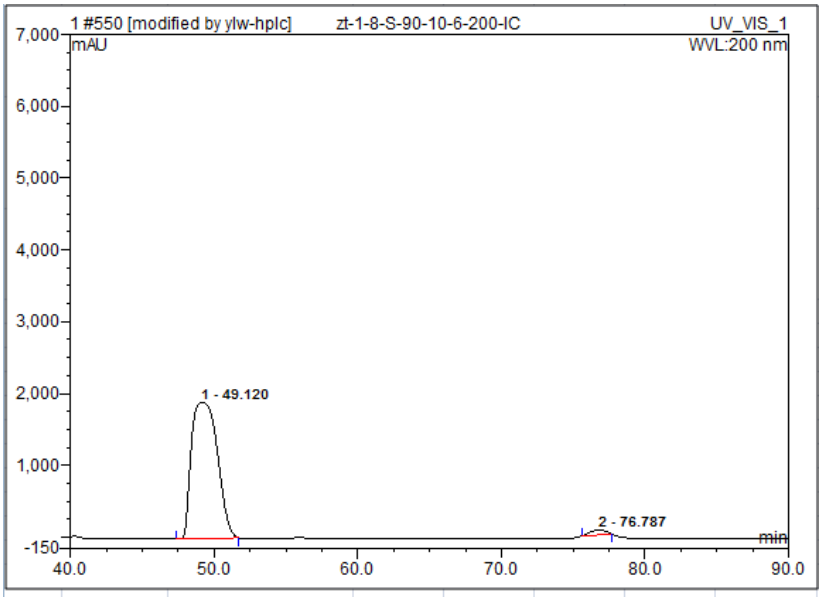
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	52.71	n.a.	0.025	0.066	0.00	n.a.	BMB*
2	57.76	n.a.	1565.861	4492.377	100.00	n.a.	BMB*
Total:			1565.887	4492.443	100.00	0.000	

Compound **1j**



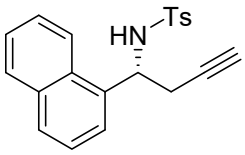


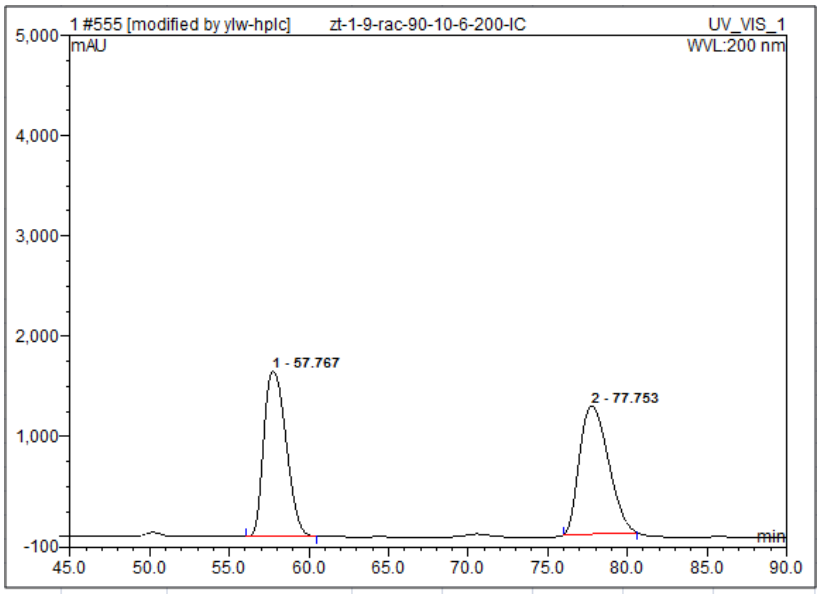
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	49.83	n.a.	925.194	1095.525	50.71	n.a.	BMB*
2	75.71	n.a.	546.210	1064.753	49.29	n.a.	BMB*
Total:			1471.404	2160.278	100.00	0.000	



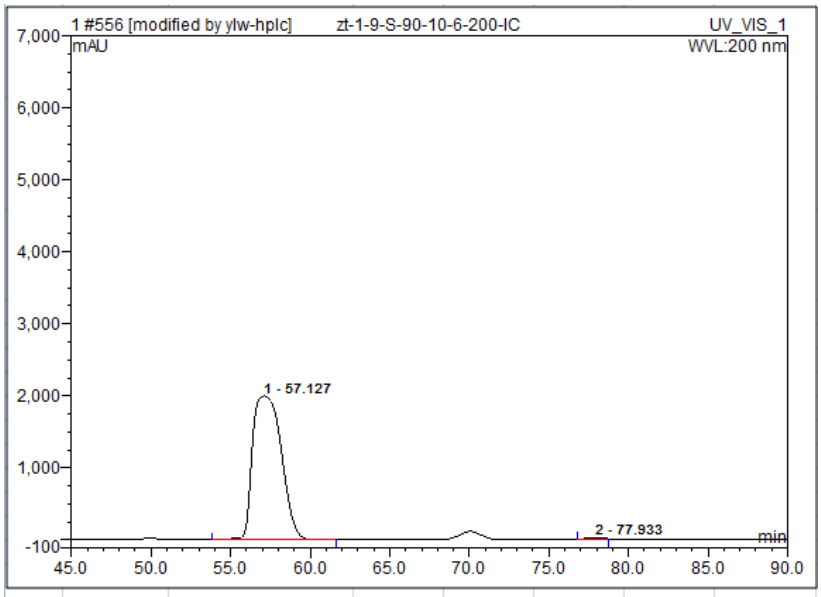
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	49.12	n.a.	1897.251	3974.794	97.86	n.a.	BMB*
2	76.79	n.a.	70.156	86.821	2.14	n.a.	BMB*
Total:			1967.407	4061.616	100.00	0.000	

Compound **1k**



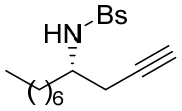


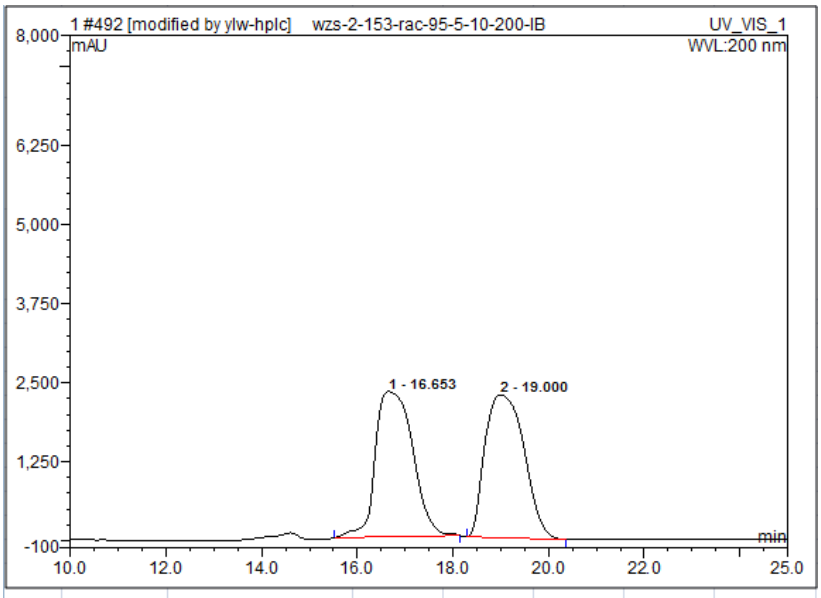
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	57.77	n.a.	1643.733	2686.002	49.91	n.a.	BMB*
2	77.75	n.a.	1276.853	2695.647	50.09	n.a.	BMB*
Total:			2920.586	5381.649	100.00	0.000	



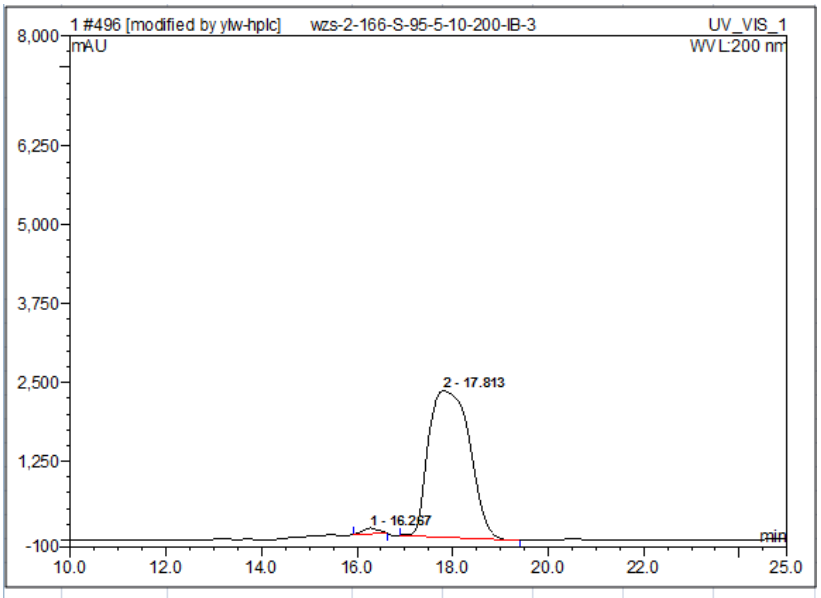
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	57.13	n.a.	1995.938	4196.194	99.56	n.a.	BMB*
2	77.93	n.a.	16.155	18.568	0.44	n.a.	BMB*
Total:			2012.093	4214.762	100.00	0.000	

Compound **1l**



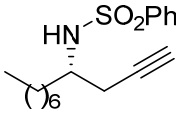


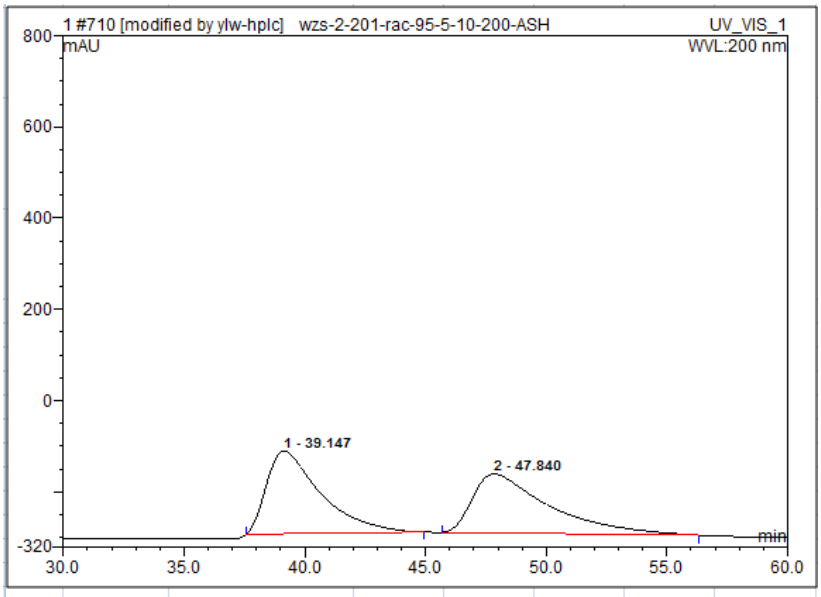
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.65	n.a.	2296.388	2088.906	49.27	n.a.	BMB*
2	19.00	n.a.	2263.569	2150.567	50.73	n.a.	BMB*
Total:			4559.957	4239.474	100.00	0.000	



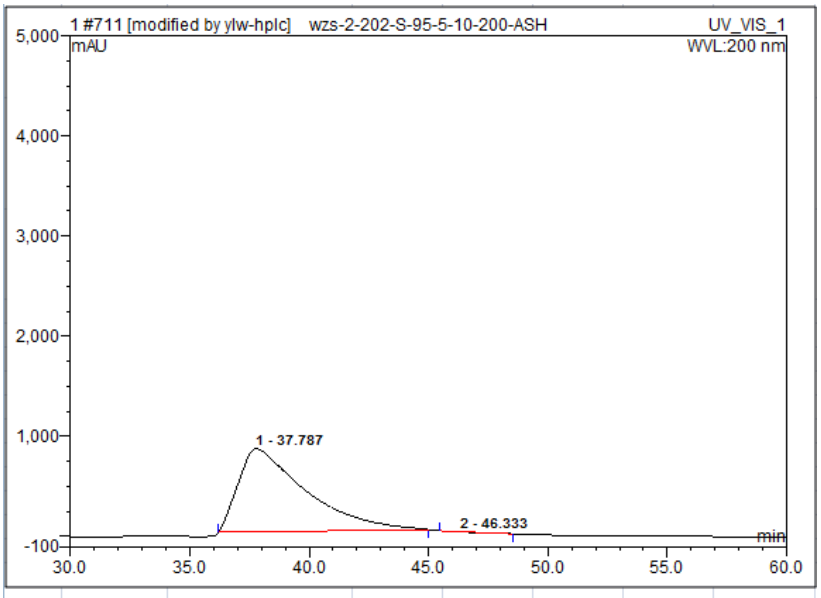
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	16.27	n.a.	90.988	32.162	1.36	n.a.	BMB*
2	17.81	n.a.	2318.559	2328.943	98.64	n.a.	BMB*
Total:			2409.546	2361.105	100.00	0.000	

Compound **1m**



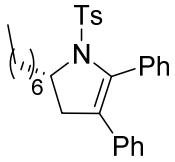


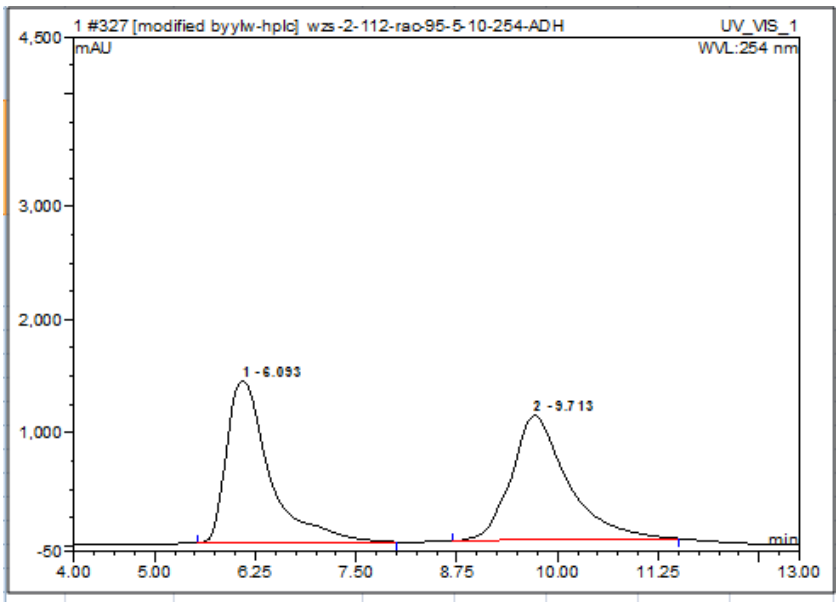
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	39.15	n.a.	181.671	469.273	49.95	n.a.	BMB*
2	47.84	n.a.	128.997	470.297	50.05	n.a.	BMB*
Total:			310.668	939.570	100.00	0.000	



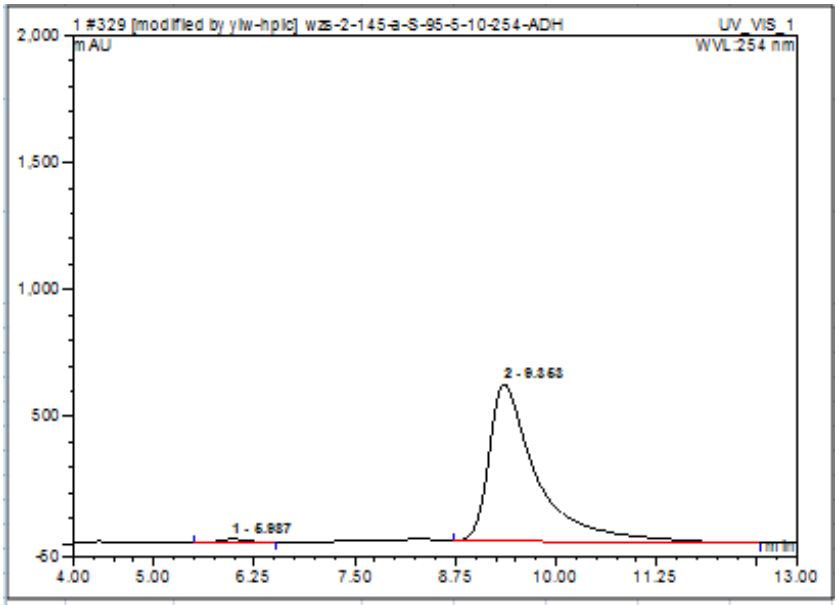
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	37.79	n.a.	828.018	2694.030	99.80	n.a.	BMB*
2	46.33	n.a.	4.249	5.383	0.20	n.a.	BMB*
Total:			832.267	2699.413	100.00	0.000	

Compound **3a**



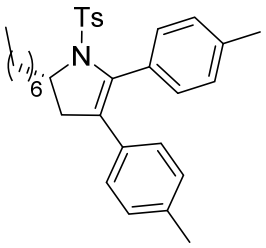


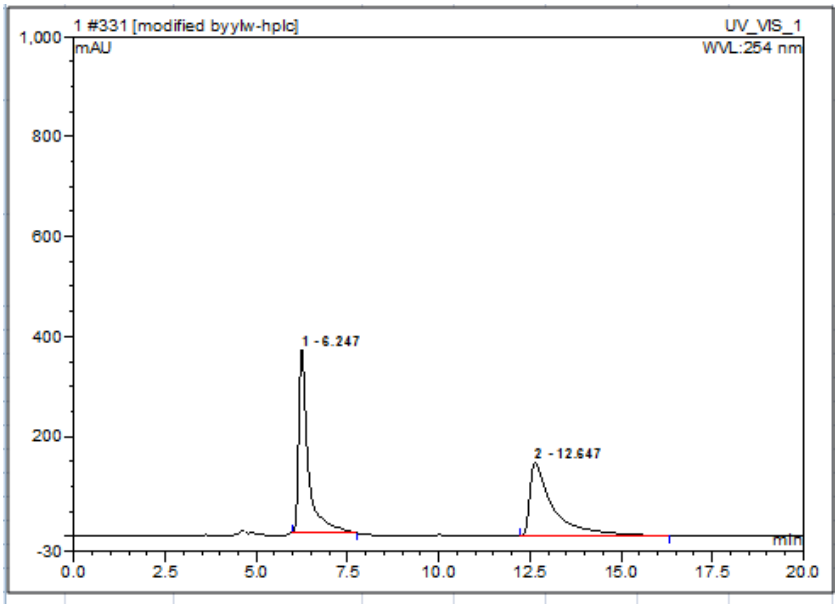
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.09	n.a.	1421.824	884.398	49.87	n.a.	BMB*
2	9.71	n.a.	1098.940	889.134	50.13	n.a.	BMB*
Total:			2520.764	1773.531	100.00	0.000	



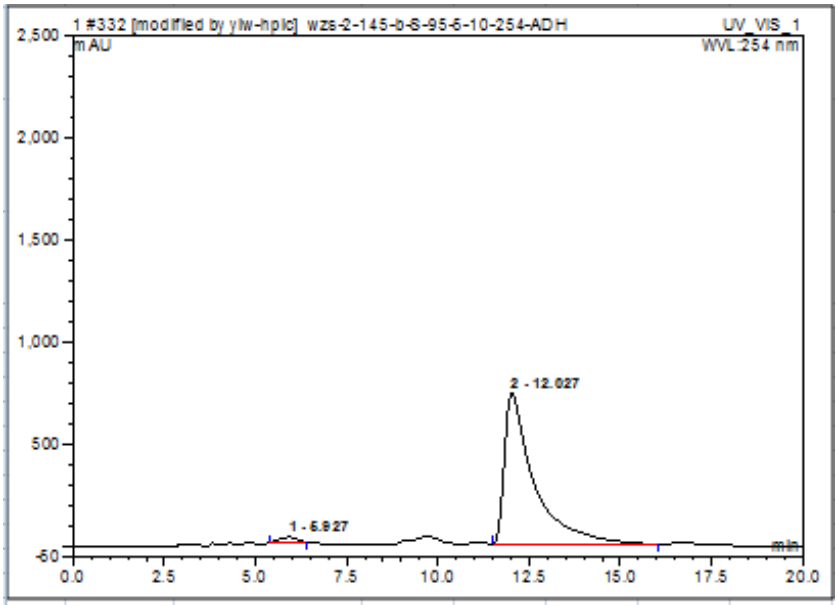
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	5.99	n.a.	11.935	4.269	0.99	n.a.	BMB*
2	9.35	n.a.	618.400	425.356	99.01	n.a.	BMB*
Total:			630.336	429.625	100.00	0.000	

Compound **3b**



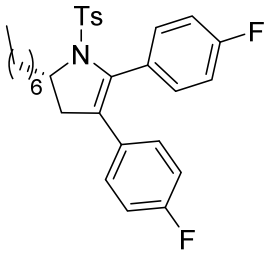


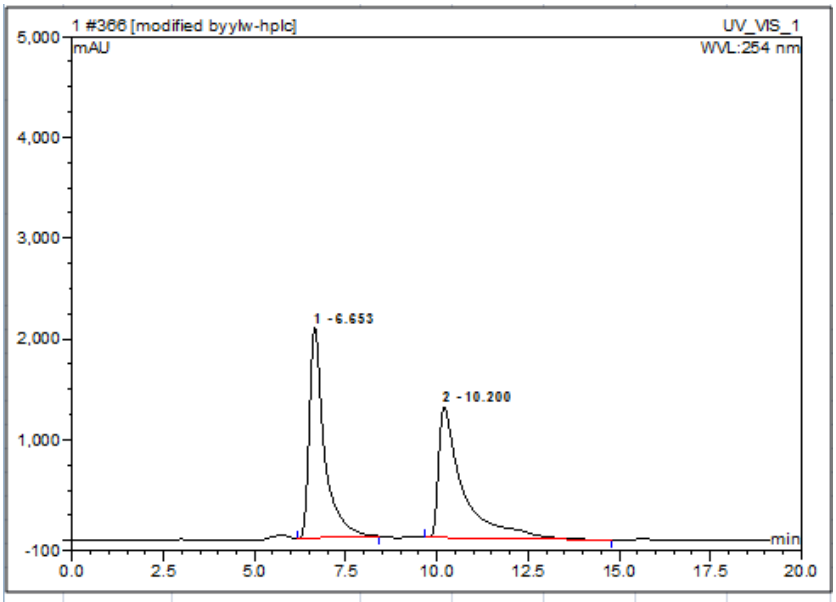
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.25	n.a.	365.041	109.258	50.76	n.a.	BMB*
2	12.65	n.a.	144.434	105.968	49.24	n.a.	BMB*
Total:			509.475	215.226	100.00	0.000	



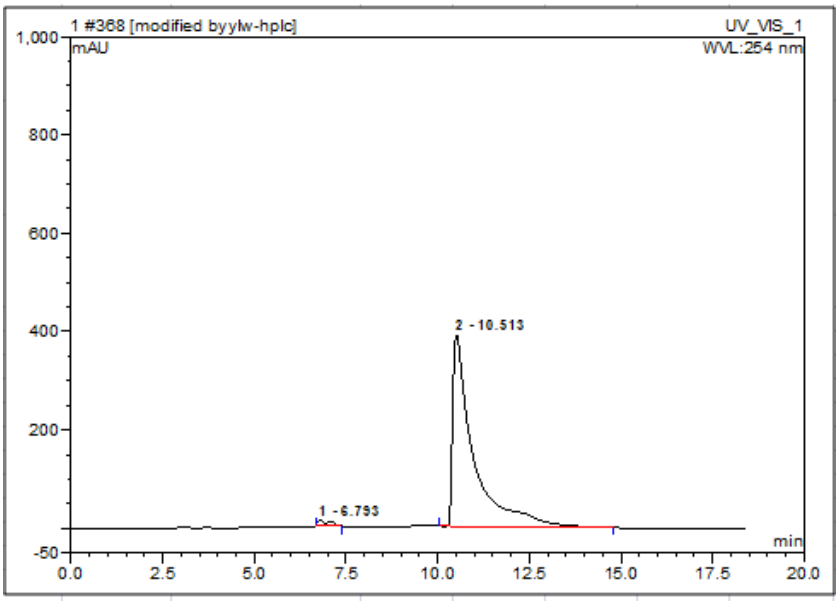
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	5.93	n.a.	25.299	14.257	2.03	n.a.	BMB*
2	12.03	n.a.	736.556	688.720	97.97	n.a.	BMB*
Total:			761.855	702.977	100.00	0.000	

Compound **3c**



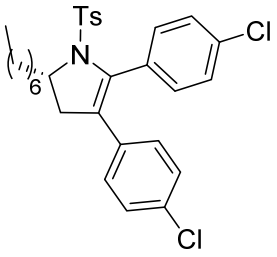


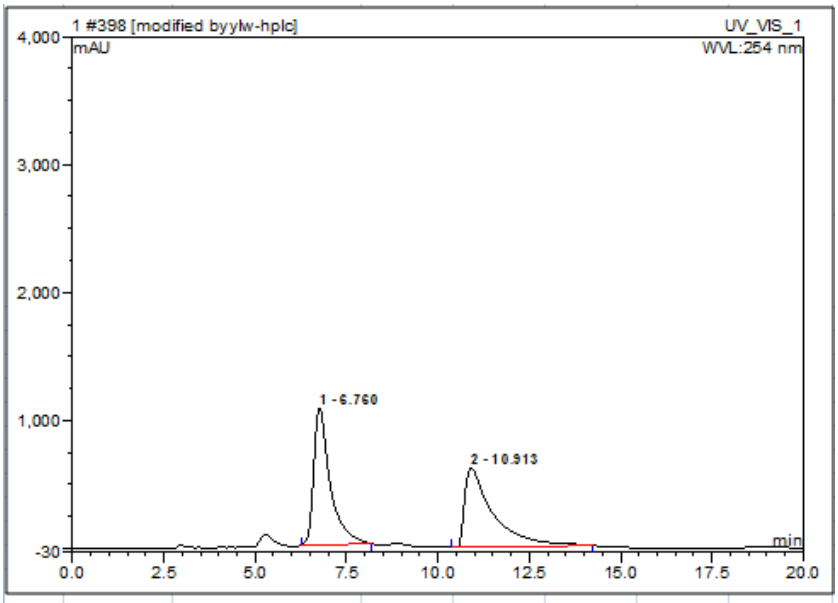
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.65	n.a.	2079.171	993.639	49.82	n.a.	BMB*
2	10.20	n.a.	1301.053	1000.963	50.18	n.a.	BMB*
Total:			3380.224	1994.602	100.00	0.000	



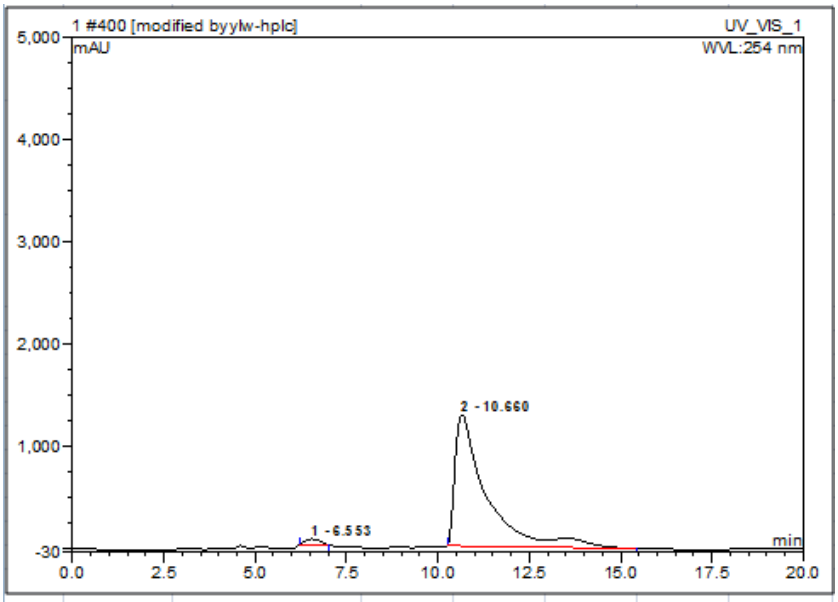
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.79	n.a.	10.785	4.032	1.55	n.a.	BMB*
2	10.51	n.a.	389.498	255.930	98.45	n.a.	BMB*
Total:			400.283	259.962	100.00	0.000	

Compound **3d**



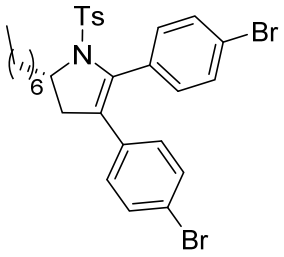


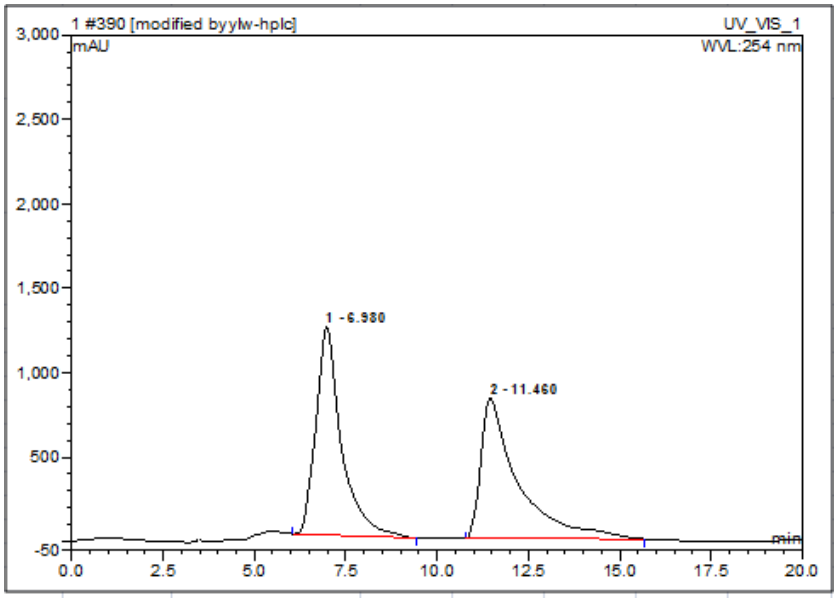
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	6.76	n.a.	1064.902	557.400	50.05	n.a.	BMB*
2	10.91	n.a.	620.212	556.253	49.95	n.a.	BMB*
Total:			1685.113	1113.652	100.00	0.000	



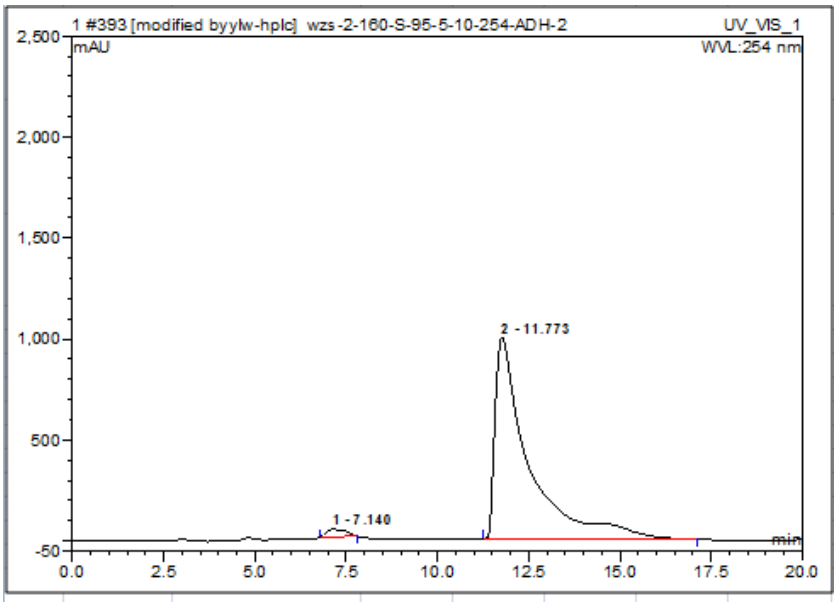
No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%	n.a.	
1	6.55	n.a.	56.427	27.303	2.10	n.a.	BMB*
2	10.66	n.a.	1281.182	1275.876	97.90	n.a.	BMB*
Total:			1337.610	1303.179	100.00	0.000	

Compound **3e**



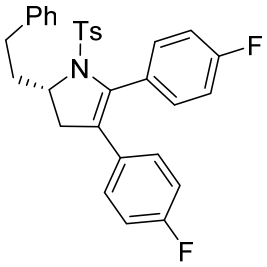


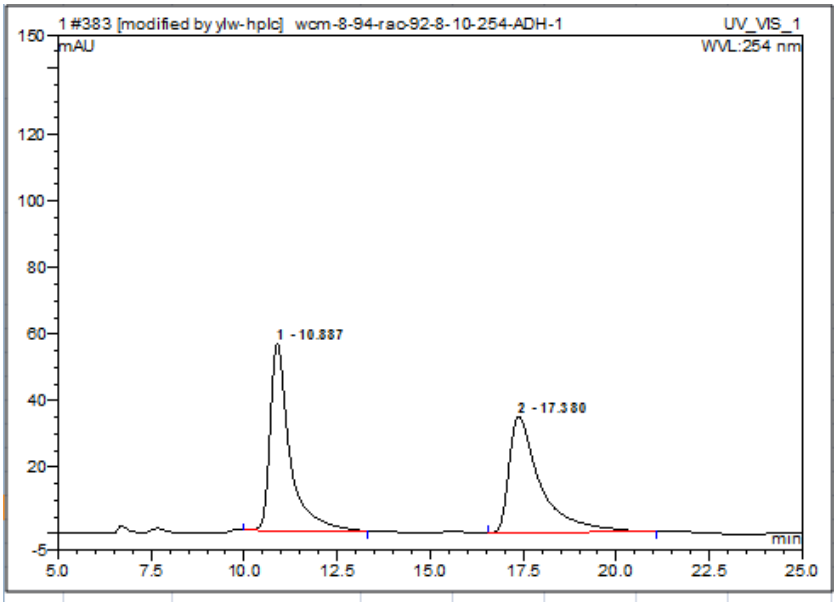
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	6.98	n.a.	1230.407	997.049	50.48	n.a.	BMB*
2	11.46	n.a.	828.699	978.158	49.52	n.a.	BMB*
Total:			2059.106	1975.206	100.00	0.000	



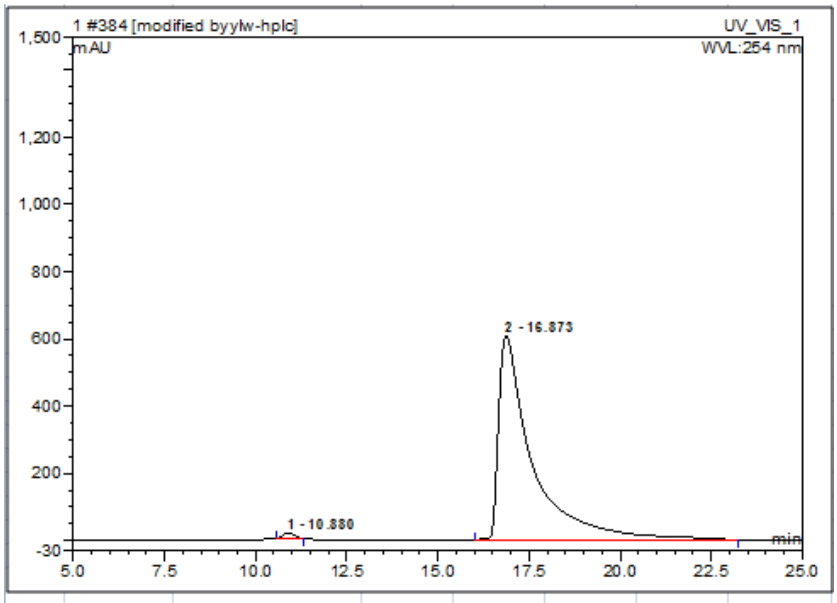
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.14	n.a.	36.686	22.683	2.09	n.a.	BMB*
2	11.77	n.a.	994.711	1064.043	97.91	n.a.	BMB*
Total:			1031.397	1086.726	100.00	0.000	

Compound **3g**



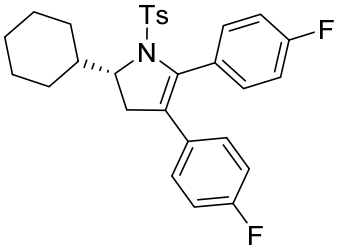


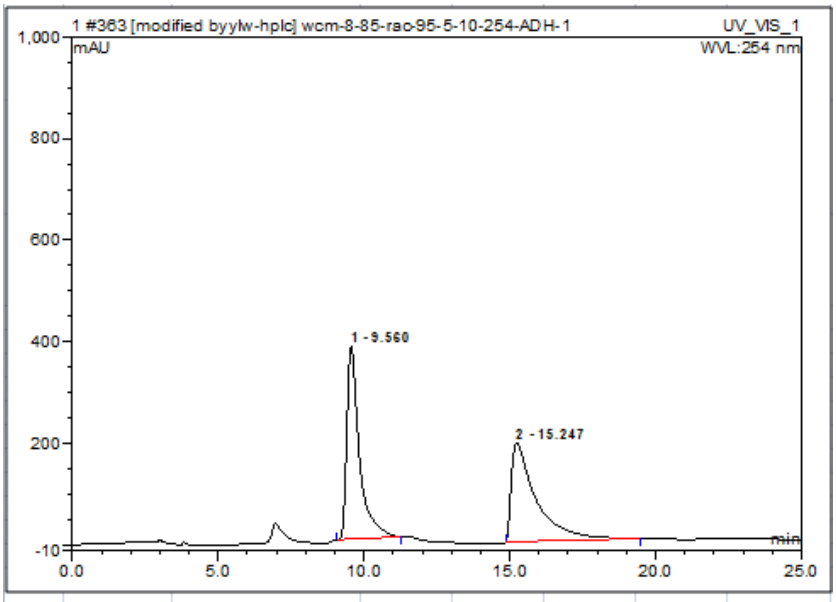
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.89	n.a.	56.358	34.393	50.23	n.a.	BMB*
2	17.38	n.a.	34.971	34.072	49.77	n.a.	BMB*
Total:			91.329	68.465	100.00	0.000	



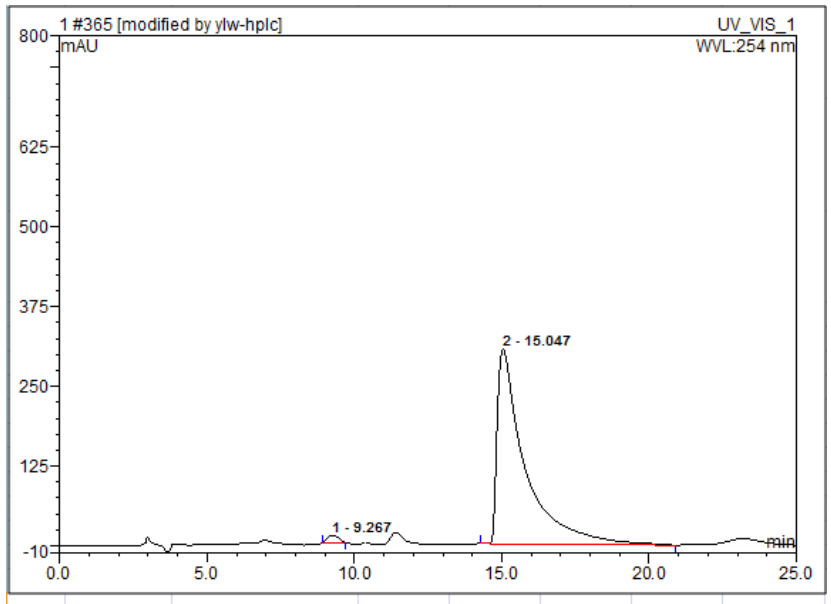
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.88	n.a.	16.901	6.164	0.94	n.a.	BMB*
2	16.87	n.a.	605.245	647.003	99.06	n.a.	BMB*
Total:			622.146	653.167	100.00	0.000	

Compound **3h**



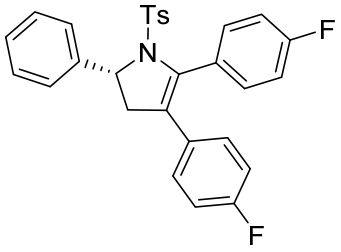


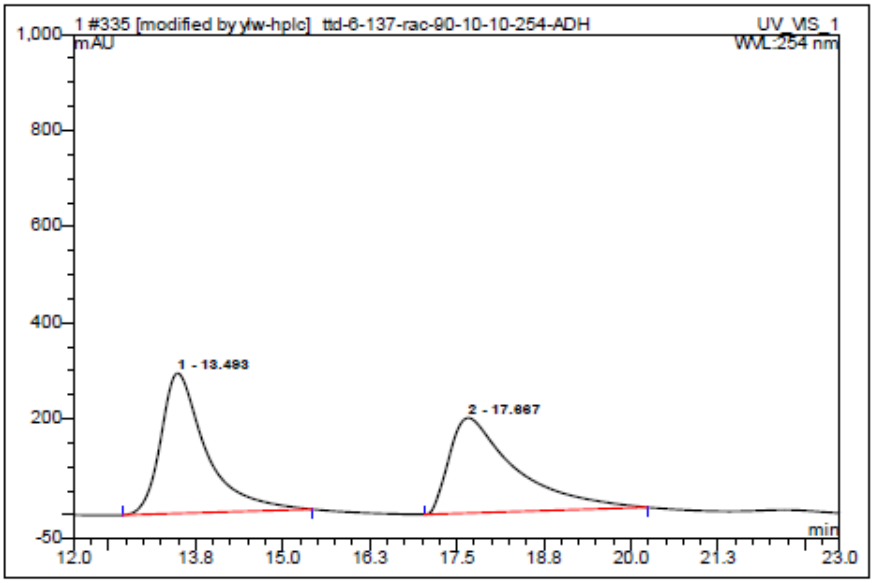
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.56	n.a.	378.675	190.252	49.92	n.a.	BMB*
2	15.25	n.a.	193.288	190.862	50.08	n.a.	BMB*
Total:			571.963	381.114	100.00	0.000	



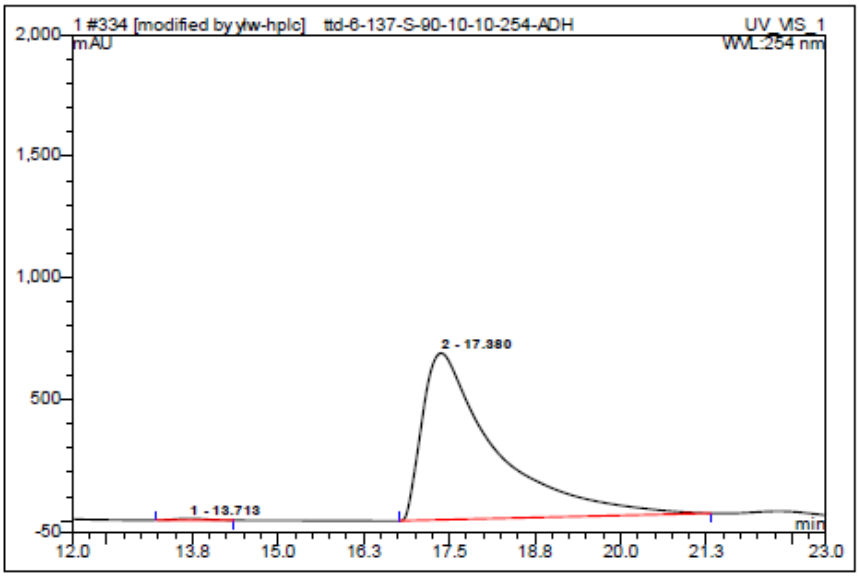
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	9.27	n.a.	11.726	5.035	1.48	n.a.	BMB*
2	15.05	n.a.	305.184	334.299	98.52	n.a.	BMB*
Total:			316.911	339.334	100.00	0.000	

Compound **3i**



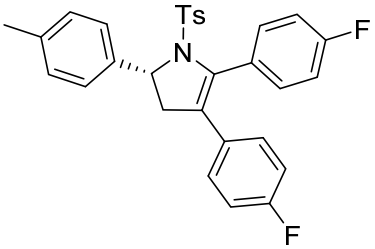


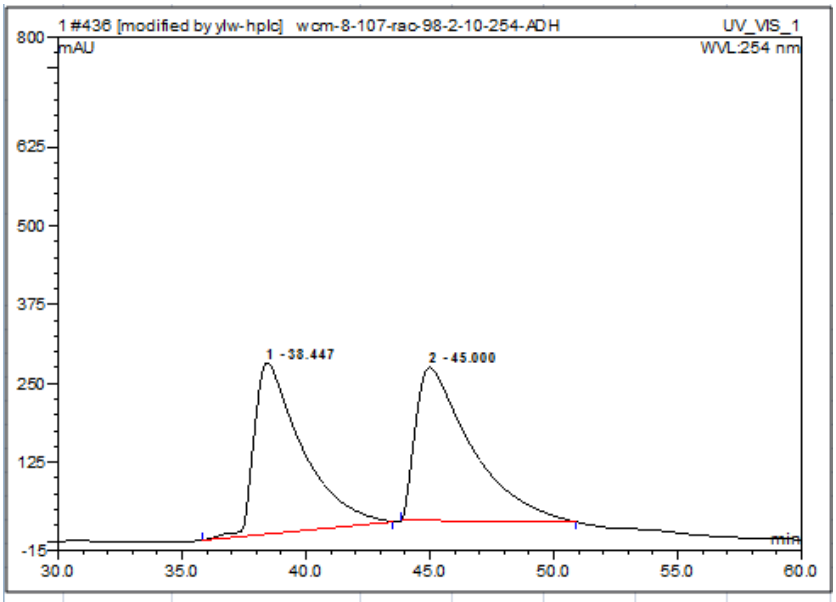
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.49	n.a.	291.573	219.524	50.26	n.a.	BMB*
2	17.67	n.a.	197.815	217.256	49.74	n.a.	BMB*
Total:			489.388	436.780	100.00	0.000	



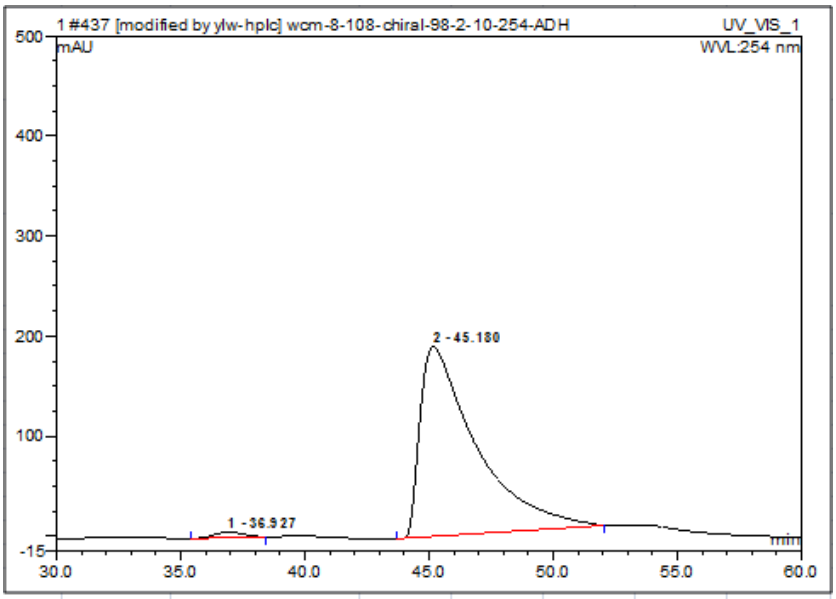
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.71	n.a.	6.323	3.330	0.39	n.a.	BMB*
2	17.38	n.a.	685.767	844.133	99.61	n.a.	BMB*
Total:			692.090	847.463	100.00	0.000	

Compound **3j**



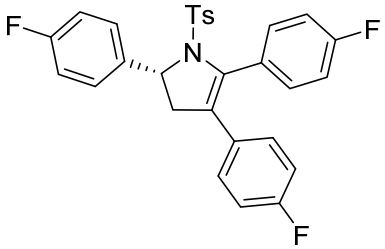


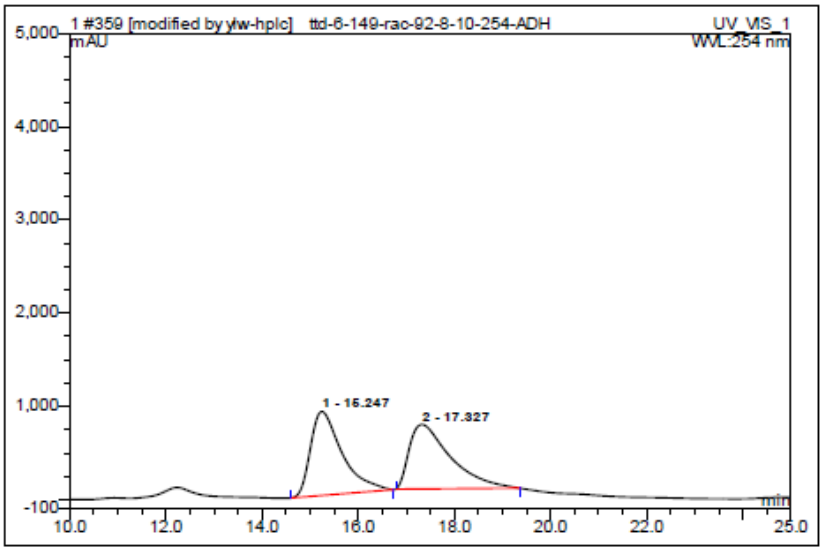
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	38.45	n.a.	271.275	611.373	49.10	n.a.	BMB*
2	45.00	n.a.	242.595	633.837	50.90	n.a.	BMB*
Total:			513.870	1245.210	100.00	0.000	



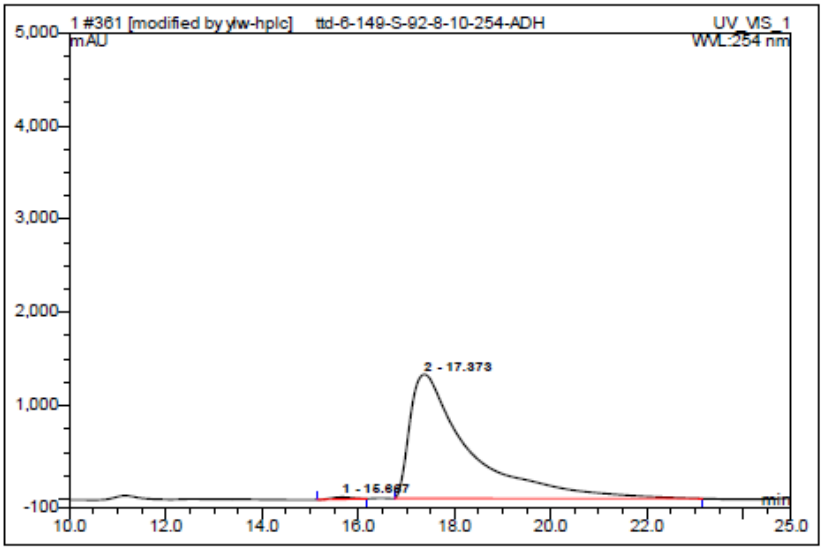
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	36.93	n.a.	5.735	7.695	1.53	n.a.	BMB*
2	45.18	n.a.	189.544	496.884	98.47	n.a.	BMB*
Total:			195.279	504.579	100.00	0.000	

Compound **3k**



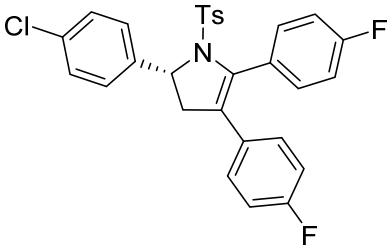


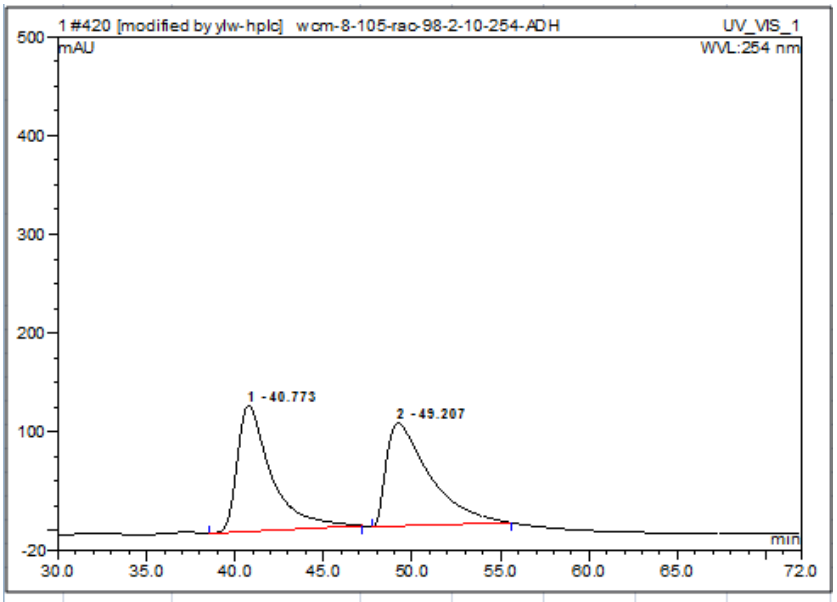
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.25	n.a.	899.443	685.287	49.89	n.a.	BMB*
2	17.33	n.a.	689.461	688.227	50.11	n.a.	BMB*
Total:			1588.904	1373.514	100.00	0.000	



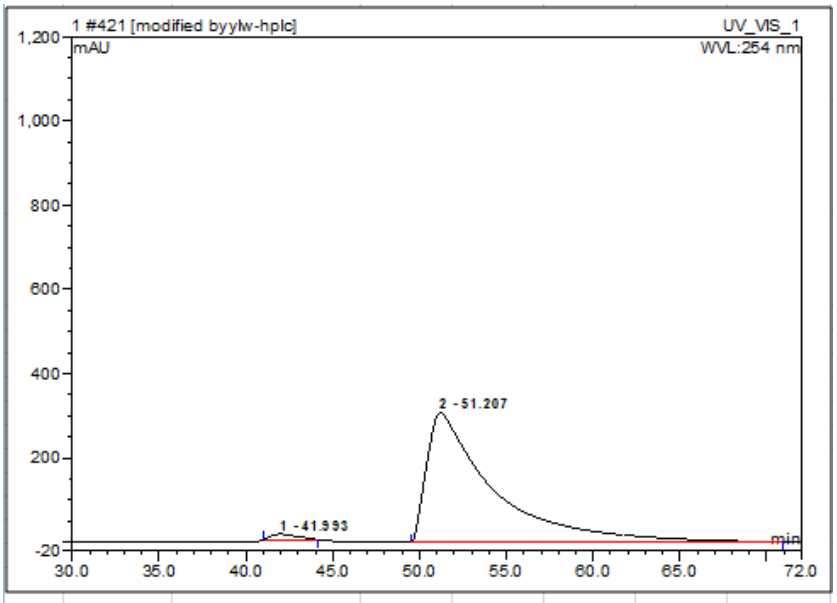
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.67	n.a.	21.965	10.992	0.58	n.a.	BMB*
2	17.37	n.a.	1328.609	1894.812	99.42	n.a.	BMB*
Total:			1350.574	1905.805	100.00	0.000	

Compound **3l**



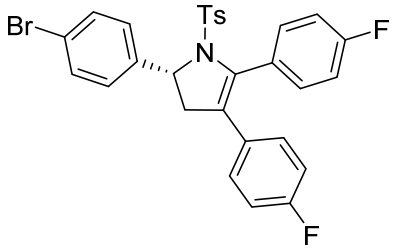


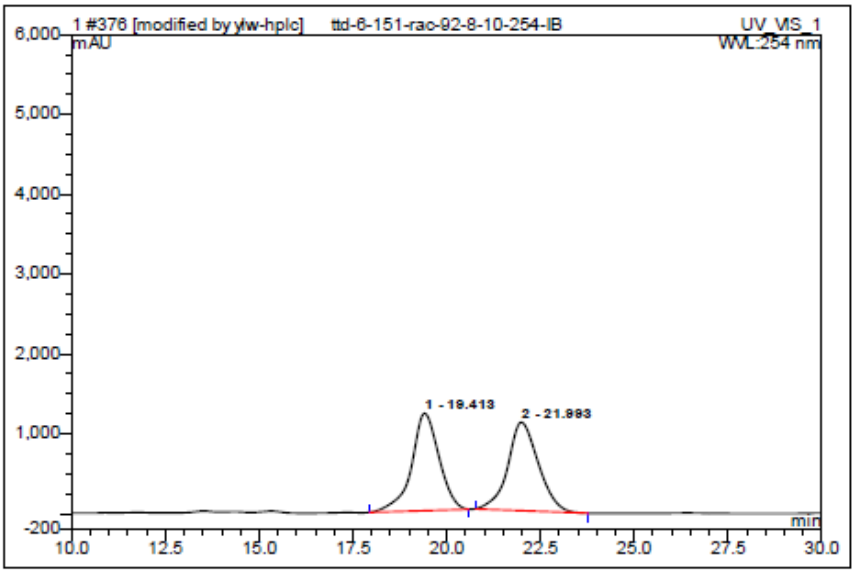
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	40.77	n.a.	127.530	284.541	49.10	n.a.	BMB*
2	49.21	n.a.	103.584	294.938	50.90	n.a.	BMB*
Total:			231.115	579.478	100.00	0.000	



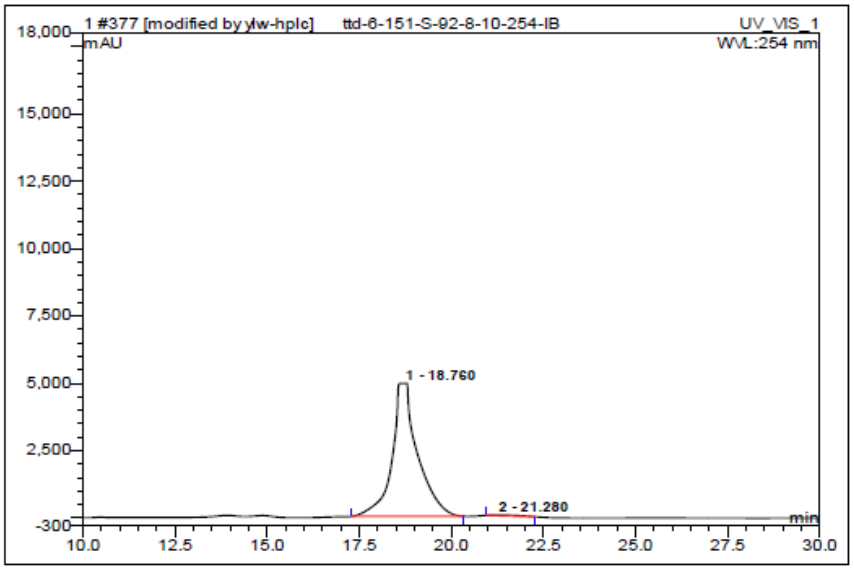
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	41.99	n.a.	12.893	21.706	1.59	n.a.	BMB*
2	51.21	n.a.	304.941	1342.279	98.41	n.a.	BMB*
Total:			317.834	1363.985	100.00	0.000	

Compound **3m**



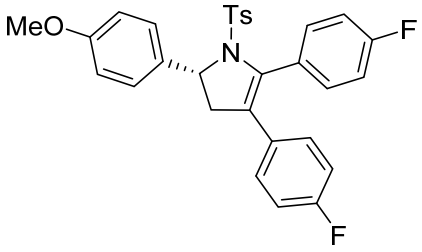


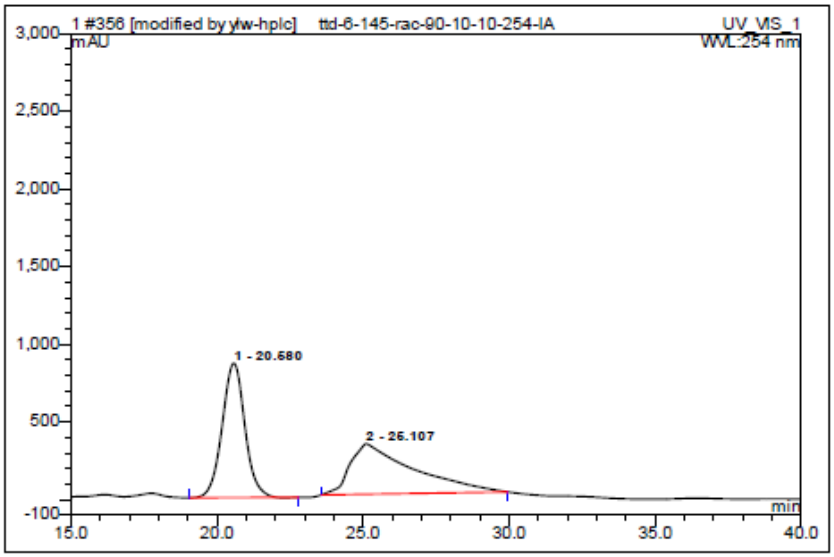
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.41	n.a.	1218.695	1039.725	49.78	n.a.	BMB*
2	21.99	n.a.	1106.164	1049.100	50.22	n.a.	BMB*
Total:			2324.859	2088.825	100.00	0.000	



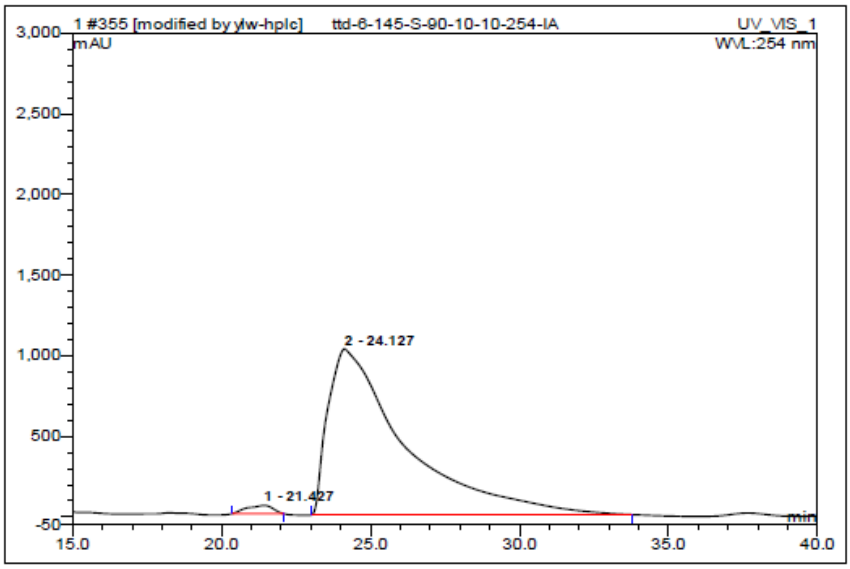
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.76	n.a.	4938.862	4005.392	99.24	n.a.	BMB*
2	21.28	n.a.	33.788	30.668	0.76	n.a.	BMB*
Total:			4972.650	4036.060	100.00	0.000	

Compound **3n**



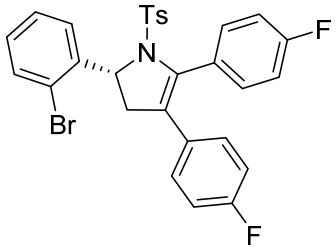


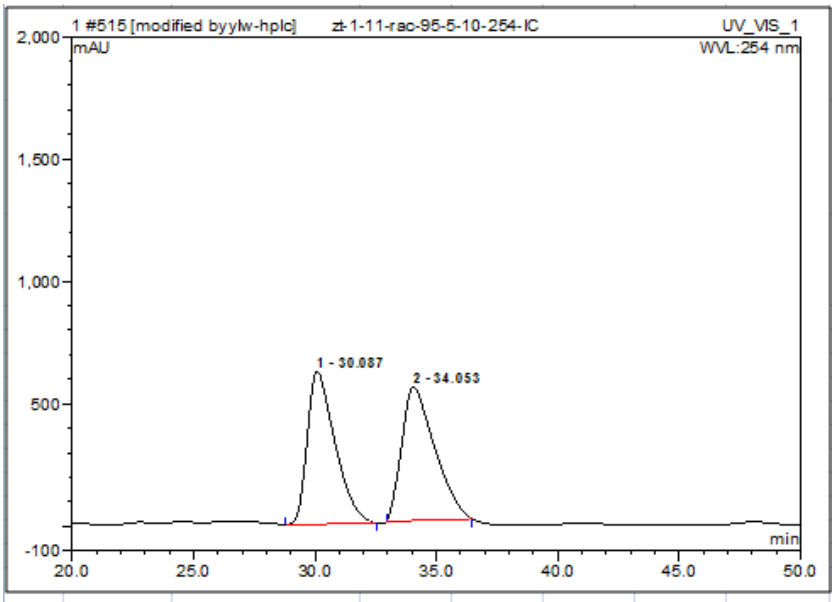
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	20.58	n.a.	865.039	779.374	49.13	n.a.	BMB*
2	25.11	n.a.	324.793	806.967	50.87	n.a.	BMB*
Total:			1189.832	1586.342	100.00	0.000	



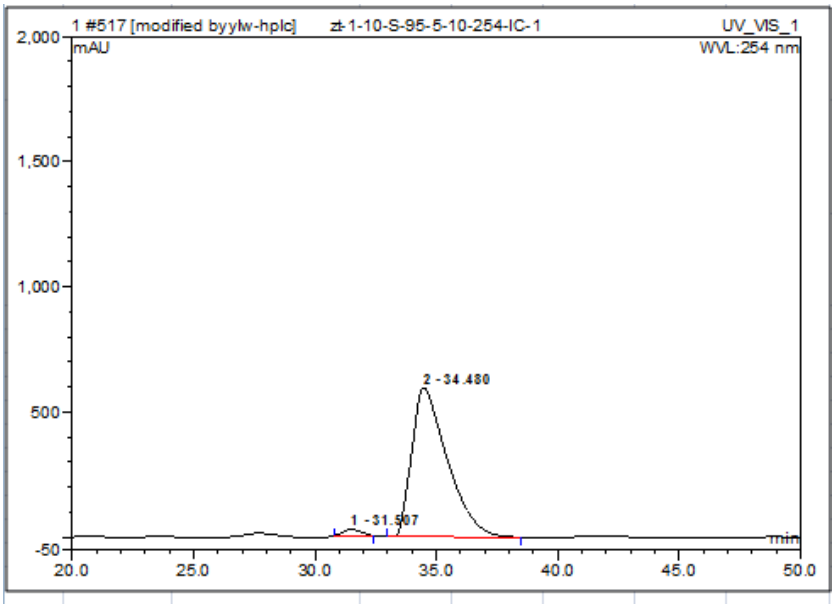
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	21.43	n.a.	51.316	51.875	1.66	n.a.	BMB*
2	24.13	n.a.	1029.079	3076.415	98.34	n.a.	BMB*
Total:			1080.395	3128.289	100.00	0.000	

Compound **3o**



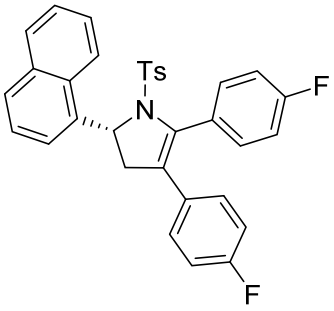


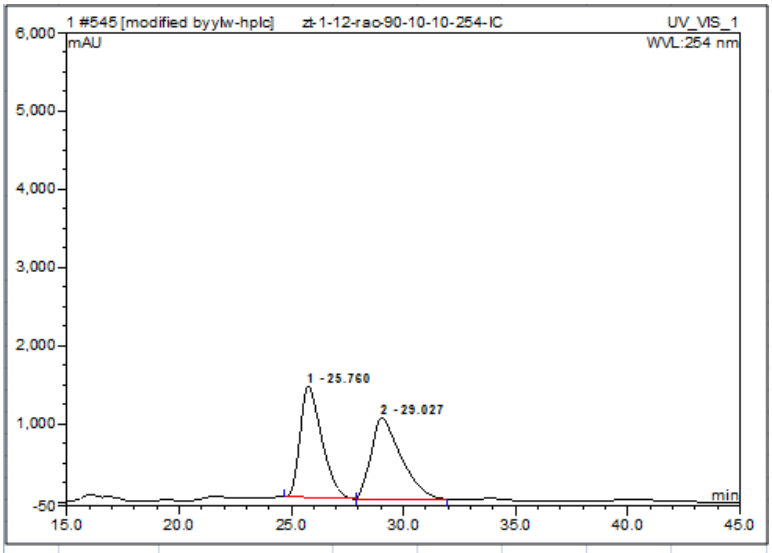
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	30.09	n.a.	625.126	827.872	49.08	n.a.	BMB*
2	34.05	n.a.	545.979	859.037	50.92	n.a.	BMB*
Total:			1171.106	1686.909	100.00	0.000	



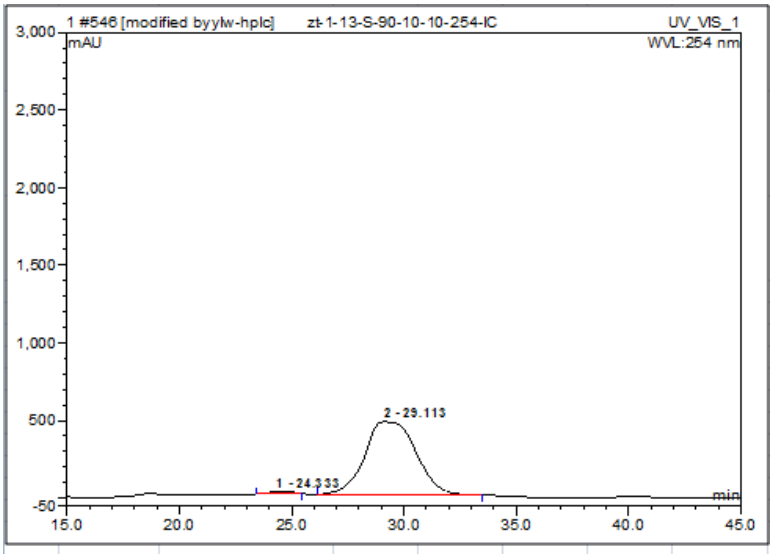
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	31.51	n.a.	24.667	21.934	2.13	n.a.	BMB*
2	34.48	n.a.	595.754	1008.155	97.87	n.a.	BMB*
Total:			620.420	1030.090	100.00	0.000	

Compound **3p**



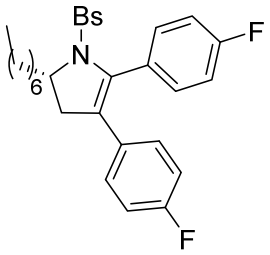


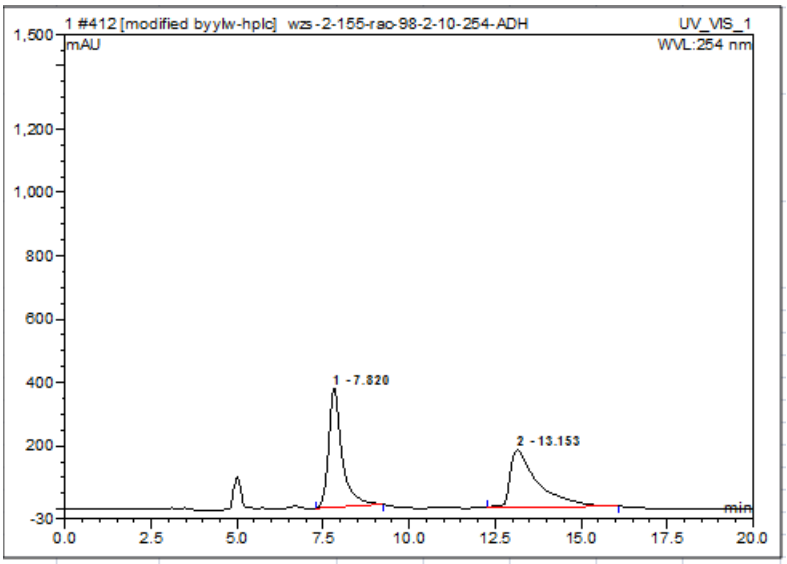
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	25.76	n.a.	1417.779	1580.352	49.61	n.a.	BMb*
2	29.03	n.a.	1037.462	1605.517	50.39	n.a.	bMB*
Total:			2455.241	3185.869	100.00	0.000	



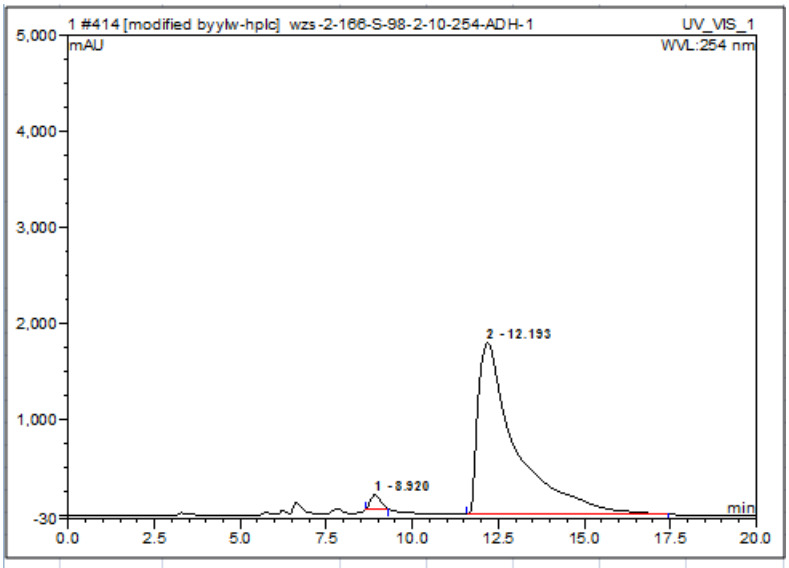
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	24.33	n.a.	11.386	13.704	1.09	n.a.	BMB*
2	29.11	n.a.	470.239	1247.344	98.91	n.a.	BMB*
Total:			481.625	1261.048	100.00	0.000	

Compound **3q**



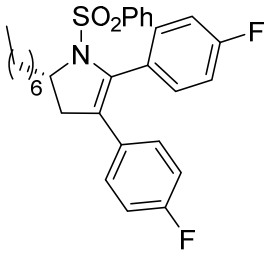


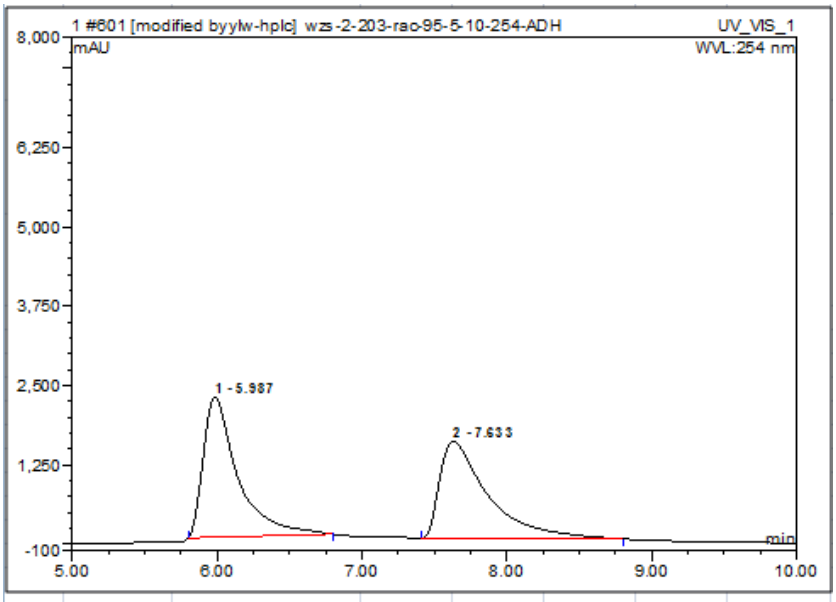
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.82	n.a.	375.555	170.117	50.46	n.a.	BMB*
2	13.15	n.a.	178.905	167.005	49.54	n.a.	BMB*
Total:			554.460	337.122	100.00	0.000	



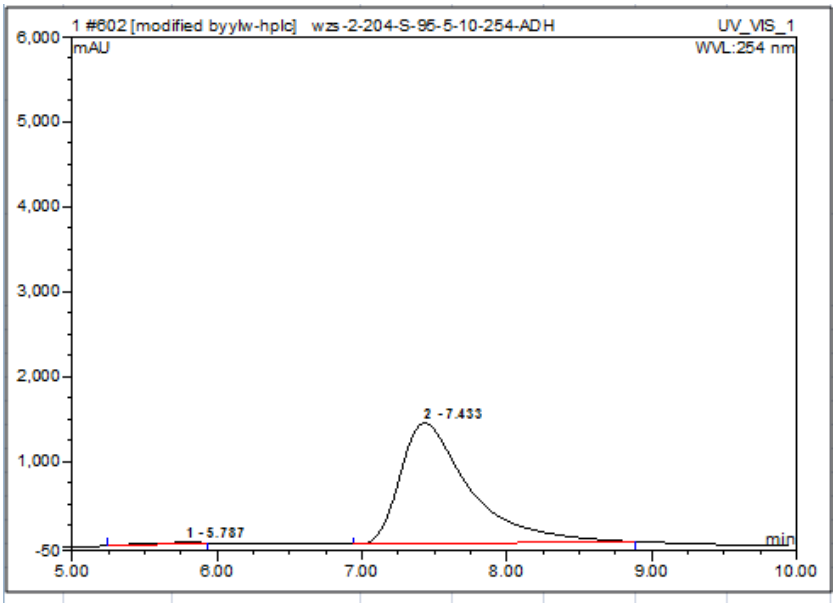
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	8.92	n.a.	150.597	49.059	2.12	n.a.	BMB*
2	12.19	n.a.	1773.490	2262.491	97.88	n.a.	BMB*
Total:			1924.087	2311.550	100.00	0.000	

Compound **3r**

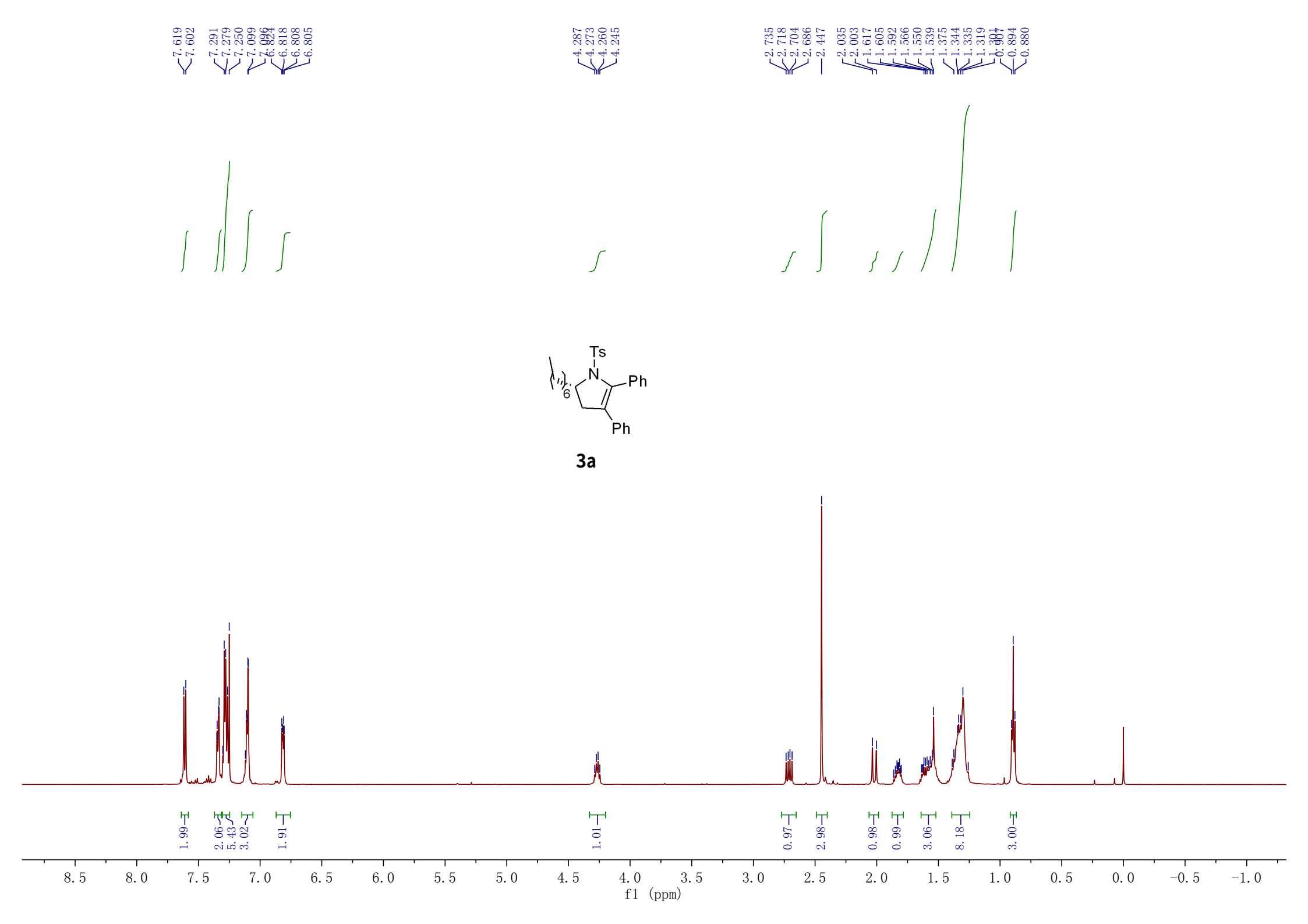




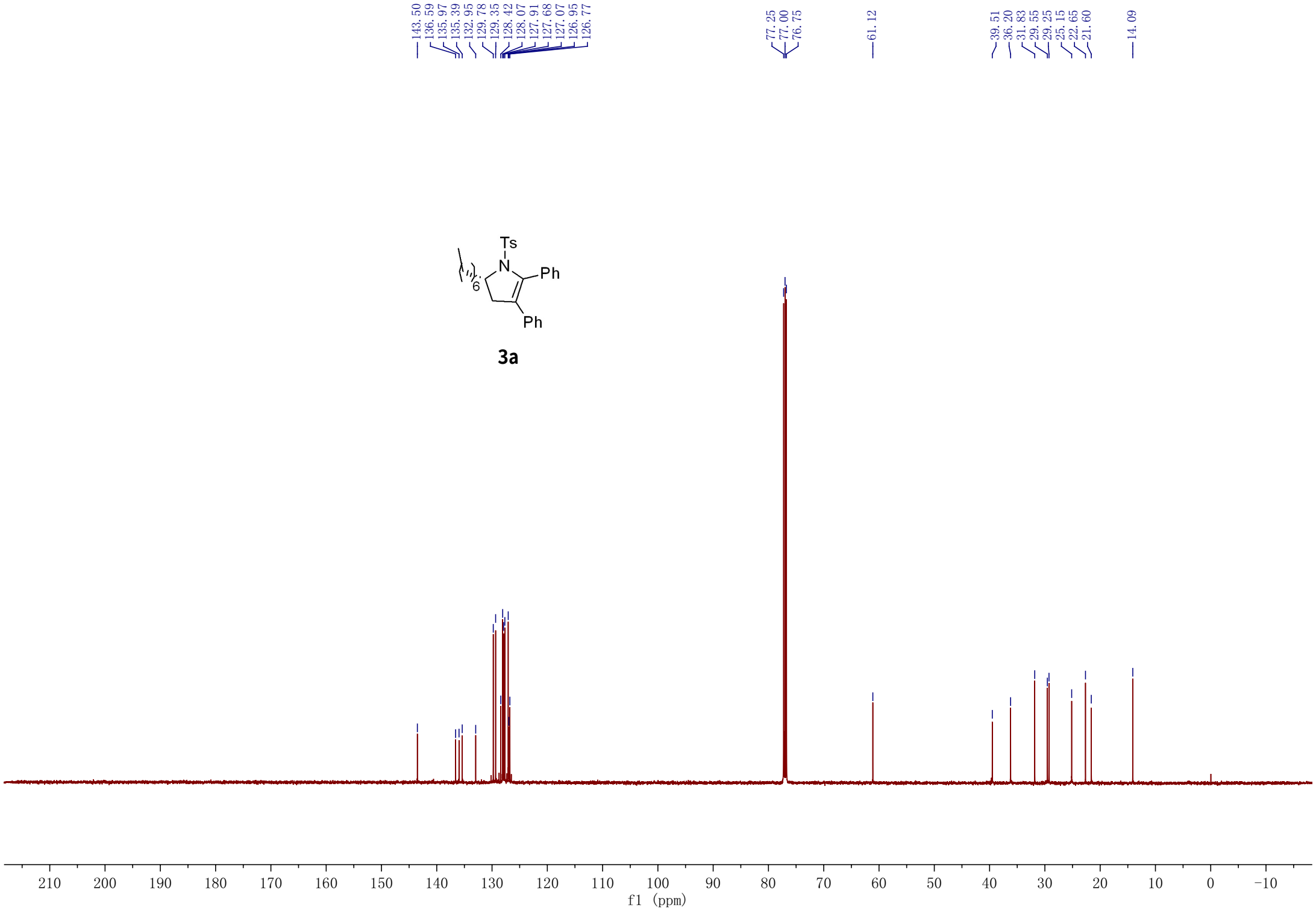
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	5.99	n.a.	2217.194	611.077	50.57	n.a.	BMB*
2	7.63	n.a.	1529.976	597.214	49.43	n.a.	BMB*
Total:			3747.170	1208.291	100.00	0.000	

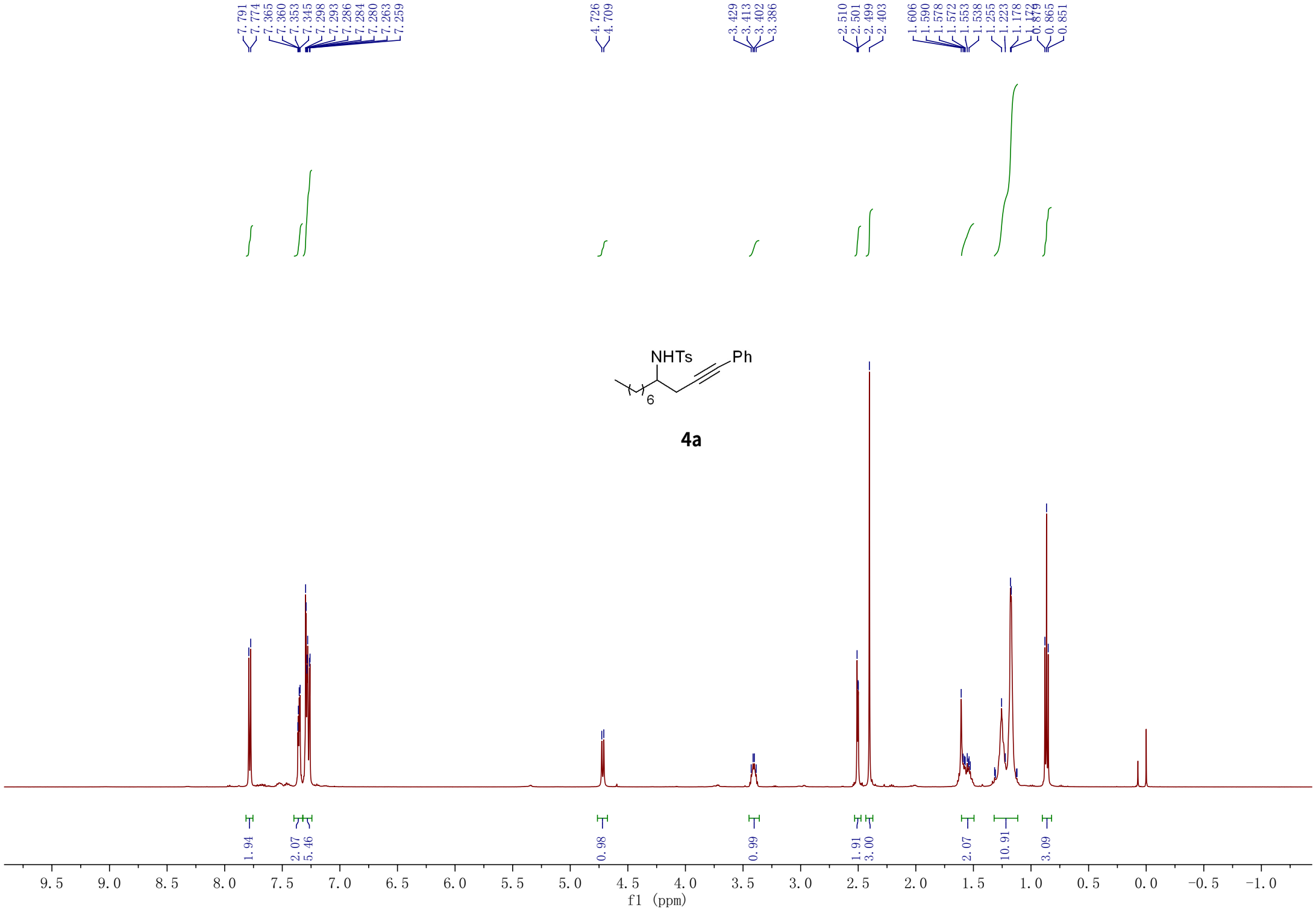


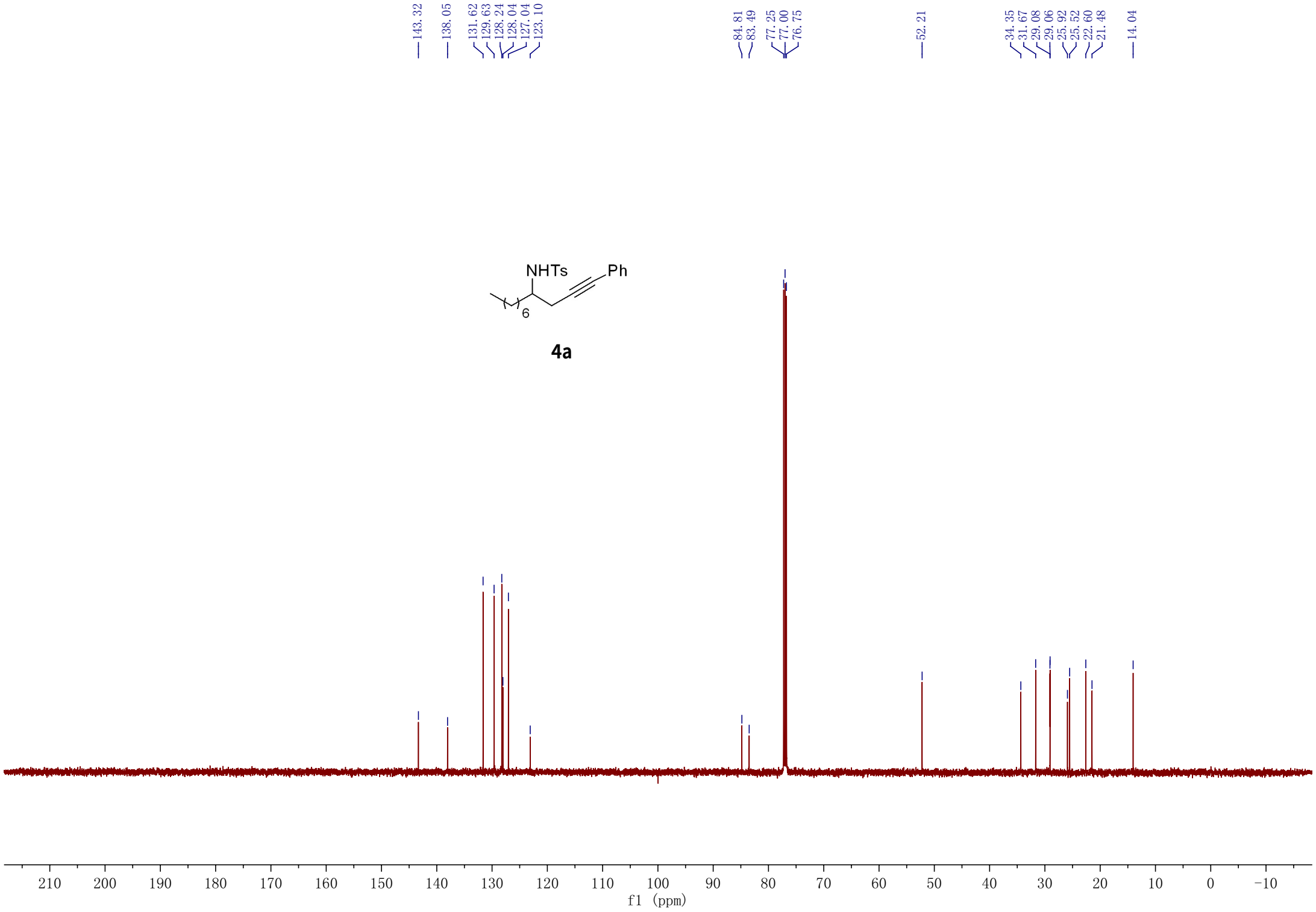
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	5.79	n.a.	17.244	6.454	0.81	n.a.	BMB*
2	7.43	n.a.	1416.285	787.134	99.19	n.a.	BMB*
Total:			1433.529	793.588	100.00	0.000	

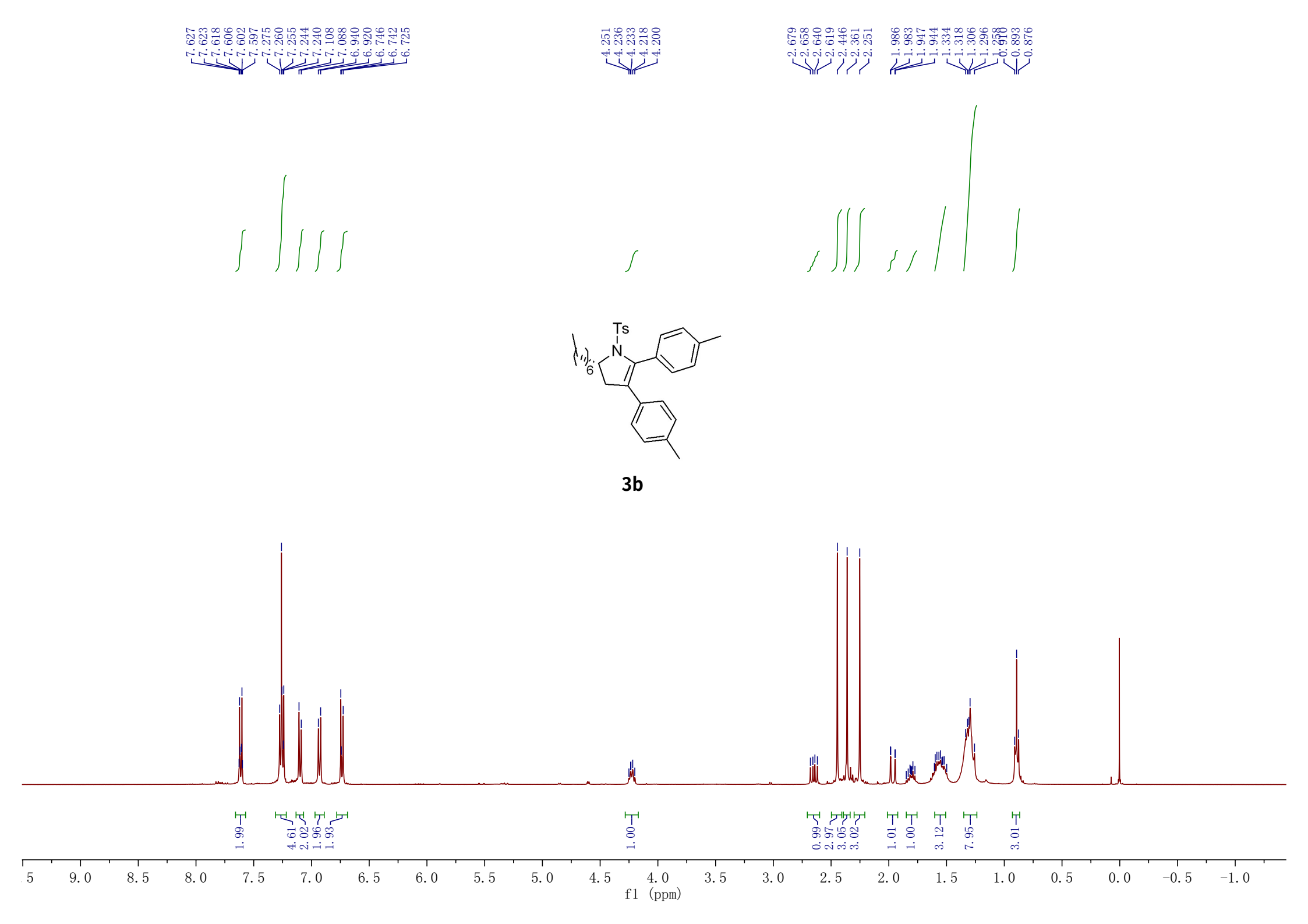

7.619
7.602
7.291
7.279
7.250
7.099
7.096
6.824
6.818
6.808
6.805
4.287
4.273
4.260
4.245
2.735
2.718
2.704
2.686
2.447
2.035
2.003
1.617
1.605
1.592
1.566
1.550
1.539
1.375
1.344
1.335
1.319
0.894
0.880
Ts
N
Ph
Ph
6
1.99
2.06
5.43
3.02
1.91
1.01
0.97
2.98
0.98
0.99
3.06
8.18
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

3a

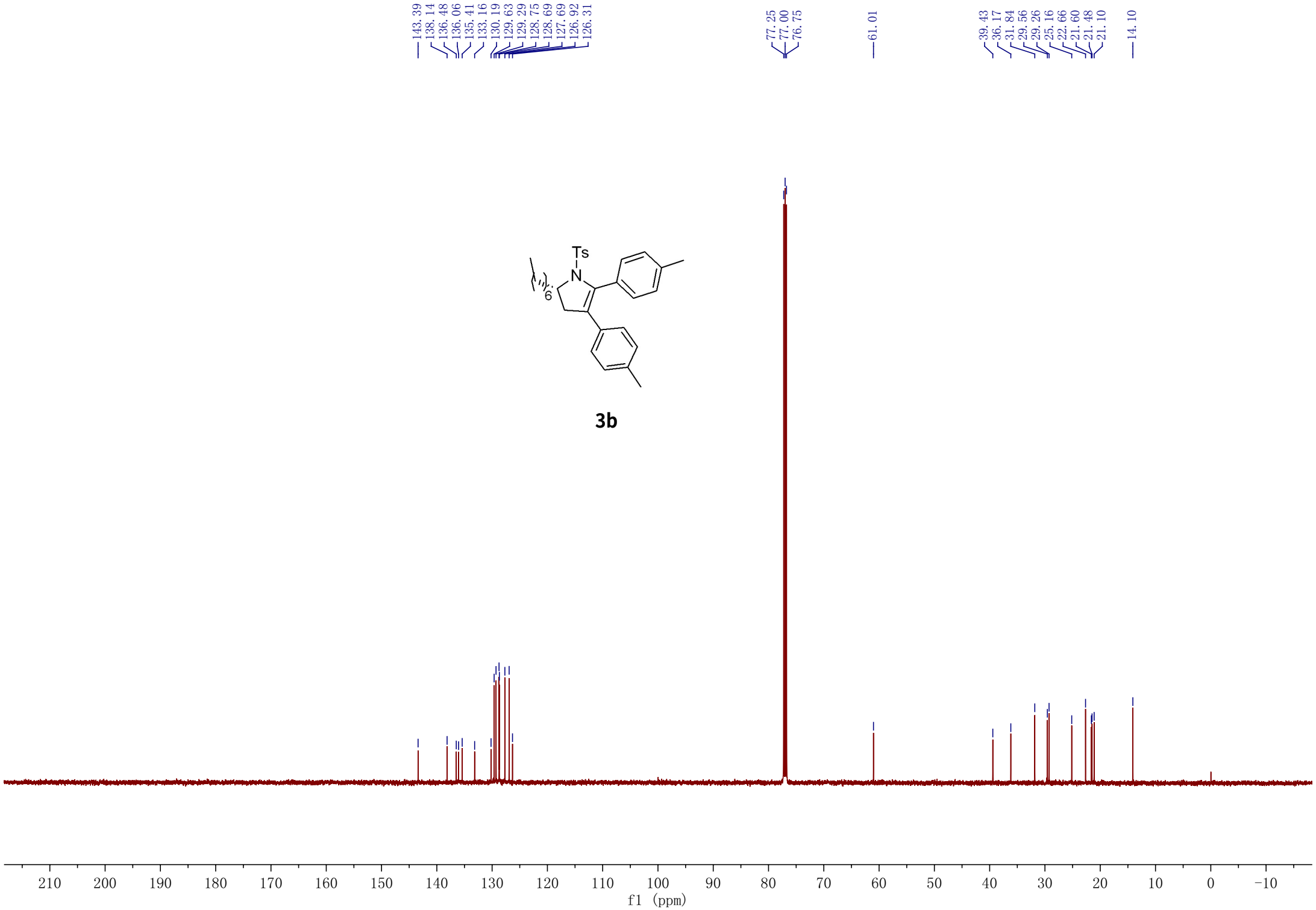

143.50
136.59
135.97
135.39
132.95
129.78
129.35
128.42
128.07
127.91
127.68
127.07
126.95
126.77
77.25
77.00
76.75
61.12
39.51
36.20
31.83
29.55
29.25
25.15
22.65
21.60
14.09
Ts
N
Ph
Ph
6
3a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

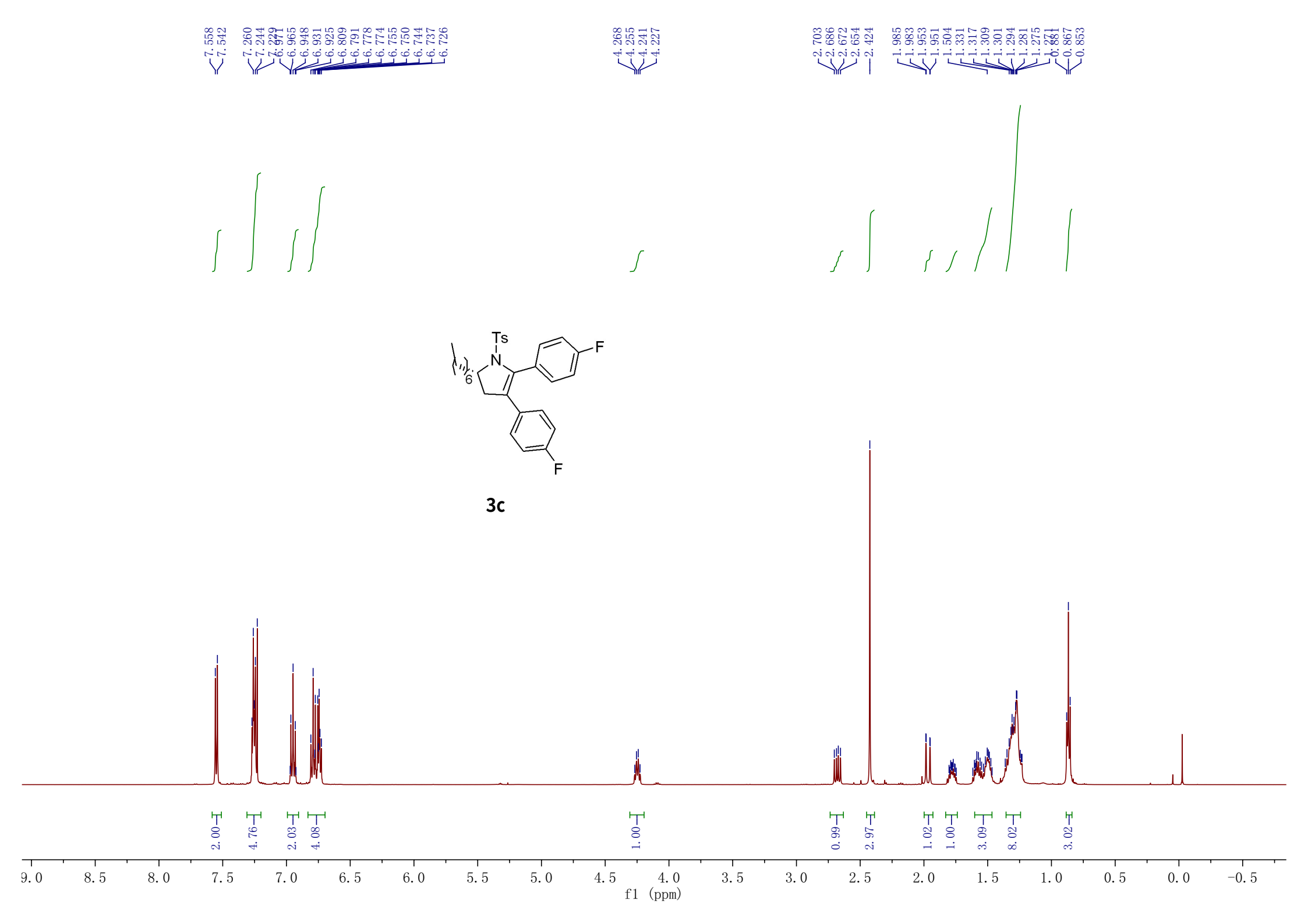

7.791
7.774
7.365
7.360
7.353
7.345
7.298
7.293
7.286
7.284
7.280
7.263
7.259
4.726
4.709
3.429
3.413
3.402
3.386
2.510
2.501
2.499
2.403
1.606
1.590
1.578
1.572
1.553
1.538
1.255
1.223
1.178
0.879
0.865
0.851
NHTs
Ph
6
4a
1.94
2.07
5.46
0.98
0.99
1.91
3.00
2.07
10.91
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

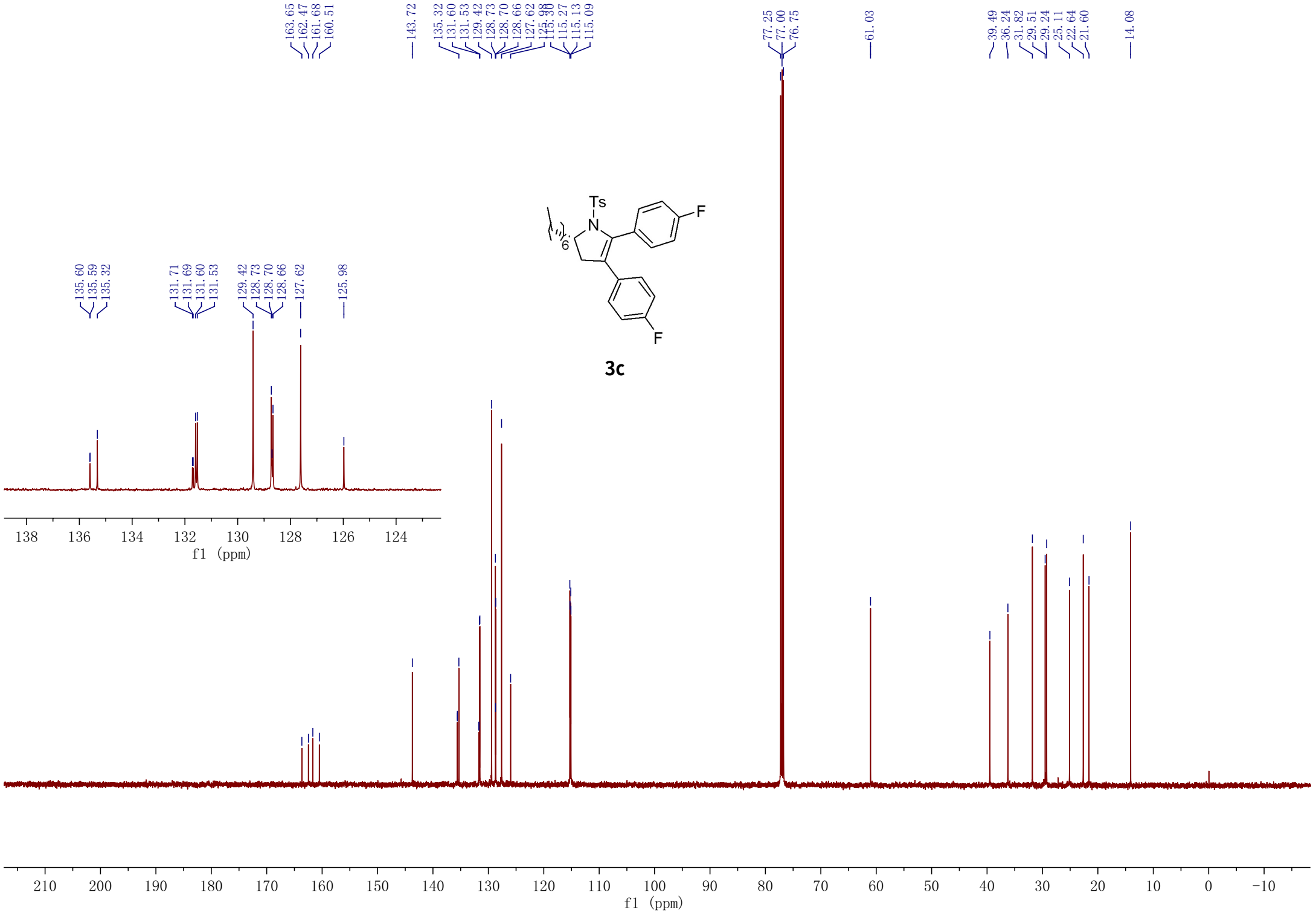

143.32
138.05
131.62
129.63
128.24
128.04
127.04
123.10
84.81
83.49
77.25
77.00
76.75
52.21
34.35
31.67
29.08
29.06
25.92
25.52
22.60
21.48
14.04
NHTs
Ph
6
4a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

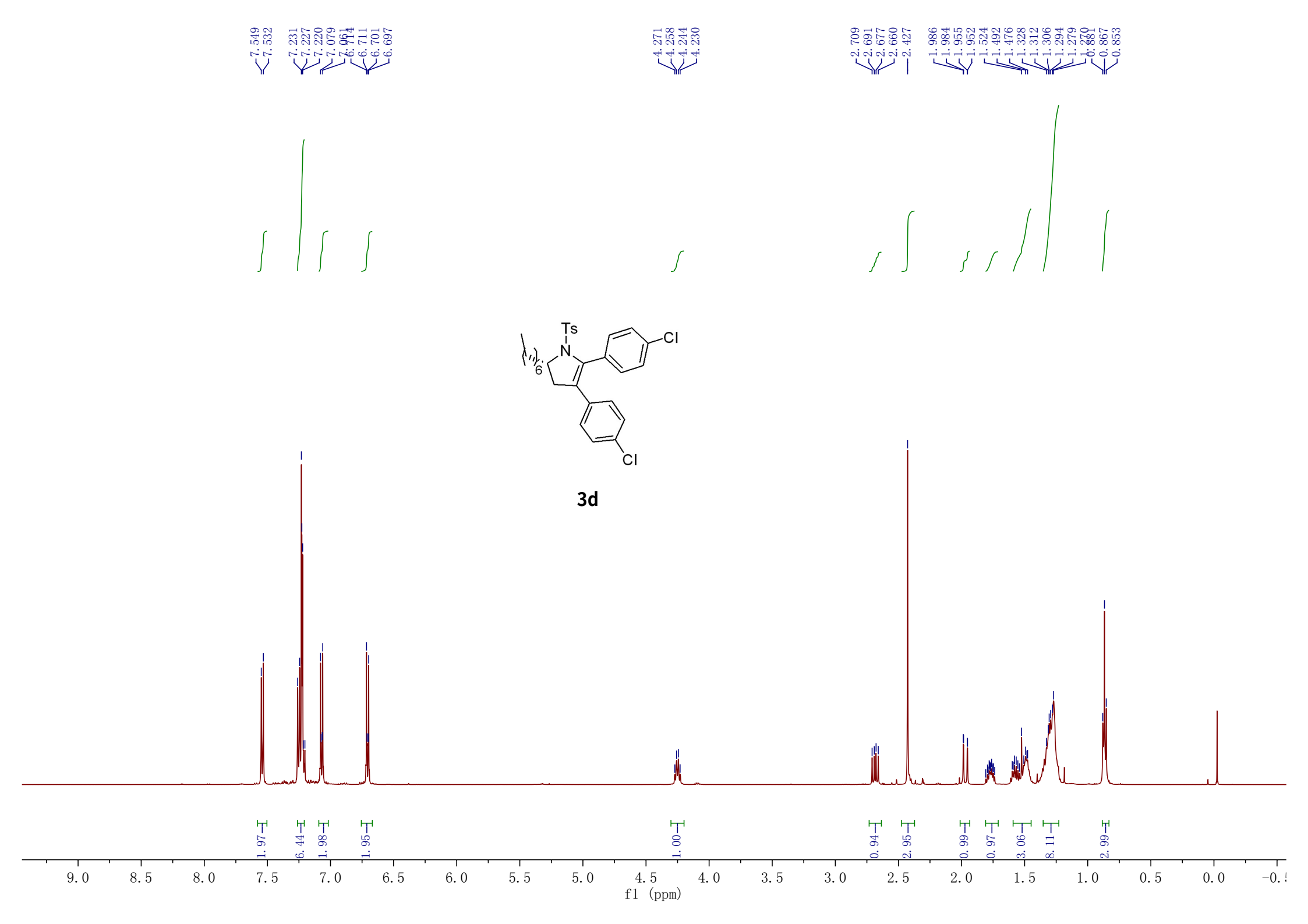

7.627
7.623
7.618
7.606
7.602
7.597
7.275
7.260
7.255
7.244
7.240
7.108
7.088
6.940
6.920
6.746
6.742
6.725
4.251
4.236
4.233
4.218
4.200
2.679
2.658
2.640
2.619
2.446
2.361
2.251
1.986
1.983
1.947
1.944
1.334
1.318
1.306
1.296
0.910
0.893
0.876
Ts
N
6
1.99
4.61
2.02
1.96
1.93
1.00
0.99
2.97
3.05
3.02
1.01
1.00
3.12
7.95
3.01
f1 (ppm)

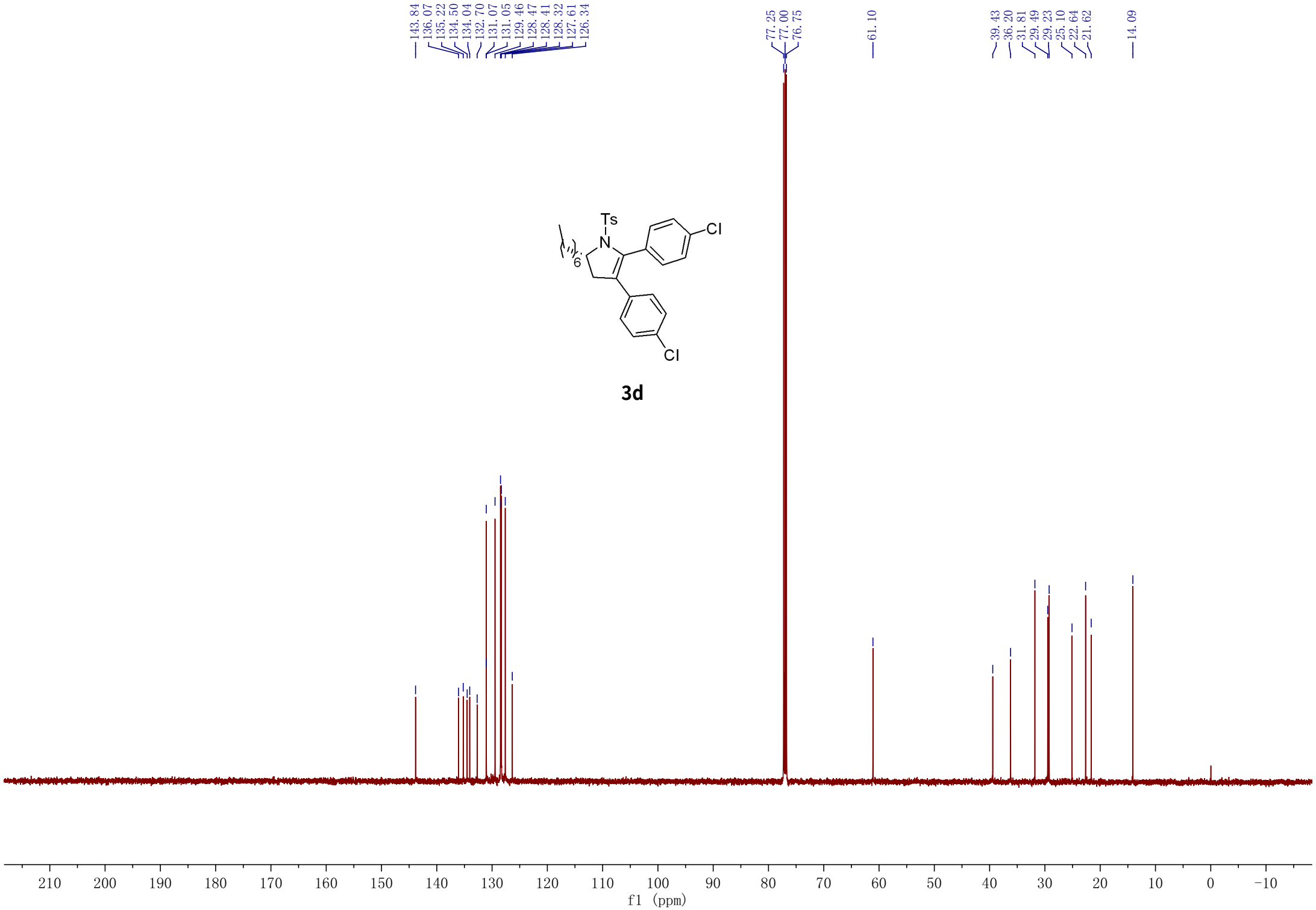
3b

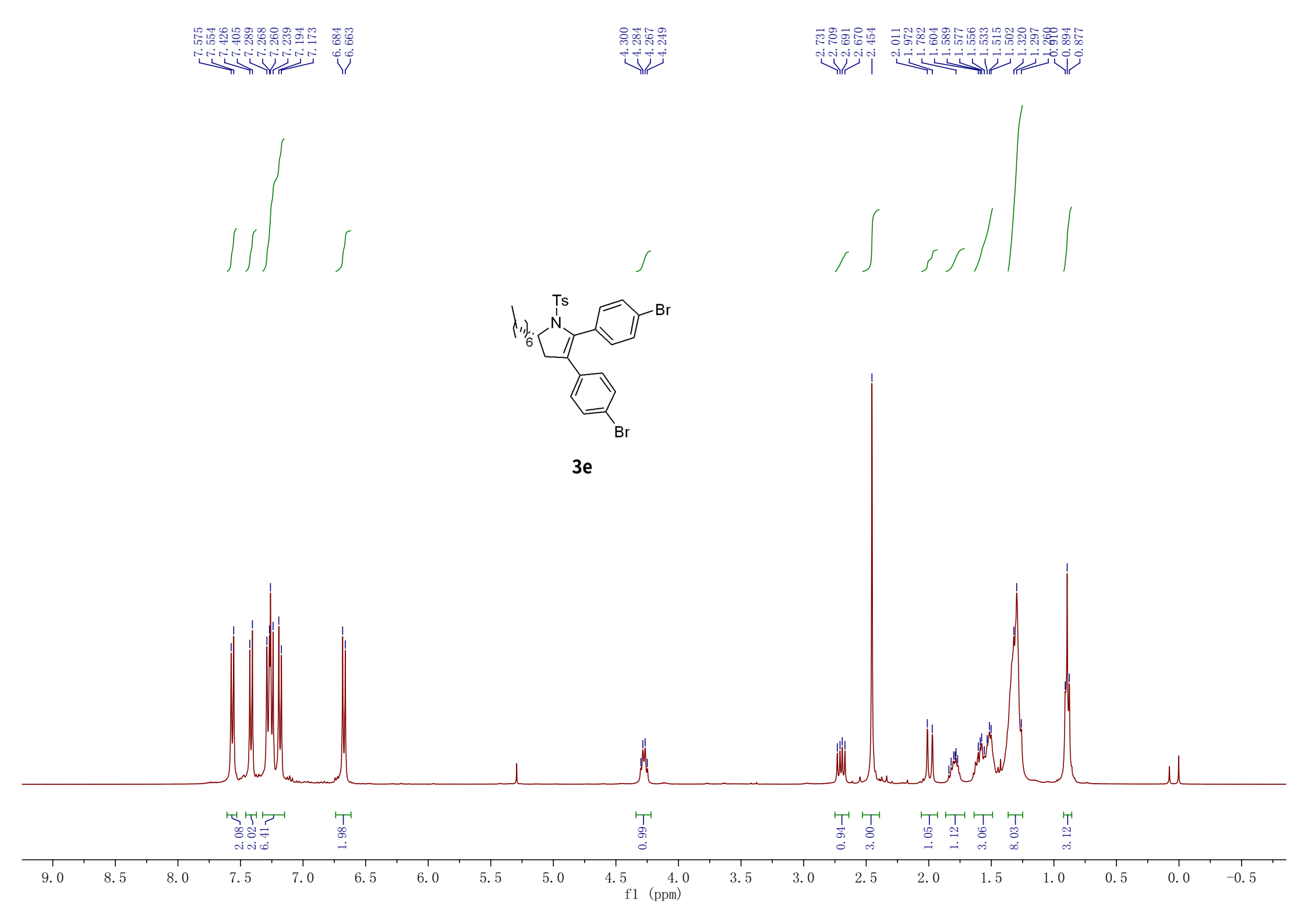

143.39
138.14
136.48
136.06
135.41
133.16
130.19
129.63
129.29
128.75
128.69
127.69
126.92
126.31
77.25
77.00
76.75
61.01
39.43
36.17
31.84
29.56
29.26
25.16
22.66
21.60
21.48
21.10
14.10
Ts
N
6
3b
f1 (ppm)

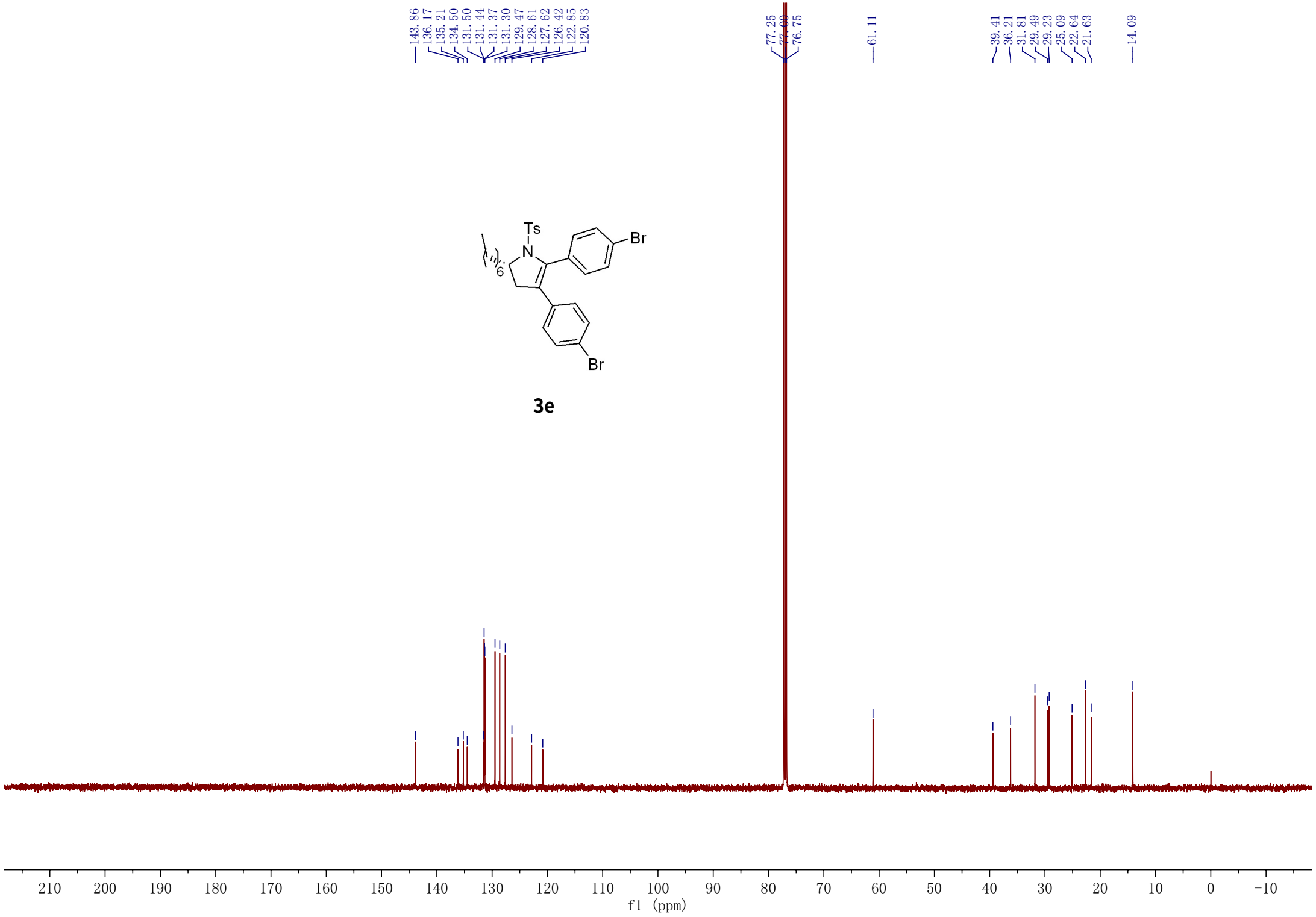

7.558
7.542
7.260
7.244
6.965
6.948
6.931
6.925
6.809
6.791
6.778
6.774
6.755
6.750
6.744
6.737
6.726
4.268
4.255
4.241
4.227
2.703
2.686
2.672
2.654
2.424
1.985
1.983
1.953
1.951
1.504
1.331
1.317
1.309
1.301
1.294
1.281
1.275
0.867
0.853
Ts
N
F
F
6
3c
2.00
4.76
2.03
4.08
1.00
0.99
2.97
1.02
1.00
3.09
8.02
3.02
f1 (ppm)

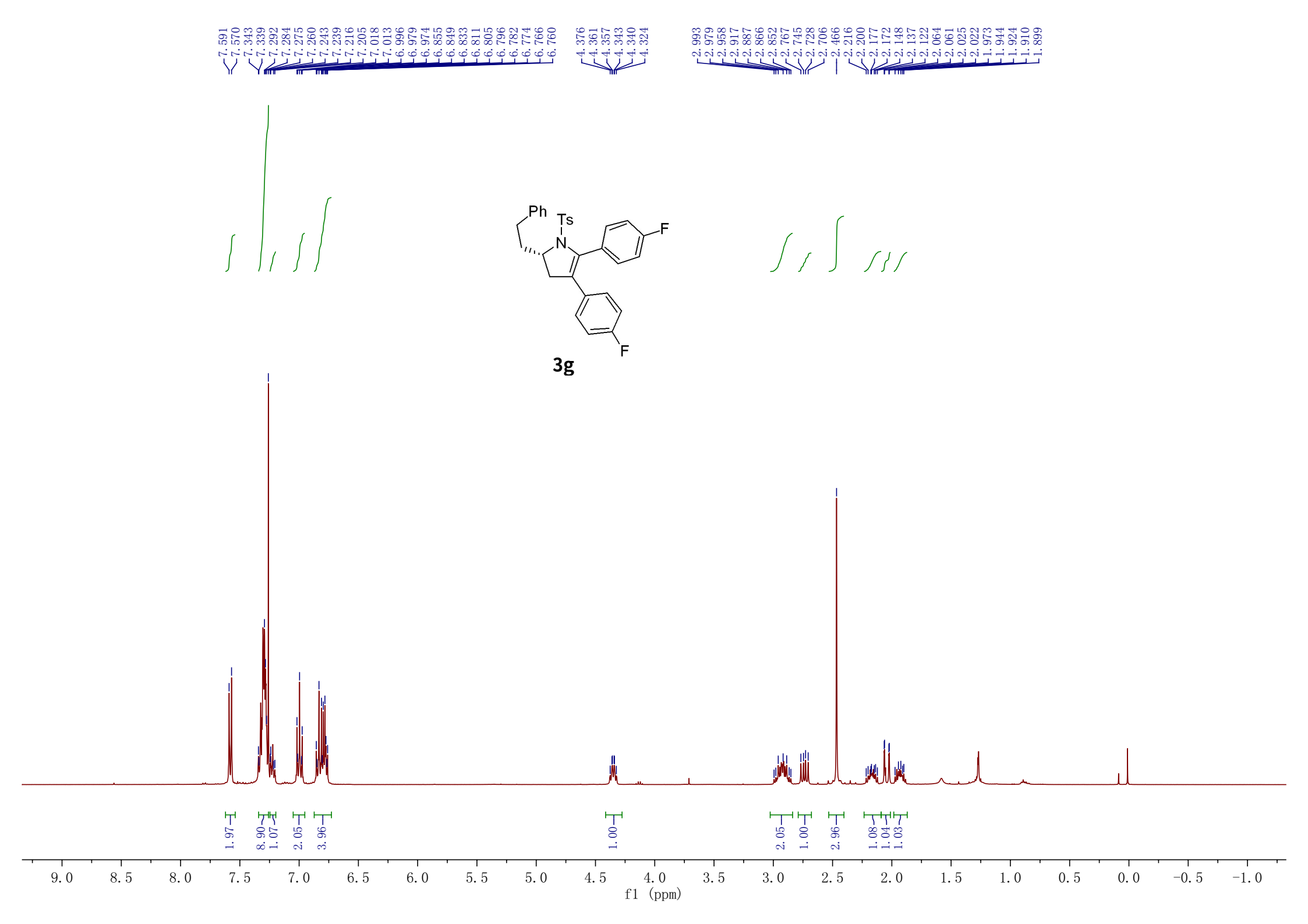

163.65
162.47
161.68
160.51
143.72
135.32
131.60
131.53
129.42
128.73
128.70
128.66
127.62
125.98
125.30
115.27
115.13
115.09
77.25
77.00
76.75
61.03
39.49
36.24
31.82
29.51
29.24
25.11
22.64
21.60
14.08
Ts
N
6
F
F
3c
135.60
135.59
135.32
131.71
131.69
131.60
131.53
129.42
128.73
128.70
128.66
127.62
125.98
138
136
134
132
130
128
126
124
f1 (ppm)
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)

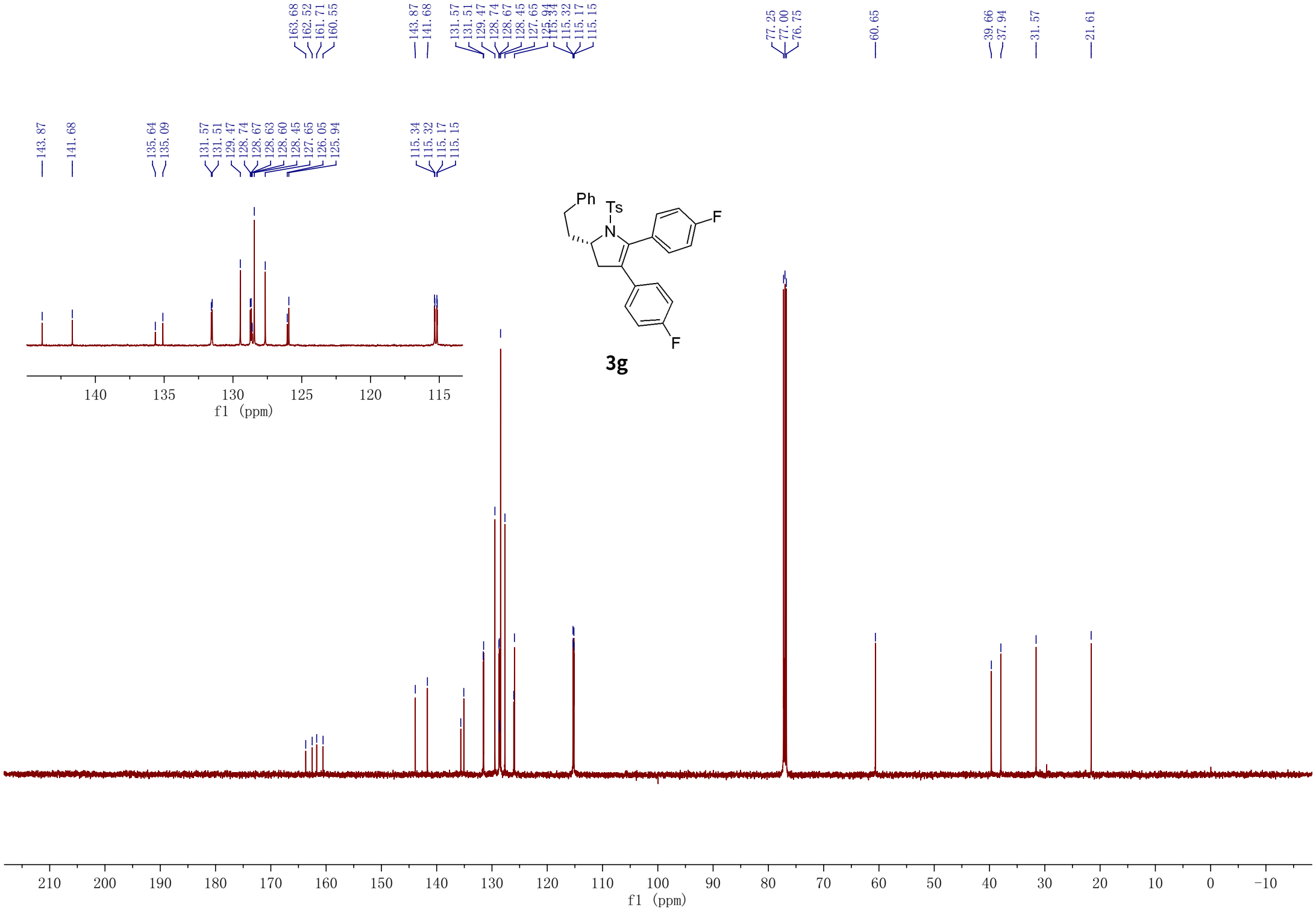

7.549
7.532
7.231
7.227
7.220
7.079
7.061
6.714
6.711
6.701
6.697
4.271
4.258
4.244
4.230
2.709
2.691
2.677
2.660
2.427
1.986
1.984
1.955
1.952
1.524
1.492
1.476
1.328
1.312
1.306
1.294
1.279
1.270
0.881
0.867
0.853
Ts
N
6
Cl
Cl
3d
1.97
6.44
1.98
1.95
1.00
0.94
2.95
0.99
0.97
3.06
8.11
2.99
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

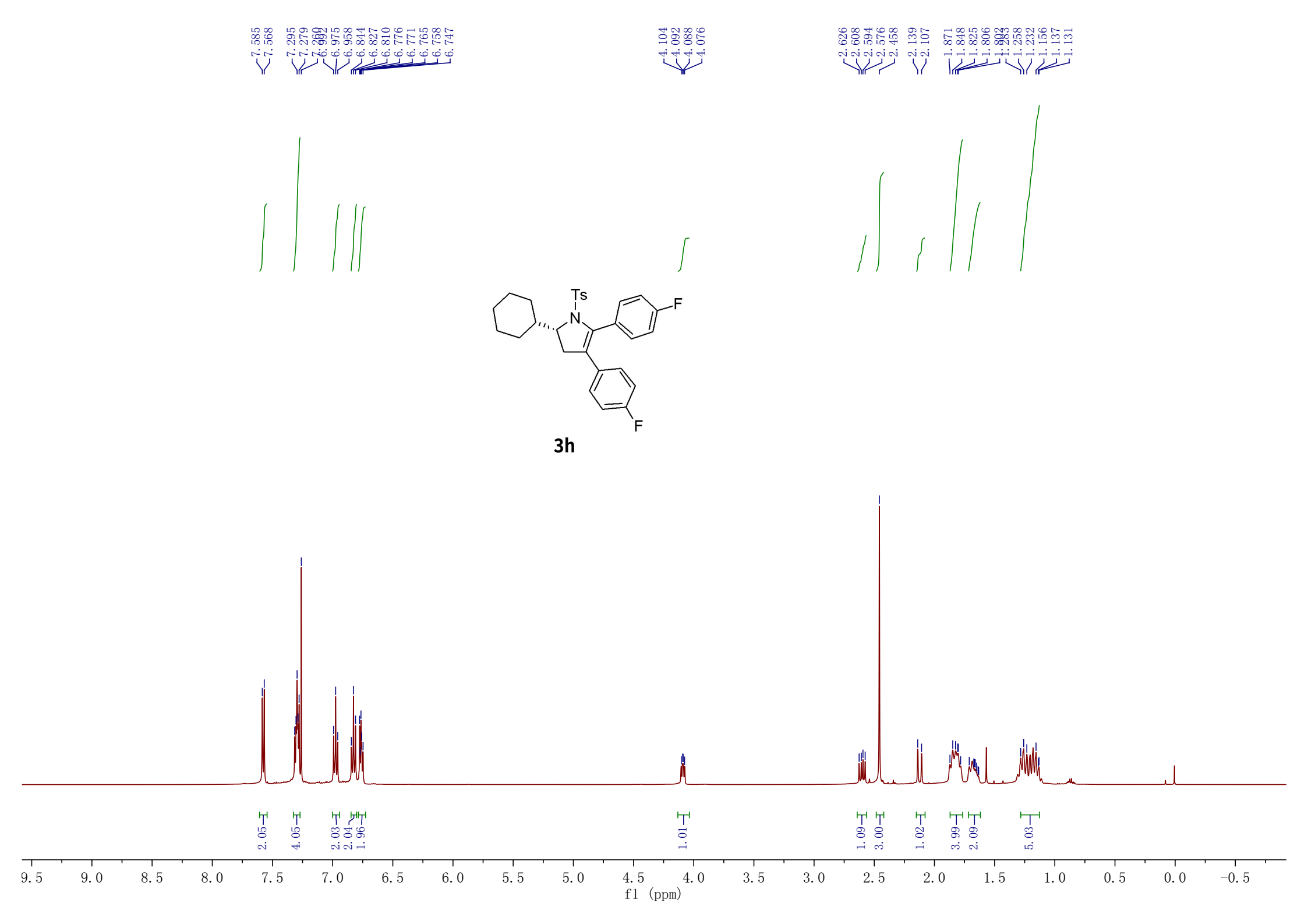

143.84
136.07
135.22
134.50
134.04
132.70
131.07
131.05
129.46
128.47
128.41
128.32
127.61
126.34
77.25
77.00
76.75
61.10
39.43
36.20
31.81
29.49
29.23
25.10
22.64
21.62
14.09
Ts
N
6
Cl
Cl
3d
f1 (ppm)

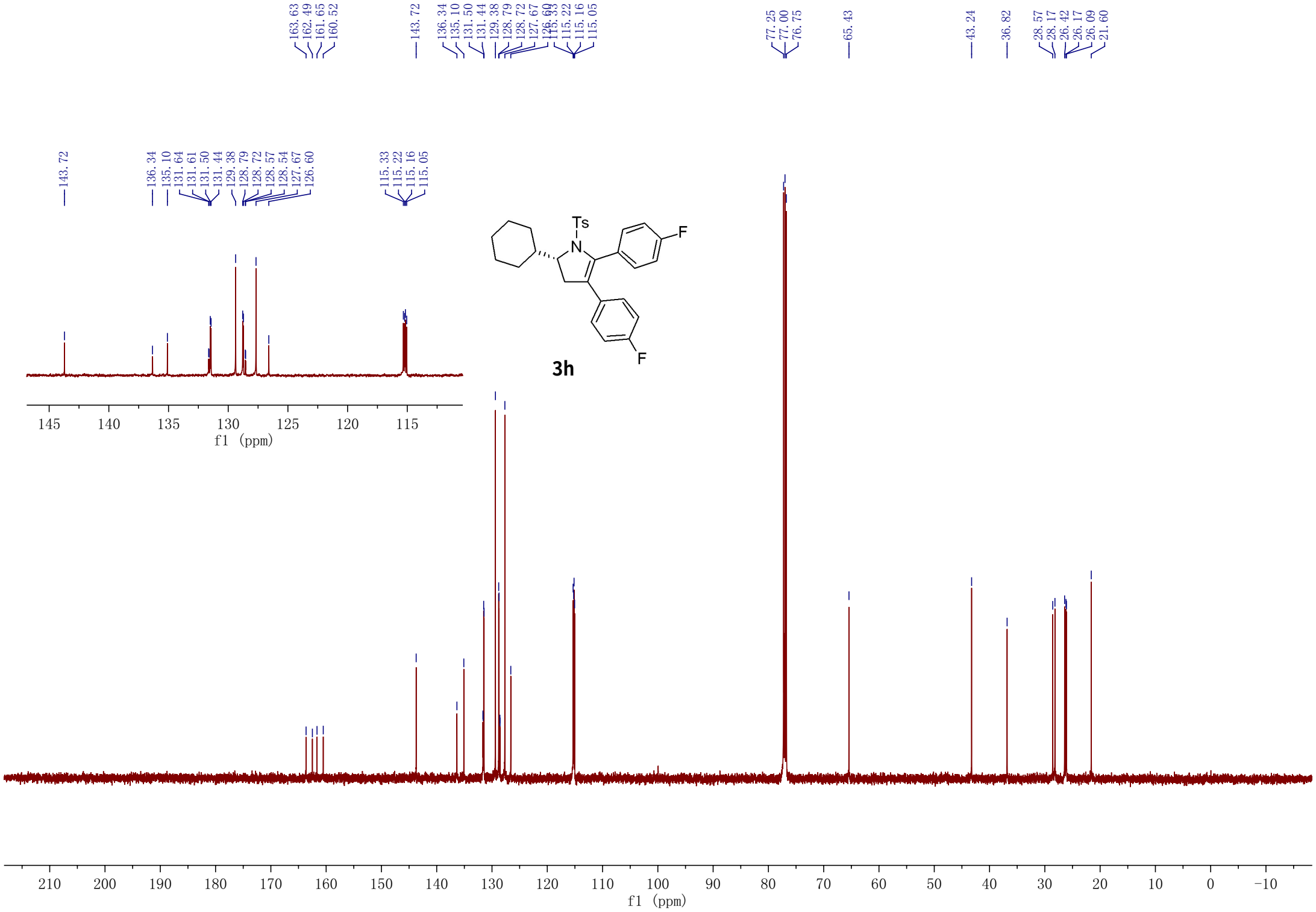

7.575
7.554
7.426
7.405
7.289
7.268
7.260
7.239
7.194
7.173
6.684
6.663
4.300
4.284
4.267
4.249
2.731
2.709
2.691
2.670
2.454
2.011
1.972
1.782
1.604
1.589
1.577
1.556
1.533
1.515
1.502
1.320
1.297
0.910
0.894
0.877
Ts
N
6
Br
Br
3e
2.08
2.02
6.41
1.98
0.99
0.94
3.00
1.05
1.12
3.06
8.03
3.12
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

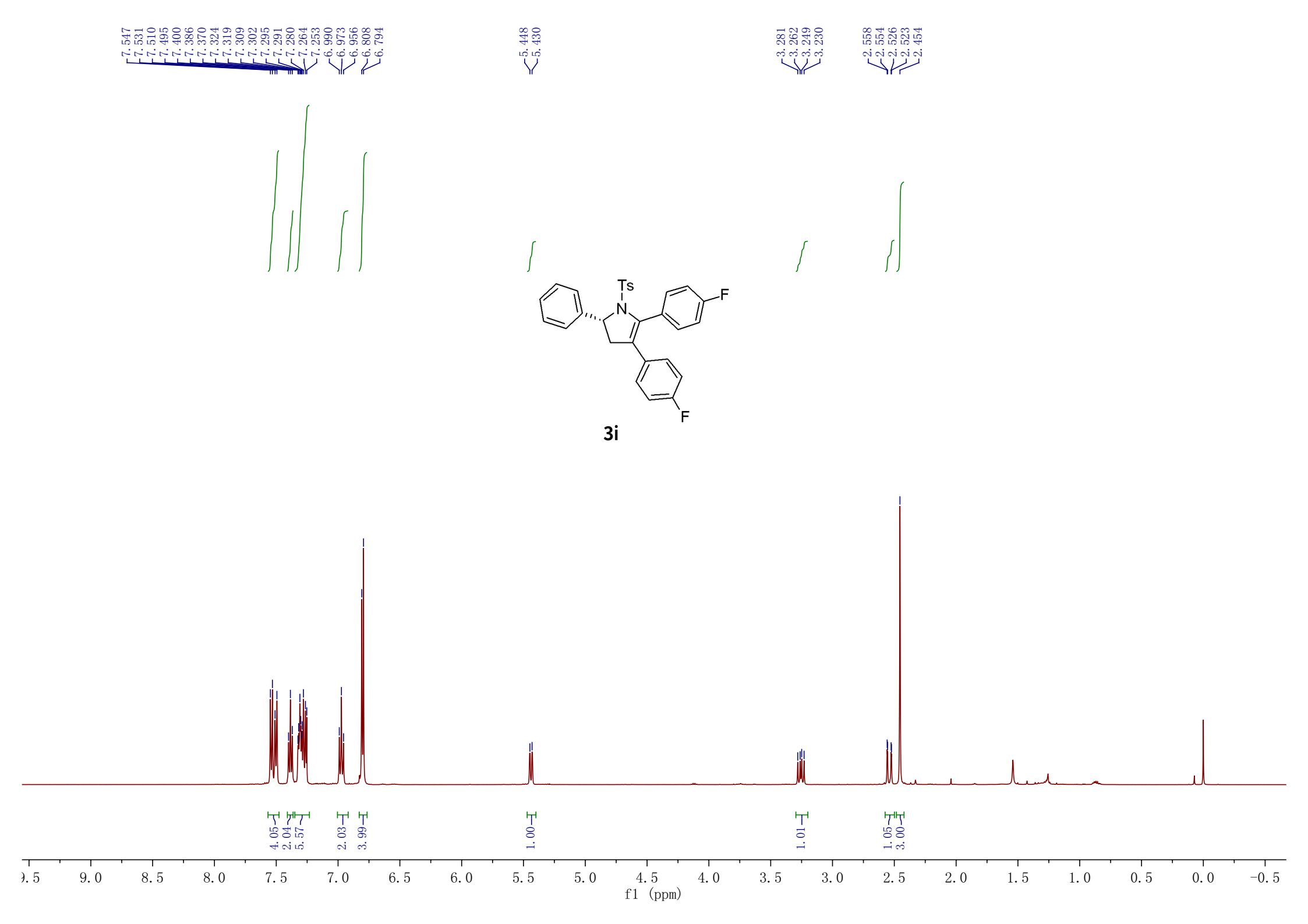

143.86
136.17
135.21
134.50
131.50
131.44
131.37
131.30
129.47
128.61
127.62
126.42
122.85
120.83
77.25
77.00
76.75
61.11
39.41
36.21
31.81
29.49
29.23
25.09
22.64
21.63
14.09
Ts
N
Br
Br
6
3e
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

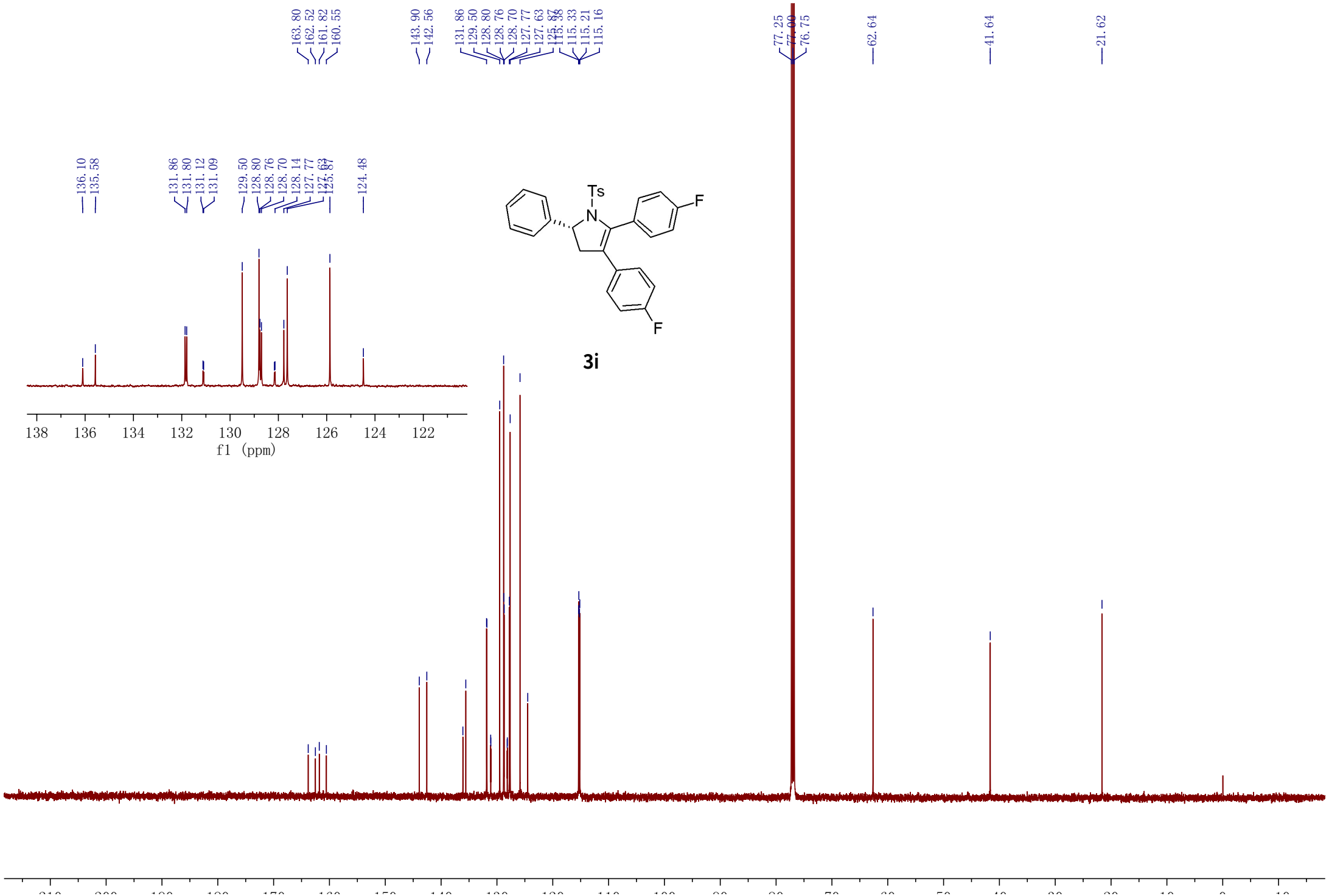

7.591
7.570
7.343
7.339
7.292
7.284
7.275
7.260
7.243
7.239
7.216
7.205
7.018
7.013
6.996
6.979
6.974
6.855
6.849
6.833
6.811
6.805
6.796
6.782
6.774
6.766
6.760
4.376
4.361
4.357
4.343
4.340
4.324
2.993
2.979
2.958
2.917
2.887
2.866
2.852
2.767
2.745
2.728
2.706
2.466
2.216
2.200
2.177
2.172
2.148
2.137
2.122
2.064
2.061
2.025
2.022
1.973
1.944
1.924
1.910
1.899
Ph
Ts
N
F
F
3g
1.97
8.90
1.07
2.05
3.96
1.00
2.05
1.00
2.96
1.08
1.04
1.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

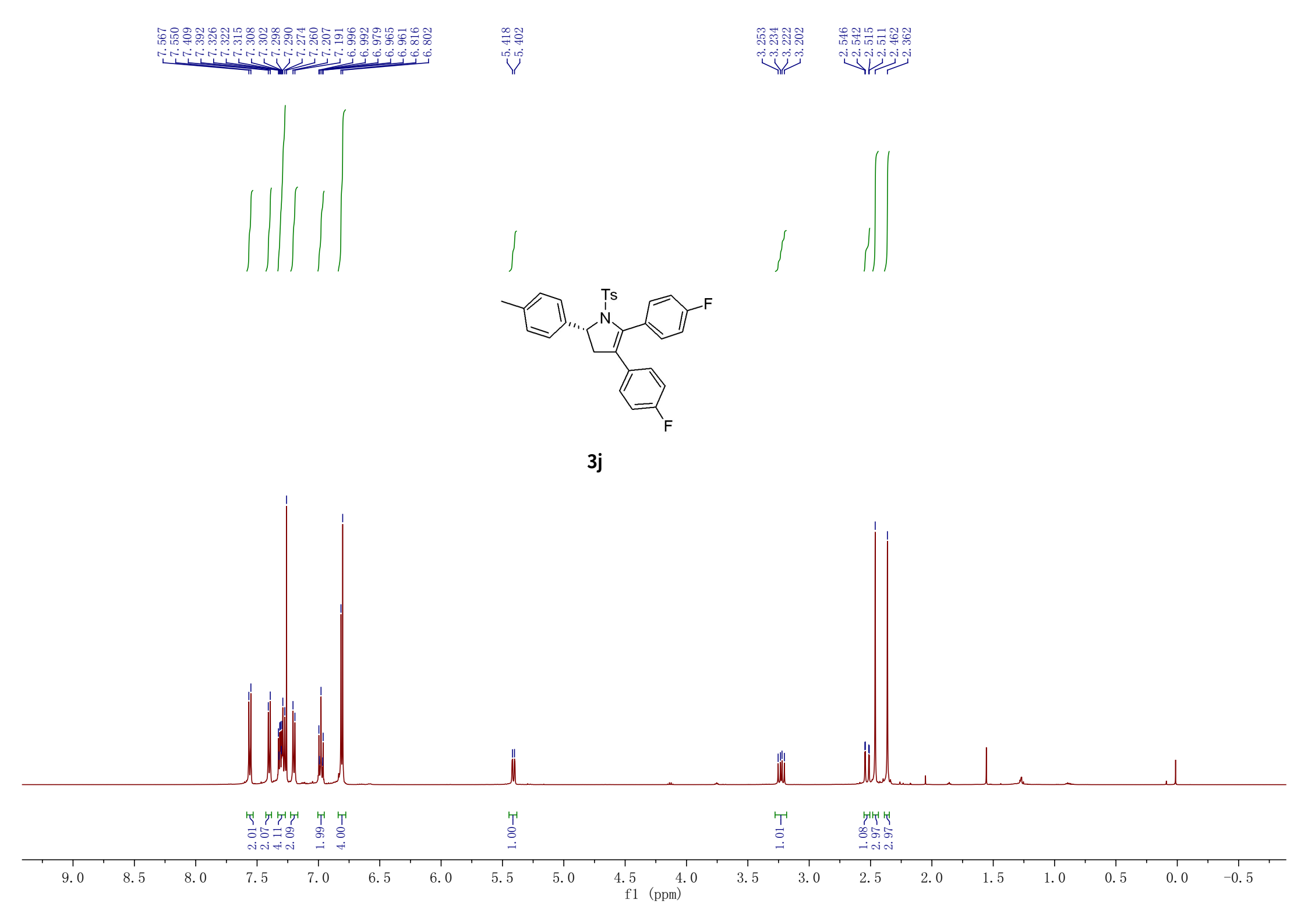

163.68
162.52
161.71
160.55
143.87
141.68
131.57
131.51
129.47
128.74
128.67
128.45
127.65
125.94
115.34
115.32
115.17
115.15
77.25
77.00
76.75
60.65
39.66
37.94
31.57
21.61
143.87
141.68
135.64
135.09
131.57
131.51
129.47
128.74
128.67
128.63
128.60
128.45
127.65
126.05
125.94
115.34
115.32
115.17
115.15
140
135
130
125
120
115
f1 (ppm)
Ph
Ts
N
F
F
3g
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)

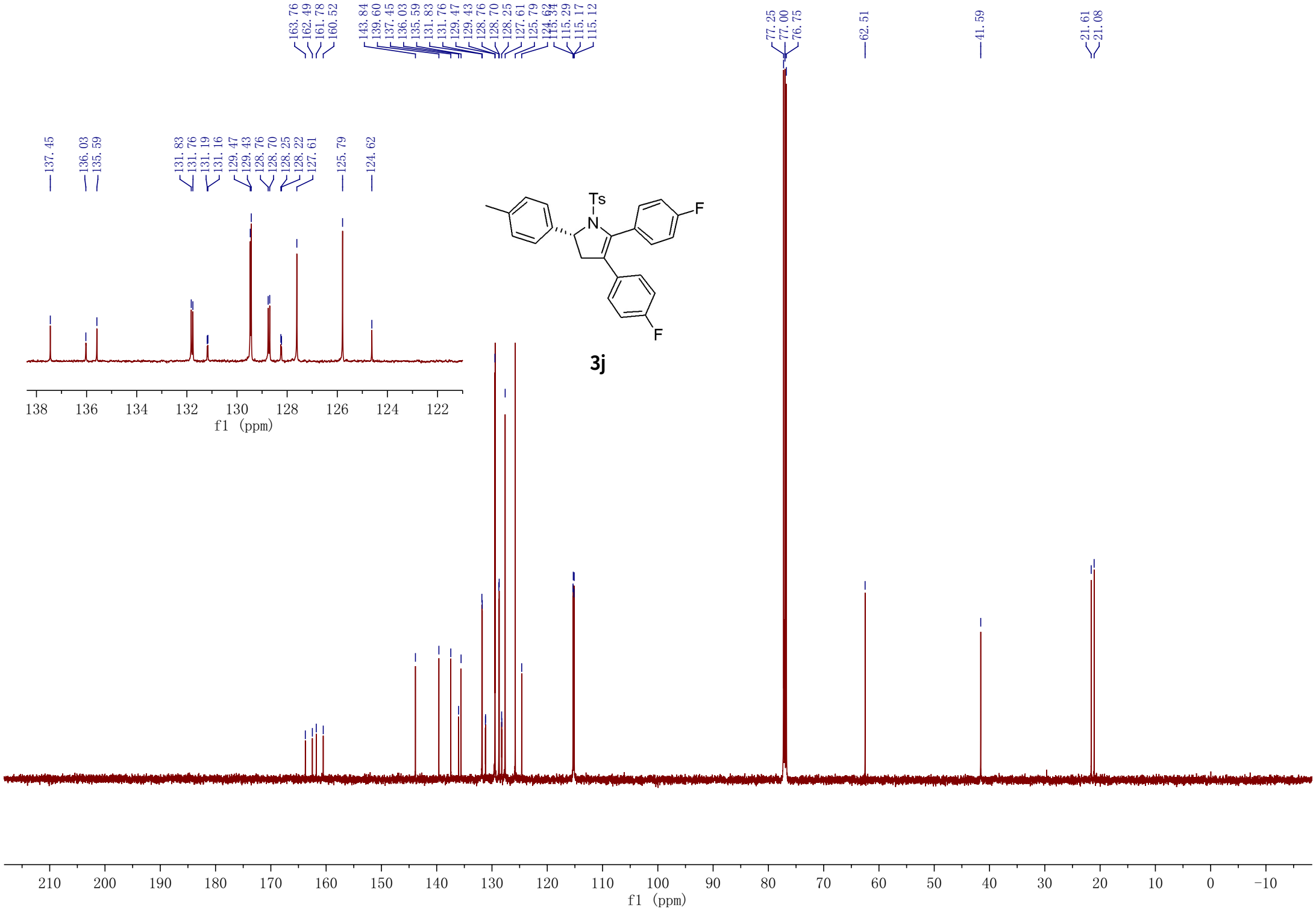

7.585
7.568
7.295
7.279
6.975
6.958
6.844
6.827
6.810
6.776
6.771
6.765
6.758
6.747
4.104
4.092
4.088
4.076
2.626
2.608
2.594
2.576
2.458
2.139
2.107
1.871
1.848
1.825
1.806
1.258
1.232
1.156
1.137
1.131
Ts
N
F
F
3h
2.05
4.05
2.03
2.04
1.96
1.01
1.09
3.00
1.02
3.99
2.09
5.03
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

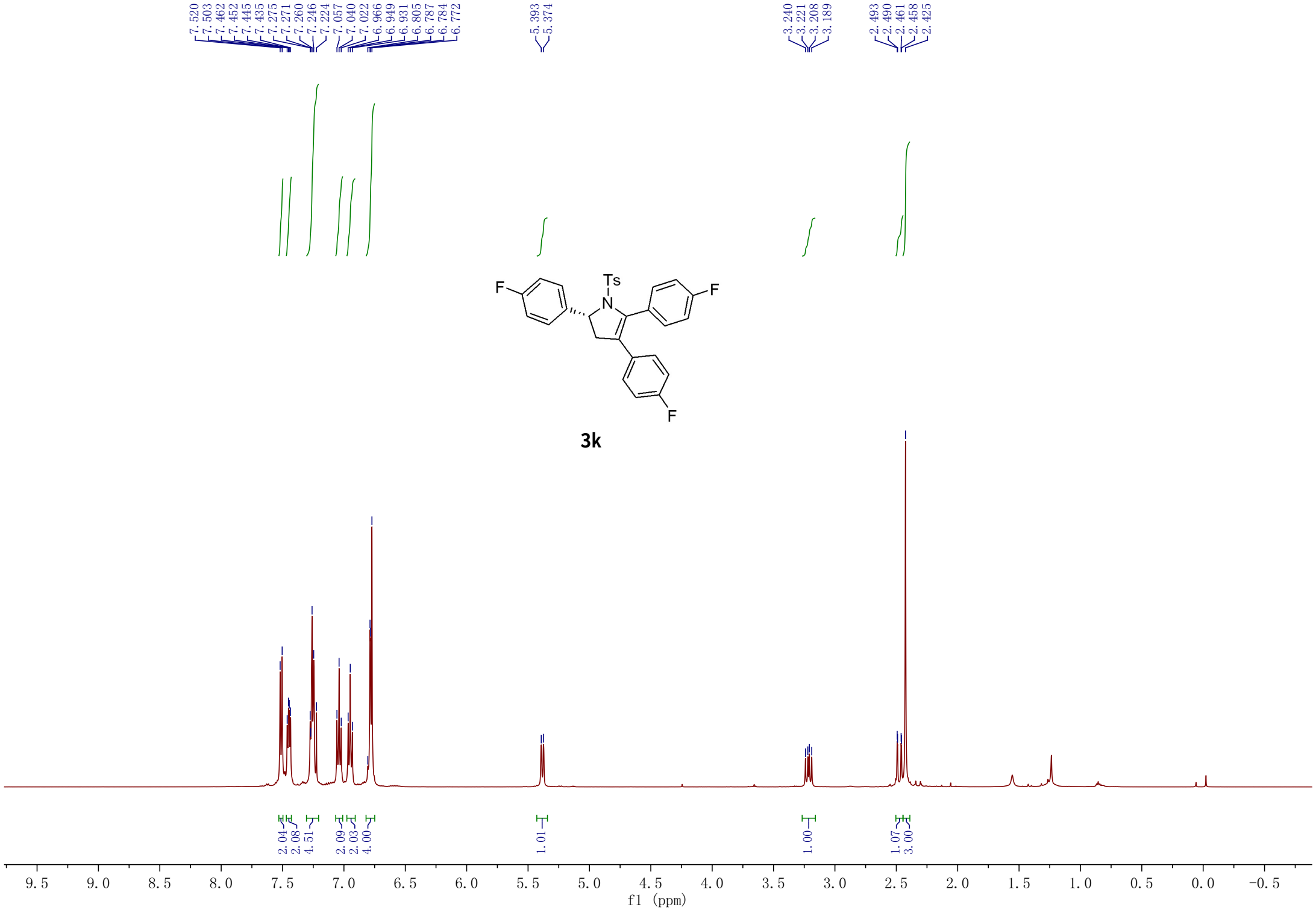

163.63
162.49
161.65
160.52
143.72
136.34
135.10
131.50
131.44
129.38
128.79
128.72
127.67
126.60
115.33
115.22
115.16
115.05
77.25
77.00
76.75
65.43
43.24
36.82
28.57
28.17
26.42
26.17
26.09
21.60
Ts
N
F
F
3h
f1 (ppm)


7.547
7.531
7.510
7.495
7.400
7.386
7.370
7.324
7.319
7.309
7.302
7.295
7.291
7.280
7.264
7.253
6.990
6.973
6.956
6.808
6.794
5.448
5.430
3.281
3.262
3.249
3.230
2.558
2.554
2.526
2.523
2.454
Ts
N
F
F
3i
4.05
2.04
5.57
2.03
3.99
1.00
1.01
1.05
3.00
f1 (ppm)

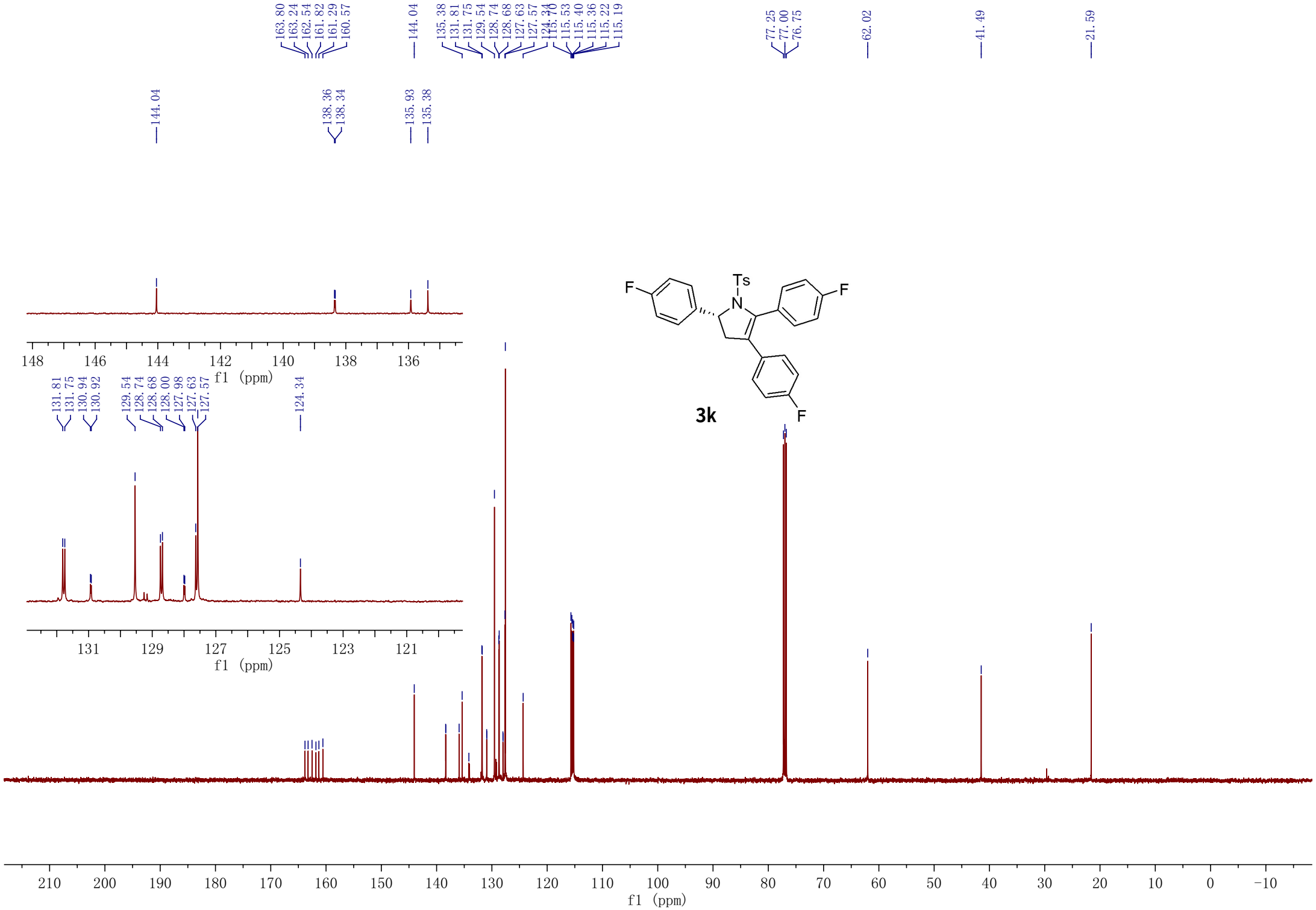

163.80
162.52
161.82
160.55
143.90
142.56
131.86
129.50
128.80
128.76
128.70
127.77
127.63
125.87
115.33
115.21
115.16
77.25
77.00
76.75
62.64
41.64
21.62
136.10
135.58
131.86
131.80
131.12
131.09
129.50
128.80
128.76
128.70
128.14
127.77
127.63
125.87
124.48
Ts
N
F
F
3i
138
136
134
132
130
128
126
124
122
f1 (ppm)

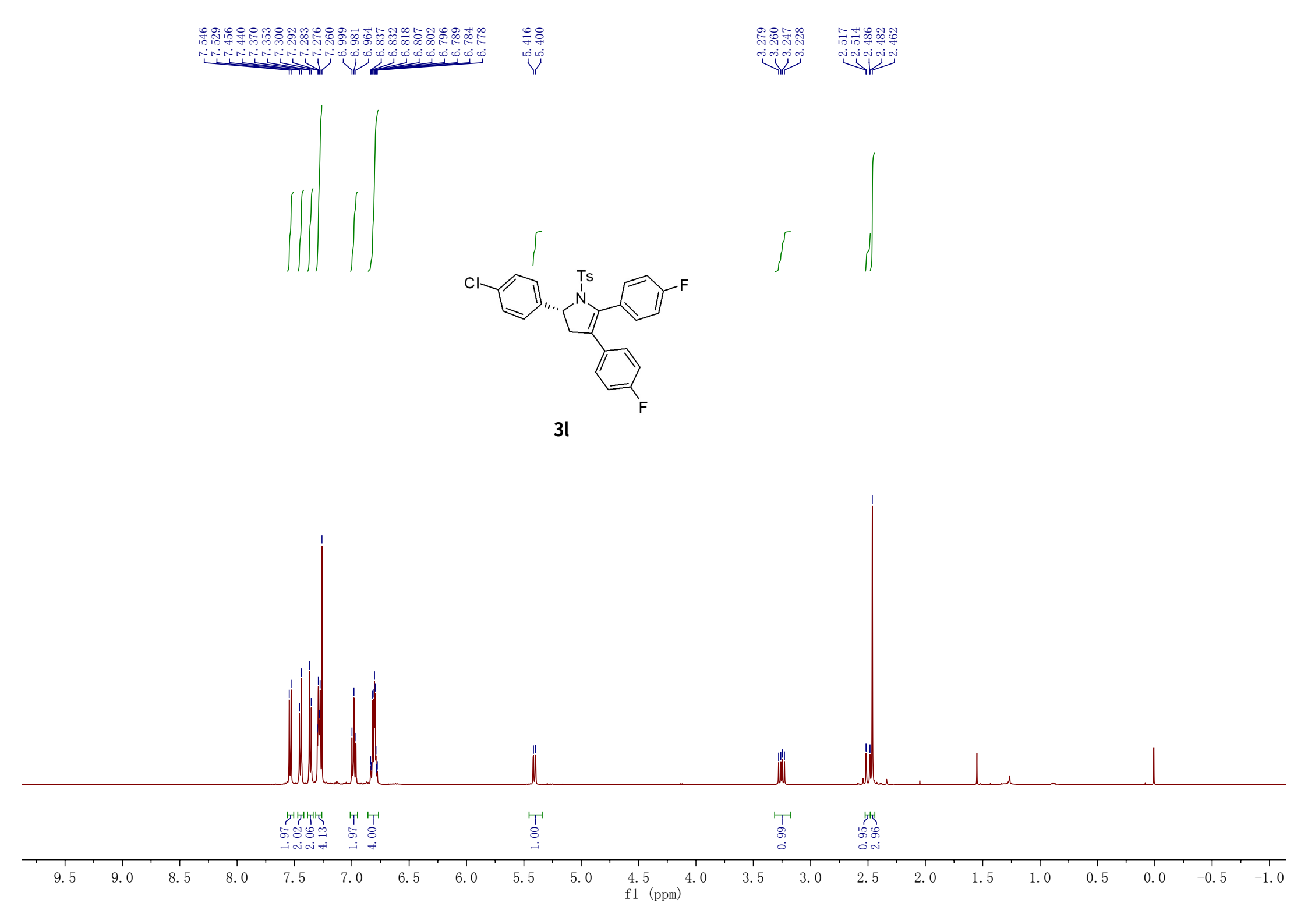

7.567
7.550
7.409
7.392
7.326
7.322
7.315
7.308
7.302
7.298
7.290
7.274
7.260
7.207
7.191
6.996
6.992
6.979
6.965
6.961
6.816
6.802
5.418
5.402
3.253
3.234
3.222
3.202
2.546
2.542
2.515
2.511
2.462
2.362
Ts
N
F
F
3j
2.01
2.07
4.11
2.09
1.99
4.00
1.00
1.01
1.08
2.97
2.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

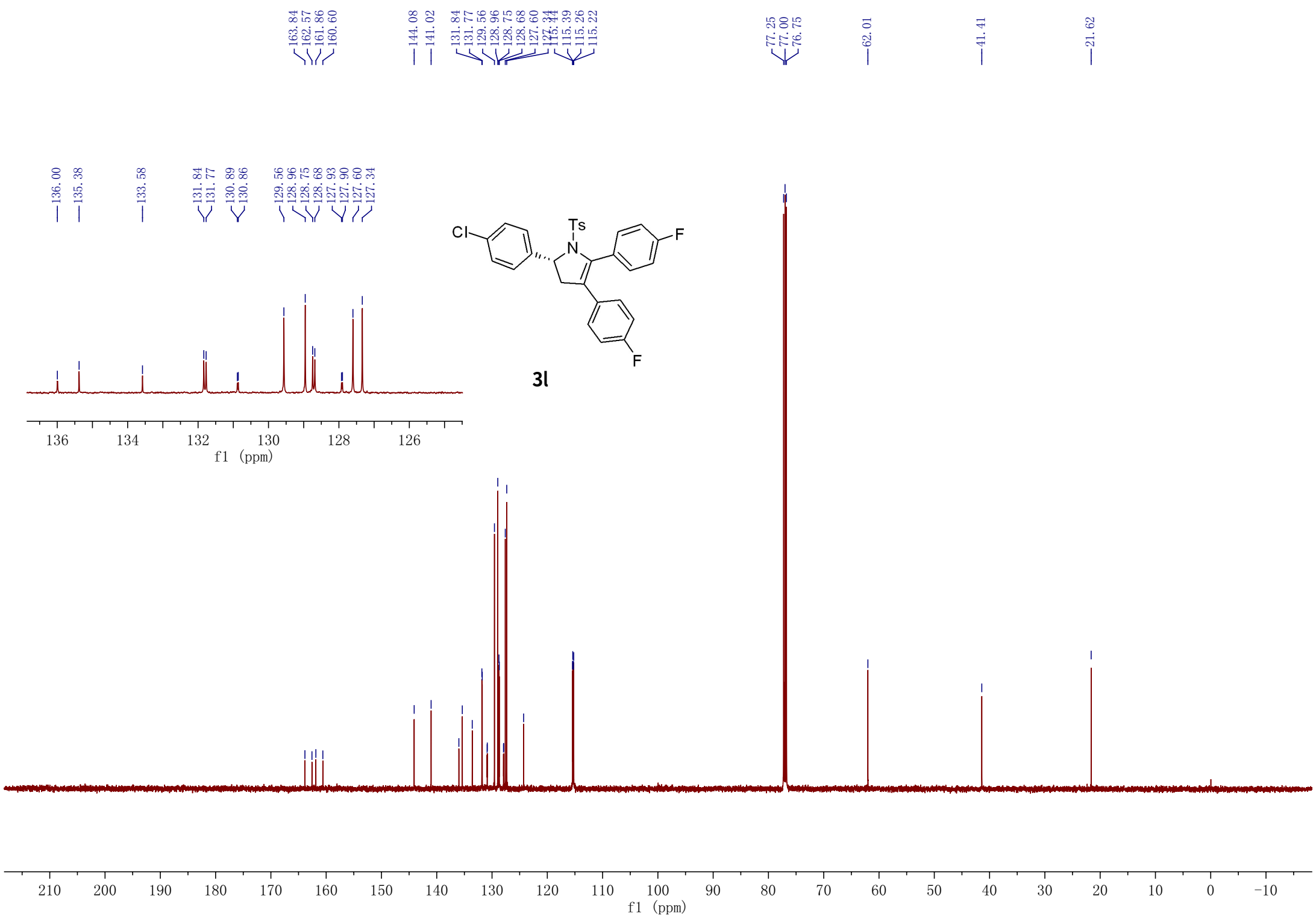

163.76
162.49
161.78
160.52
143.84
139.60
137.45
136.03
135.59
131.83
131.76
129.47
129.43
128.76
128.70
128.25
127.61
125.79
124.62
115.29
115.17
115.12
77.25
77.00
76.75
62.51
41.59
21.61
21.08
137.45
136.03
135.59
131.83
131.76
131.19
131.16
129.47
129.43
128.76
128.70
128.25
128.22
127.61
125.79
124.62
Ts
N
F
F
3j
f1 (ppm)
f1 (ppm)

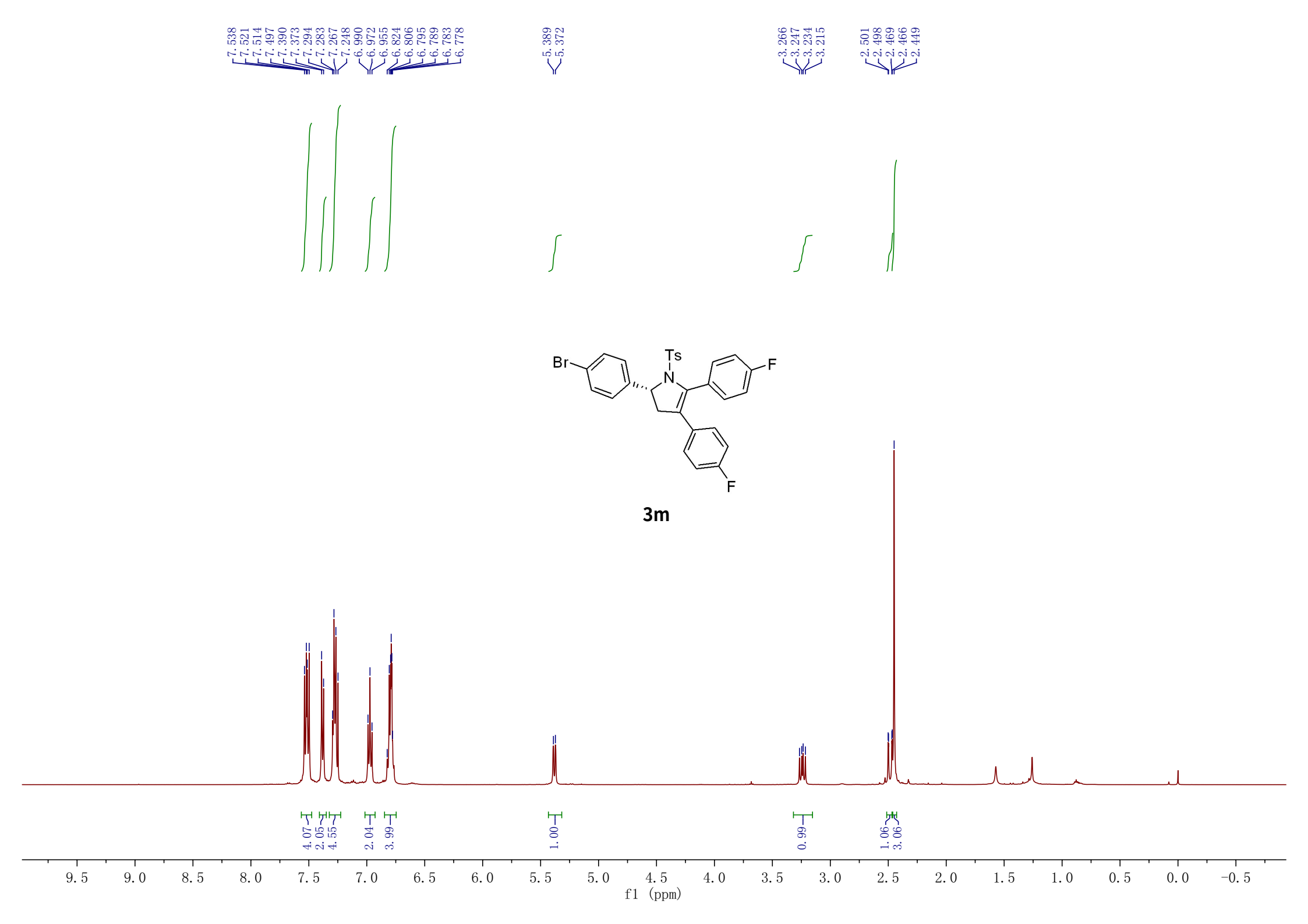

7.520
7.503
7.462
7.452
7.445
7.435
7.275
7.271
7.260
7.246
7.224
7.057
7.040
7.022
6.966
6.949
6.931
6.805
6.787
6.784
6.772
5.393
5.374
3.240
3.221
3.208
3.189
2.493
2.490
2.461
2.458
2.425
F
Ts
N
F
F
2.04
2.08
4.51
2.09
2.03
4.00
1.01
1.00
1.07
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

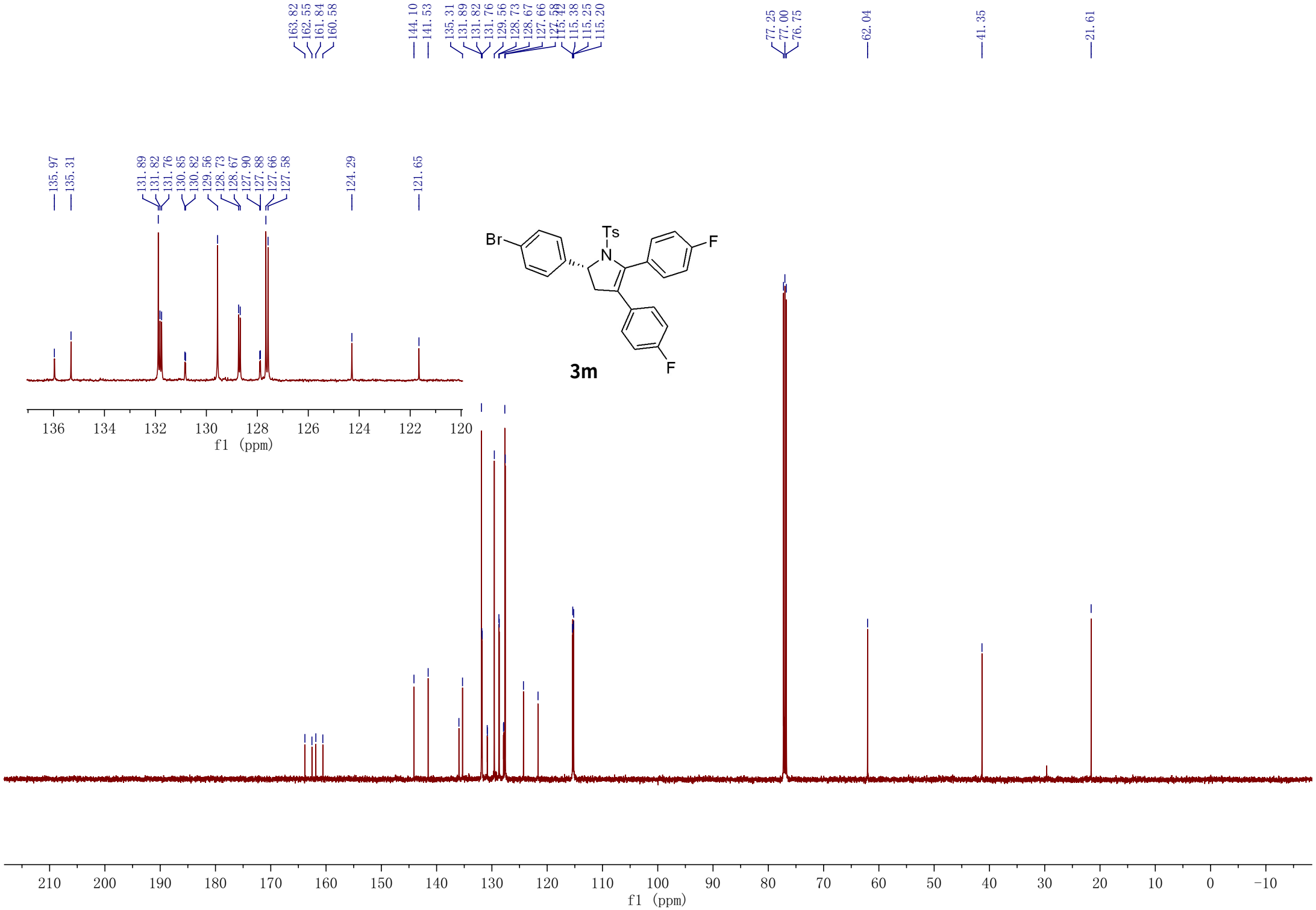
3k

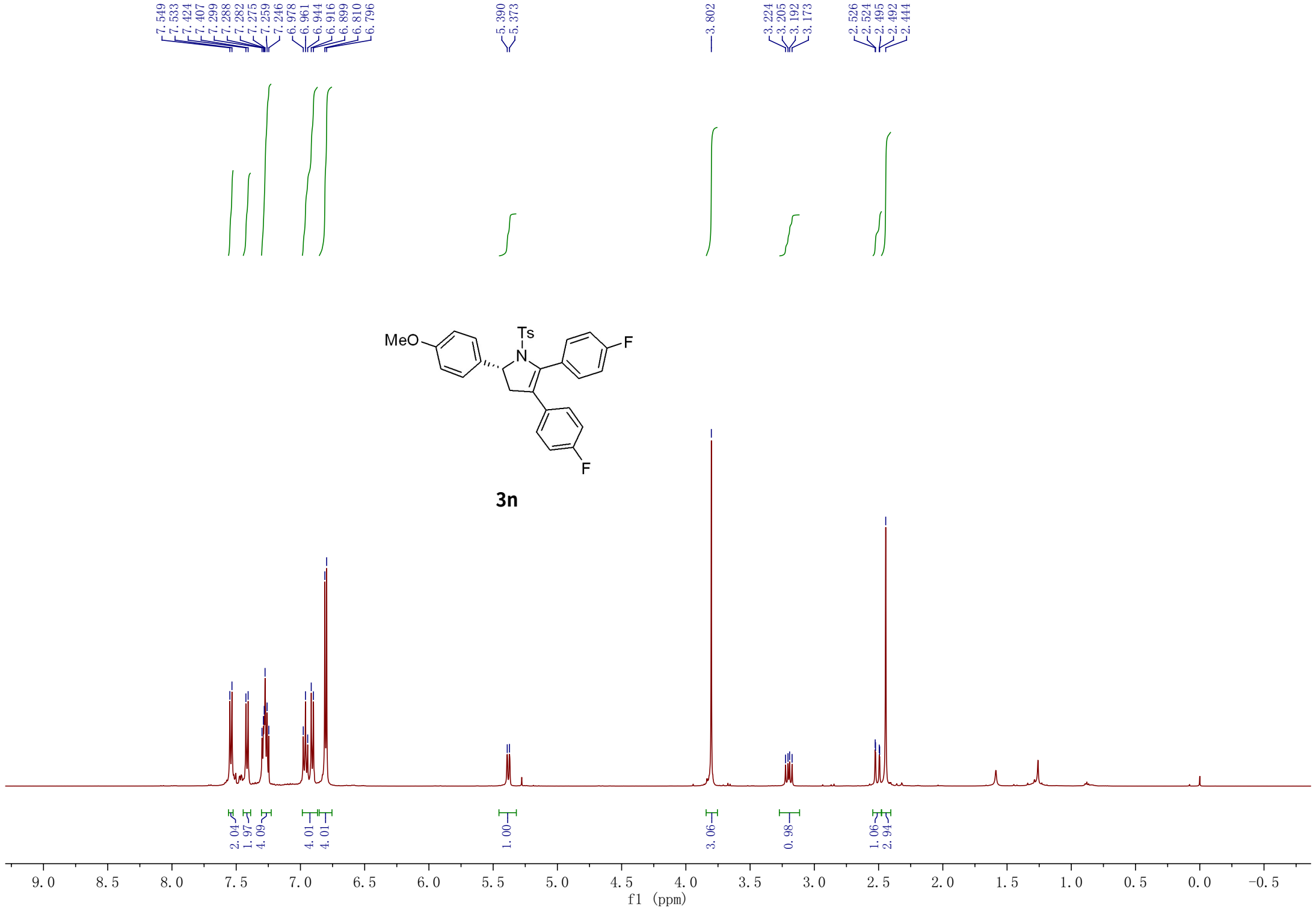

163.80
163.24
162.54
161.82
161.29
160.57
144.04
135.38
131.81
131.75
131.54
129.54
128.74
128.68
127.98
127.63
127.57
124.34
115.53
115.40
115.36
115.22
115.19
77.25
77.00
76.75
62.02
41.49
21.59
144.04
138.36
138.34
135.93
135.38
131.81
131.75
130.94
130.92
129.54
128.74
128.68
128.00
127.98
127.63
127.57
124.34
F
Ts
N
F
F
3k
f1 (ppm)
f1 (ppm)
f1 (ppm)

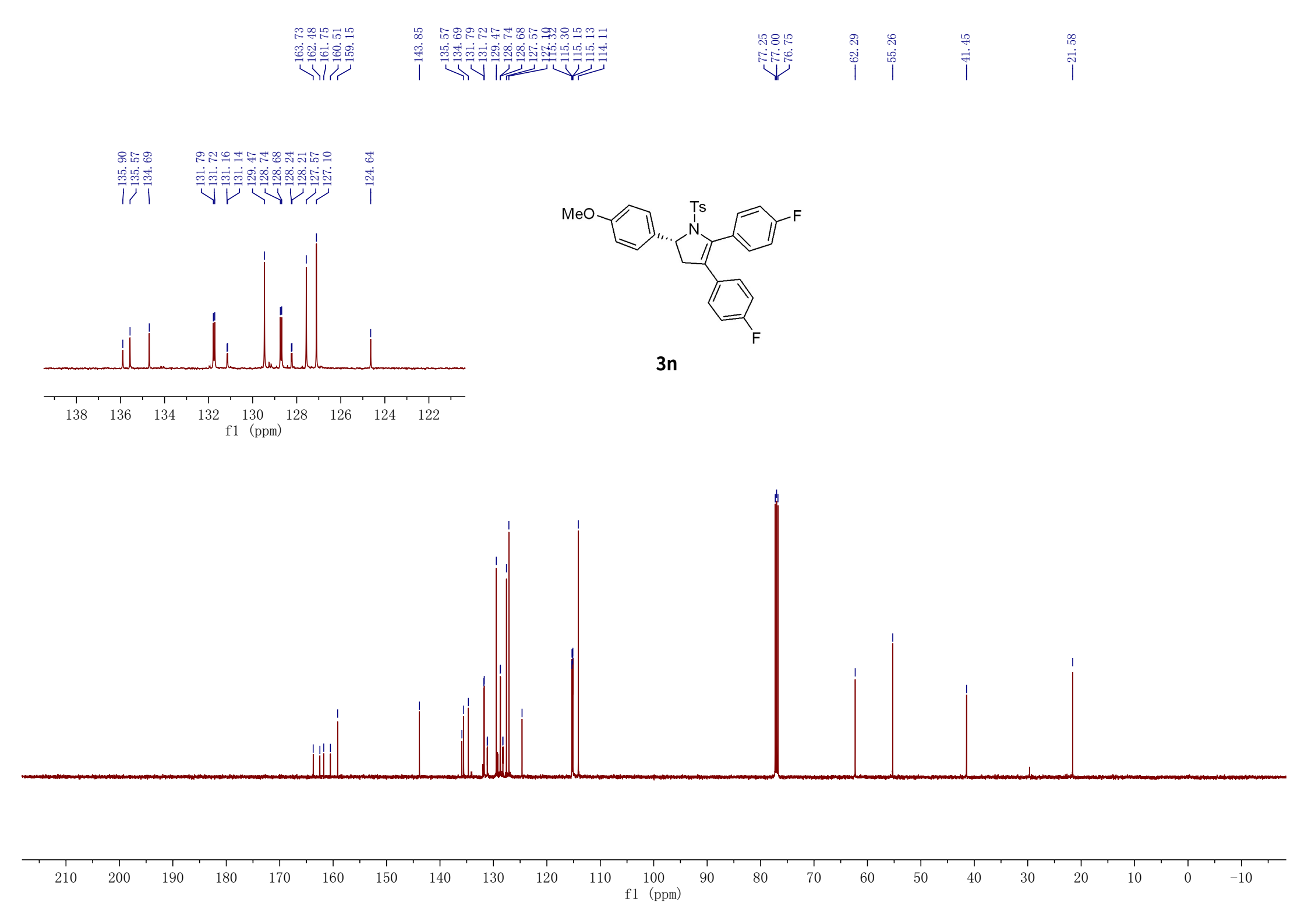

7.546
7.529
7.456
7.440
7.370
7.353
7.300
7.292
7.283
7.276
7.260
6.999
6.981
6.964
6.837
6.832
6.818
6.807
6.802
6.796
6.789
6.784
6.778
5.416
5.400
3.279
3.260
3.247
3.228
2.517
2.514
2.486
2.482
2.462
Cl
Ts
N
F
F
3l
1.97
2.02
2.06
4.13
1.97
4.00
1.00
0.99
0.95
2.96
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

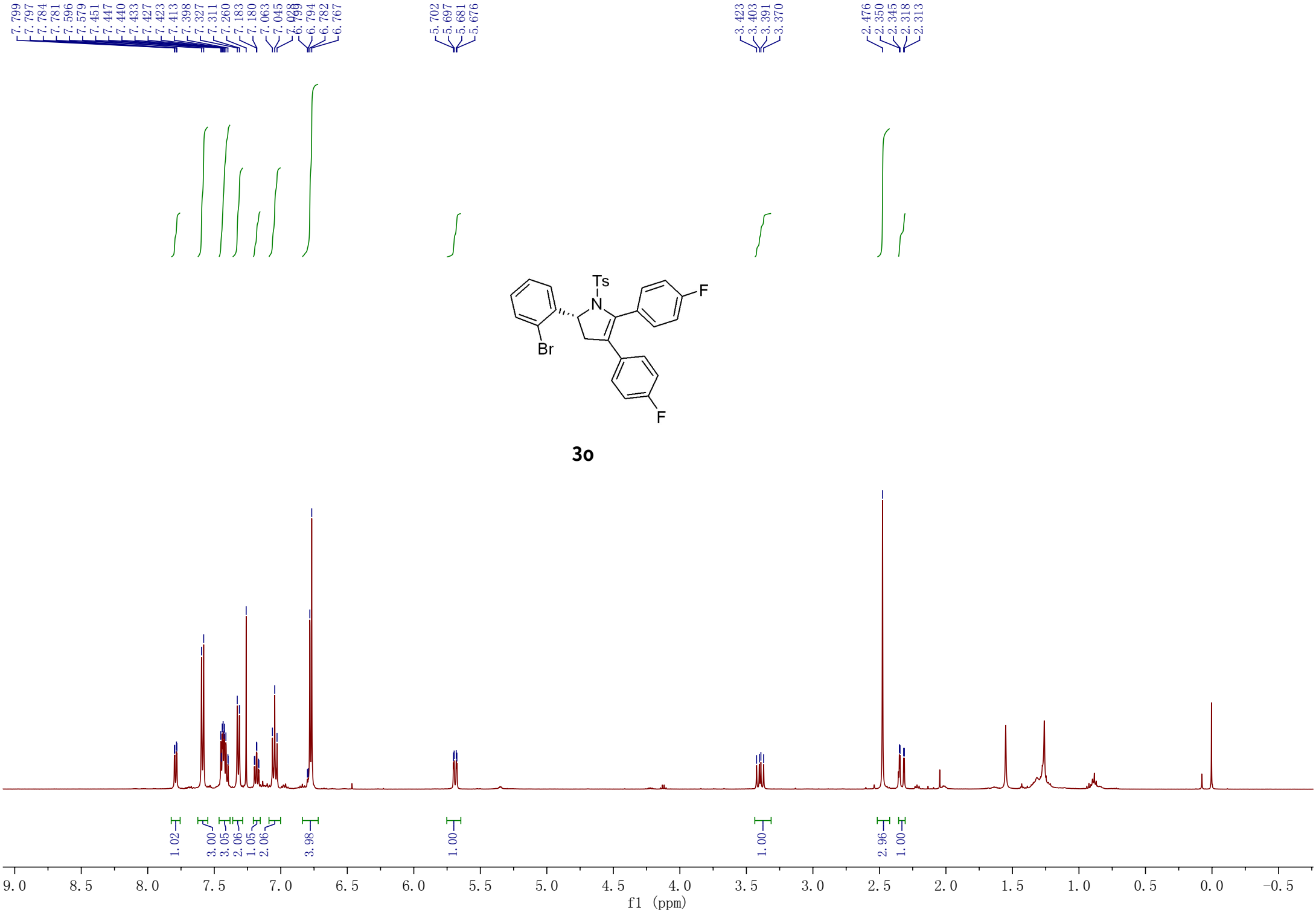

163.84
162.57
161.86
160.60
144.08
141.02
131.84
131.77
129.56
128.96
128.75
128.68
127.60
127.34
115.39
115.26
115.22
77.25
77.00
76.75
62.01
41.41
21.62
136.00
135.38
133.58
131.84
131.77
130.89
130.86
129.56
128.96
128.75
128.68
127.93
127.90
127.60
127.34
Cl
Ts
N
F
F
3l
136
134
132
130
128
126
f1 (ppm)
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)


7.538
7.521
7.514
7.497
7.390
7.373
7.294
7.283
7.267
7.248
6.990
6.972
6.955
6.824
6.806
6.795
6.789
6.783
6.778
5.389
5.372
3.266
3.247
3.234
3.215
2.501
2.498
2.469
2.466
2.449
Br
Ts
N
F
F
3m
4.07
2.05
4.55
2.04
3.99
1.00
0.99
1.06
3.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

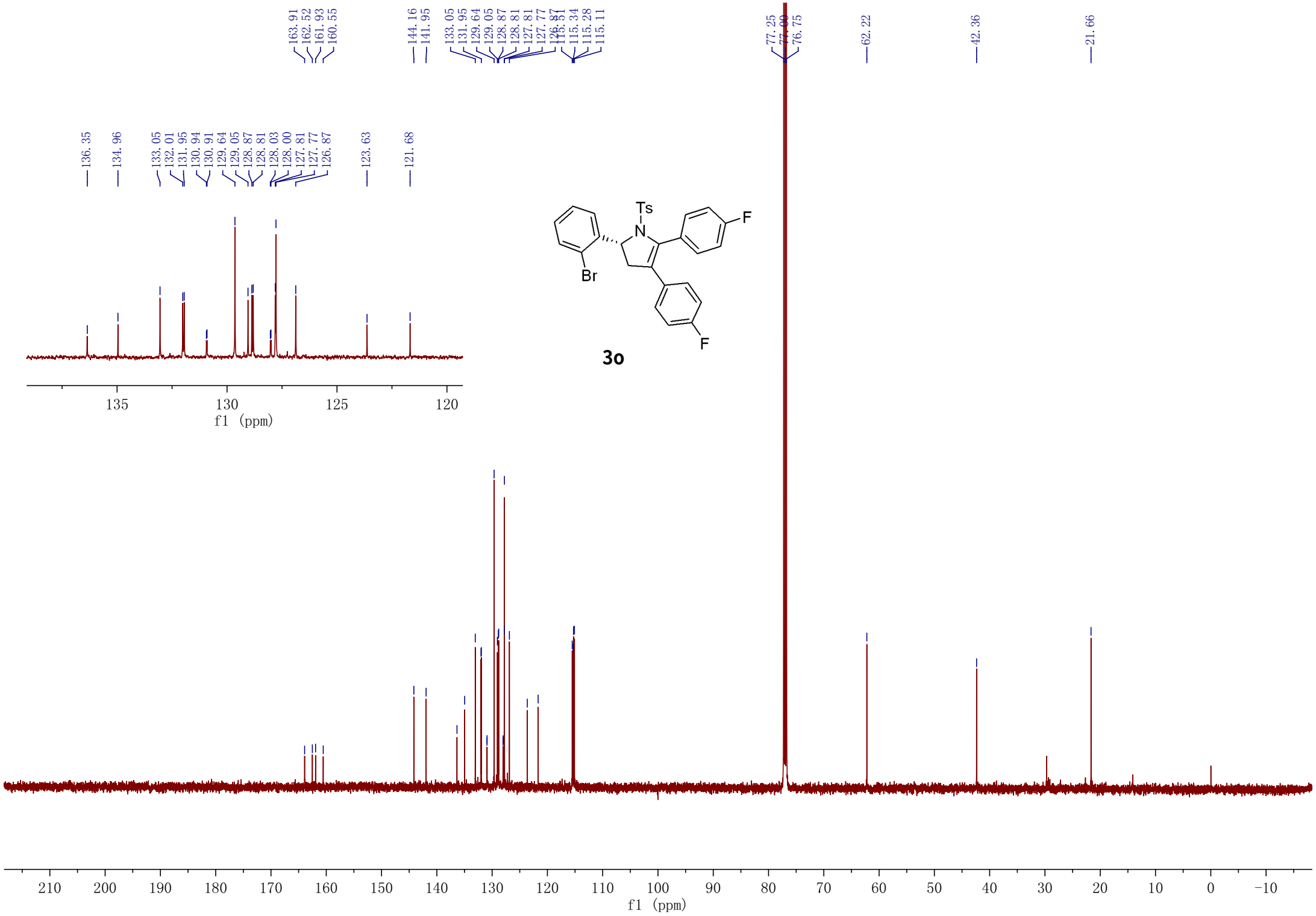

163.82
162.55
161.84
160.58
144.10
141.53
135.31
131.89
131.82
131.76
129.56
128.73
128.67
127.66
115.38
115.25
115.20
77.25
77.00
76.75
62.04
41.35
21.61
135.97
135.31
131.89
131.82
131.76
130.85
130.82
129.56
128.73
128.67
127.90
127.88
127.66
127.58
124.29
121.65
Br
Ts
N
F
F
3m
136
134
132
130
128
126
124
122
120
f1 (ppm)
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)

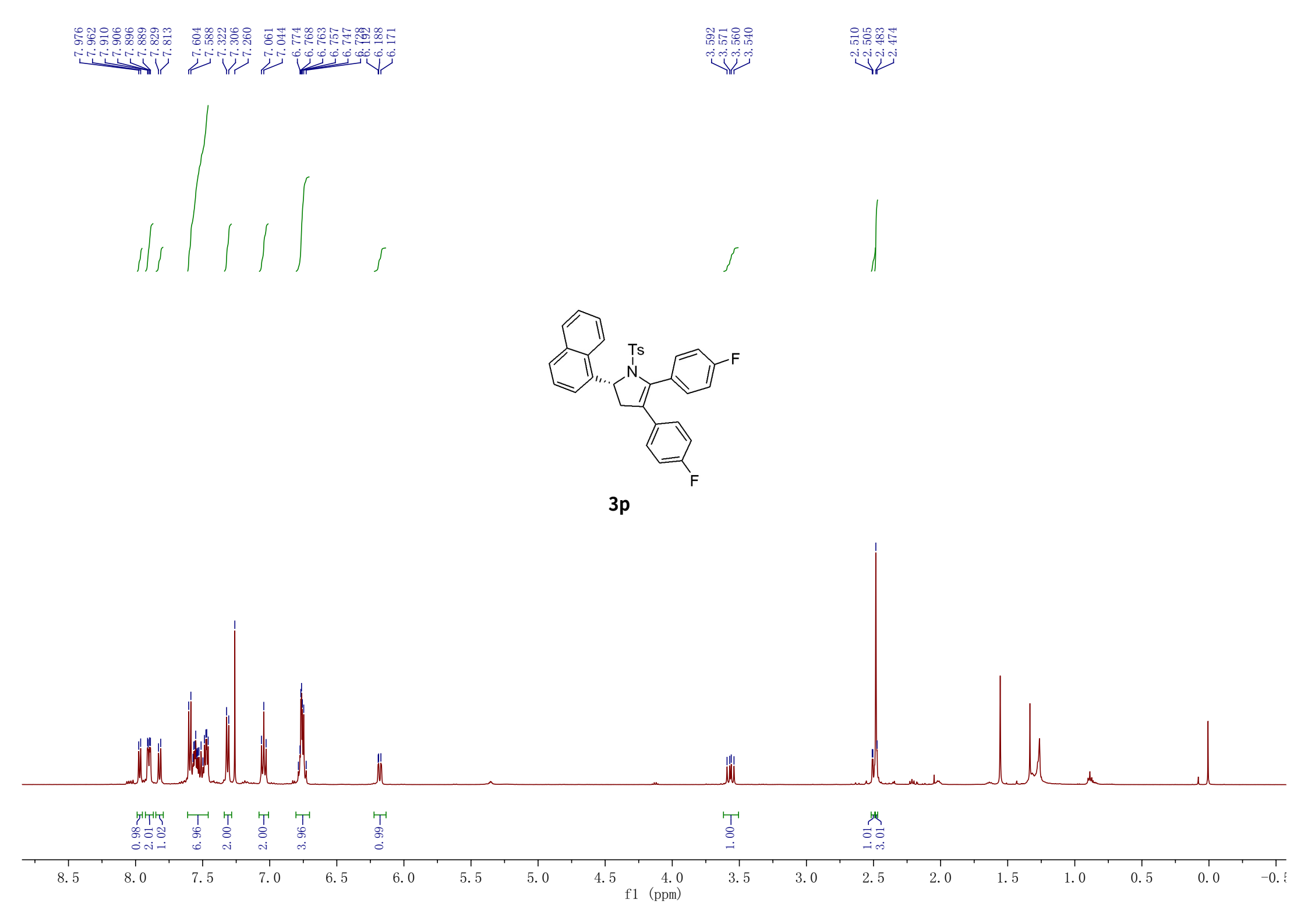

7.549
7.533
7.424
7.407
7.299
7.288
7.282
7.275
7.259
7.246
6.978
6.961
6.944
6.916
6.899
6.810
6.796
5.390
5.373
3.802
3.224
3.205
3.192
3.173
2.526
2.524
2.495
2.492
2.444
MeO
Ts
N
F
F
3n
2.04
1.97
4.09
4.01
4.01
1.00
3.06
0.98
1.06
2.94
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

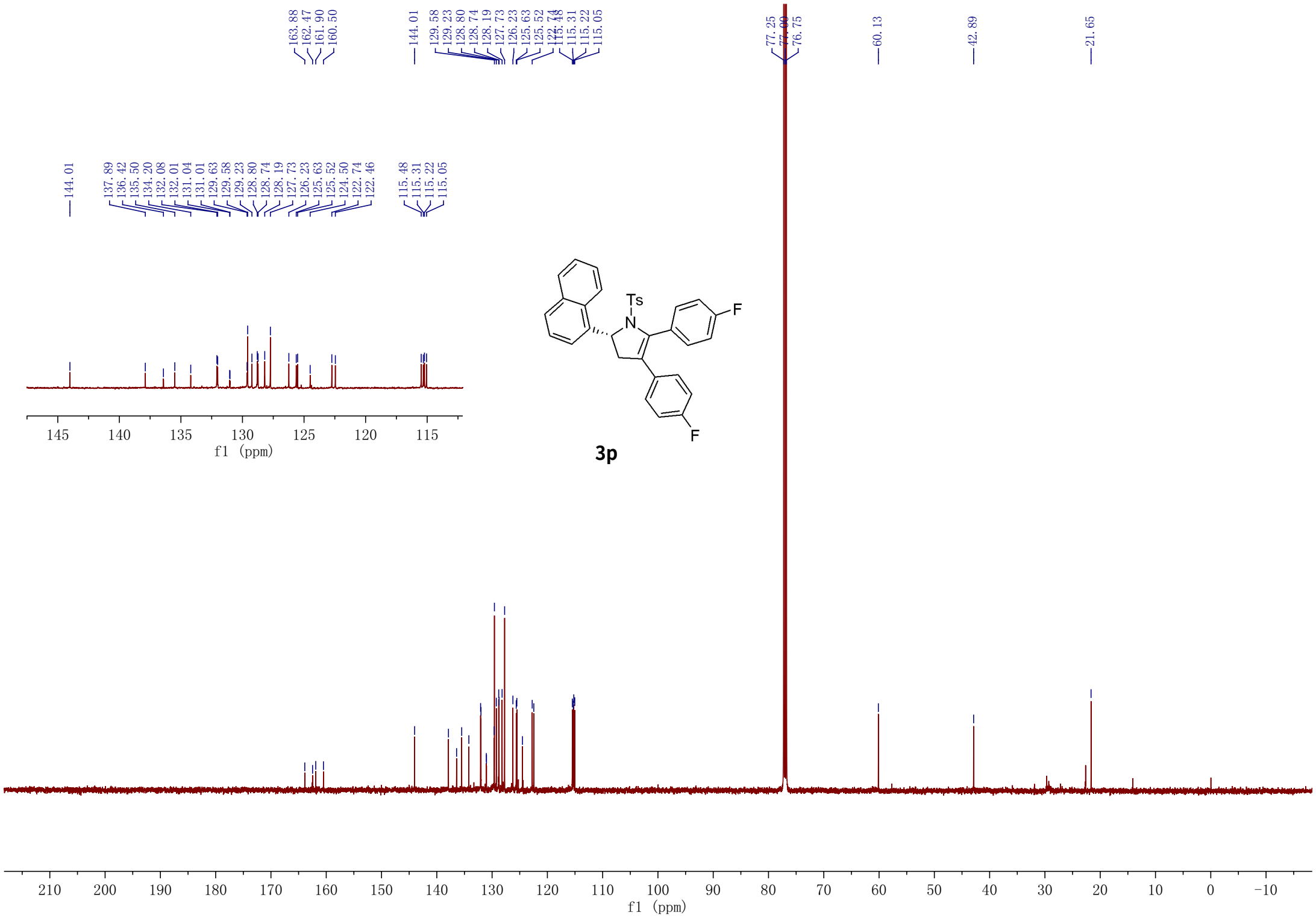

163.73
162.48
161.75
160.51
159.15
143.85
135.57
134.69
131.79
131.72
129.47
128.74
128.68
127.57
127.10
115.30
115.15
115.13
114.11
77.25
77.00
76.75
62.29
55.26
41.45
21.58
135.90
135.57
134.69
131.79
131.72
131.16
131.14
129.47
128.74
128.68
128.24
128.21
127.57
127.10
124.64
MeO
Ts
N
F
F
3n
138
136
134
132
130
128
126
124
122
f1 (ppm)
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)

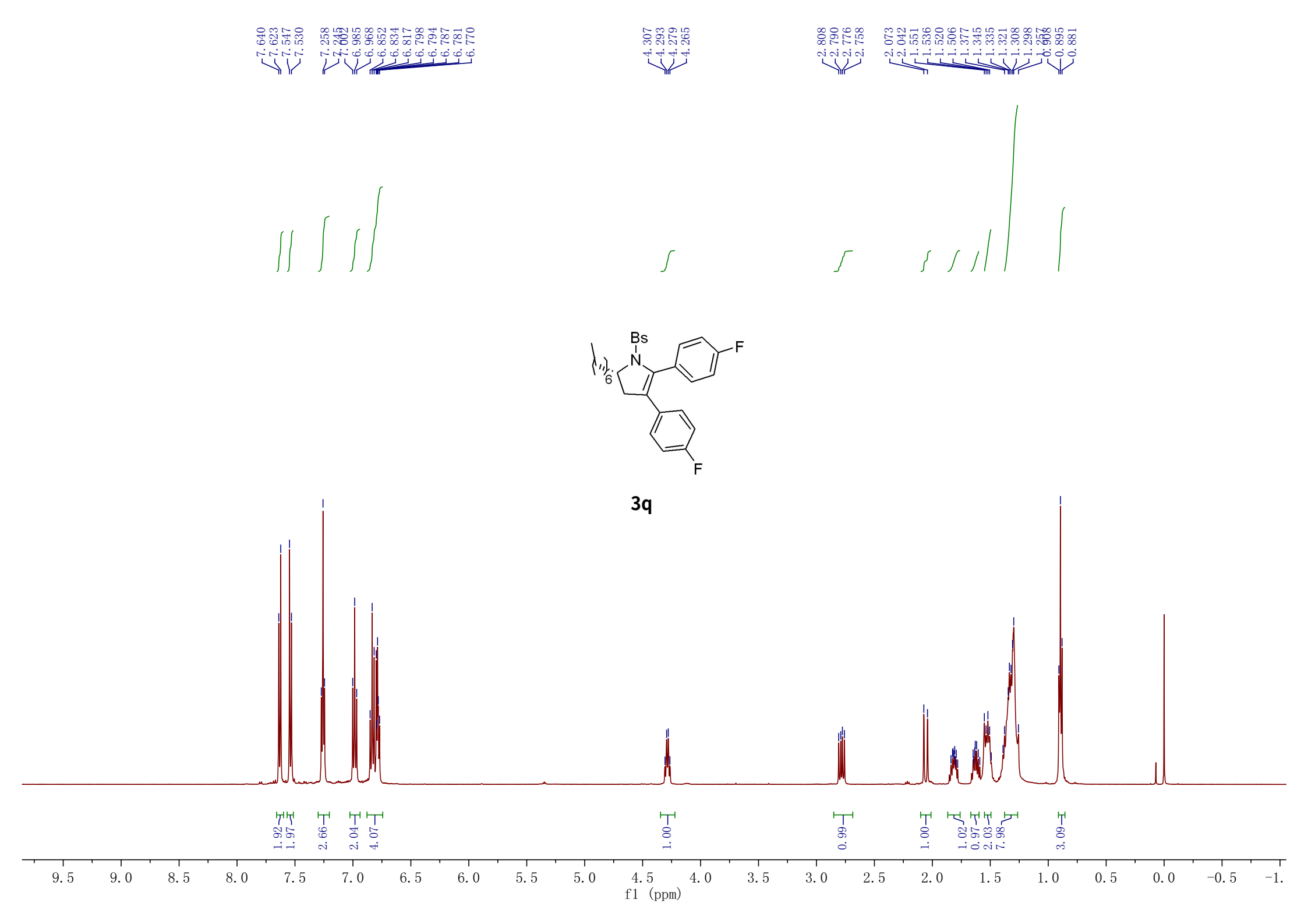

7.799
7.797
7.784
7.781
7.596
7.579
7.451
7.447
7.440
7.433
7.427
7.423
7.413
7.398
7.327
7.311
7.260
7.183
7.180
7.063
7.045
6.794
6.782
6.767
5.702
5.697
5.681
5.676
3.423
3.403
3.391
3.370
2.476
2.350
2.345
2.318
2.313
Ts
N
F
Br
F
1.02
3.00
3.05
2.06
1.05
2.06
3.98
1.00
1.00
2.96
1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

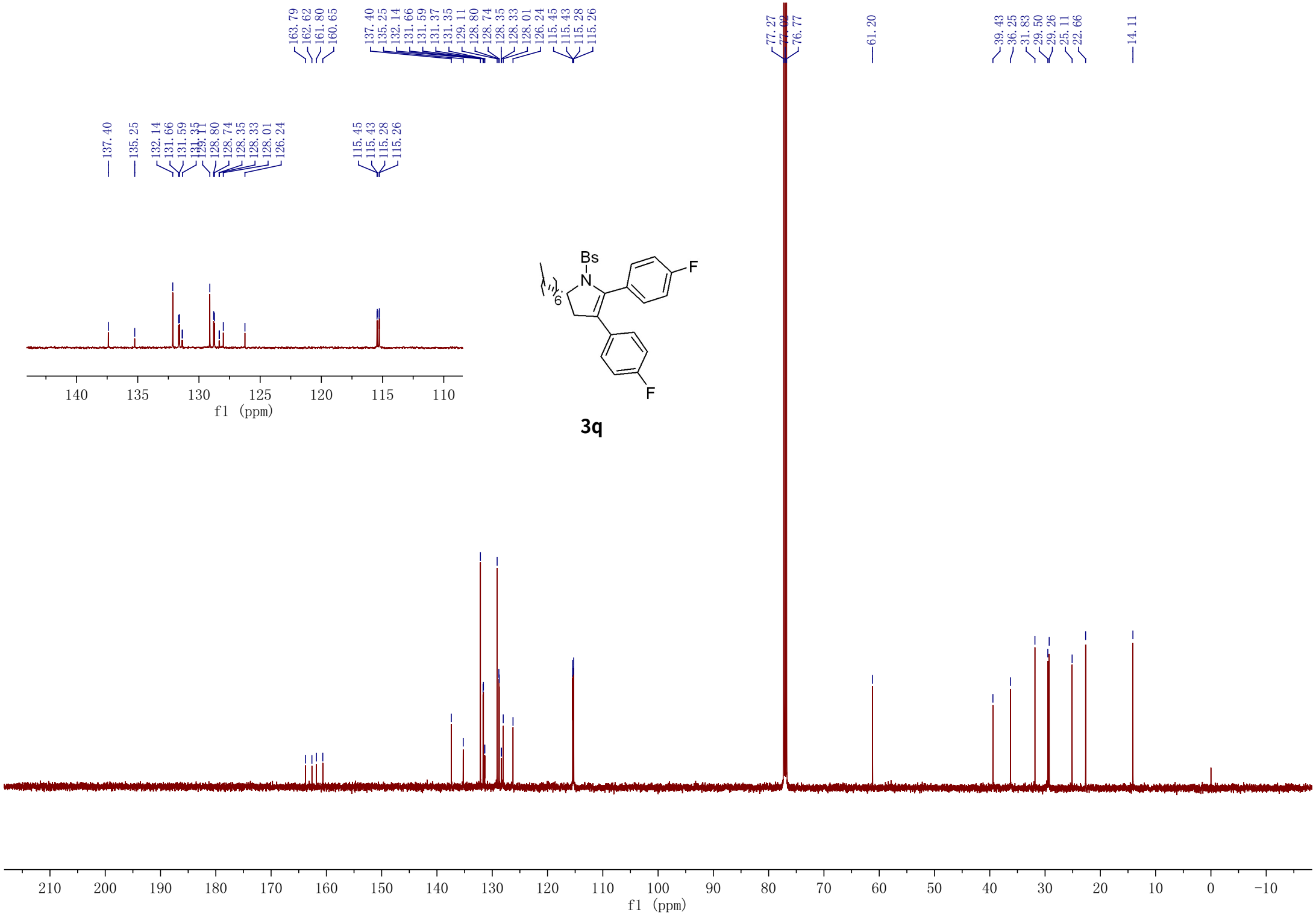
3o

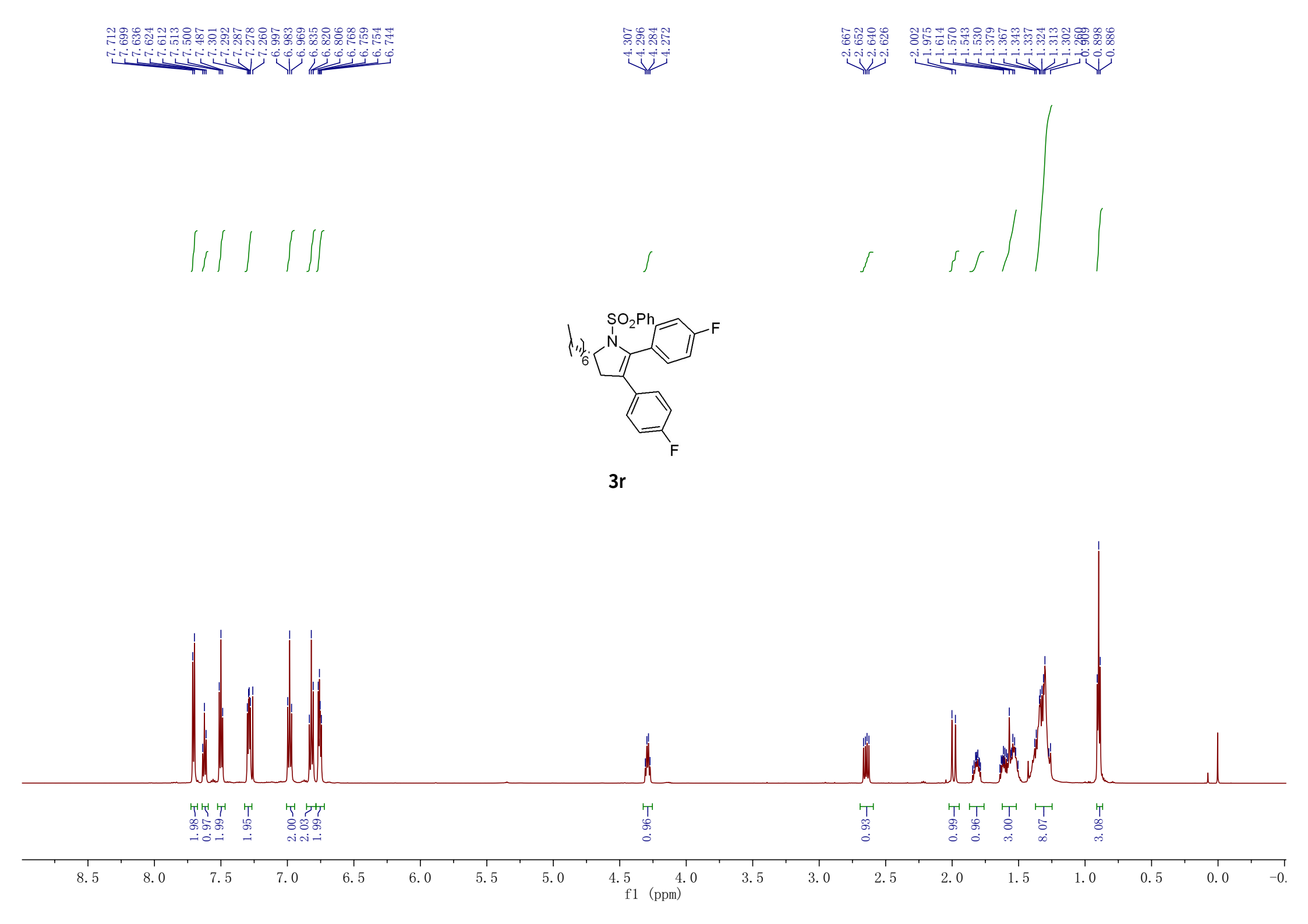

163.91
162.52
161.93
160.55
144.16
141.95
133.05
131.95
129.64
129.05
128.87
128.81
127.81
127.77
126.87
115.34
115.28
115.11
77.25
77.00
76.75
62.22
42.36
21.66
136.35
134.96
133.05
132.01
131.95
130.94
130.91
129.64
129.05
128.87
128.81
128.03
128.00
127.81
127.77
126.87
123.63
121.68
Ts
N
F
Br
F
3o
135
130
125
120
f1 (ppm)
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)


7.976
7.962
7.910
7.906
7.896
7.889
7.829
7.813
7.604
7.588
7.322
7.306
7.260
7.061
7.044
6.774
6.768
6.763
6.757
6.747
6.192
6.188
6.171
3.592
3.571
3.560
3.540
2.510
2.505
2.483
2.474
Ts
N
F
F
3p
0.98
2.01
1.02
6.96
2.00
2.00
3.96
0.99
1.00
1.01
3.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

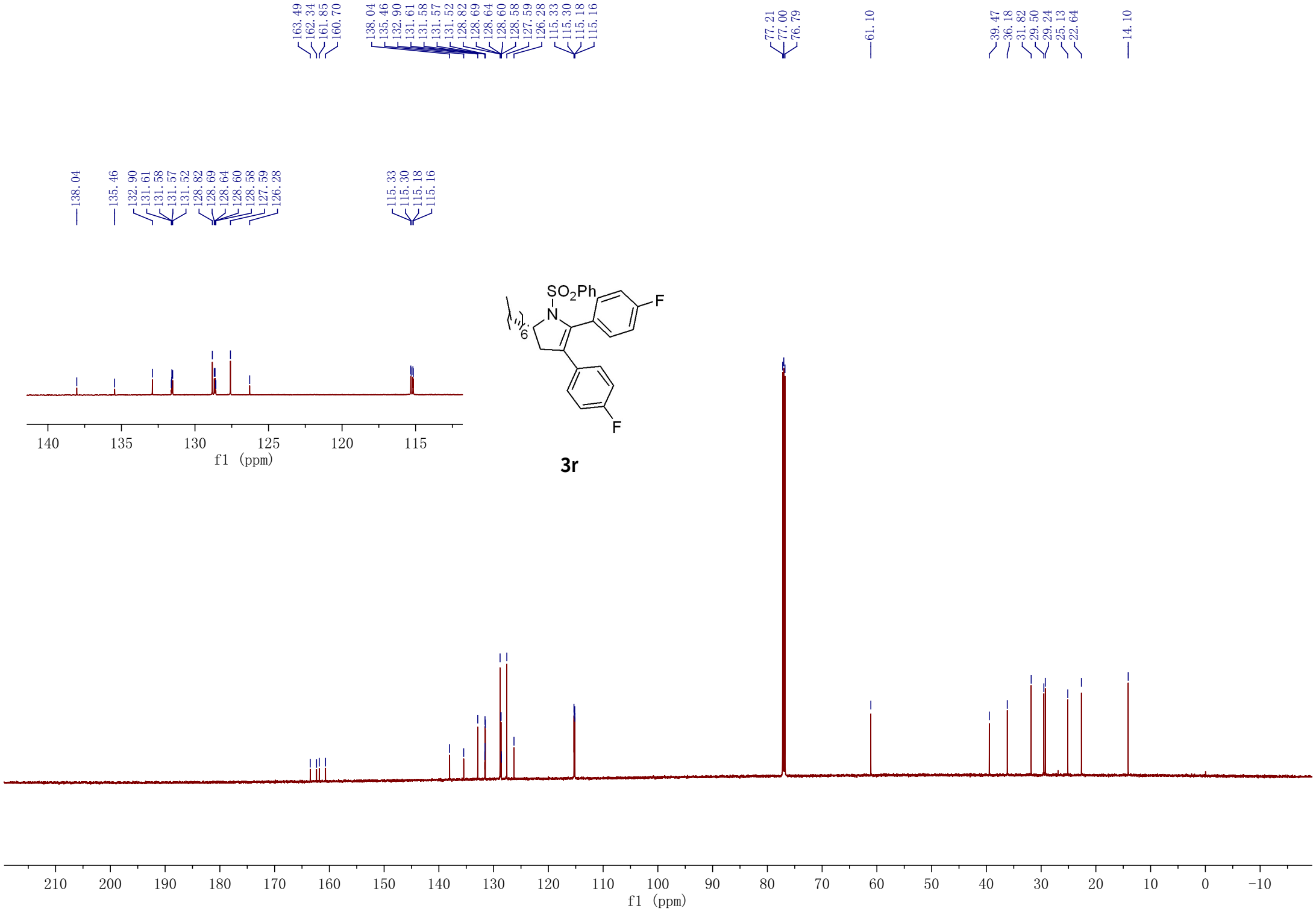

163.88
162.47
161.90
160.50
144.01
129.58
129.23
128.80
128.74
128.19
127.73
126.23
125.63
125.52
122.74
115.48
115.31
115.22
115.05
77.25
77.00
76.75
60.13
42.89
21.65
144.01
137.89
136.42
135.50
134.20
132.08
132.01
131.04
131.01
129.63
129.58
129.23
128.80
128.74
128.19
127.73
126.23
125.63
125.52
124.50
122.74
122.46
115.48
115.31
115.22
115.05
145
140
135
130
125
120
115
f1 (ppm)
Ts
N
F
F
3p
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)

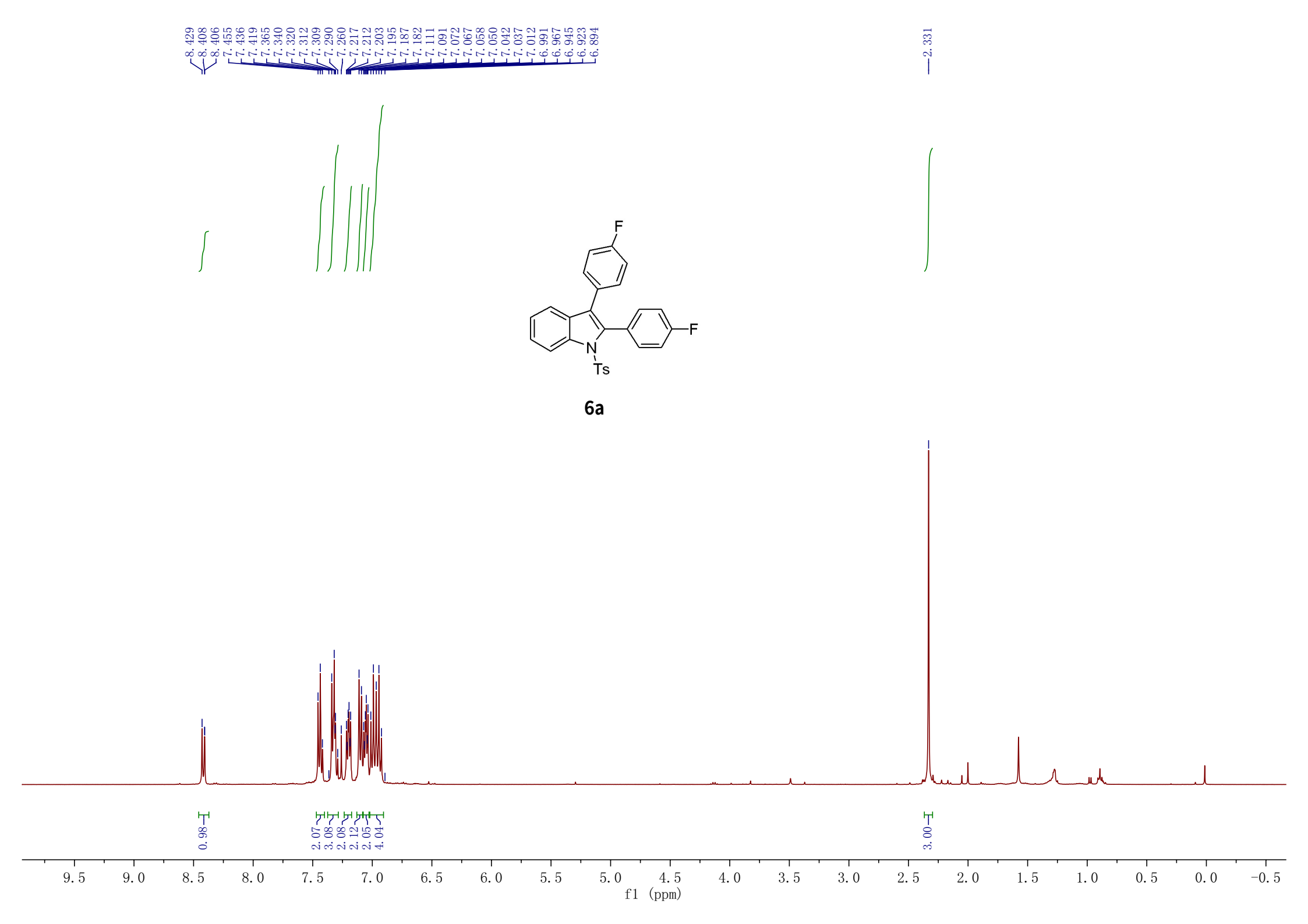

7.640
7.623
7.547
7.530
7.258
7.245
7.002
6.985
6.968
6.852
6.834
6.817
6.798
6.794
6.787
6.781
6.770
4.307
4.293
4.279
4.265
2.808
2.790
2.776
2.758
2.073
2.042
1.551
1.536
1.520
1.506
1.377
1.345
1.335
1.321
1.308
1.298
0.895
0.881
Bs
N
6
F
F
3q
1.92
1.97
2.66
2.04
4.07
1.00
0.99
1.00
1.02
0.97
2.03
7.98
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)


163.79
162.62
161.80
160.65
137.40
135.25
132.14
131.66
131.59
131.37
131.35
129.11
128.80
128.74
128.35
128.33
128.01
126.24
115.45
115.43
115.28
115.26
77.27
77.02
76.77
61.20
39.43
36.25
31.83
29.50
29.26
25.11
22.66
14.11
Bs
N
6
F
F
3q
f1 (ppm)
f1 (ppm)

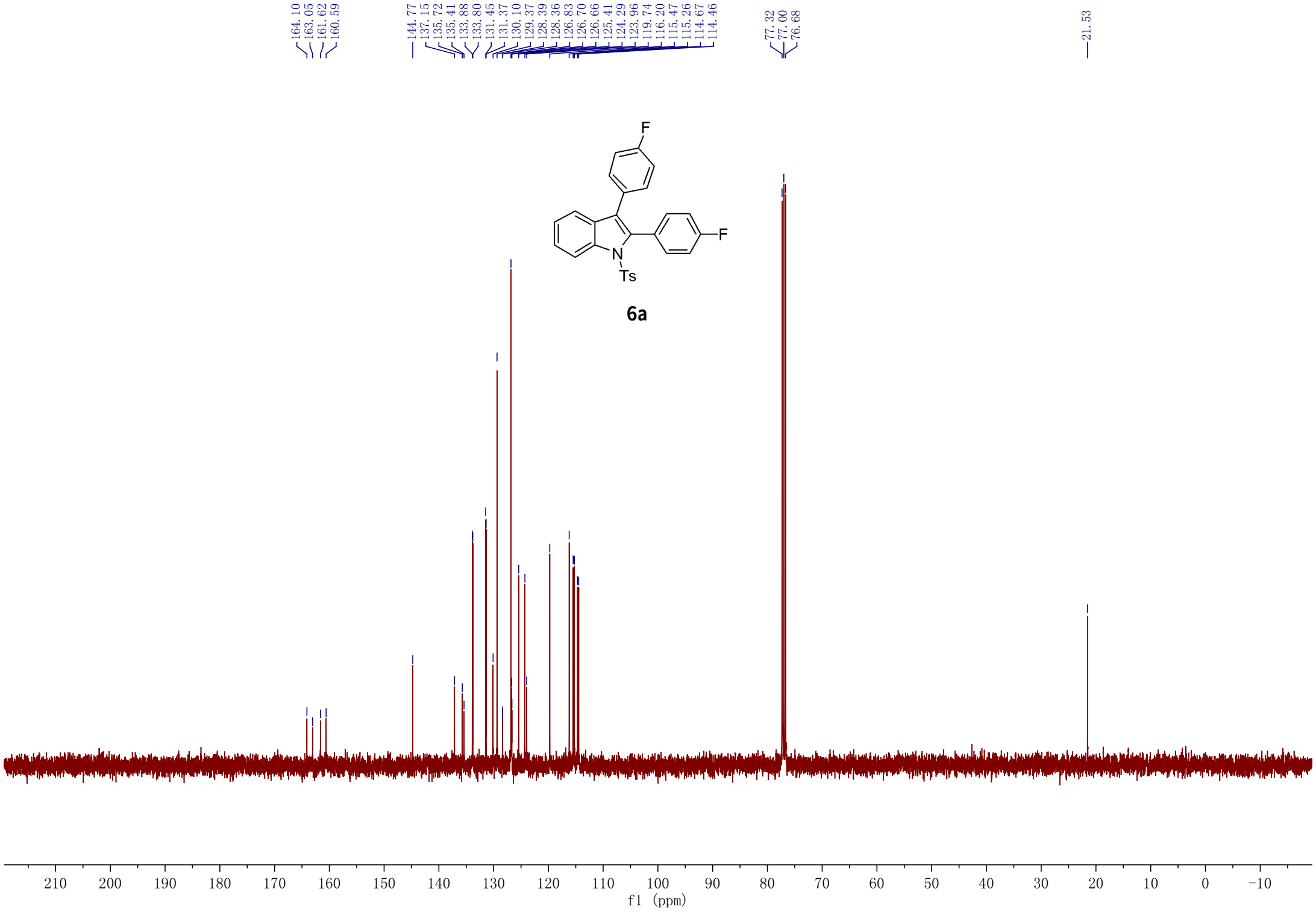

7.712
7.699
7.636
7.624
7.612
7.513
7.500
7.487
7.301
7.292
7.287
7.278
7.260
6.997
6.983
6.969
6.835
6.820
6.806
6.768
6.759
6.754
6.744
4.307
4.296
4.284
4.272
2.667
2.652
2.640
2.626
2.002
1.975
1.614
1.570
1.543
1.530
1.379
1.367
1.343
1.337
1.324
1.313
1.302
0.909
0.898
0.886
SO2Ph
N
F
F
6
1.98
0.97
1.99
1.95
2.00
2.03
1.99
0.96
0.93
0.99
0.96
3.00
8.07
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

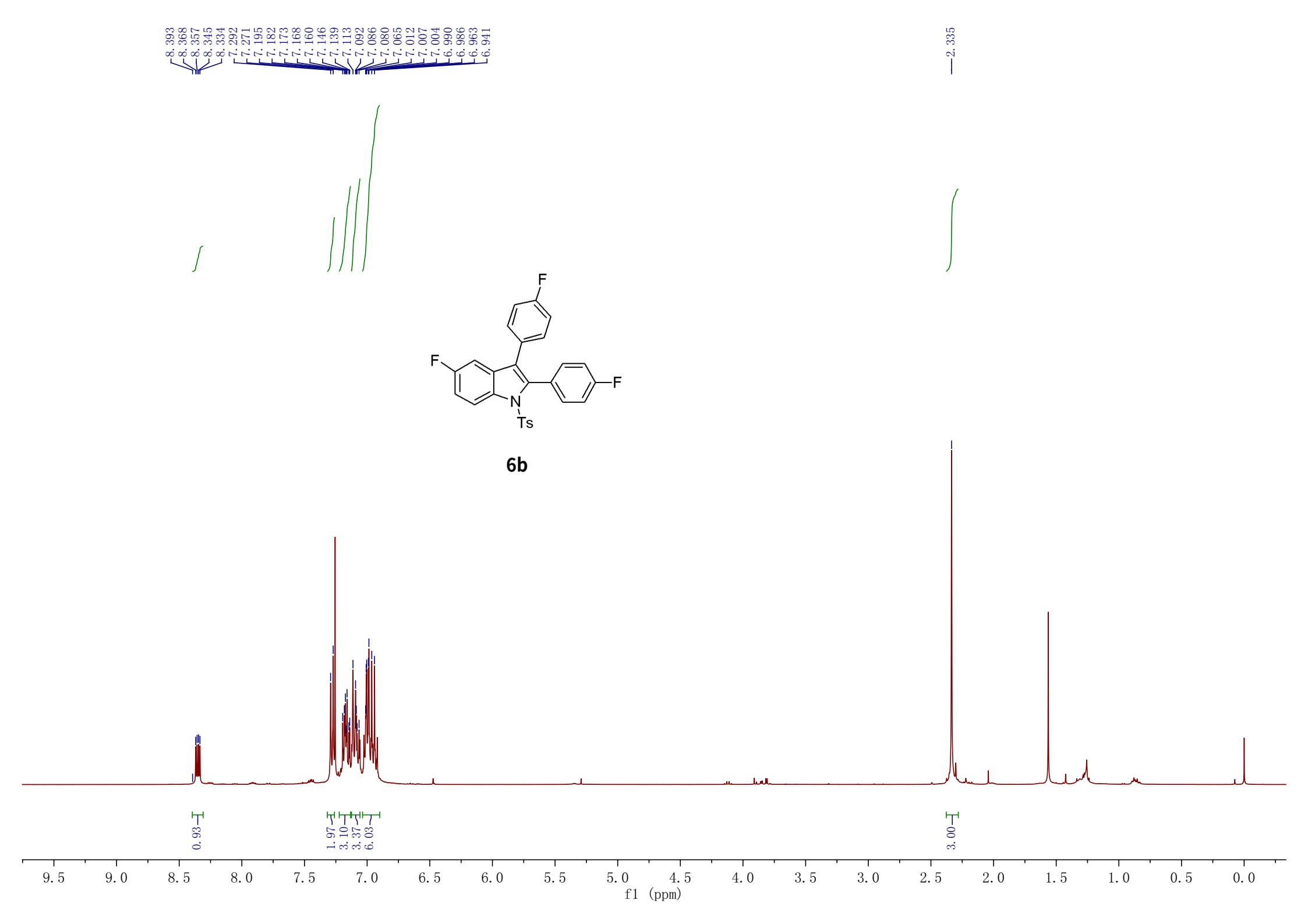
3r

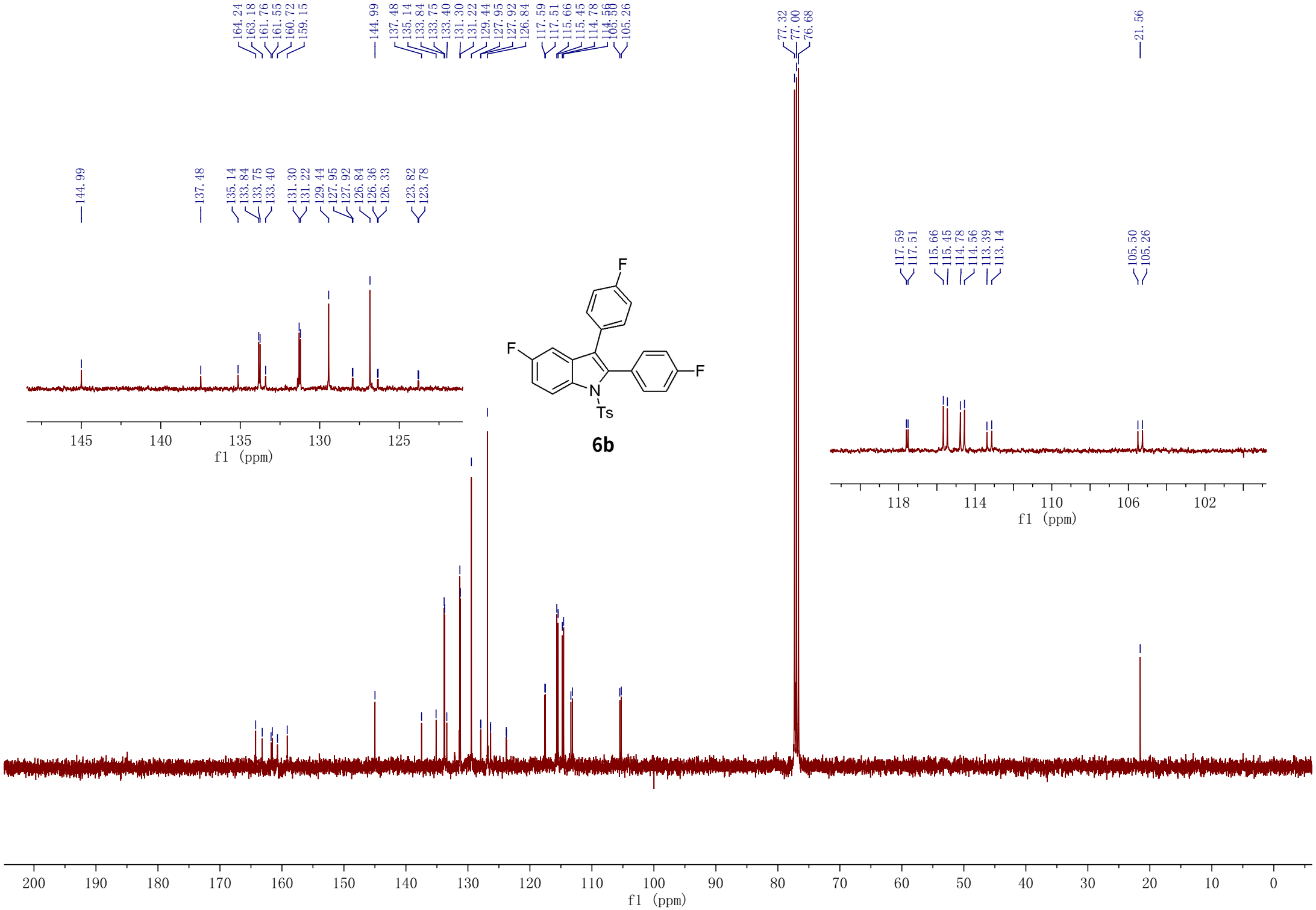

163.49
162.34
161.85
160.70
138.04
135.46
132.90
131.61
131.58
131.57
131.52
128.82
128.69
128.64
128.60
128.58
127.59
126.28
115.33
115.30
115.18
115.16
77.21
77.00
76.79
61.10
39.47
36.18
31.82
29.50
29.24
25.13
22.64
14.10
SO2Ph
N
F
F
6
3r
f1 (ppm)
f1 (ppm)

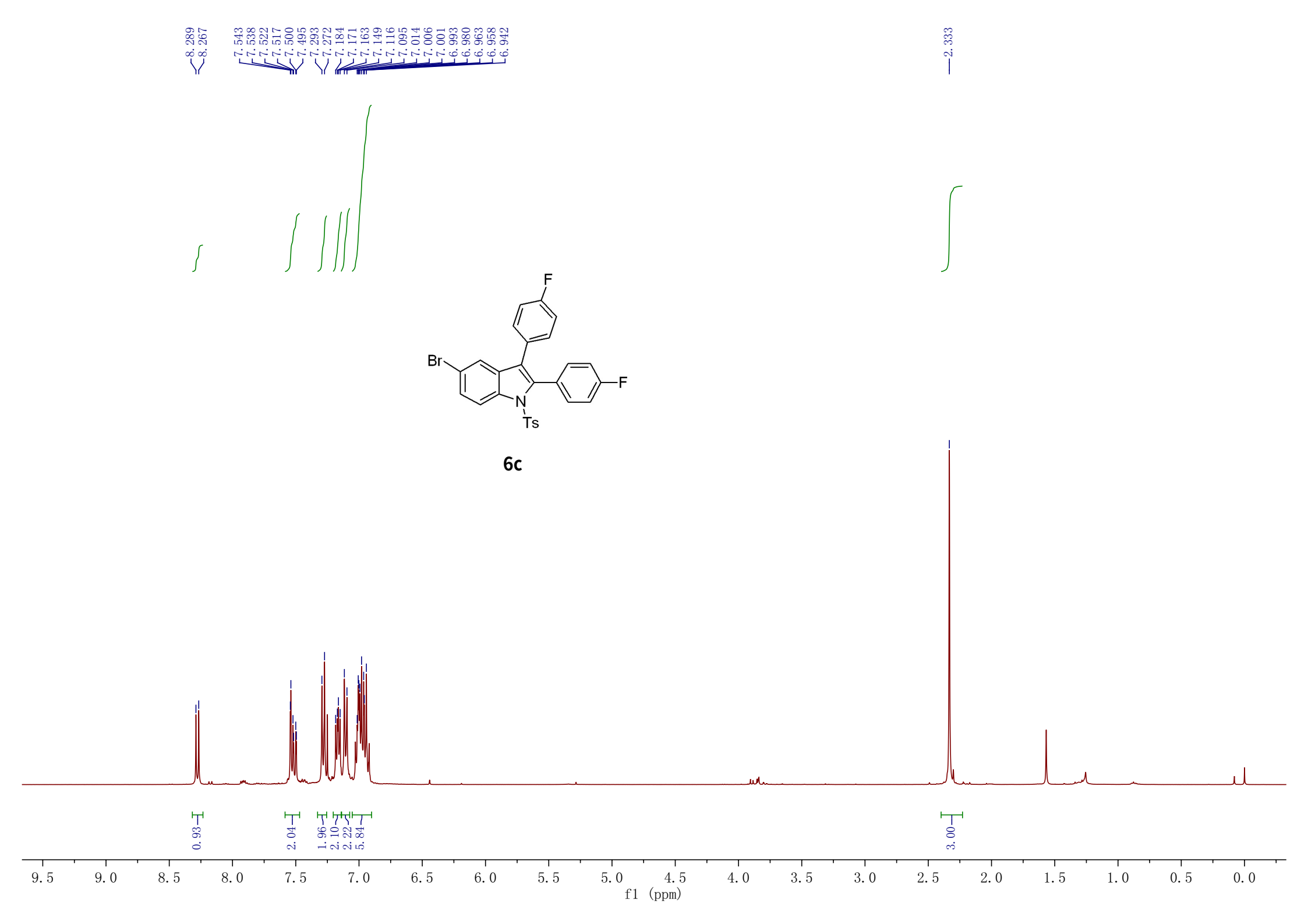

8.429
8.408
8.406
7.455
7.436
7.419
7.365
7.340
7.320
7.312
7.309
7.290
7.260
7.217
7.212
7.203
7.195
7.187
7.182
7.111
7.091
7.072
7.067
7.058
7.050
7.042
7.037
7.012
6.991
6.967
6.945
6.923
6.894
2.331
F
F
N
Ts
0.98
2.07
3.08
2.08
2.12
2.05
4.04
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

6a

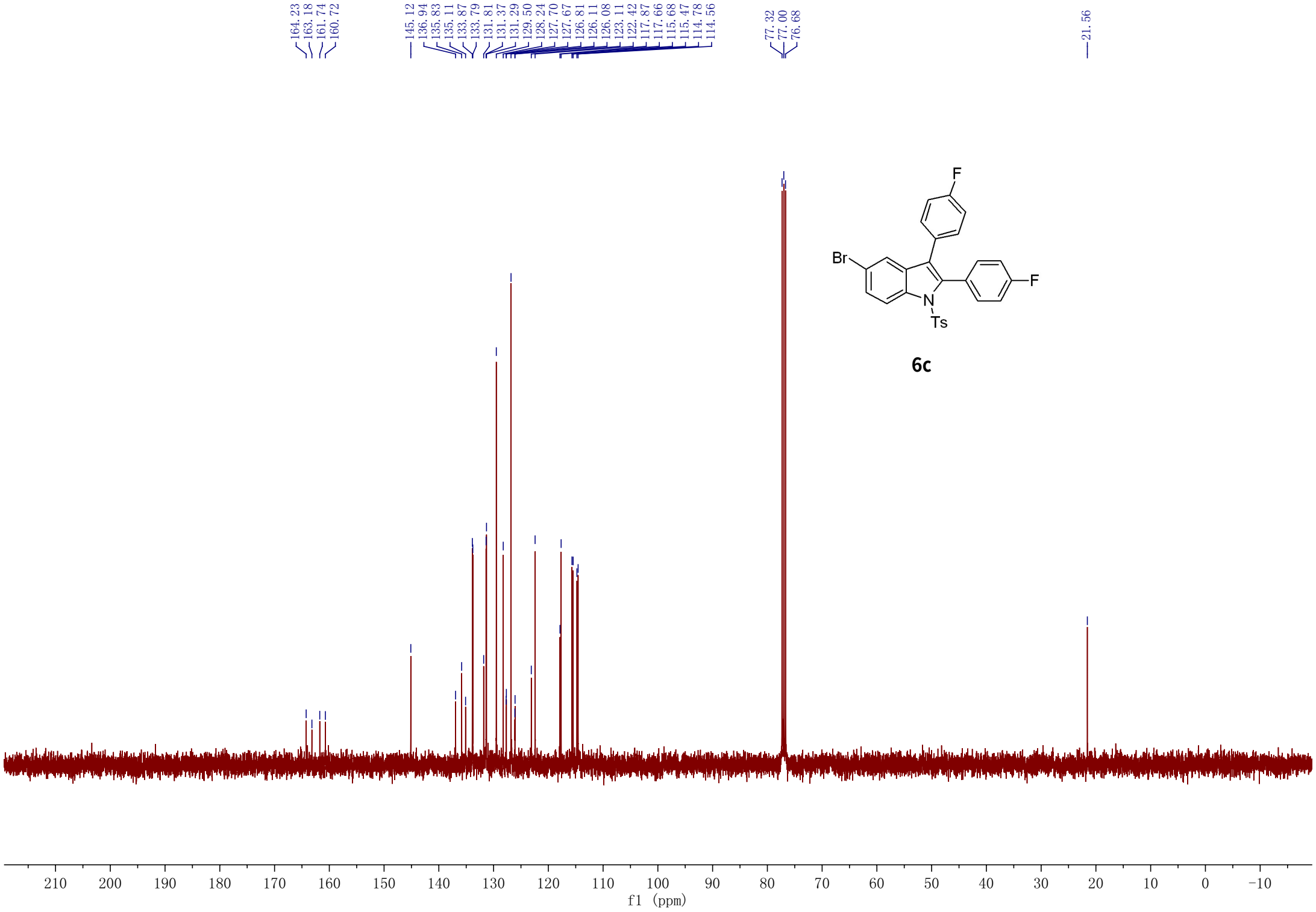

164.10
163.05
161.62
160.59
144.77
137.15
135.72
135.41
133.88
133.80
131.45
131.37
130.10
129.37
128.39
128.36
126.83
126.70
126.66
125.41
124.29
123.96
119.74
116.20
115.47
115.26
114.67
114.46
77.32
77.00
76.68
21.53
F
F
N
Ts
6a
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

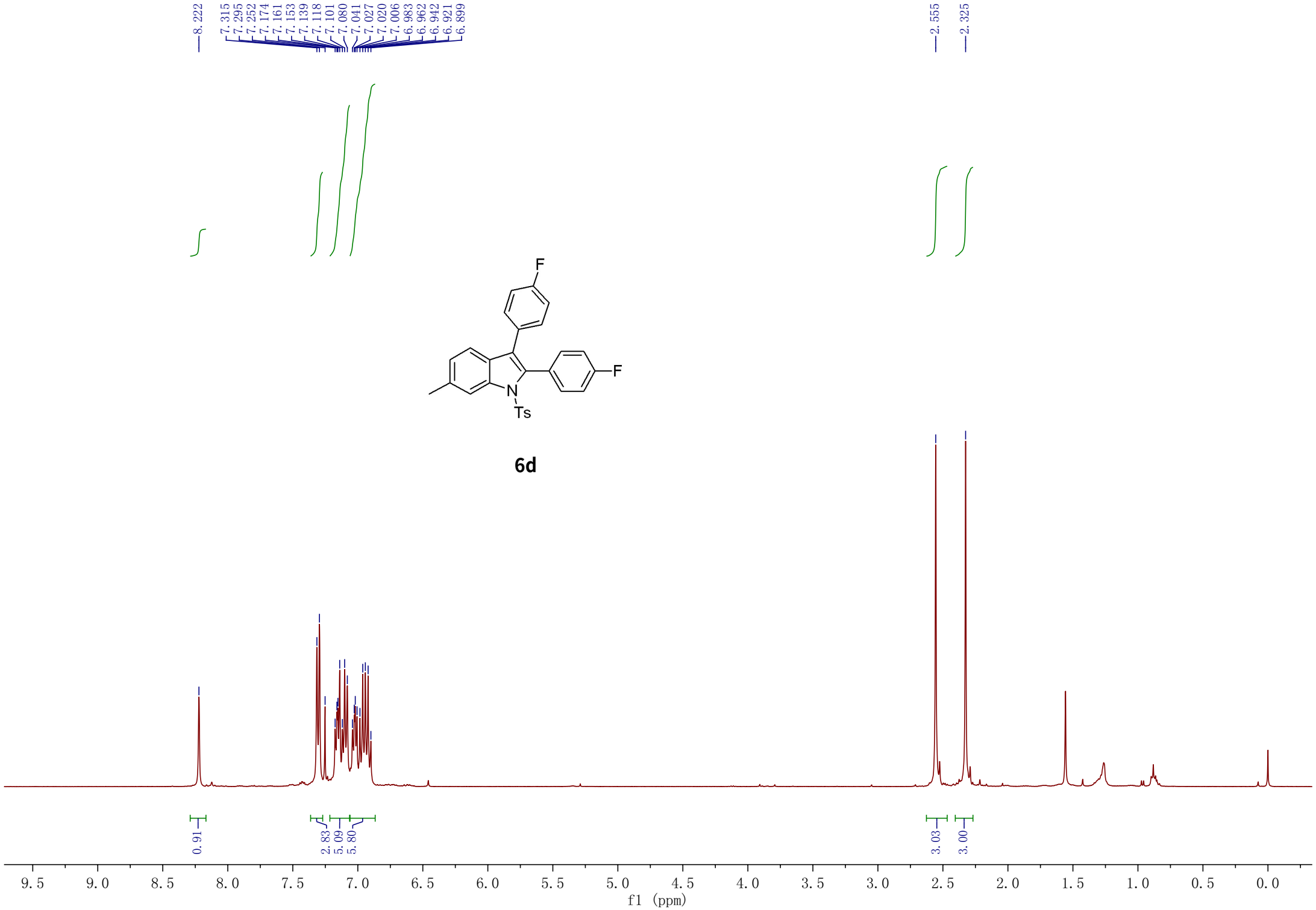

8.393
8.368
8.357
8.345
8.334
7.292
7.271
7.195
7.182
7.173
7.168
7.160
7.146
7.139
7.113
7.092
7.086
7.080
7.065
7.012
7.007
7.004
6.990
6.986
6.963
6.941
2.335
F
F
F
N
Ts
6b
0.93
1.97
3.10
3.37
6.03
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

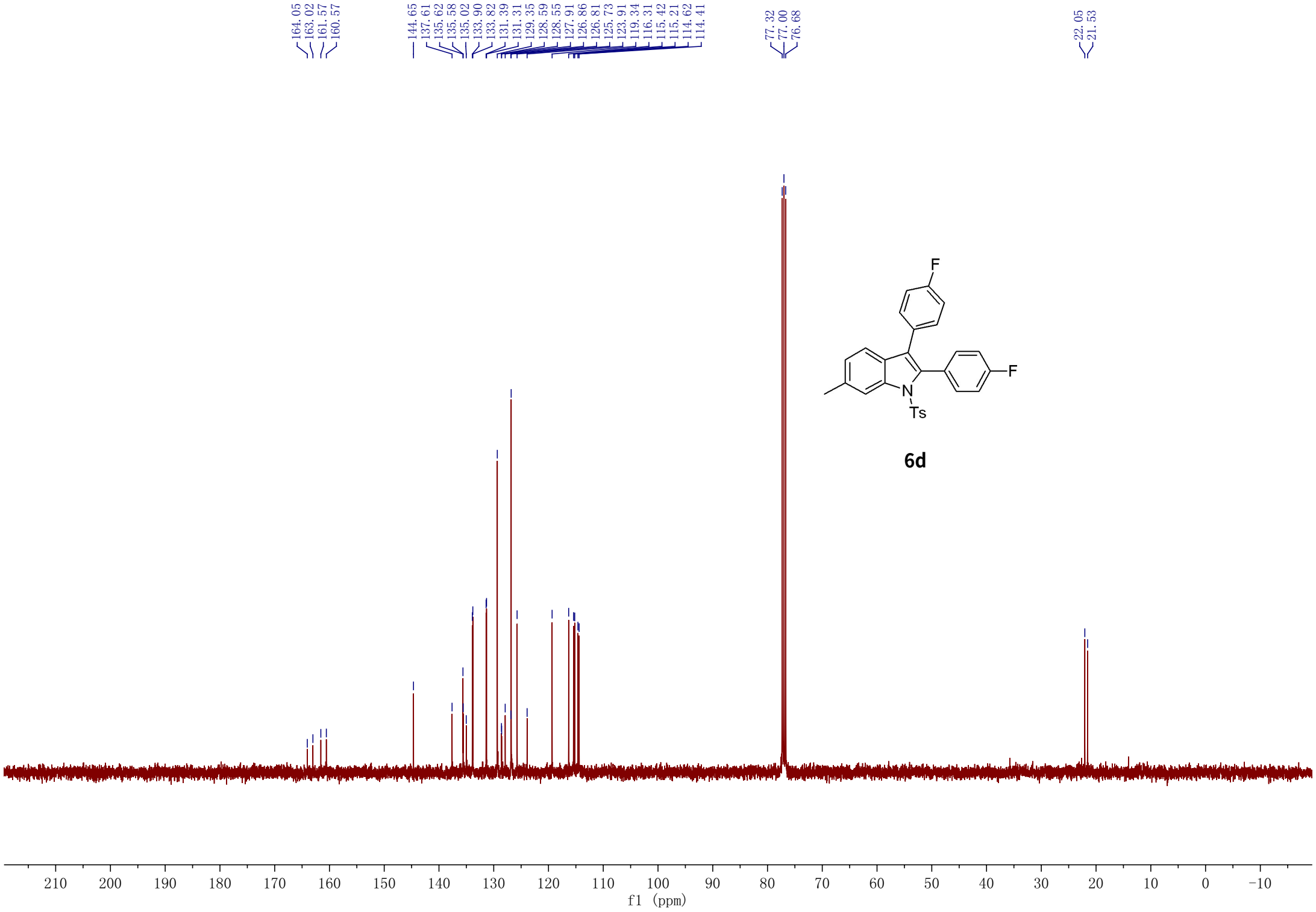

164.24
163.18
161.76
161.55
160.72
159.15
144.99
137.48
135.14
133.84
133.75
133.40
131.30
131.22
129.44
127.95
127.92
126.84
117.59
117.51
115.66
115.45
114.78
114.56
105.50
105.26
77.32
77.00
76.68
21.56
F
F
F
N
Ts
6b
f1 (ppm)

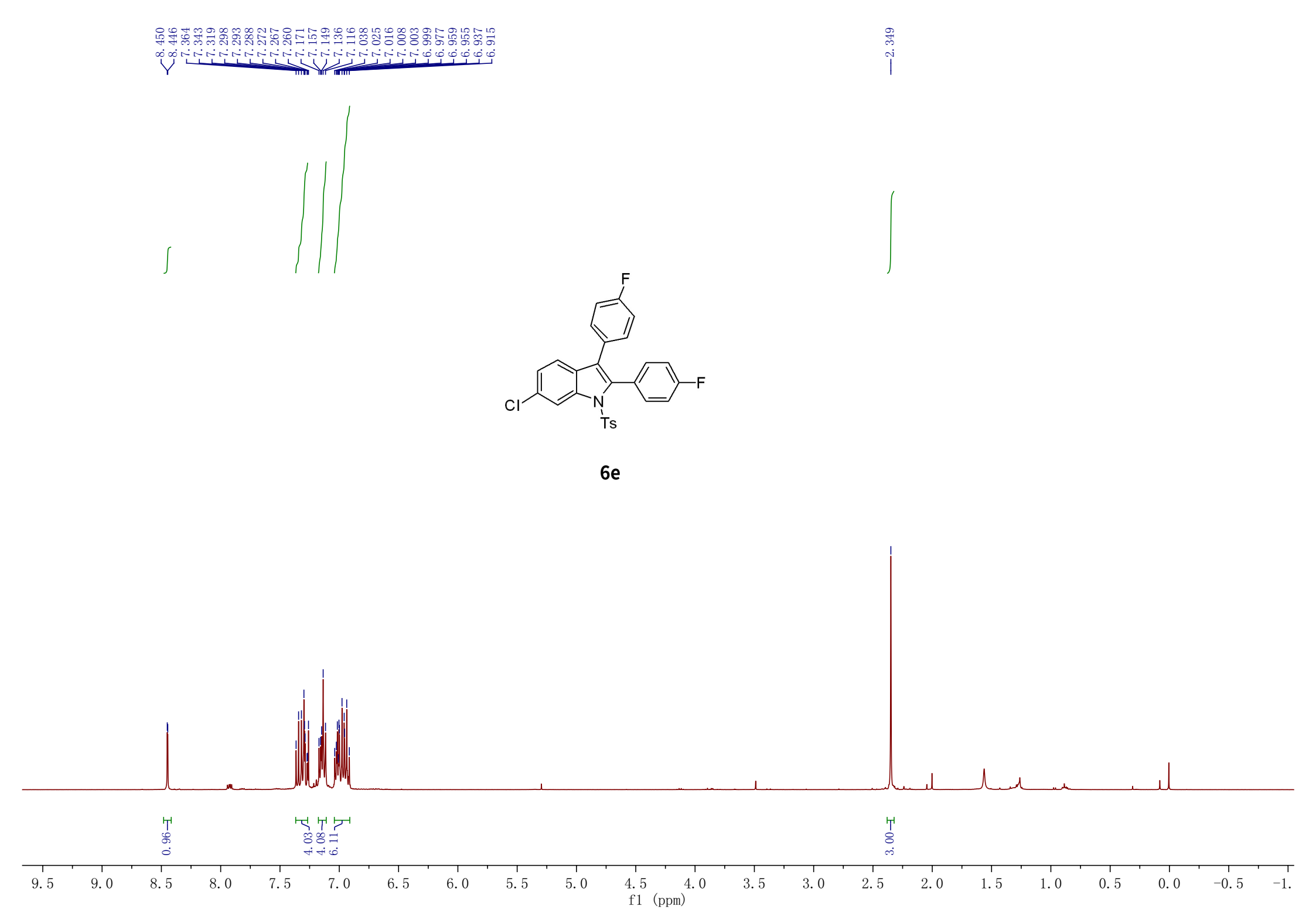

8.289
8.267
7.543
7.538
7.522
7.517
7.500
7.495
7.293
7.272
7.184
7.171
7.163
7.149
7.116
7.095
7.014
7.006
7.001
6.993
6.980
6.963
6.958
6.942
2.333
F
Br
F
N
Ts
0.93
2.04
1.96
2.10
2.22
5.84
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

6c

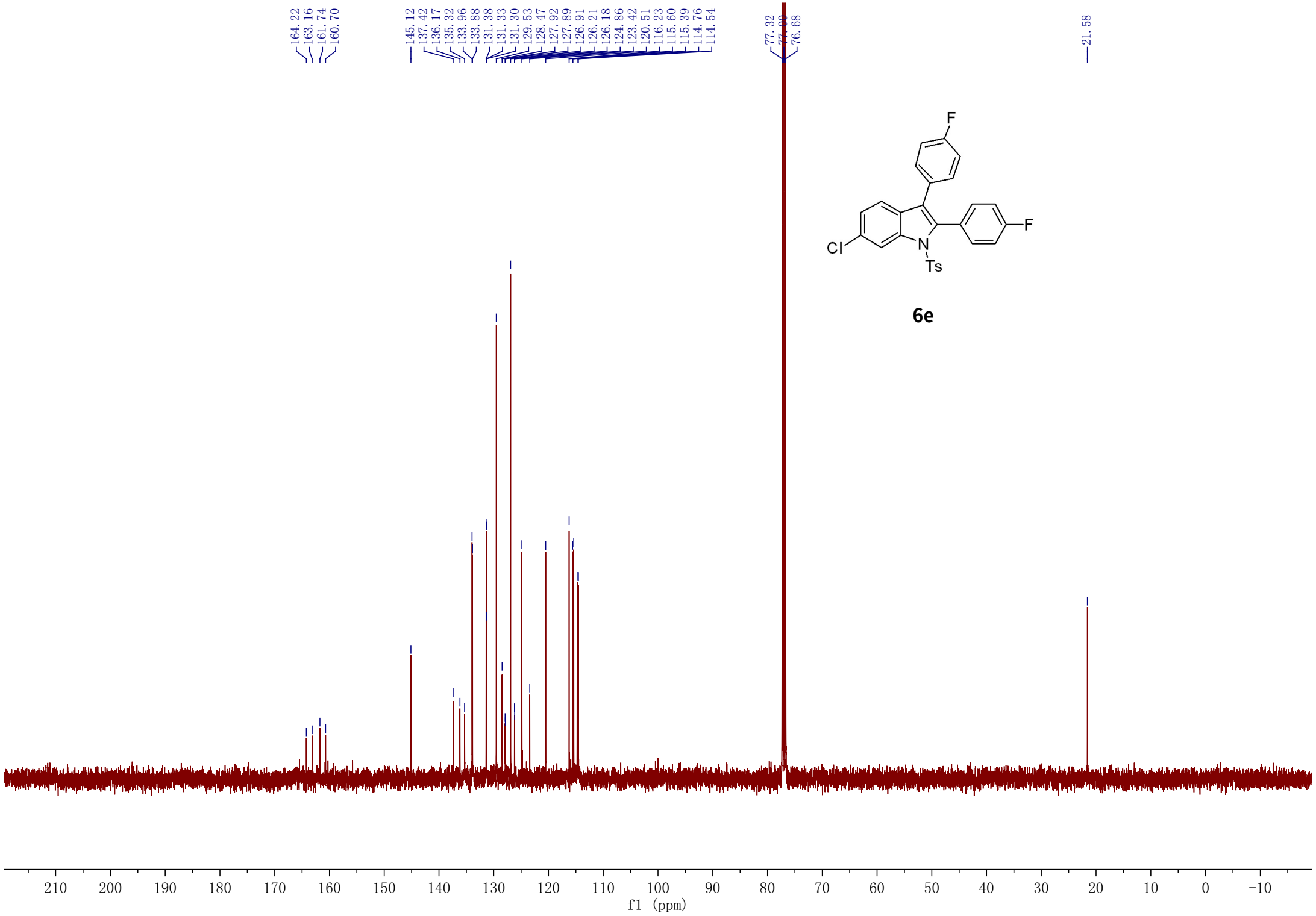

164.23
163.18
161.74
160.72
145.12
136.94
135.83
135.11
133.87
133.79
131.81
131.37
131.29
129.50
128.24
127.70
127.67
126.81
126.11
126.08
123.11
122.42
117.87
117.66
115.68
115.47
114.78
114.56
77.32
77.00
76.68
21.56
F
Br
F
N
Ts
6c
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

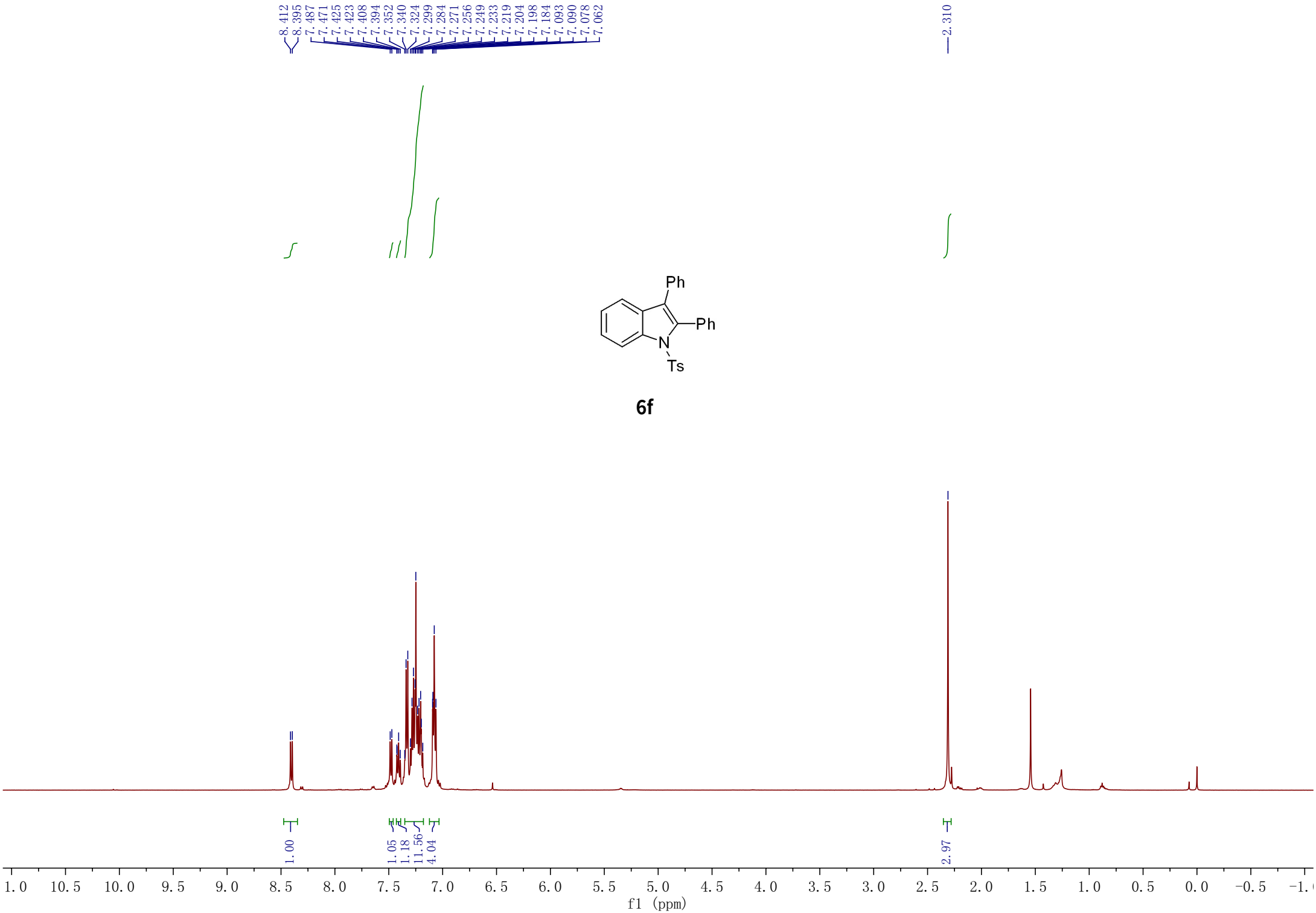

8.222
7.315
7.295
7.252
7.174
7.161
7.153
7.139
7.118
7.101
7.080
7.041
7.027
7.020
7.006
6.983
6.962
6.942
6.921
6.899
2.555
2.325
F
F
N
Ts
6d
0.91
2.83
5.09
5.80
3.03
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


164.05
163.02
161.57
160.57
144.65
137.61
135.62
135.58
135.02
133.90
133.82
131.39
131.31
129.35
128.59
128.55
127.91
126.86
126.81
125.73
123.91
119.34
116.31
115.42
115.21
114.62
114.41
77.32
77.00
76.68
22.05
21.53
F
F
N
Ts
6d
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)

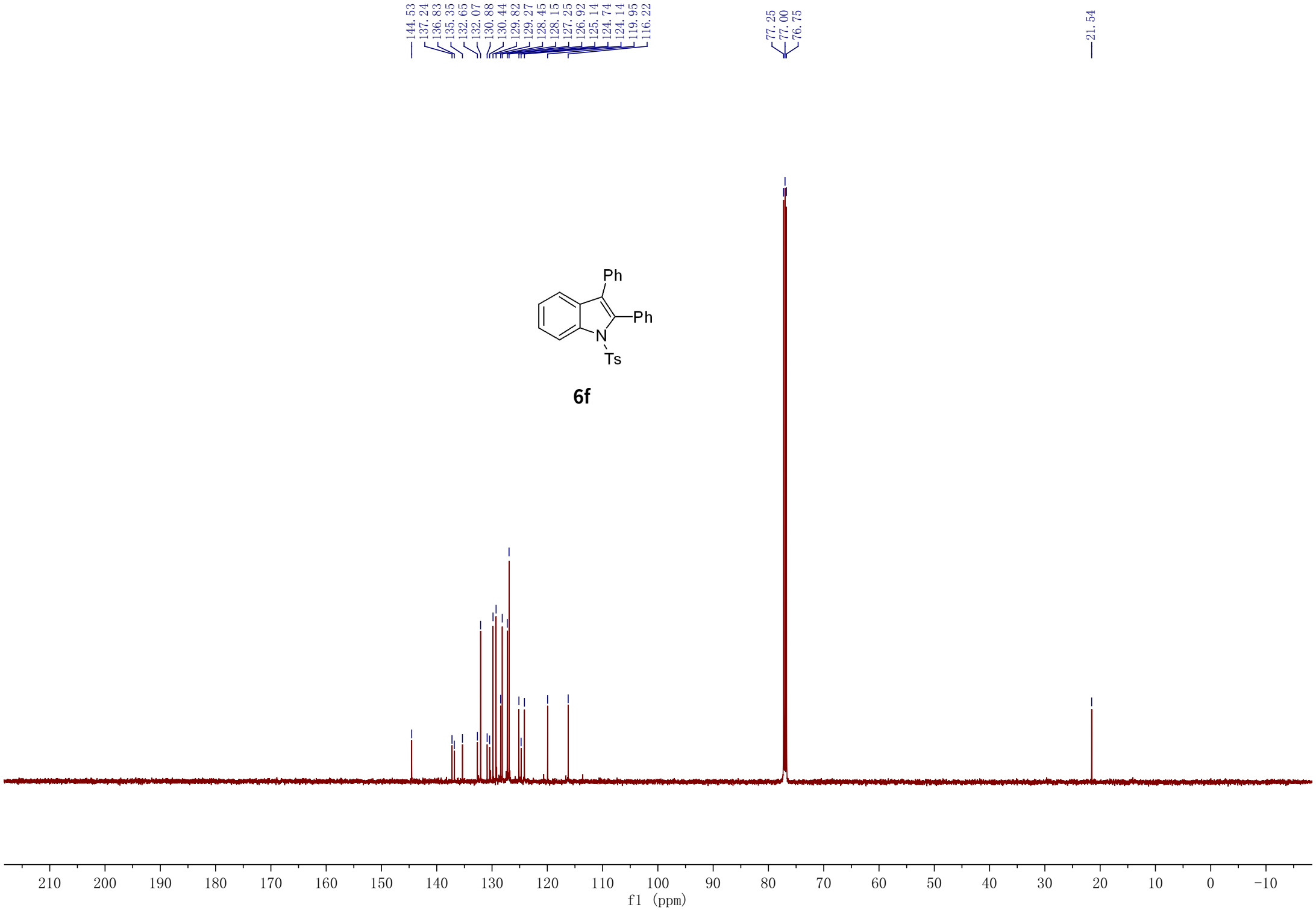

8.450
8.446
7.364
7.343
7.319
7.298
7.293
7.288
7.272
7.267
7.260
7.171
7.157
7.149
7.136
7.116
7.038
7.025
7.016
7.008
7.003
6.999
6.977
6.959
6.955
6.937
6.915
2.349
F
F
Cl
N
Ts
0.96
4.03
4.08
6.11
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.
f1 (ppm)

6e


164.22
163.16
161.74
160.70
145.12
137.42
136.17
135.32
133.96
133.88
131.38
131.33
131.30
129.53
128.47
127.92
127.89
126.91
126.21
126.18
124.86
123.42
120.51
116.23
115.60
115.39
114.76
114.54
77.32
77.00
76.68
21.58
F
F
Cl
N
Ts
6e
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)


8.412
8.395
7.487
7.471
7.425
7.423
7.408
7.394
7.352
7.340
7.324
7.299
7.284
7.271
7.256
7.249
7.233
7.219
7.204
7.198
7.184
7.093
7.090
7.078
7.062
2.310
Ph
Ph
N
Ts
1.00
1.05
1.18
11.56
4.04
2.97
f1 (ppm)

6f


144.53
137.24
136.83
135.35
132.65
132.07
130.88
130.44
129.82
129.27
128.45
128.15
127.25
126.92
125.14
124.74
124.14
119.95
116.22
77.25
77.00
76.75
21.54
Ph
Ph
N
Ts
6f
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)