melenSupporting Information

$B(3,4,5\text{-}F_3H_2C_6)_3$ Lewis acid-catalysed C3-allylation of indoles

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Contents

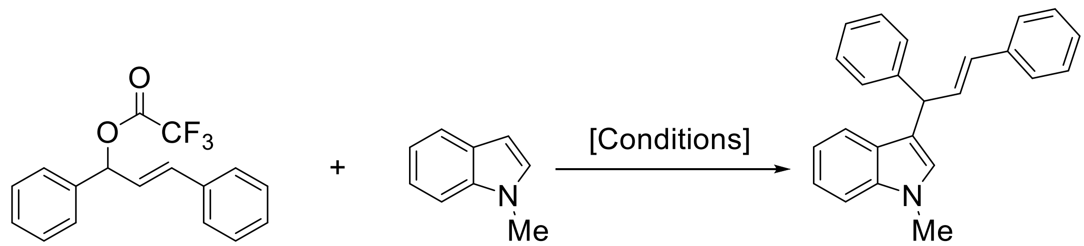
1. Experimental

1.1 General experimental

Except for the starting materials, all reactions and manipulations were carried out under an atmosphere of dry, O_2-free nitrogen using standard double-manifold techniques with a rotary oil pump. A nitrogen-filled glove box (MBraun) was used to manipulate solids including the storage of starting materials, ambient temperature reactions, product recovery and sample preparation for analysis. Dichloromethane was dried by employing a solvent purification system MB SPS-800 and stored under a nitrogen atmosphere. Anhydrous (with Sure/Seal) 1,2-dichloroethane (1,2-$C_2H_4Cl_2$) was purchased from Merck and dried over molecular sieves before use. Chloroform was dried over calcium hydride followed by distillation under nitrogen atmosphere before use. Chemicals were purchased from commercial suppliers and used as received. All the triarylfluoroboranes were prepared as per the standard literature report.[1] Thin-layer chromatography (TLC) was performed on pre-coated aluminium sheets of Merck silica gel 60 F254 (0.20 mm). ^{1}H, ^{13}C{^{1}H}, and ^{19}F NMR spectra were recorded on a Bruker Avance II 400 or Bruker Avance 500 spectrometer. All coupling constants are absolute values and are expressed in Hertz (Hz). ^{13}C{^{1}H} NMR was measured as ^{1}H decoupled. Yields are given as isolated yields. Chemical shifts are expressed as parts per million (ppm, δ) downfield of tetramethylsilane (TMS) and are referenced to $CDCl_3$ (7.26/77.16 ppm) as internal standard. The description of signals includes s = singlet, d = doublet, t = triplet, q = quartet, and m = multiplet, br = broad. All coupling constants are absolute values and are expressed in Hertz (Hz). All spectra were analysed assuming a first order approximation. IR-Spectra were measured on a Shimadzu IRAffinity-1 photo-spectrometer. Mass spectra were measured on a Waters LCT Premier/XE or a Waters GCT Premier spectrometer. Ions were generated by the Atmospheric Solids, Analysis Probe (ASAP), Electrospray (ES) or Electron Ionisation (EI). The molecular ion peaks values quoted for either molecular ion (M^+), molecular ion plus or minus hydrogen ($M+H^+$, $M-H^-$), molecular ion plus sodium ($M+Na^+$).

2. Reaction Optimisation

Table S1. Optimisation of the reaction conditions.



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

Entry	Catalyst	Loading (mol%)	Solvent	Temp (°C)	Time (h)	Yield[a] (%)
1	$B(C_6F_5)_3$	20	$1,2\text{-}C_2H_4Cl_2$	80	24	62
2	$B(C_6F_5)_3$	20	$1,2\text{-}C_2H_4Cl_2$	45	24	56
3	$B(C_6F_5)_3$	20	CH_2Cl_2	45	24	59
4	$B(C_6F_5)_3$	20	$CHCl_3$	45	24	73
5	$B(C_6F_5)_3$	20	$CHCl_3$	60	24	87
6	-	-	$CHCl_3$	60	24	n.d.
7	$B(C_6F_5)_3$	15	$CHCl_3$	60	24	90
8	$B(C_6F_5)_3$	10	$CHCl_3$	60	24	62
9	$B(C_6F_5)_3$	15	$CHCl_3$	60	15	84
10	$B(C_6F_5)_3$	15	$CHCl_3$	60	7	65
11	$B(C_6F_5)_3$[b]	15	$CHCl_3$	60	24	90
12	$B(C_6F_5)_3$[b,c]	15	$CHCl_3$	60	24	40
13	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	$CHCl_3$	60	24	97
14	$B(2,4,6\text{-}F_3H_2C_6)_3$[b]	15	$CHCl_3$	60	24	53
15	$BF_3{\bullet}OEt_2$[b]	15	$CHCl_3$	60	24	68
16	BPh_3[b]	15	$CHCl_3$	60	24	46
17	TFA	17	$CHCl_3$	60	24	68
18	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	10	$CHCl_3$	60	24	71
19	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	5	$CHCl_3$	60	24	65
20	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	$CHCl_3$	r.t	24	63
21	$B(3,4,5\text{-}F_3H_2C_6)_3$[b,c]	15	$CHCl_3$	r.t	24	n.d.
22	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	5	$CHCl_3$	60	24	65
23	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	10	$CHCl_3$	60	24	71
24	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	CH_2Cl_2	45	24	35
25	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	$1,2\text{-}C_2H_4Cl_2$	80	24	71
26	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	$CHCl_3$ (0.5mL)	60	24	69
27	$B(3,4,5\text{-}F_3H_2C_6)_3$[b]	15	$CHCl_3$ (2 mL)	60	24	94
28	$B(3,4,5\text{-}F_3H_2C_6)_3$[b,d]	15	$CHCl_3$	60	24	97
29	$B(3,4,5\text{-}F_3H_2C_6)_3$[b,e]	15	$CHCl_3$	60	24	91
30	TFA[b]	17	$CHCl_3$	60	24	56

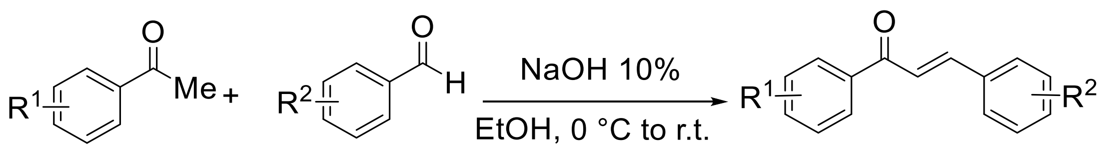
[a]Reported yields are isolated yields. [b]2 equiv. of $MgSO_4$ was added.[c]The alcohol derivative of **1a** was used. All the reactions were carried out in the dark on a 0.1 mmol scale. 2-methyl indole (1 equiv.), **1a** (1 equiv.), and catalyst, and 1.0 mL of solvent were used. n.d.= not

detected. TFA = trifluoroacetic acid, [d]1.5 equiv. of 2-methyl indole **2a** was used, [e]1.5 equiv. of **1a** was used.

3. Synthesis and characterization of starting materials

3.1 Synthesis of allylic ketone

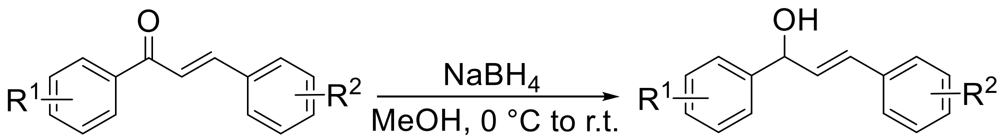
General procedure a: All the ketone compounds were prepared using literature procedures.[2] To a stirred solution of the corresponding ketone (20 mmol, 1 equiv.) in EtOH (50 mL), an aqueous solution of NaOH 10% (24 mL) was added dropwise at 0 ºC. After 5 min, the corresponding aldehyde (20 mmol, 1 equiv.)was added dropwise and the mixture allowed to stir at room temperature until complete consumption. The mixture was diluted with water (40 mL). If the allylic ketone precipitated at this stage, it was filtered and washed with water and with the minimum amount of EtOH, dried and used in the next step without further purification. If the product did not precipitate, the reaction mixture was extracted three times with DCM (40 mL). The combined organic phases were dried over $MgSO_4$ and the solvent evaporated under reduced pressure. The crude oil was used in the next step without further purification.



3.2 Synthesis of allylic alcohol

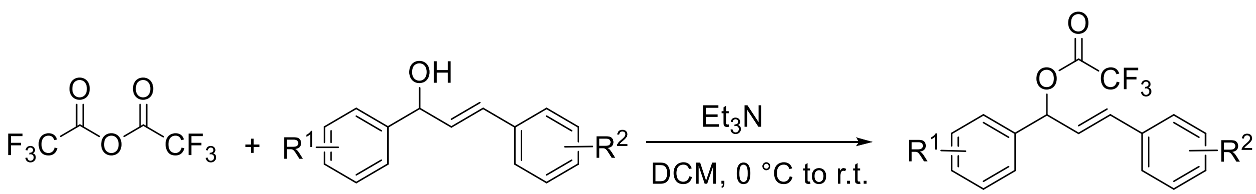
General procedure b:

To a stirred solution of the corresponding ketone in MeOH (20 mL) at 0 ºC, $NaBH_4$ (1.51 g, 40 mmol, 2 equiv.) was added portion wise. The mixture was then stirred at room temperature for 6 h. The reaction was quenched with water (10 mL) and extracted with DCM (3 × 40 mL). The combined organic phases were dried over $MgSO_4$ and the solvent evaporated under reduced pressure. The crude was used in the next step without further purification.



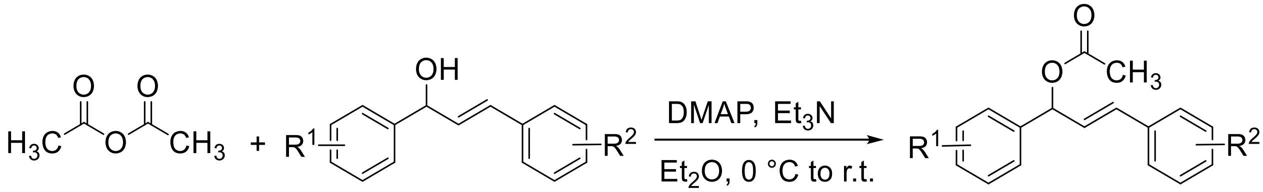
3.3 Synthesis of allylic esters

General procedure c: ester **1a** was prepared using a slightly modified literature procedure.[3] Triethylamine (1.2 mL, 14.3 mmol, 1.5 equiv.) was added to a stirred CH_2Cl_2 (25 mL) solution of the allylic alcohol (1 equiv.) at 0 °C. The reaction mixture was allowed to stir for 15 min under nitrogen at same temperature. Trifluoroacetic anhydride (2 mL, 14.3 mmol, 1.5 equiv.) was added to the reaction mixture dropwise at 0 °C. The reaction mixture was allowed to stir over night at ambient temperature and quenched the reaction with saturated aq. NaHCO3 solution (1 × 30 mL). The organic compounds were extracted with ethyl acetate (3 × 25 mL), the combined organic fractions were washed with brine solution (1 × 30 mL), dried over $MgSO_4$ and concentrated using vacuum. The crude compound was purified via column chromatography using silica gel and hexane/ethyl acetate (95:5 v/v) as eluent.



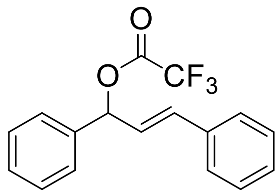
General procedure d:

All esters except **1a** were prepared according to a literature procedure.[2] To a vigorously stirred solution of the corresponding alcohol (15 mmol, 1 equiv.), DMAP (59 mg, 0.49 mmol, 0.03 equiv.) and Et_3N (6.6 mL, 47 mmol, 3.13 equiv.) in Et_2O (35 mL) at 0 ºC, acetic anhydride was added dropwise (4.3 mL, 45.5 mmol, 3.03 equiv.). The reaction was stirred at room temperature for 2 h. The reaction mixture was quenched with sat. solution of $NaHCO_3$ (50 mL). The organic phase was separated and the aqueous layer extracted with EtOAc (3 × 50 mL). The combined organic phases were dried over $MgSO_4$ and the solvent evaporated under reduced pressure. The crude was used in the allylation reaction without further purification.



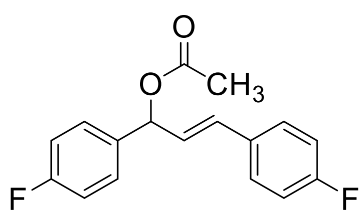
3.4 Synthesis and spectral characterization of allylic ester compounds:

Synthesis of (E)-1,3-diphenylallyl 2,2,2-trifluoroacetate **(1a)**[3]



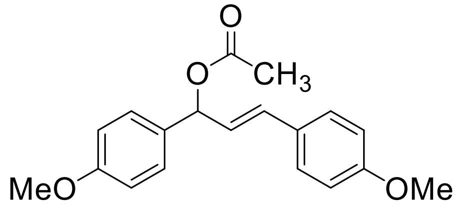
Synthesized in accordance with General Procedure c using (*E*)-1,3-diphenylprop-2-en-1-ol (2 g, 9.5 mmol, 1 equiv.). The desired product **1a** was obtained as a colorless oil, which was recrystallized using pentane at -30 ^{o}C. A white solid was obtained as a pure compound. Yield: 1.8 g, 5.9 mmol, 62%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.47–7.42 (m, 2H, Ar–CH), 7.42–7.34 (m, 4H, Ar–CH), 7.34–7.27 (m, 3H, Ar–CH), 7.26–7.19 (m, 1H, Ar–CH), 6.61 (dd, *J* = 15.9, 4.9 Hz, 1H, $H_{vinylic}$), 6.35 (ddd, *J* = 26.2, 15.9, 7.1 Hz, 1H, CH), 5.11 (dd, *J* = 9.6, 7.2 Hz, 1H, $H_{vinylic}$); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ:141.4, 141.3, 136.8 (d, $J_{C–F}$ = 2.0 Hz), 131.6 (d, $J_{C–F}$ = 23.2 Hz), 130.5 (d, $J_{C–F}$ = 21.1 Hz), 128.67, 128.65, 127.9 (d, $J_{C–F}$ = 2.1 Hz), 127.8, 127.2, 126.8 (d, $J_{C–F}$ = 2.5 Hz), 79.4, 79.2; ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -75.1. (CF_3). Data agrees with literature values.[3]

Synthesis of (E)-1,3-bis(4-fluorophenyl)allyl acetate **(1b)**[4]



Synthesized in accordance with General Procedure d using (*E*)-1,3-bis(4-fluorophenyl)prop-2-en-1-ol (3.69 g, 15 mmol, 1 equiv.). The desired product **1b** was obtained as a pale yellow oil. Yield: 3.5 g, 12.14 mmol, 81%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.42–7.32 (m, 4H, Ar–CH), 7.11–7.03 (m, 2H, Ar–CH), 7.03–6.97 (m, 2H, Ar–CH), 6.58 (d, *J* = 15.9 Hz, 1H, $H_{vinylic}$), 6.41 (d, *J* = 6.7 Hz, 1H, CH), 6.25 (dd, *J* = 15.5, 7.1 Hz, 1H, $H_{vinylic}$), 2.14 (s, 3H, Me); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 170.1, 162.7 (d, J_{C-F} = 247.7 Hz), 162.6 (d, J_{C-F} = 246.9 Hz), 135.1 (d, J_{C-F} = 3.2 Hz), 132.3 (d, J_{C-F} = 3.3 Hz), 131.7, 129.0 (d, J_{C-F} = 8.2 Hz), 128.4 (d, J_{C-F} = 8.1 Hz), 127.2 (d, J_{C-F} = 2.3 Hz), 115.7 (d, J_{C-F} = 21.7 Hz), 75.5 (CH), 21.4 (Me); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -113.4, -113.7. Data agrees with literature values.[4]

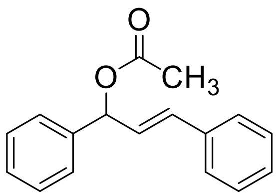
Synthesis of (E)-1,3-bis(4-methoxyphenyl)allyl acetate **(1c)**[5,4]



Synthesized in accordance with General Procedure d using (*E*)-1,3-bis(4-methoxyphenyl)prop-2-en-1-ol (4.05 g, 15 mmol, 1 equiv.). The desired product **1c** was obtained as a pale yellow oil. Yield: 3.5 g, 11.2 mmol, 75%. ^{1}H NMR (500

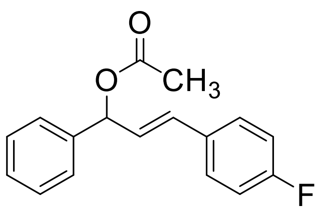
MHz, $CDCl_3$, 298 K) δ: 7.38–7.31 (m, 4H, Ar–CH), 6.93–6.90 (m, 2H, Ar–CH), 6.87–6.83 (m, 2H, Ar–CH), 6.57 (d, J = 15.7 Hz, 1H, $H_{vinylic}$), 6.41 (d, J = 7.8 Hz, 1H, CH), 6.24 (dd, J = 15.8, 6.8 Hz, 1H, $H_{vinylic}$), 3.81 (s, 3H, OMe), 3.80 (s, 3H, OMe), 2.12 (s, 3H, Me); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 170.2, 159.6, 159.5, 132.0, 131.7, 129.1, 128.6, 128.0, 125.6, 114.06, 114.05, 76.1 (CH), 55.37 (OMe), 55.35 (OMe), 21.5 (Me). Data agrees with literature values.[5,4]

Synthesis of (E)-1,3-diphenylallyl acetate **(1d)**[6]



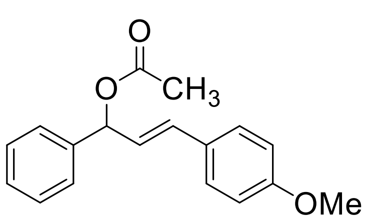
Synthesized in accordance with General Procedure d using (*E*)-1,3-diphenylprop-2-en-1-ol (3.15 g, 15 mmol, 1 equiv.). The desired product **1d** was obtained as a pale yellow oil. Yield: 3.1 g, 12.29 mmol, 82%. ^1H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.34–7.11 (m, 10H, Ar–CH), 6.54 (d, J = 15.9 Hz, 1H, $H_{vinylic}$), 6.35 (d, J = 7.0 Hz, 1H, CH), 6.25 (ddd, J = 15.8, 6.8, 2.5 Hz, 1H, $H_{vinylic}$), 2.04 (s, 3H, Me); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 170.2, 139.4, 136.3, 132.7, 128.8, 128.7, 128.3, 128.2, 127.6, 127.2, 126.8, 76.3 (CH), 21.5 (Me). Data agrees with literature values.[6]

Synthesis of (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **(1e)**[2]



Synthesized in accordance with General Procedure d using (*E*)-3-(4-fluorophenyl)-1-phenylprop-2-en-1-ol (3.42 g, 15 mmol, 1 equiv.). The desired product **1e** was obtained as a pale yellow oil. Yield: 3 g, 11.1 mmol, 75%. ^1H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.44–7.30 (m, 7H, Ar–CH), 7.03–6.97 (m, 2H, Ar–CH), 6.60 (d, J = 15.9 Hz, 1H, $H_{vinylic}$), 6.43 (d, J = 6.9 Hz, 1H, CH), 6.27 (dd, J = 15.8, 6.8 Hz, 1H, $H_{vinylic}$), 2.14 (s, 3H, Me); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 170.2, 162.7 (d, $J_{C\text{-}F}$ = 247.6 Hz), 139.3, 132.5 (d, $J_{C\text{-}F}$ = 3.3 Hz), 131.6, 128.8, 128.41 (d, $J_{C\text{-}F}$ = 8.1 Hz), 128.36, 127.4 (d, $J_{C\text{-}F}$ = 2.3 Hz), 127.1, 115.7 (d, $J_{C\text{-}F}$ = 21.6 Hz), 76.2 (CH), 21.5 (Me); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -113.7. Data agrees with literature values.[2]

Synthesis of (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **(1f)**[7]



Synthesized in accordance with General Procedure d using (*E*)-3-(4-methoxyphenyl)-1-phenylprop-2-en-1-ol (3.57 g, 15 mmol, 1 equiv.). The desired product **1f** was obtained as a pale yellow oil. Yield: 3.3 g, 11.69 mmol, 78%. ^1H NMR (500 MHz, $CDCl_3$, 298

K) δ: 7.44–7.30 (m, 7H, Ar–CH), 6.85 (d, *J* = 8.7 Hz, 2H, Ar–CH), 6.60 (d, *J* = 15.9 Hz, 1H, $H_{vinylic}$), 6.44 (d, *J* = 7.1 Hz, 1H, CH), 6.23 (dd, *J* = 15.9, 6.9 Hz, 1H, $H_{vinylic}$), 3.80 (s, 3H, OMe), 2.14 (s, 3H, Me); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 170.2, 159.7, 139.6, 132.5, 129.0, 128.7, 128.2, 128.1, 127.1, 125.4, 114.1, 76.5 (CH), 55.4 (OMe), 21.5 (Me). Data agrees with literature values.[7]

4. Synthesis and characterization of products:

4.1 General procedure

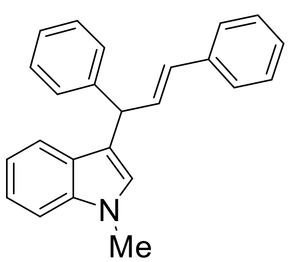
General procedure e:

In the glovebox, glass microwave vials were separately charged with indole (1 equiv.) allylic ester (1 equiv.), and $B(3,4,5\text{-}Ar^F)_3$ (15 mol%). The vials were brought outside the glovebox and 0.3 mL of $CHCl_3$ were added to each vial using a syringe. Indole solution was added to the ester solution. The solution of $B(3,4,5\text{-}Ar^F)_3$ was added to the mixture dropwise with vigorous stirring at room temperature. All the reactions were carried out at an optimum temperature 60 °C for 24 h. All volatiles were removed in vacuo and the crude compound was purified via preparative thin layer chromatography using hexane/ethyl acetate as eluent.

NB. $MgSO_4$ (2 equiv.) was used during the reactions for all substrates to eliminate the residual water from the reaction mixture.

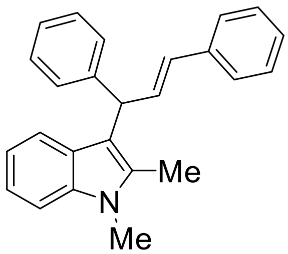
4.2 Synthesis and spectral characterization of allylic indole derivatives:

Synthesis of (E)-3-(1,3-diphenylallyl)-1-methyl-1H-indole **(3a)**[8]



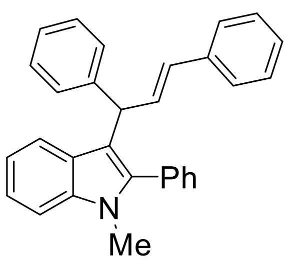
Synthesized in accordance with General Procedure e using $B(3,4,5\text{-}Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-diphenylallyl 2,2,2-trifluoroacetate **1a** (31 mg, 0.1 mmol, 1 equiv.), and 1-methylindole (13 µL, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3a**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3a** was obtained as a yellow oil. Yield: 31 mg, 0.1 mmol, 97%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.49–7.44 (m, 1H, Ar–CH), 7.43–7.30 (m, 9H, Ar–CH), 7.29–7.21 (m, 3H, Ar–CH), 7.06 (t, *J* = 7.5 Hz, 1H, Ar–CH), 6.82–6.71 (m, 2H, overlapped indole CH and $H_{vinylic}$), 6.48 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.16 (d, *J* = 7.4 Hz, 1H, CH), 3.76 (s, 3H, NMe); $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 143.7, 137.7, 137.5, 132.8, 130.6, 128.6, 128.5, 127.5, 127.34, 127.26, 126.5, 126.4, 121.8, 120.1, 119.0, 117.2, 109.3, 46.3 (CH), 32.8 (NMe). Data agrees with literature values.[8]

Synthesis of (E)-3-(1,3-diphenylallyl)-1,2-dimethyl-1H-indole **(3b)**



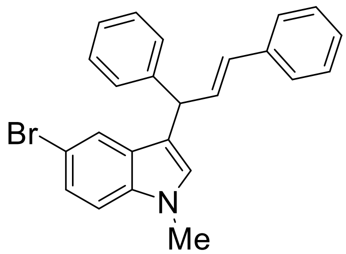
Synthesized in accordance with General Procedure e using B(3,4,5-$Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-diphenylallyl 2,2,2-trifluoroacetate **1a** (31 mg, 0.1 mmol, 1 equiv.), and 1,2-dimethyl-1*H*-indole (15 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3b**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3b** was obtained as a yellow oil. Yield: 22 mg, 0.07 mmol, 65%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.41–7.34 (m, 5H, Ar–CH), 7.31–7.26 (m, 5H, Ar–CH), 7.22–7.18 (m, 2H, Ar–CH), 7.14 (t, *J* = 7.6 Hz, 1H, Ar–CH), 6.98 (t, *J* = 7.1 Hz, 1H, Ar–CH), 6.85 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.43 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.19 (d, *J* = 7.2 Hz, 1H, CH), 3.69 (s, 3H, NMe), 2.39 (s, 3H, Me); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 143.8, 137.7, 137.0, 133.6, 132.5, 130.6, 128.6, 128.38, 128.35, 127.2, 127.1, 126.4, 126.2, 120.6, 119.6, 119.0, 112.3, 108.8, 45.5 (CH), 29.7 (NMe), 10.9 (Me); IR ν_{max} (cm^{-1}): 3055, 3024, 2924, 1687, 1599, 1490, 1471. HRMS (CI) [M] [$C_{25}H_{23}N$]: calculated 337.1825, found 337.1822.

Synthesis of (E)-3-(1,3-diphenylallyl)-1-methyl-2-phenyl-1H-indole **(3c)**[9]



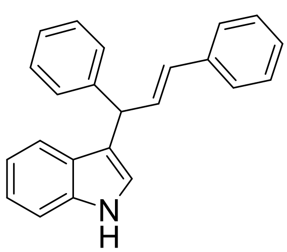
Synthesized in accordance with General Procedure e using B(3,4,5-$Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-diphenylallyl 2,2,2-trifluoroacetate **1a** (31 mg, 0.1 mmol, 1 equiv.), and 1-methyl-2-phenyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3c**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3c** was obtained as a yellow oil. Yield: 20 mg, 0.05 mmol, 50%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.5–7.26 (m, 13H, Ar–CH), 7.26–7.15 (m, 5H, Ar–CH), 7.06–7.01 (m, 1H, Ar–CH), 6.83 (dd, *J* = 15.8, 7.6 Hz, 1H, $H_{vinylic}$), 6.35 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.01 (d, *J* = 7.6 Hz, 1H, CH), 3.62 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 144.0, 138.8, 137.8, 137.6, 132.6, 132.1, 131.0, 130.8, 128.6, 128.5, 128.32, 128.28, 127.2, 126.7, 126.4, 126.1, 121.7, 121.0, 119.4, 114.2, 109.6, 45.7 (CH), 31.0 (NMe). Data agrees with literature values.[9]

Synthesis of (E)-5-bromo-3-(1,3-diphenylallyl)-1-methyl-1H-indole **(3d)**



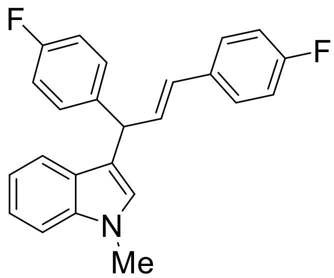
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-diphenylallyl 2,2,2-trifluoroacetate **1a** (31 mg, 0.1 mmol, 1 equiv.), and 5-bromo-1-methyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3d**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3d** was obtained as a yellow oil. Yield: 37 mg, 0.09 mmol, 93%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.48 (d, *J* = 1.4 Hz, 1H, Ar–CH), 7.33–7.29 (m, 2H, Ar–CH), 7.28–7.26 (m, 1H, Ar–CH), 7.26–7.12 (m, 8H, Ar–CH), 7.10 (d, *J* = 8.1 Hz, 1H), 6.70 (s, 1H, indole CH), 6.62 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.35 (d, *J* = 15.9 Hz, 1H, $H_{vinylic}$), 5.00 (d, *J* = 7.3 Hz, 1H, CH), 3.66 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 143.2, 137.5, 136.2, 132.4, 130.8, 129.0, 128.68, 128.65, 128.64, 128.5, 127.4, 126.7, 126.5, 124.7, 122.4, 116.92, 112.5, 110.9, 46.0 (CH), 33.0 (NMe); IR ν_{max} (cm^{-1}): 3059, 3024, 2924, 1697, 1599, 1475. HRMS (CI) [M] [$C_{24}H_{20}N^{79}Br$]: calculated 401.0774, found 401.0765.

Synthesis of (E)-3-(1,3-diphenylallyl)-1H-indole **(3e)**[10]



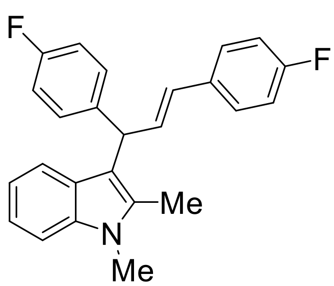
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-diphenylallyl 2,2,2-trifluoroacetate **1a** (31 mg, 0.1 mmol, 1 equiv.), and indole (12 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3e**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3e** was obtained as a yellow oil. Yield: 13 mg, 0.04 mmol, 42%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.99 (s, br, 1H, NH), 7.45 (d, *J* = 8.5 Hz, 1H, Ar–CH), 7.40–7.28 (m, 9H, Ar–CH), 7.25–7.16 (m, 3H, Ar–CH), 7.08–7.01 (m, 1H, Ar–CH), 6.91 (d, *J* = 2.4 Hz, 1H, indole CH), 6.75 (dd, J = 15.8, 7.4 Hz, 1H, $H_{vinylic}$), 6.46 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.14 (d, *J* = 7.4 Hz, 1H, CH); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 143.5, 137.6, 136.8, 132.7, 130.7, 128.63, 128.61, 128.6, 127.3, 126.9, 126.52, 126.45, 122.7, 122.2, 120.0, 119.6, 118.8, 111.2, 46.3 (CH). Data agrees with literature values.[10]

Synthesis of (E)-3-(1,3-bis(4-fluorophenyl)allyl)-1-methyl-1H-indole **(3f)**



Synthesized in accordance with General Procedure e using B(3,4,5-$Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-fluorophenyl)allyl acetate **1b** (29 mg, 0.1 mmol, 1 equiv.), and 1-methylindole (13 µL, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3f**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3f** was obtained as a yellow oil. Yield: 27 mg, 0.08 mmol, 75%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.40 (d, *J* = 8.1 Hz, 1H, Ar–CH), 7.36–7.28 (m, 5H, Ar–CH), 7.25–7.21 (m, 1H, Ar–CH), 7.07–6.96 (m, 5H, Ar–CH), 6.76 (s, 1H, indole CH), 6.62 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.38 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.10 (d, *J* = 7.3 Hz, 1H, CH), 3.76 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.3 (d, $J_{C\text{-}F}$ = 246.3 Hz), 161.7 (d, $J_{C\text{-}F}$ = 244.3 Hz), 139.2 (d, $J_{C\text{-}F}$ = 3.1 Hz), 137.6, 133.6 (d, $J_{C\text{-}F}$ = 3.3 Hz), 132.4 (d, $J_{C\text{-}F}$ = 2.3 Hz), 130.0 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.6, 127.9 (d, $J_{C\text{-}F}$ = 8.0 Hz), 127.4, 127.2, 121.9, 119.9, 119.1, 116.9, 115.5 (d, $J_{C\text{-}F}$ = 21.5 Hz), 115.3 (d, $J_{C\text{-}F}$ = 21.2 Hz), 109.4, 45.5 (CH), 32.9 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.0, -116.9; IR ν_{max} (cm^{-1}): 3049, 2930, 1601, 1506, 1223. HRMS (CI) [M] [$C_{24}H_{19}NF_2$]: calculated 359.1480, found 359.1478.

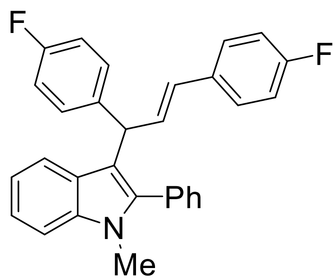
Synthesis of (E)-3-(1,3-bis(4-fluorophenyl)allyl)-1,2-dimethyl-1H-indole **(3g)**



Synthesized in accordance with General Procedure e using B(3,4,5-$Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-fluorophenyl)allyl acetate **1b** (29 mg, 0.1 mmol, 1 equiv.), and and 1,2-dimethyl-1*H*-indole (15 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3g**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3g** was obtained as a yellow oil. Yield: 31 mg, 0.08 mmol, 84%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.36–7.26 (m, 6H, Ar–CH), 7.18–7.13 (m, 1H, Ar–CH), 7.01–6.93

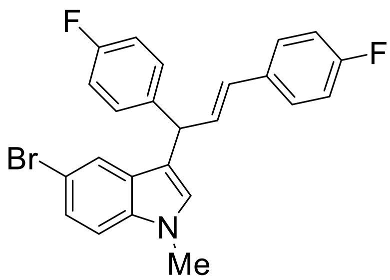
(m, 5H, Ar–CH), 6.72 (dd, J = 15.8, 7.8 Hz, 1H, $H_{vinylic}$), 6.37 (d, J = 15.8 Hz, 1H, $H_{vinylic}$), 5.13 (d, J = 7.3 Hz, 1H, CH), 3.70 (s, 3H, NMe), 2.39 (s, 3H, Me); $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$, 298 K) δ: 162.1 (d, $J_{C\text{-}F}$ = 246.2 Hz), 161.4 (d, $J_{C\text{-}F}$ = 244.0 Hz), 139.3 (d, $J_{C\text{-}F}$ = 3.1 Hz), 137.0, 133.7 (d, $J_{C\text{-}F}$ = 3.3 Hz), 133.6, 132.1 (d, $J_{C\text{-}F}$ = 2.1 Hz), 129.8 (d, $J_{C\text{-}F}$ = 7.8 Hz), 129.6, 127.9 (d, $J_{C\text{-}F}$ = 8.0 Hz), 126.9, 120.8, 119.4, 119.1, 115.5 (d, $J_{C\text{-}F}$ = 21.5 Hz), 115.1 (d, $J_{C\text{-}F}$ = 21.1 Hz), 112.0, 108.9, 44.8 (CH), 29.7 (NMe), 10.9 (Me); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.2, -117.4; IR ν_{max} (cm^{-1}): 3046, 2932, 1600, 1506, 1471, 1223, 1157. HRMS (CI) [M] [$C_{25}H_{21}NF_2$]: calculated 373.1637, found 373.1633.

Synthesis of (E)-3-(1,3-bis(4-fluorophenyl)allyl)-1-methyl-2-phenyl-1H-indole **(3h)**



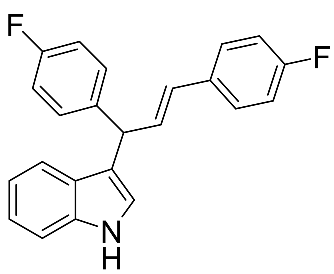
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-fluorophenyl)allyl acetate **1b** (29 mg, 0.1 mmol, 1 equiv.), and 1-methyl-2-phenyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3h**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3h** was obtained as a pale yellow oil. Yield: 37 mg, 0.08 mmol, 84%. ^1H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.49–7.32 (m, 7H, Ar–CH), 7.27–7.18 (m, 5H, Ar–CH), 7.06–7.00 (m, 1H, Ar–CH), 6.96–6.86 (m, 4H, Ar–CH), 6.68 (ddd, J = 15.8, 7.0, 1.5 Hz, 1H, $H_{vinylic}$), 6.27 (d, J = 15.8 Hz, 1H, $H_{vinylic}$), 4.94 (d, J = 7.6 Hz, 1H, CH), 3.59 (s, 3H, NMe); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.8 (d, $J_{C\text{-}F}$ = 92.5 Hz), 160.9 (d, $J_{C\text{-}F}$ = 90.5 Hz), 139.5 (d, $J_{C\text{-}F}$ = 3.1 Hz), 138.8, 137.6, 133.7 (d, $J_{C\text{-}F}$ = 3.3 Hz), 132.2 (d, $J_{C\text{-}F}$ = 2.3 Hz), 131.9, 130.9, 129.74, 129.66, 128.60, 128.57, 127.9 (d, $J_{C\text{-}F}$ = 7.9 Hz), 126.5, 121.9, 120.7, 119.6, 115.4 (d, $J_{C\text{-}F}$ = 21.5 Hz), 115.0 (d, $J_{C\text{-}F}$ = 21.0 Hz), 113.9, 109.7, 45.0 (CH), 31.0 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.2, -117.5; IR ν_{max} (cm^{-1}): 3049, 2941, 1601, 1504, 1223. HRMS (CI) [M] [$C_{30}H_{23}NF_2$]: calculated 435.1793, found 435.1792.

Synthesis of (E)-3-(1,3-bis(4-fluorophenyl)allyl)-5-bromo-1-methyl-1H-indole **(3i)**



Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-fluorophenyl)allyl acetate **1b** (29 mg, 0.1 mmol, 1 equiv.), and 5-bromo-1-methyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3i**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3i** was obtained as a yellow oil. Yield: 40 mg, 0.09 mmol, 91%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.52 (d, *J* = 1.3 Hz, 1H, Ar–CH), 7.36–7.24 (m, 5H, Ar–CH), 7.17 (d, *J* = 8.7 Hz, 1H, Ar–CH), 7.05–6.97 (m, 4H, Ar–CH), 6.77 (s, 1H, indole CH), 6.57 (dd, *J* = 15.8, 7.2 Hz, 1H, $H_{vinylic}$), 6.36 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.04 (d, *J* = 7.2 Hz, 1H, CH), 3.73 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.3 (d, J_{C-F} = 246.5 Hz), 161.7 (d, J_{C-F} = 244.7 Hz), 138.8 (d, J_{C-F} = 3.1 Hz), 136.2, 133.5 (d, J_{C-F} = 3.3 Hz), 131.9 (d, J_{C-F} = 2.2 Hz), 129.9 (d, J_{C-F} = 7.9 Hz), 129.8, 128.8, 128.6, 127.9 (d, J_{C-F} = 7.9 Hz), 124.8, 122.3, 116.6, 115.5 (d, J_{C-F} = 21.5 Hz), 115.4 (d, J_{C-F} = 21.2 Hz), 112.6, 111.0, 45.1 (CH), 33.0 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -114.8, -116.5; IR ν_{max} (cm^{-1}): 2349, 2326, 1601, 1504, 1474, 1221, 1155. HRMS (CI) [M] [$C_{24}H_{18}N^{79}BrF_2$]: calculated 437.0585, found 437.0583.

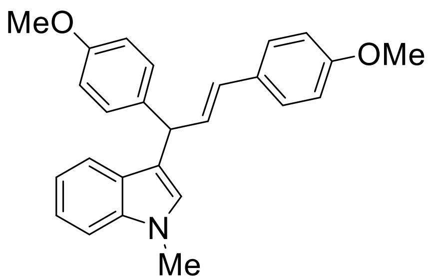
Synthesis of (E)-3-(1,3-bis(4-fluorophenyl)allyl)-1H-indole **(3j)**



Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-fluorophenyl)allyl acetate **1b** (29 mg, 0.1 mmol, 1 equiv.), and indole (12 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3j**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3j** was obtained as a yellow oil. Yield: 19 mg, 0.05 mmol, 54%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 8.00 (s, br, 1H, NH), 7.44–7.27 (m, 6H, Ar–CH), 7.24–7.18 (m, 1H, Ar–CH), 7.10–6.96 (m, 5H, Ar–CH), 6.91 (dd, *J* = 2.4, 1.0 Hz, 1H, indole CH), 6.63 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.39 (d, *J* = 15.9 Hz, 1H, $H_{vinylic}$), 5.11 (d, *J* = 7.3 Hz, 1H, CH); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.2 (d, J_{C-F} = 246.3 Hz), 161.6 (d, J_{C-F} = 244.4 Hz), 139.0 (d, J_{C-F} = 3.1 Hz), 136.8, 133.6 (d, J_{C-F} = 3.2 Hz), 132.2 (d, J_{C-F} = 2.2 Hz), 130.0 (d, J_{C-F} = 7.9 Hz), 129.7, 127.9 (d, J_{C-F} = 7.9 Hz), 126.7, 122.7, 122.4, 119.8 (d, J_{C-F} = 25.1 Hz), 118.6, 115.6, 115.4, 115.3, 111.3, 45.5 (CH); ^{19}F NMR (471 MHz, $CDCl_3$, 298

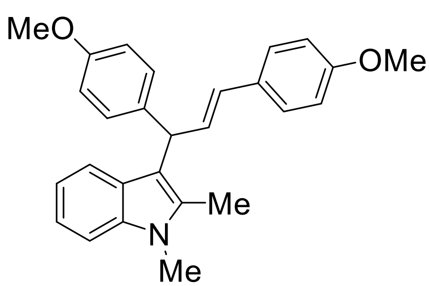
K) δ: -115.0, -116.8; IR ν_{max} (cm^{-1}): 3414, 3040, 1601, 1506, 1456, 1221, 1157. HRMS (CI) [M] [$C_{23}H_{17}NF_2$]: calculated 345.1324, found 345.1321.

Synthesis of (E)-3-(1,3-bis(4-methoxyphenyl)allyl)-1-methyl-1H-indole **(3k)**



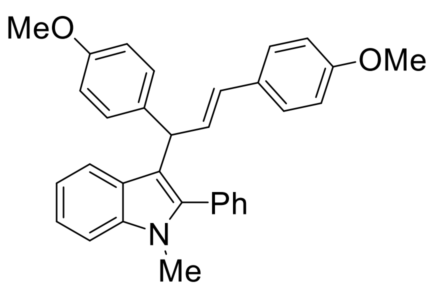
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-methoxyphenyl)allyl acetate **1c** (31 mg, 0.1 mmol, 1 equiv.), and 1-methylindole (13 μL, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3k**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3k** was obtained as a yellow oil in 1:1 inseparable regioisomeric mixture. Yield: 30 mg, 0.08 mmol, 79%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.44 (d, *J* = 7.6 Hz, 1H, Ar–CH), 7.35–7.18 (m, 6H, Ar–CH), 7.03 (t, *J* = 8.0 Hz, 1H, Ar–CH), 6.90–6.81 (m, 4H, Ar–CH), 6.76 (s, 1H, indole CH), 6.58 (ddd, *J* = 15.8, 7.3, 1.7 Hz, 1H, $H_{vinylic}$), 6.38 (d, *J* = 15.7 Hz, 1H, $H_{vinylic}$), 5.06 (d, *J* = 7.2 Hz, 1H, CH), 3.80 + 3.81 (two overlapped signals, 6H, OMe), 3.74 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.0, 158.2, 137.6, 136.0, 131.0, 130.5, 129.6, 129.5, 127.5, 127.41, 127.35, 121.7, 120.2, 118.9, 117.7, 114.01, 113.97, 113.9, 109.3, 55.41 (OMe), 55.37 (OMe), 45.4 (CH), 32.8 (NMe); IR ν_{max} (cm^{-1}): 2999, 2932, 2833, 1606, 1508, 1464, 1244, 1173, 1032. HRMS (CI) [M] [$C_{26}H_{25}O_2N$]: calculated 383.1880, found 383.1877.

Synthesis of (E)-3-(1,3-bis(4-methoxyphenyl)allyl)-1,2-dimethyl-1H-indole **(3l)**



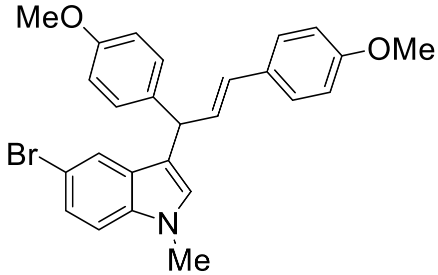
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-methoxyphenyl)allyl acetate **1c** (31 mg, 0.1 mmol, 1 equiv.), and 1,2-dimethyl-1*H*-indole (15 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3l**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3l** was obtained as a yellow oil. Yield: 26 mg, 0.07 mmol, 65%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.42 (d, *J* = 6.9 Hz, 1H, Ar–CH), 7.35–7.31 (m, 2H, Ar–CH), 7.31–7.26 (m, 3H, Ar–CH), 7.19–7.13 (m, 1H, Ar–CH), 7.04–6.97 (m, 1H, Ar–CH), 6.87– 6.82 (m, 4H, Ar–CH), 6.74–6.68 (m, 1H, $H_{vinylic}$), 6.38 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.13 (d, *J* = 7.3 Hz, 1H, CH), 3.81 (s, 3H, OMe), 3.80 (s, 3H, OMe), 3.69 (s, 3H, NMe), 2.40 (s, 3H, Me); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 158.9, 158.0, 136.9, 136.1, 133.4, 130.8, 130.6, 129.7, 129.3, 127.5, 127.1, 120.5, 119.6, 118.9, 114.0, 113.7, 112.7, 108.7, 55.39 (OMe), 55.35 (OMe), 44.7 (CH), 29.7 (NMe), 10.9 (Me); IR ν_{max} (cm^{-1}): 3028, 2932, 2833, 1606, 1508, 1470, 1244, 1173, 1032. HRMS (CI) [M] [$C_{27}H_{27}O_2N$]: calculated 397.2036, found 397.2033.

Synthesis of (E)-3-(1,3-bis(4-methoxyphenyl)allyl)-1-methyl-2-phenyl-1H-indole **(3m)**



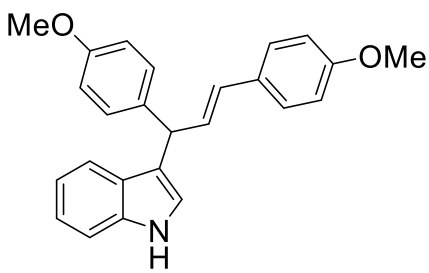
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-methoxyphenyl)allyl acetate **1c** (31 mg, 0.1 mmol, 1 equiv.), and 1-methyl-2-phenyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3m**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3m** was obtained as a yellow oil. Yield: 33 mg, 0.07 mmol, 72%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.52–7.44 (m, 4H, Ar–CH), 7.43–7.39 (m, 2H, Ar–CH), 7.37 (d, J = 8.2 Hz, 1H, Ar–CH), 7.30–7.20 (m, 5H, Ar–CH), 7.08–7.01 (m, 1H, Ar–CH), 6.86–6.77 (m, 4H, Ar–CH), 6.69 (dd, *J* = 15.8, 7.5 Hz, 1H, $H_{vinylic}$), 6.29 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 4.95 (d, *J* = 7.5 Hz, 1H, CH), 3.79 (s, 3H, OMe), 3.78 (s, 3H, OMe), 3.62 (s, 3H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 158.9, 157.9, 138.5, 137.6, 136.3, 132.1, 131.0, 130.8, 130.6, 129.8, 129.3, 128.5, 128.4, 127.5, 126.7, 121.6, 121.1, 119.4, 114.6, 114.0, 113.6, 109.5, 55.4 (OMe), 55.3 (OMe), 44.9 (CH), 31.0 (NMe); IR ν_{max} (cm^{-1}): 2999, 2932, 2833, 1605, 1508, 1464, 1244, 1173, 1032. HRMS (CI) [M] [$C_{32}H_{29}O_2N$]: calculated 459.2193, found 459.2191.

Synthesis of (E)-3-(1,3-bis(4-methoxyphenyl)allyl)-5-bromo-1-methyl-1H-indole **(3n)**



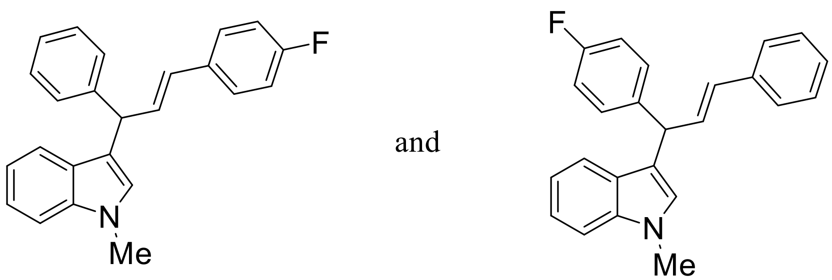
Synthesized in accordance with General Procedure e using $B(3,4,5\text{-}Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-methoxyphenyl)allyl acetate **1c** (31 mg, 0.1 mmol, 1 equiv.), and 5-bromo-1-methyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3n**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3n** was obtained as a light brown oil. Yield: 41 mg, 0.09 mmol, 89%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.55 (d, *J* = 1.3 Hz, 1H, Ar–CH), 7.33–7.27 (m, 3H, Ar–CH), 7.25–7.21 (m, 2H, Ar–CH), 7.15 (d, *J* = 8.7 Hz, 1H, Ar–CH), 6.92–6.81 (m, 4H, Ar–CH), 6.76 (s, 1H, indole CH), 6.53 (dd, *J* = 15.7, 7.2 Hz, 1H, $H_{vinylic}$), 6.34 (d, *J* = 15.7 Hz, 1H, $H_{vinylic}$), 4.99 (d, *J* = 7.2 Hz, 1H, CH), 3.81 (s, 3H, OMe), 3.80 (s, 3H, OMe), 3.71 (s, 3H, NMe); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.1, 158.3, 136.2, 135.5, 130.5, 130.3, 129.9, 129.4, 129.0, 128.6, 127.5, 124.6, 122.5, 117.4, 114.03, 113.97, 112.4, 110.8, 55.41 (OMe), 55.38 (OMe), 45.1 (CH), 33.0 (NMe); IR ν_{max} (cm^{-1}): 2930, 2833, 2349, 2326, 2139, 1607, 1508, 1474, 1298, 1244, 1173, 1032. HRMS (CI) [M] [$C_{26}H_{24}O_2N^{79}Br$]: calculated 461.0985, found 461.0982.

Synthesis of (E)-3-(1,3-bis(4-methoxyphenyl)allyl)-1H-indole **(3o)**[9]



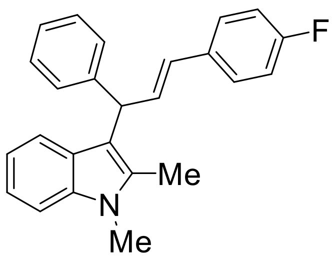
Synthesized in accordance with General Procedure e using $B(3,4,5\text{-}Ar^F)_3$ (6 mg, 0.015 mmol 0.15 equiv.), (*E*)-1,3-bis(4-methoxyphenyl)allyl acetate **1c** (31 mg, 0.1 mmol, 1 equiv.), and indole (12 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3o**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. The desired compound **3o** was obtained as a brown oil. Yield: 21 mg, 0.06 mmol, 57%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 8.02 (s, br, 1H, NH), 7.43 (d, *J* = 6.8 Hz, 1H, Ar–CH), 7.34 (d, *J* = 8.1 Hz, 1H, Ar–CH), 7.33–7.27 (m, 2H, Ar–CH), 7.27–7.22 (m, 2H, Ar–CH), 7.19–7.14 (m, 1H, Ar–CH), 7.03–6.99 (m, 1H, Ar–CH), 6.89 (dd, *J* = 2.4, 1.1 Hz, 1H, indole CH), 6.87–6.79 (m, 4H, Ar–CH), 6.57 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.36 (d, *J* = 15.4 Hz, 1H, $H_{vinylic}$), 5.05 (d, *J* = 7.3 Hz, 1H, CH), 3.79 (s, 6H, OMe); $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.0, 158.2, 136.8, 135.9, 130.9, 130.5, 129.8, 129.5, 127.5, 127.0, 122.7, 122.2, 120.1, 119.5, 119.3, 114.0, 113.9, 111.2, 55.43 (OMe), 55.38 (OMe), 45.5 (CH). Data agrees with literature values.[9]

Synthesis of (E)-3-(3-(4-fluorophenyl)-1-phenylallyl)-1-methyl-1H-indole **(3p)** *and (E)-3-(1-(4-fluorophenyl)-3-phenylallyl)-1-methyl-1H-indole* **(3p′)**

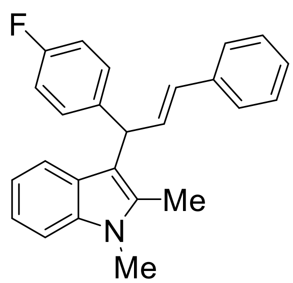


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **1e** (27 mg, 0.1 mmol, 1 equiv.), and 1-methylindole (13 µL, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3p** and **3p′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3p** and **3p′** was obtained as a yellow oil. Combined yields: 26 mg, 0.08 mmol, 76%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.47–7.27 (m, 17H, Ar–CH), 7.25–7.21 (m, 3H, Ar–CH), 7.07–6.96 (m, 6H, Ar–CH), 6.77 (s, 1H, indole CH), 6.76 (s, 1H, indole CH), 6.72 (dd, J = 15.8, 7.4 Hz, 1H, $H_{vinylic}$), 6.66 (dd, J = 15.8, 7.4 Hz, 1H, $H_{vinylic}$), 6.44 + 6.42 (two overlapped doublets, d, J = 15.8 Hz, 1H, $H_{vinylic}$ + d, J = 15.9 Hz, 1H, $H_{vinylic}$), 5.13 (d, J = 7.3 Hz, 2H, CH), 3.77 + 3.76 (two overlapped singlets, 6H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.2 (d, $J_{C\text{-}F}$ = 246.1 Hz), 161.7 (d, $J_{C\text{-}F}$ = 244.2 Hz), 161.2, 160.7, 143.6, 139.32, 139.30, 137.6, 137.54, 137.49, 133.80, 133.78, 132.61, 132.59, 130.7, 130.04, 129.98, 129.4, 128.7, 128.6, 127.9, 127.8, 127.46, 127.45, 127.4, 127.30, 127.2, 126.5, 126.4, 121.9, 121.8, 120.02, 119.99, 119.1, 119.0, 117.1, 117.0, 115.5, 115.4, 115.2, 109.38, 109.35, 46.3 (CH), 45.5 (CH), 32.84 (NMe), 32.82 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.2, -117.0; IR ν_{max} (cm^{-1}): 3055, 3026, 2928, 1599, 1506, 1472, 1223, 1155. HRMS (CI) [M] [$C_{24}H_{20}NF$]: calculated 341.1574, found 341.1566.

Synthesis of (E)-3-(3-(4-fluorophenyl)-1-phenylallyl)-1,2-dimethyl-1H-indol **(3q)** *and (E)-3-(1-(4-fluorophenyl)-3-phenylallyl)-1,2-dimethyl-1H-indole* **(3q′)**



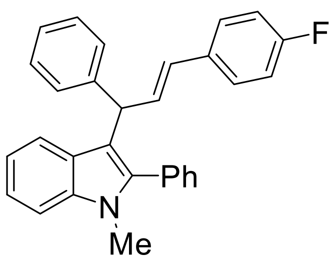
and



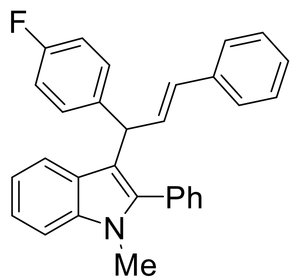
Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **1e** (27 mg, 0.1 mmol, 1 equiv.), and 1,2-dimethyl-1*H*-indole (15 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3q** and **3q′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3q** and **3q′** was obtained as a yellow oil. Combined yields: 26 mg, 0.07 mmol, 72%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.43–7.28 (m, 16H, Ar–CH), 7.25–7.20 (m, 2H, Ar–CH), 7.20–7.14 (m, 2H, Ar–CH), 7.05–6.94 (m, 6H, Ar–CH), 6.84 + 6.79 (two overlapped doublet of doublets, dd, J = 15.8, 7.3 Hz, 1H, $H_{vinylic}$ + dd, J = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.44 + 641 (two overlapped doublets, d, J = 15.8 Hz, 1H, $H_{vinylic}$ + d, J = 15.8 Hz, 1H, $H_{vinylic}$), 5.19 (d, J = 7.3 Hz, 1H, CH), 5.17(d, J = 7.3 Hz, 1H, CH), 3.70 (two overlapped singlets, 6H, NMe), 2.41 (s, 6H, Me); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.2 (d, J_{C-F} = 245.9 Hz), 161.5 (d, J_{C-F} = 244.0 Hz), 143.7, 139.40, 139.38, 137.6, 136.97, 136.95, 133.88, 133.85, 133.6, 132.3, 130.7, 129.82, 129.75, 129.4, 128.6, 128.4, 128.3, 127.9, 127.8, 127.3, 127.0, 126.9, 126.7, 126.4, 126.2, 120.7, 120.6, 119.5, 119.4, 119.1, 119.0, 115.4 (d, J_{C-F} = 21.5 Hz), 115.1 (d, J_{C-F} = 21.1 Hz), 112.2, 112.1, 108.9, 108.8, 45.4 (CH), 44.8 (CH), 29.7 (NMe), 10.90 (Me), 10.88 (Me); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.4, -117.5; IR ν_{max} (cm^{-1}):

3057, 3026, 1601, 1506, 1472, 1367, 1223, 1157. HRMS (CI) [M] [$C_{25}H_{22}NF$]: calculated 355.1731, found 355.1728.

Synthesis of (E)-3-(3-(4-fluorophenyl)-1-phenylallyl)-1-methyl-2-phenyl-1H-indole **(3r)** *and (E)-3-(1-(4-fluorophenyl)-3-phenylallyl)-1-methyl-2-phenyl-1H-indole* **(3r′)**

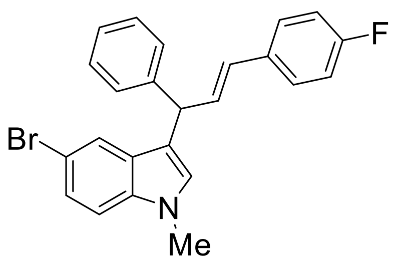


and

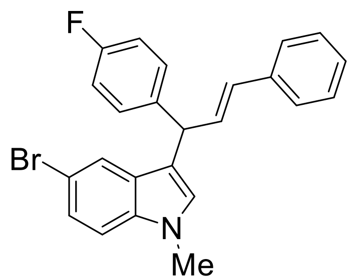


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **1e** (27 mg, 0.1 mmol, 1 equiv.), and 1-methyl-2-phenyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3r** and **3r′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3r** and **3r′** was obtained as a yellow oil. Combined yields: 29 mg, 0.07 mmol, 69%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.54–7.24 (m, 28H, Ar–CH), 7.24–7.17 (m, 2H, Ar–CH), 7.11–7.03 (m, 2H, Ar–CH), 7.00–6.91 (m, 4H, Ar–CH), 6.82 (dd, *J* = 15.8, 7.5 Hz, 1H, $H_{vinylic}$), 6.76 (dd, J = 15.8, 7.6 Hz, 1H, $H_{vinylic}$), 6.37 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 6.32 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.01 (d, *J* = 7.5 Hz, 1H, CH), 4.99 (d, *J* = 7.5 Hz, 1H, CH), 3.64 (s, 6H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.6 (d, $J_{C\text{-}F}$ = 245.9 Hz), 161.3 (d, $J_{C\text{-}F}$ = 243.9 Hz), 143.9, 139.63, 139.60, 138.76, 138.75, 137.61, 137.59, 133.90, 133.88, 132.42, 132.40, 132.38, 132.0, 131.95, 130.97, 130.93, 130.89, 129.8, 129.70, 129.5, 128.58, 128.55, 128.54, 128.48, 128.31, 128.28, 127.9, 127.8, 127.3, 126.6, 126.5, 126.4, 126.1, 121.81, 121.75, 120.9, 120.8, 119.53, 119.47, 115.4 (d, $J_{C\text{-}F}$ = 21.5 Hz), 115.0 (d, $J_{C\text{-}F}$ = 21.1 Hz), 114.1, 114.0, 109.7, 109.6, 45.7 (CH), 45.0 (CH), 31.0 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.4, -117.6; IR ν_{max} (cm^{-1}): 3057, 2926, 1601, 1506, 1468, 1223, 1157. HRMS (CI) [M] [$C_{30}N_{24}NF$]: calculated 417.1887, found 417.1885.

Synthesis of (E)-5-bromo-3-(3-(4-fluorophenyl)-1-phenylallyl)-1-methyl-1H-indole **(3s)** *and (E)-5-bromo-3-(1-(4-fluorophenyl)-3-phenylallyl)-1-methyl-1H-indole* **(3s′)**

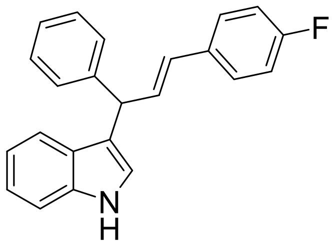


and

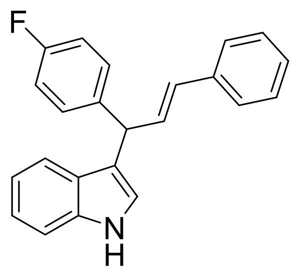


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **1e** (27 mg, 0.1 mmol, 1 equiv.), and 5-bromo-1-methyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3s** and **3s′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3s** and **3s′** was obtained as an orange oil. Combined yields: 32 mg, 0.08 mmol, 76%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.55 (d, J = 1.9 Hz, 1H, Ar–CH), 7.51 (d, J = 1.3 Hz, 1H, Ar–CH), 7.40–7.26 (m, 15H, Ar–CH), 7.25–7.21 (m, 1H, Ar–CH), 7.18 (d, J = 2.9 Hz, 1H, Ar–CH), 7.16 (d, J = 2.9 Hz, 1H), 7.04 – 6.96 (m, 4H, Ar–CH), 6.77 (s, 1H, indole CH), 6.76 (s, 1H, indole CH), 6.66 (dd, J = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.60 (dd, J = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.39 + 6.38 (two overlapped doublets, d, J = 15.9 Hz, 1H, $H_{vinylic}$ + d, J = 15.9 Hz, 1H, $H_{vinylic}$), 5.05 (d, J = 7.2 Hz, 2H, CH), 3.73 + 3.72 (two overlapped singlets, 6H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.2 (d, $J_{C\text{-}F}$ = 246.2 Hz), 161.7 (d, $J_{C\text{-}F}$ = 244.6 Hz), 143.1, 138.84, 138.82, 137.3, 136.22, 136.18, 133.62, 133.60, 132.13, 132.12, 131.0, 130.0, 129.9, 129.7, 128.9, 128.8, 127.94, 127.88, 127.5, 126.72, 126.66, 126.5, 124.8, 124.7, 122.4, 122.3, 116.8, 116.7, 115.5 (d, $J_{C\text{-}F}$ = 21.5 Hz), 115.4 (d, $J_{C\text{-}F}$ = 21.2 Hz), 112.6, 112.5, 110.94, 110.90, 45.9 (CH) 45.2 (CH), 33.02 (NMe) 33.01 (NMe); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.0, -116.6; IR ν_{max} (cm^{-1}): 3057, 3024, 2922, 2349, 2326, 1600, 1506, 1476, 1422, 1223, 1157. HRMS (CI) [M] [$C_{24}H_{19}N^{79}BrF$]: calculated 419.0679, found 419.0676.

Synthesis of (E)-3-(3-(4-fluorophenyl)-1-phenylallyl)-1H-indole **(3t)** *and (E)-3-(1-(4-fluorophenyl)-3-phenylallyl)-1H-indole* **(3t′)**

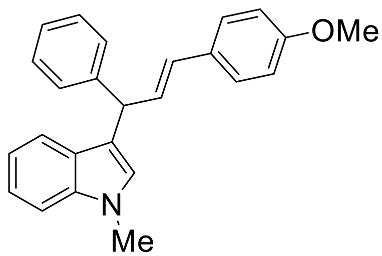


and

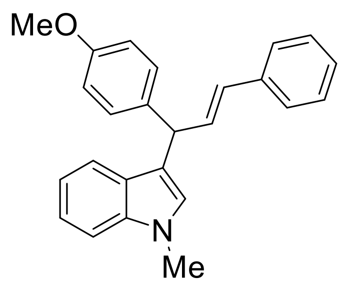


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-fluorophenyl)-1-phenylallyl acetate **1e** (27 mg, 0.1 mmol, 1 equiv.), and indole (12 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3t** and **3t′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3t** and **3t′** was obtained as a yellow oil. Combined yields: 20 mg, 0.06 mmol, 61%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 8.00 (s, br, 2H, NH), 7.46–7.26 (m, 16H, Ar–CH), 7.26–7.16 (m, 4H, Ar–CH), 7.08–7.03 (m, 2H, Ar–CH), 7.03–6.95 (m, 4H, Ar–CH), 6.92 (dd, *J* = 2.4, 0.9 Hz, 1H, indole CH), 6.91 (dd, *J* = 2.4, 0.8 Hz, 1H, indole CH), 6.71 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.66 (dd, *J* = 15.7, 7.3 Hz, 1H, $H_{vinylic}$), 6.43 + 6.41 (two overlapped doublets, d, *J* = 15.8 Hz, 1H, $H_{vinylic}$ + d, *J* = 15.9 Hz, 1H, $H_{vinylic}$), 5.12 (d, *J* = 7.4 Hz, 2H, CH); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 162.2 (d, J_{C-F} = 246.1 Hz), 161.7 (d, J_{C-F} = 244.3 Hz), 143.4, 139.14, 139.12, 137.5, 136.83, 136.80, 133.8, 133.7, 132.43, 132.41, 130.9, 130.1, 130.0, 129.5, 128.7, 128.6, 127.92, 127.85, 127.4, 126.9, 126.8, 126.6, 126.5, 122.72, 122.69, 122.4, 122.3, 120.0, 119.9, 119.7, 119.6, 118.8, 118.7, 115.5 (d, J_{C-F} = 20.0 Hz), 115.3 (d, J_{C-F} = 19.8 Hz), 111.30, 111.27, 46.3 (CH), 45.5 (CH); ^{19}F NMR (471 MHz, $CDCl_3$, 298 K) δ: -115.2, -116.9; IR ν_{max} (cm^{-1}): 3418, 3057, 3026, 1601, 1506, 1456, 1221, 1157, 1096. HRMS (ES-) [M-H]$^-$ [$C_{23}H_{17}NF$]: calculated 326.1345, found 326.1346.

Synthesis of (E)-3-(3-(4-methoxyphenyl)-1-phenylallyl)-1-methyl-1H-indole **(3u)** *and (E)-3-(1-(4-methoxyphenyl)-3-phenylallyl)-1-methyl-1H-indole* **(3u′)**

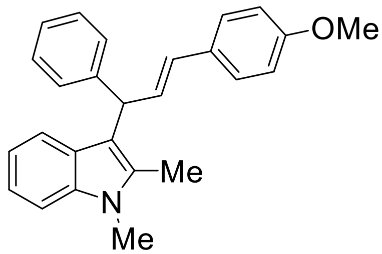


and

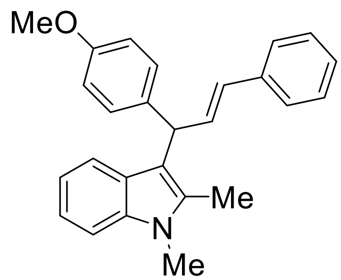


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **1f** (28 mg, 0.1 mmol, 1 equiv.), and 1-methylindole (13 µL, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3u** and **3u′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3u** and **3u′** was obtained as a yellow oil. Combined yields: 18 mg, 0.05 mmol, 51%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.48–7.44 (m, 2H, Ar–CH), 7.42–7.31 (m, 12H, Ar–CH), 7.31–7.26 (m, 3H, Ar–CH), 7.26–7.22 (m, 3H, Ar–CH), 7.08–7.02 (m, 2H, Ar–CH), 6.91–6.84 (m, 4H, Ar–CH), 6.78 (two overlapped singlets, 2H, indole CH), 6.74 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.61 (dd, *J* = 15.8, 7.4 Hz, 1H, $H_{vinylic}$), 6.45 + 6.42 (two overlapped doublets, d, *J* = 15.8 Hz, 1H, $H_{vinylic}$ + d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.12 + 5.10 (two overlapped doublets, d, *J* = 7.5 Hz, 1H, CH + d, *J* = 7.5 Hz, 1H, CH), 3.82 (two overlapped singlets, 6H, OMe), 3.76 (two overlapped singlets, 6H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.0, 158.2, 143.9, 137.7, 137.6, 137.5, 135.8, 133.1, 130.7, 130.5, 130.28, 130.27, 129.9, 129.5, 128.60, 128.59, 128.5, 127.54, 127.48, 127.44, 127.36, 127.33, 127.2, 126.42, 126.39, 121.73, 121.71, 120.13, 120.11, 119.0, 117.5, 117.4, 114.1, 114.0, 113.9, 109.29, 109.28, 55.42 (OMe), 55.38 (OMe), 46.3 (CH), 45.4 (CH), 32.8 (NMe); IR ν_{max} (cm^{-1}): 3024, 2932, 2833, 1736, 1606, 1508, 1464, 1244, 1175, 1030. HRMS (CI) [M] [$C_{25}H_{23}ON$]: calculated 353.1774, found 353.1772.

Synthesis of (E)-3-(3-(4-methoxyphenyl)-1-phenylallyl)-1,2-dimethyl-1H-indole **(3v)** *and (E)-3-(1-(4-methoxyphenyl)-3-phenylallyl)-1,2-dimethyl-1H-indole* **(3v′)**

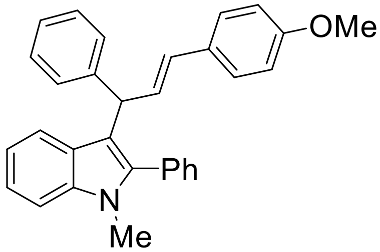


and

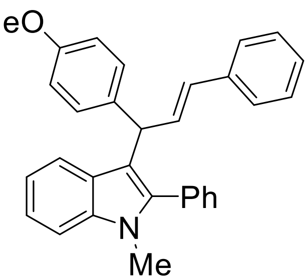


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **1f** (28 mg, 0.1 mmol, 1 equiv.), and 1,2-dimethyl-1*H*-indole (15 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3v** and **3v′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3v** and **3v′** was obtained as a pale yellow oil. Combined yields: 24 mg, 0.07 mmol, 65%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.44–7.36 (m, 6H, Ar–CH), 7.35–7.27 (m, 10H, Ar–CH), 7.25–7.19 (m, 2H, Ar–CH), 7.19–7.14 (m, 2H, Ar–CH), 7.03–6.98 (m, 2H, Ar–CH), 6.89–6.82 (m, 5H, Ar–CH + $H_{vinylic}$), 6.74 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.44 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 6.40 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.19 (d, *J* = 7.2 Hz, 1H, CH), 5.16 (d, *J* = 7.2 Hz, 1H, CH), 3.81 (two overlapped singlets, 6H, OMe), 3.70 (s, 6H, NMe), 2.41 (s, 6H, Me); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 158.9, 158.0, 144.0, 137.8, 136.94, 136.93, 135.8, 133.50, 133.48, 132.9, 130.6, 130.4, 130.34, 130.26, 130.0, 129.3, 128.58, 128.4, 128.3, 127.5, 127.12, 127.10, 127.06, 126.4, 126.1, 120.6, 120.5, 119.58, 119.57, 118.92, 118.91, 114.1, 114.0, 113.7, 112.53, 112.49, 108.8, 55.39 (OMe), 55.35 (OMe), 45.4 (CH), 44.7 (CH), 29.7 (NMe), 10.90 (Me), 10.89 (Me); IR ν_{max} (cm^{-1}): 3024, 2932, 2833, 2349, 1736, 1607, 1508, 1470, 1366, 1246, 1175, 1030. HRMS (CI) [M] [$C_{26}H_{25}ON$]: calculated 367.1931, found 367.1926.

Synthesis of (E)-3-(3-(4-methoxyphenyl)-1-phenylallyl)-1-methyl-2-phenyl-1H-indole **(3w)** *and (E)-3-(1-(4-methoxyphenyl)-3-phenylallyl)-1-methyl-2-phenyl-1H-indole* **(3w′)**

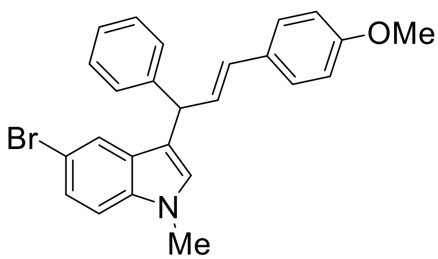


and

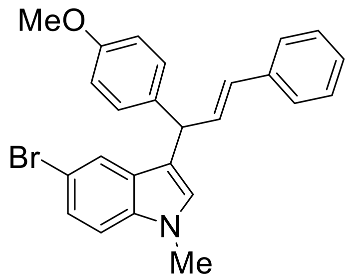


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **1f** (28 mg, 0.1 mmol, 1 equiv.), and 1-methyl-2-phenyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3w**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3w** and **3w′** was obtained as a pale yellow oil. Combined yields: 28 mg, 0.07 mmol, 65%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.53–7.45 (m, 8H, Ar–CH), 7.45–7.36 (m, 6H, Ar–CH), 7.36–7.31 (m, 4H, Ar–CH), 7.31–7.23 (m, 10H, Ar–CH), 7.22–7.16 (m, 2H, Ar–CH), 7.09–7.02 (m, 2H, Ar–CH), 6.88–6.78 (m, 5H, Ar–CH + $H_{vinylic}$), 6.71 (dd, *J* = 15.8, 7.6 Hz, 1H, $H_{vinylic}$), 6.35 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 6.31 (d, *J* = 15.8 Hz, 1H, $H_{vinylic}$), 5.01 (d, *J* = 7.6 Hz, 1H, CH), 4.98 (d, *J* = 7.5 Hz, 1H, CH), 3.81 (s, 3H, NMe), 3.79 (s, 3H, NMe), 3.63 (s, 6H, OMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 158.9, 157.9, 144.2, 138.7, 138.6, 137.8, 137.62, 137.61, 136.1, 133.0, 132.08, 132.07, 130.99, 130.97, 130.6, 130.5, 130.1, 129.3, 128.53, 128.51, 128.4, 128.3, 128.2, 127.5, 127.1, 126.68, 126.66, 126.4, 126.0, 121.68, 121.67, 121.02, 121.01, 119.40, 119.39, 114.40, 114.38, 114.0, 113.7, 109.56, 109.55, 55.4 (OMe), 55.3 (OMe), 45.7 (CH), 44.9 (CH), 31.0 (NMe); IR ν_{max} (cm^{-1}): 3057, 3026, 2930, 2833, 2349, 2326, 1607, 1508, 1466, 1248, 1175, 1034. HRMS (CI) [M] [$C_{31}H_{27}ON$]: calculated 429.2087, found 429.2081.

Synthesis of (E)-5-bromo-3-(3-(4-methoxyphenyl)-1-phenylallyl)-1-methyl-1H-indole **(3x)** *and (E)-5-bromo-3-(1-(4-methoxyphenyl)-3-phenylallyl)-1-methyl-1H-indole* **(3x′)**

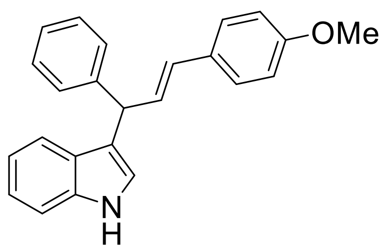


and

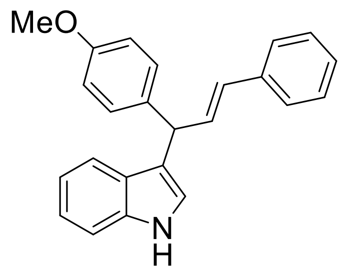


Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **1f** (28 mg, 0.1 mmol, 1 equiv.), and 5-bromo-1-methyl-1*H*-indole (21 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **3x** and **3x′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **3x** and **3x′** was obtained as a yellow oil. Combined yields: 34 mg, 0.08 mmol, 79%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.48 (t, *J* = 2.2 Hz, 2H, Ar–CH), 7.34–7.27 (m, 4H, Ar–CH), 7.26–7.13 (m, 12H, Ar–CH), 7.09 (dd, *J* = 8.7, 1.8 Hz, 2H, Ar–CH), 6.83–6.75 (m, 4H, Ar–CH), 6.70 (s, 2H, indole CH), 6.61 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.48 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.32 (two overlapped doublets, t, *J* = 15.6 Hz, 2H, $H_{vinylic}$), 5.00–4.94 (m, 2H, CH), 3.74 + 3.75 (two overlapped singlets, 6H, OMe), 3.65 (two overlapped singlets, 6H, NMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.1, 158.4, 143.5, 137.3, 136.20, 136.18, 135.3, 132.7, 130.5, 130.28, 130.26, 130.25, 130.2, 129.4, 128.98, 128.95, 128.7, 128.62, 128.61, 128.5, 127.6, 127.3, 126.6, 126.4, 124.62, 124.60, 122.4, 117.2, 117.1, 114.09, 114.05, 114.0, 112.46, 112.45, 110.85, 110.84, 55.42 (OMe), 55.39 (OMe), 46.0 (CH), 45.1 (CH), 33.0 (NMe); IR ν_{max} (cm^{-1}): 3024, 2930, 2833, 1732, 1606, 1508, 1474, 1422, 1246, 1175, 1031. HRMS (CI) [M] [$C_{25}H_{22}ON^{79}Br$]: calculated 431.0879, found 431.0874.

Synthesis of (E)-3-(3-(4-methoxyphenyl)-1-phenylallyl)-1H-indole **(3y)** *and (E)-3-(1-(4-methoxyphenyl)-3-phenylallyl)-1H-indole* **(3y′)**



and



Synthesized in accordance with General Procedure e using B(3,4,5-Ar^F)$_3$ (6 mg, 0.015 mmol 0.15 equiv.), (E)-3-(4-methoxyphenyl)-1-phenylallyl acetate **1f** (28 mg, 0.1 mmol, 1 equiv.), and indole (12 mg, 0.1 mmol, 1 equiv.) in $CHCl_3$ to afford **2y** and **2y′**. The crude reaction mixture was purified via preparative thin layer chromatography using hexane/ethyl acetate (92:8 v/v) as eluent. A 1:1 inseparable regioisomeric mixture of **2y** and **2y′** was obtained as a yellow oil. Combined yields: 23 mg, 0.07 mmol, 68%. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ: 7.97 (s, br, 2H, NH), 7.46 (d, *J* = 8.0, 2H, Ar–CH), 7.41–7.26 (m, 14H, Ar–CH), 7.26–7.17 (m, 4H, Ar–CH), 7.08–7.02 (m, 2H, Ar–CH), 6.91–6.90 (m, 2H, indole CH), 6.90–6.83 (m, 4H, Ar–CH), 6.74 (dd, *J* = 15.8, 7.3 Hz, 1H, $H_{vinylic}$), 6.61 (dd, *J* = 15.8, 7.4 Hz, 1H, $H_{vinylic}$), 6.43 (t, *J* = 15.7 Hz, 2H, $H_{vinylic}$), 5.12 + 5.10 (two overlapped doublets, d, *J* = 7.4 Hz, 1H, CH, d, *J* = 7.4 Hz, 1H, CH), 3.81 (two overlapped singlets, 6H, OMe); ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) δ: 159.0, 158.2, 143.8, 137.7, 136.81, 136.79, 135.6, 133.0, 130.6, 130.5, 130.4, 130.0, 129.6, 128.61, 128.56, 128.52, 127.6, 127.2, 127.0, 126.9, 126.4, 122.72, 122.66, 122.20, 122.18, 120.07, 120.05, 119.5, 119.10, 119.05, 114.0, 113.9, 111.22, 111.21, 55.42 (OMe), 55.38 (OMe), 46.3 (CH), 45.5 (CH); IR ν_{max} (cm^{-1}): 3416, 3026, 2932, 2835, 1607, 1508, 1456, 1246, 1175, 1032. HRMS (CI) [M] [$C_{24}H_{21}ON$]: calculated 339.1618, found 339.1615.

5. NMR Spectra

Figure S1: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1a**.

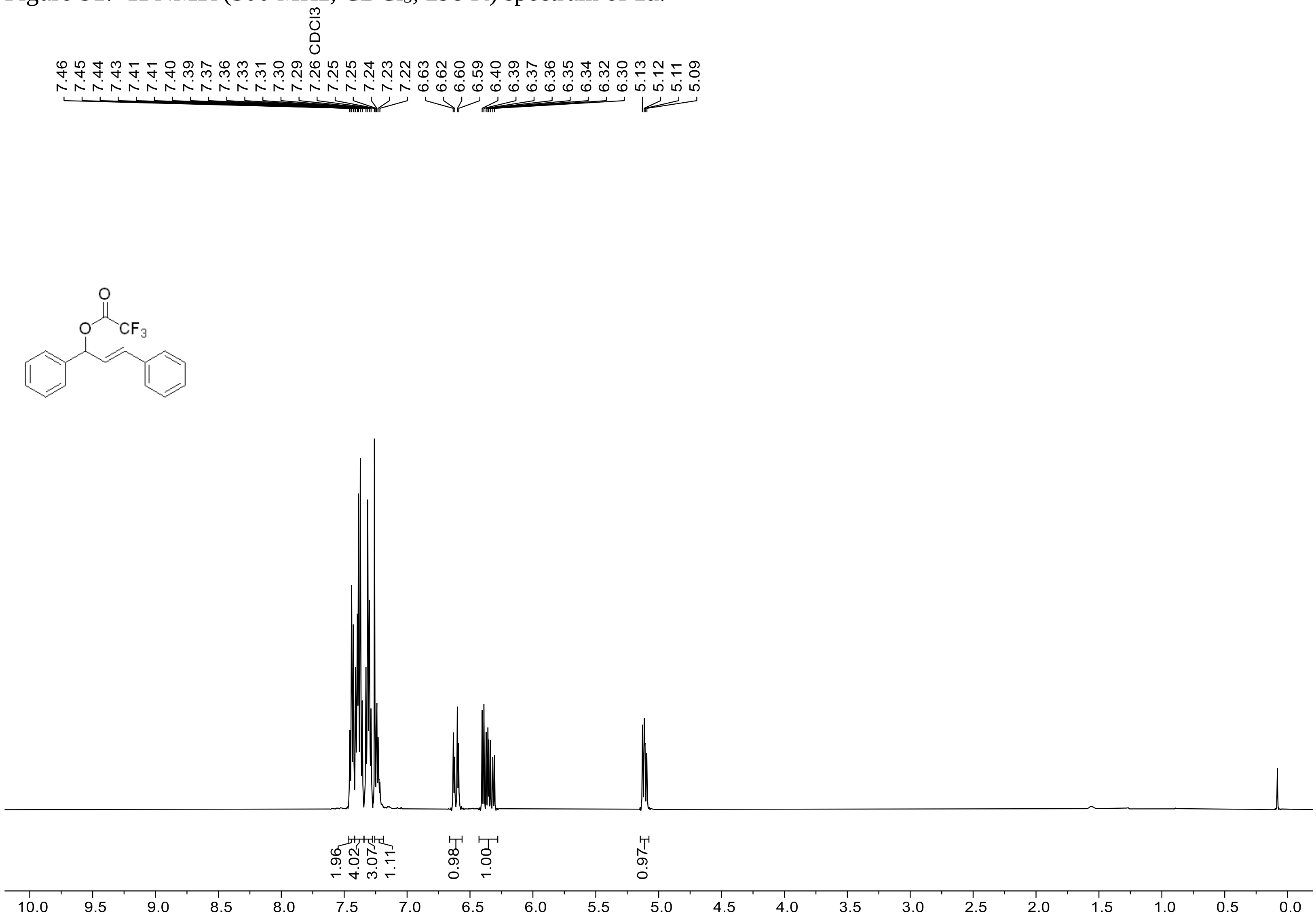


Figure S2: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1a**.

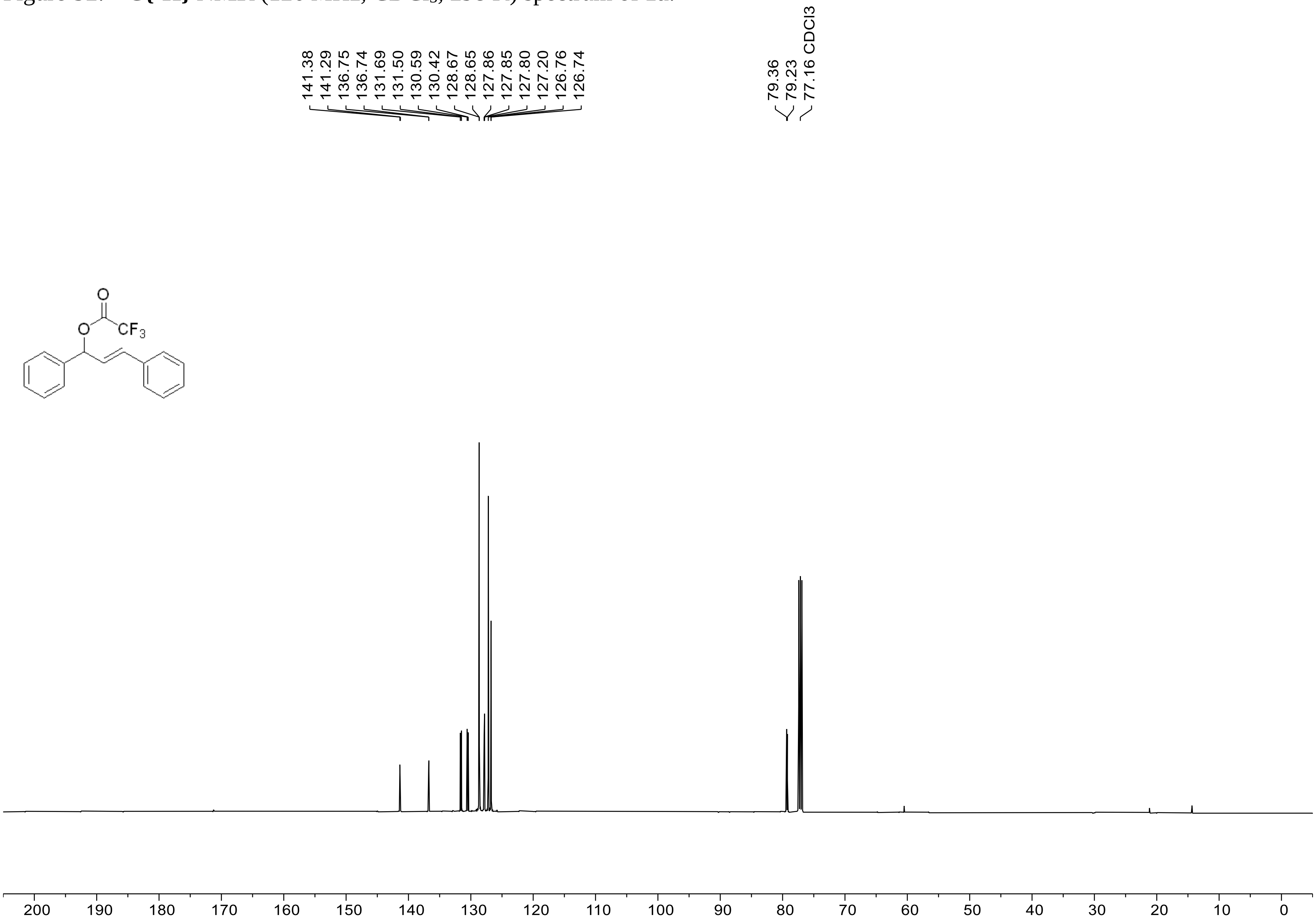


Figure S3: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **1a**.

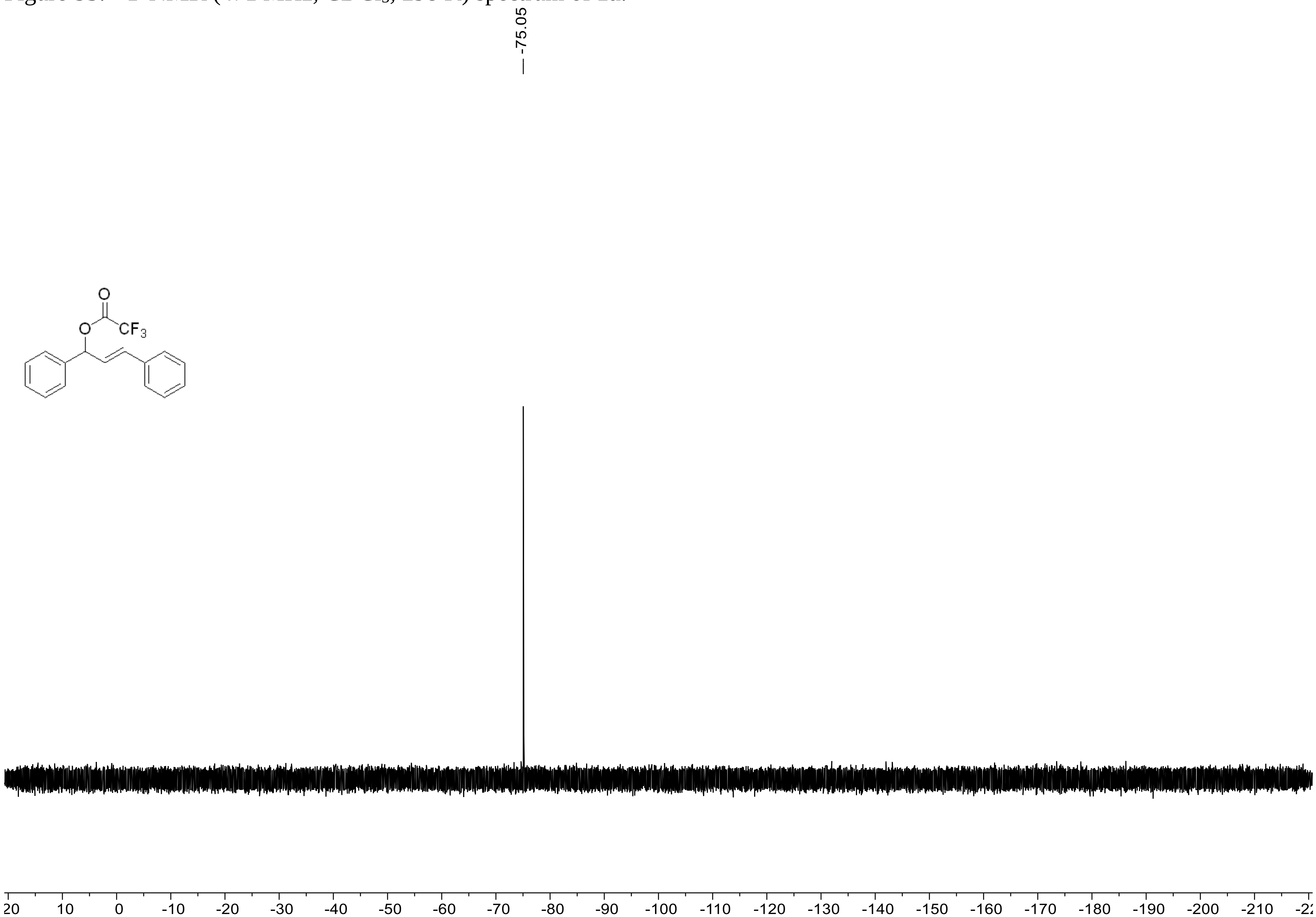


Figure S4: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1b**.

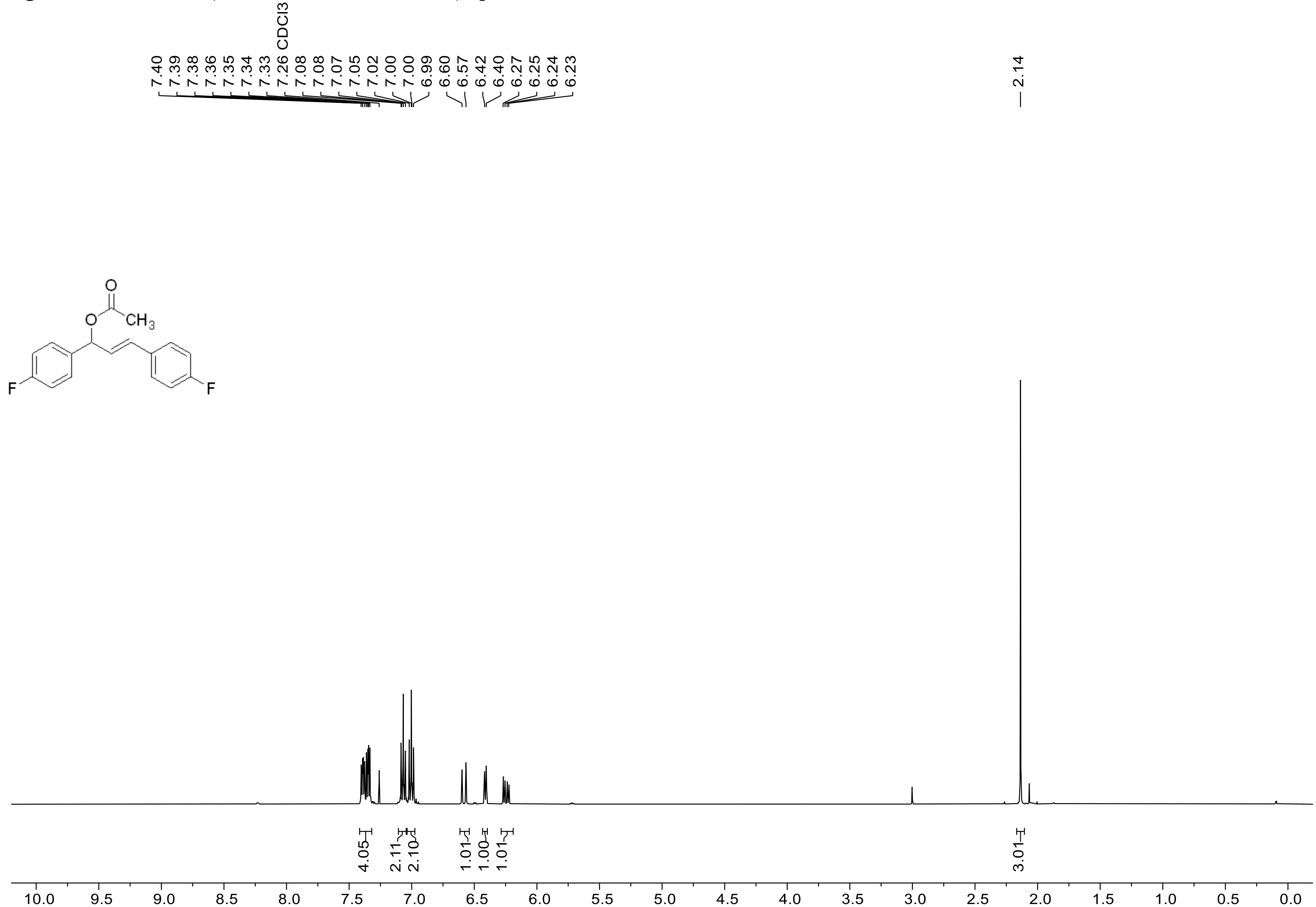


Figure S5: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1b**.

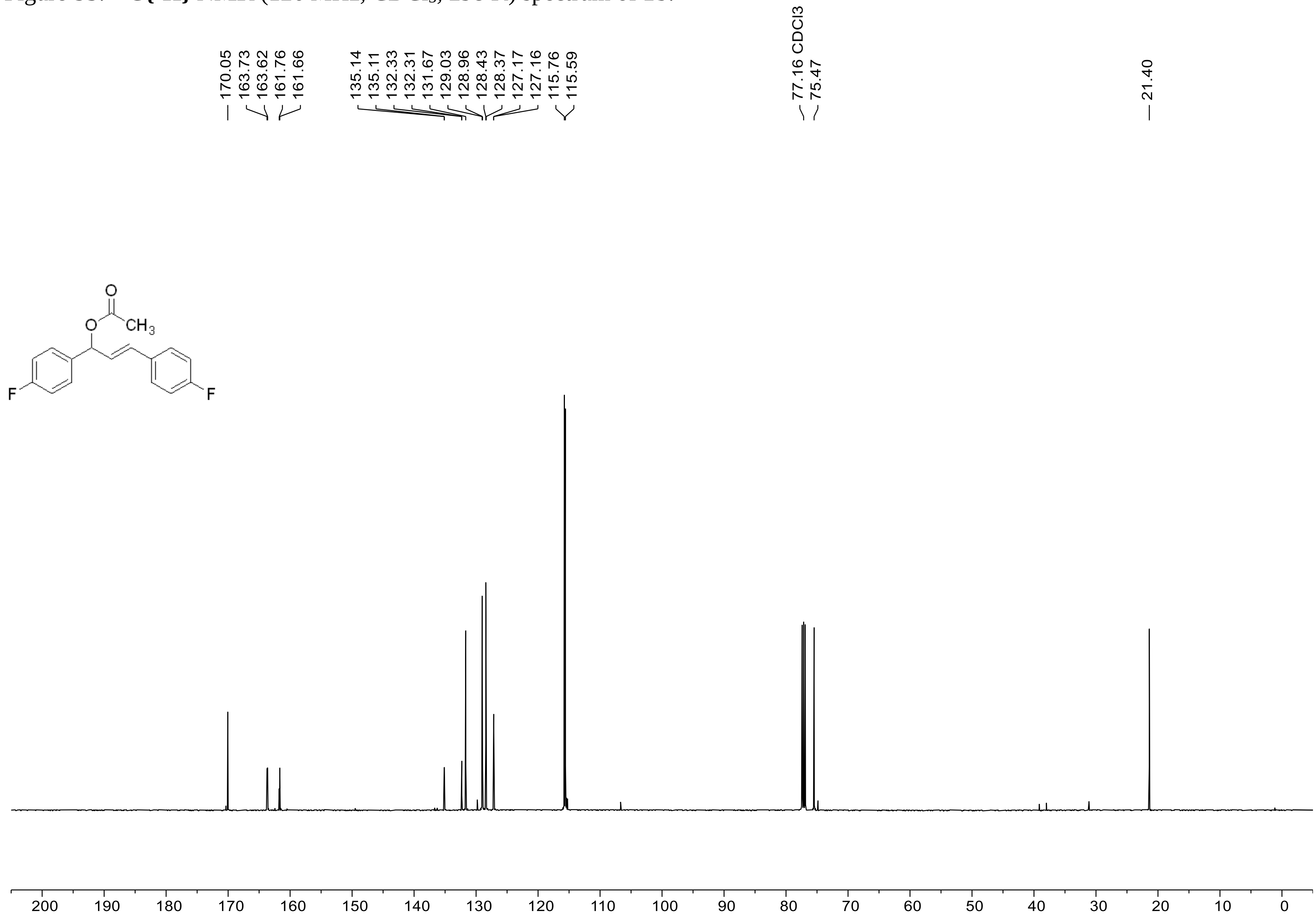


Figure S6: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **1b**.

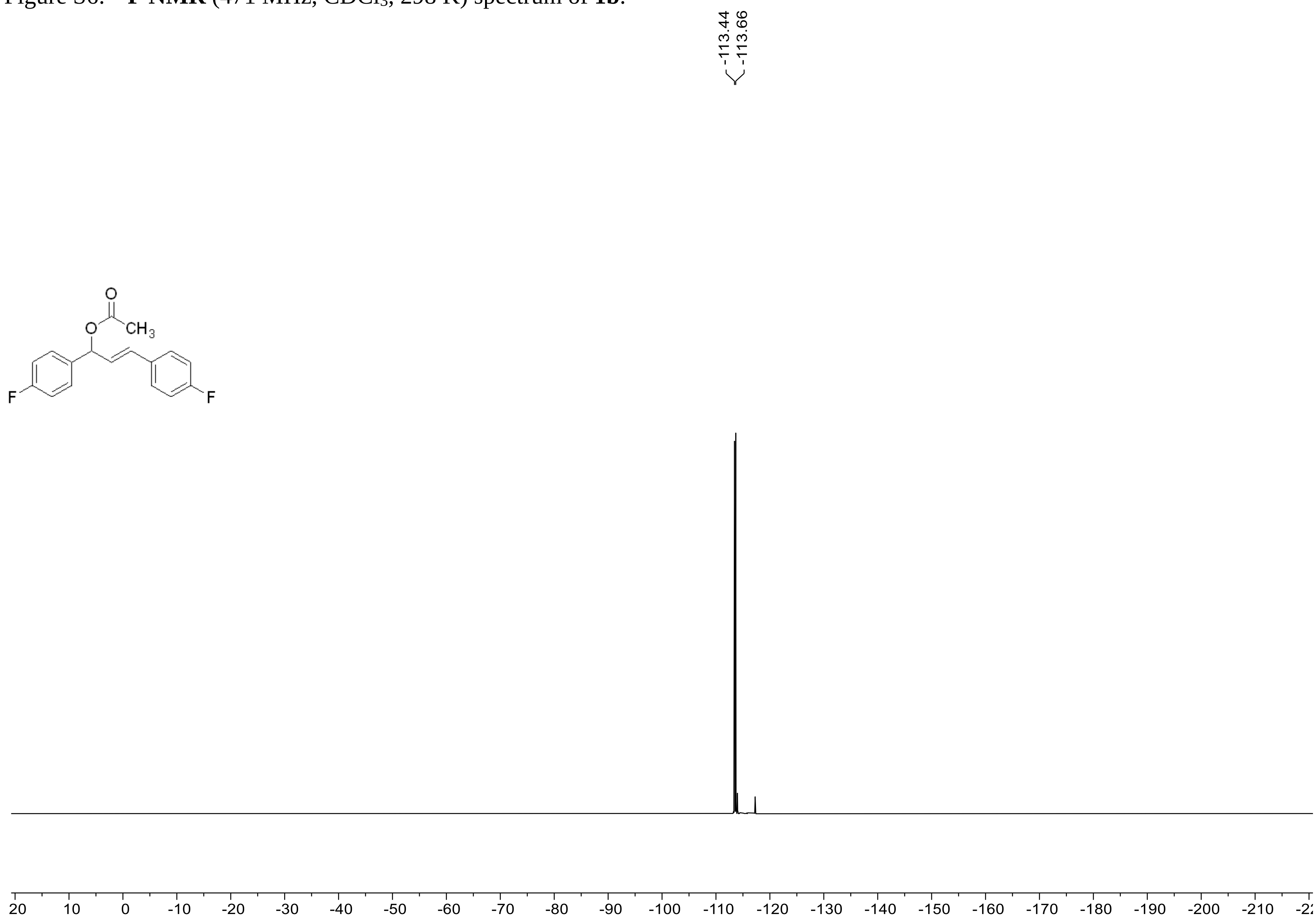


Figure S7: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1c**.

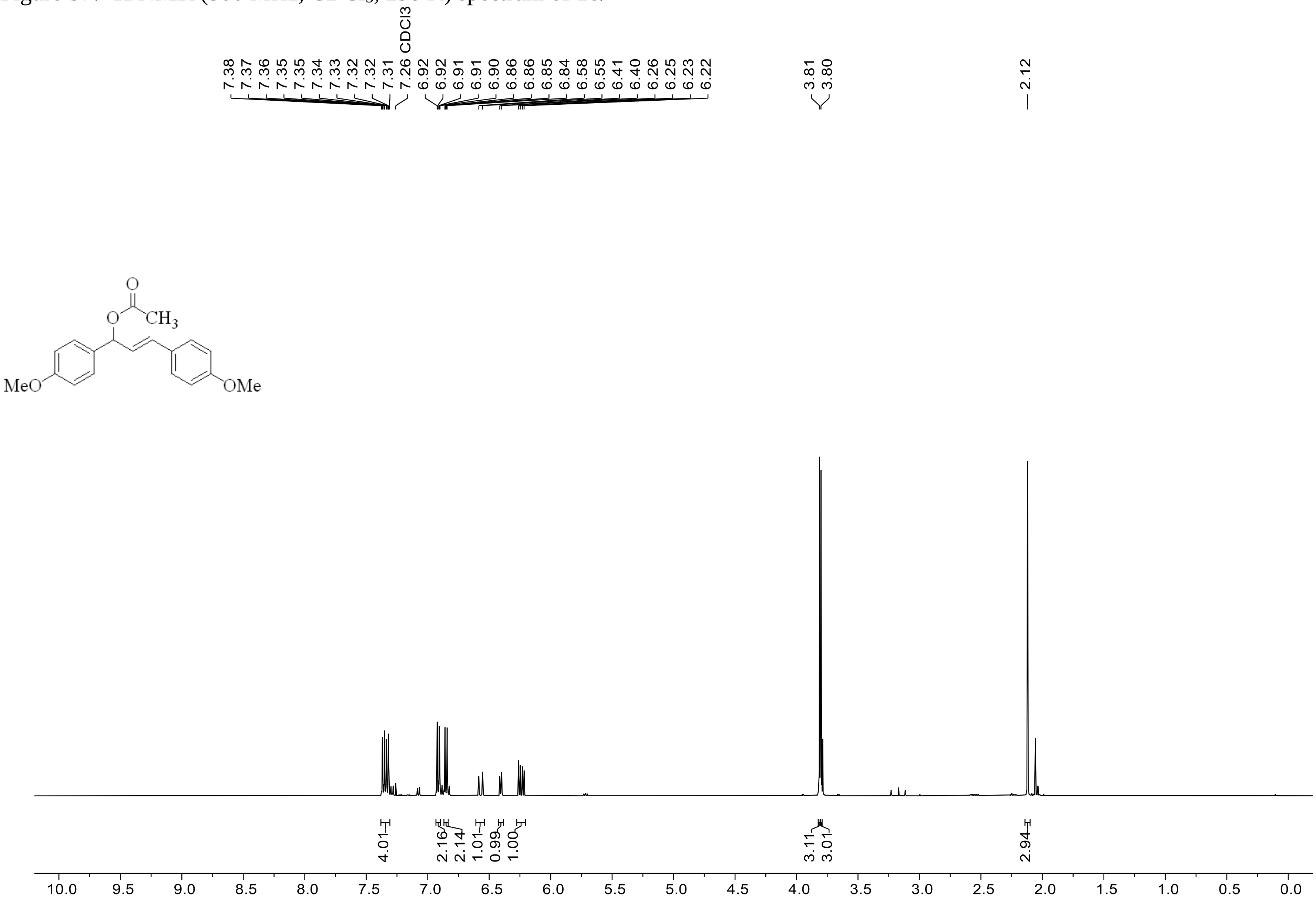


Figure S8: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1c**.

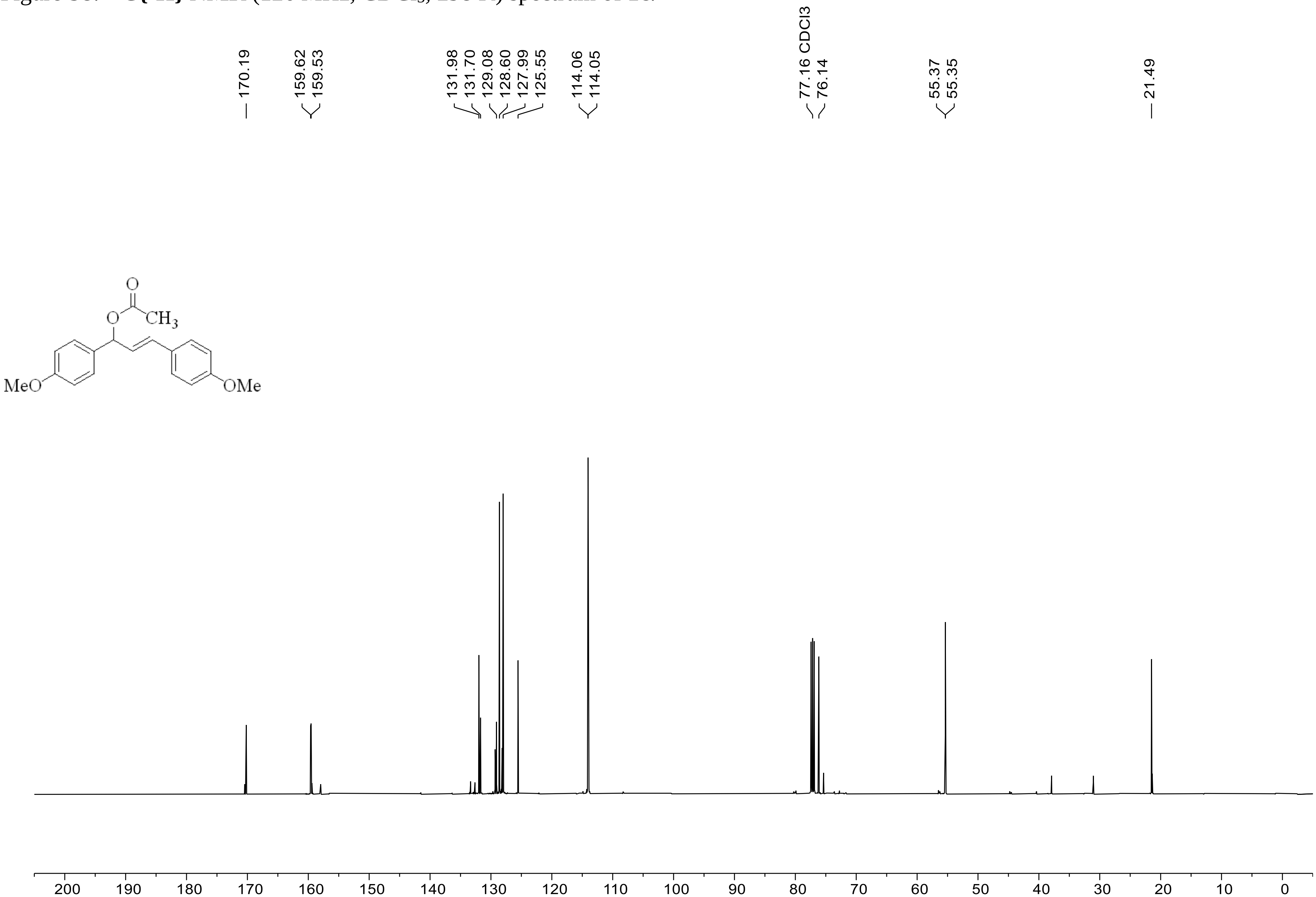


Figure S9: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1d**.

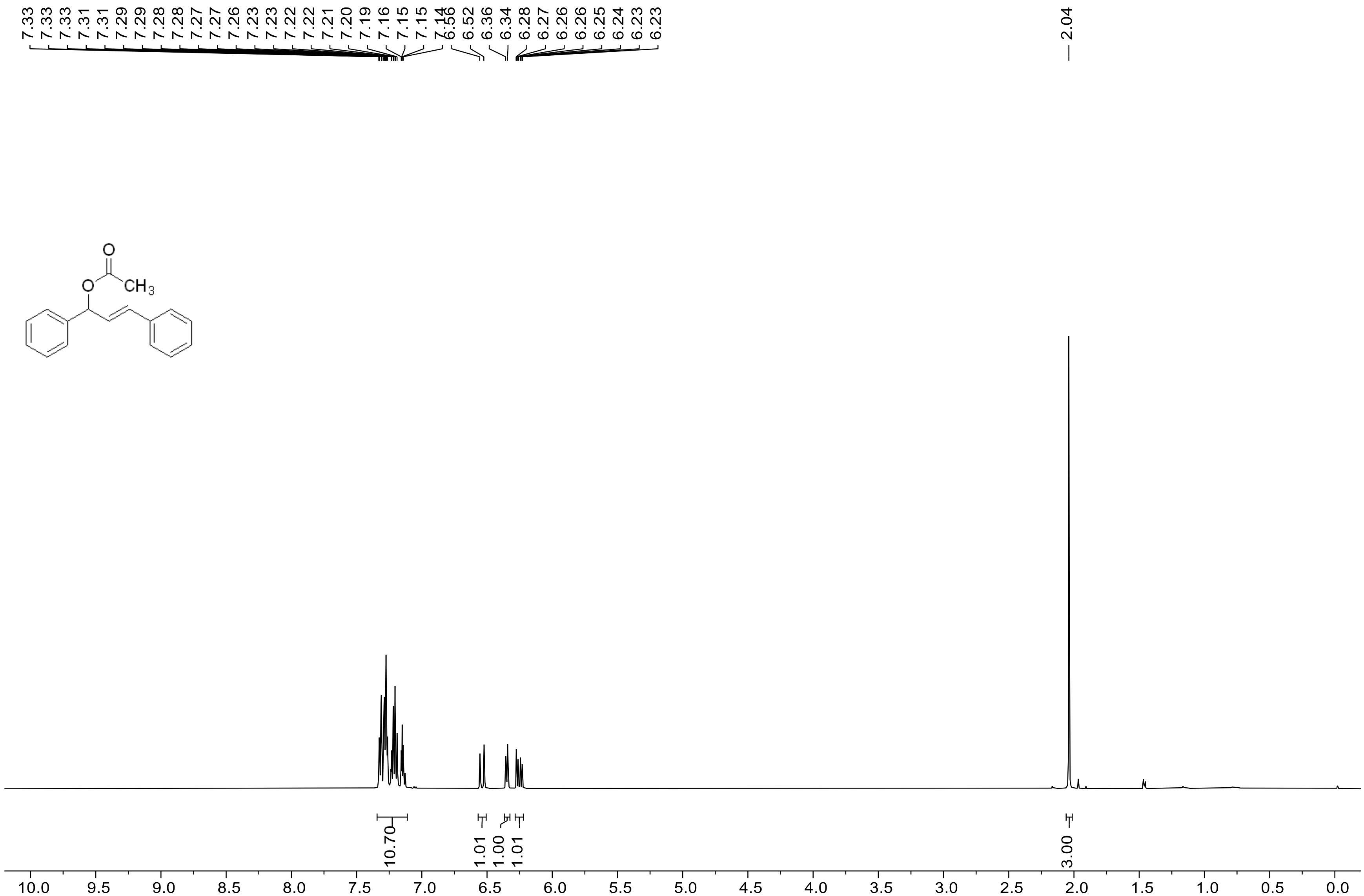


Figure S10: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1d**.

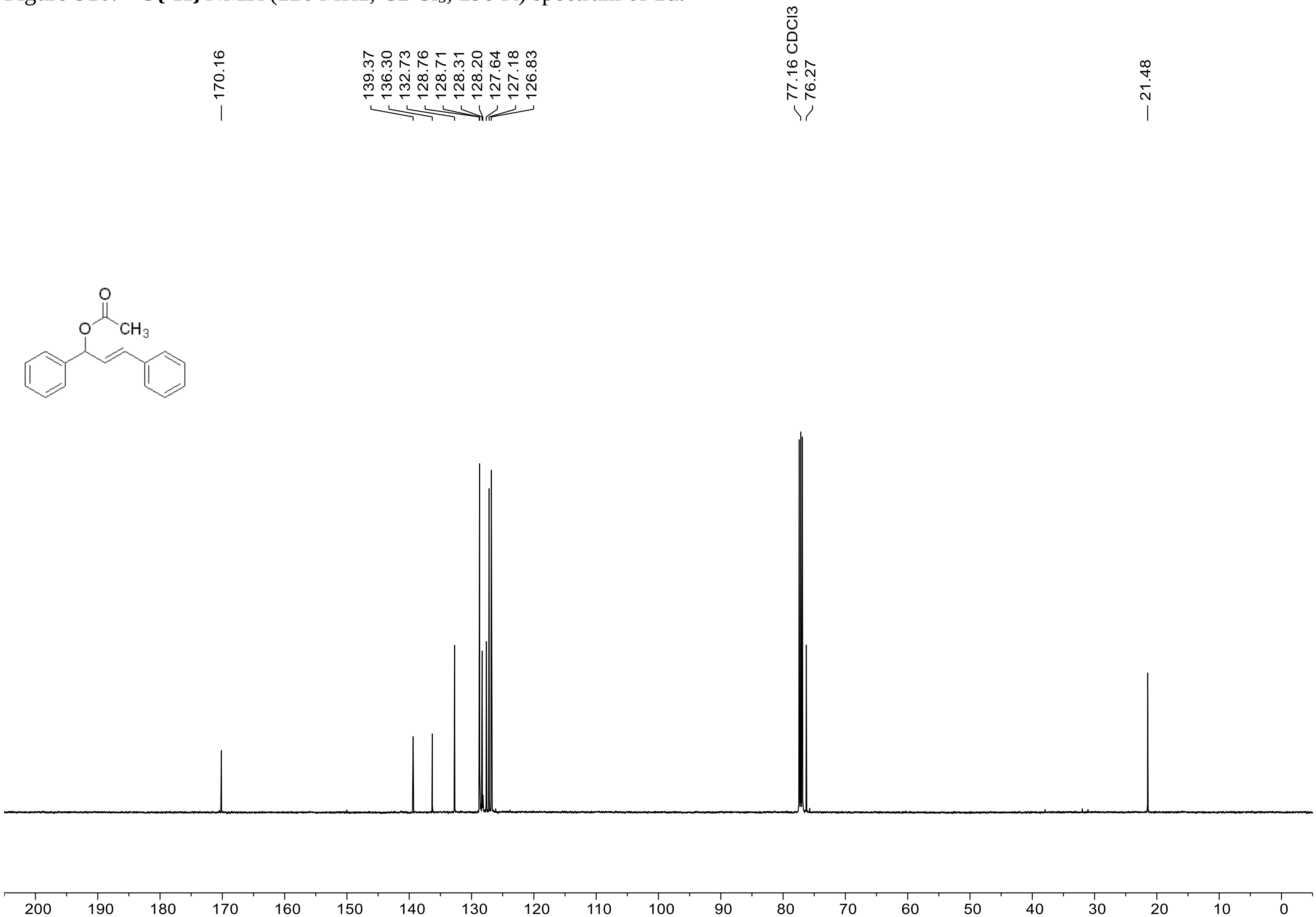


Figure S11: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1e**.

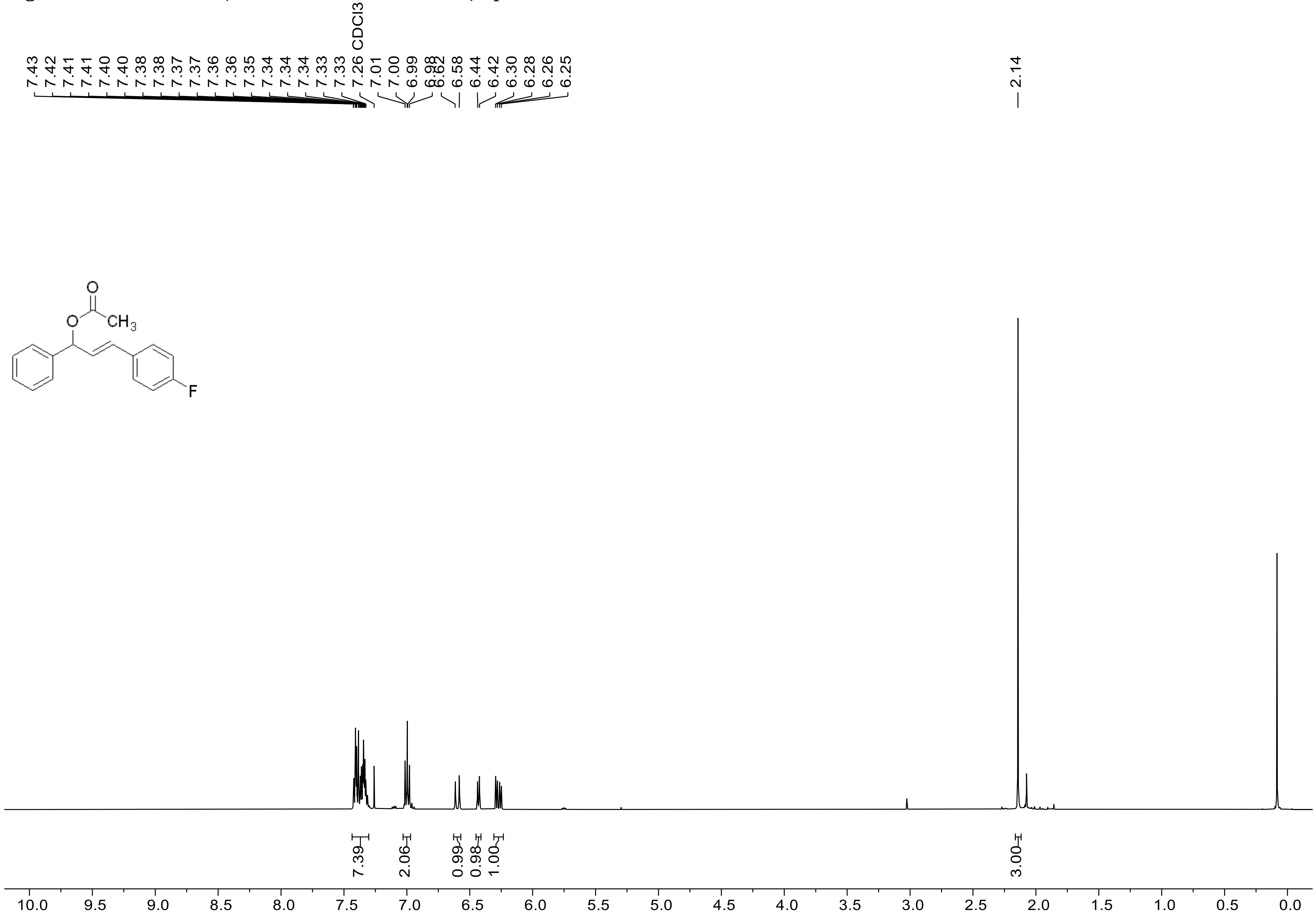


Figure S12: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1e**.

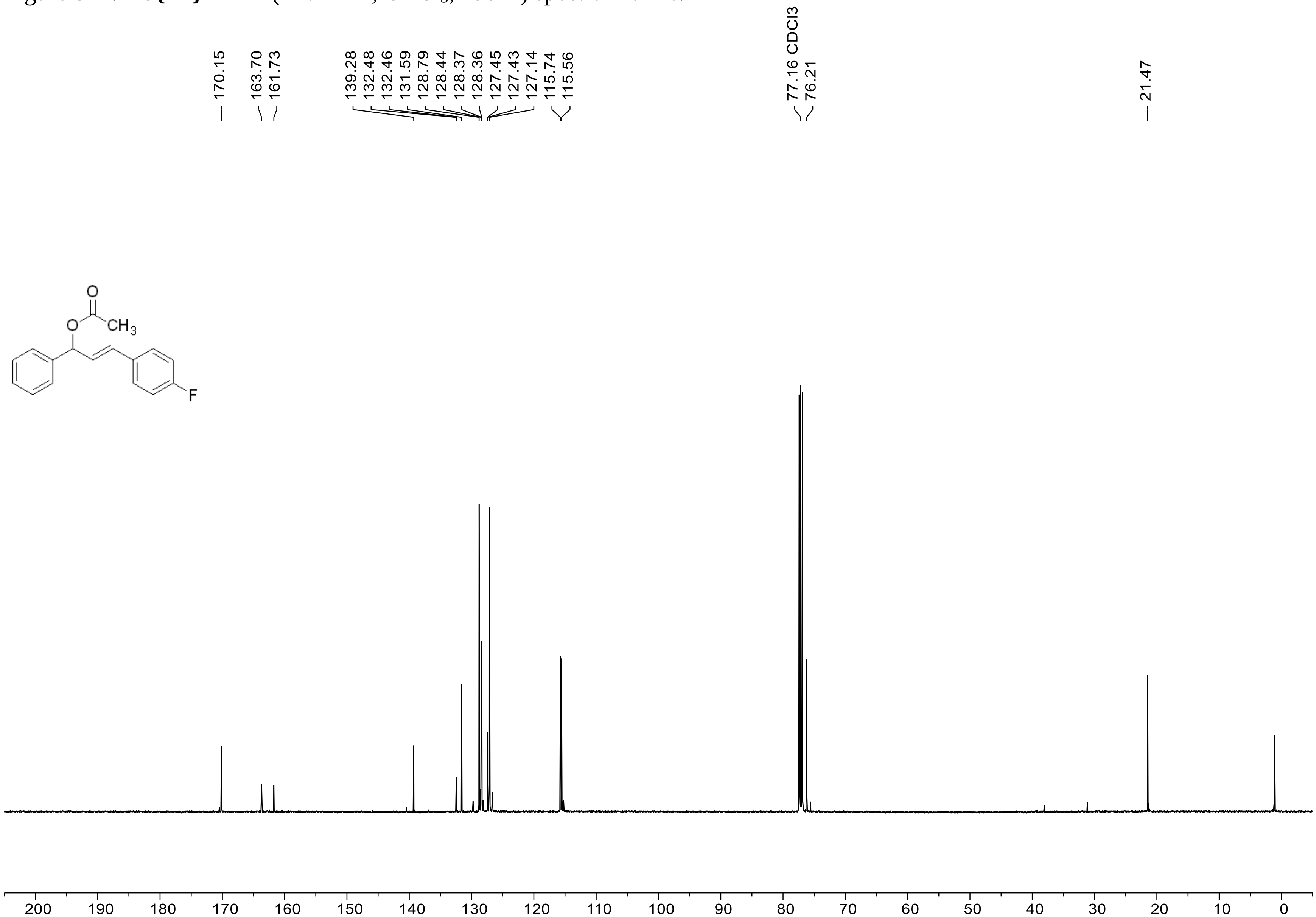


Figure S13: ^{19}**F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **1e**.

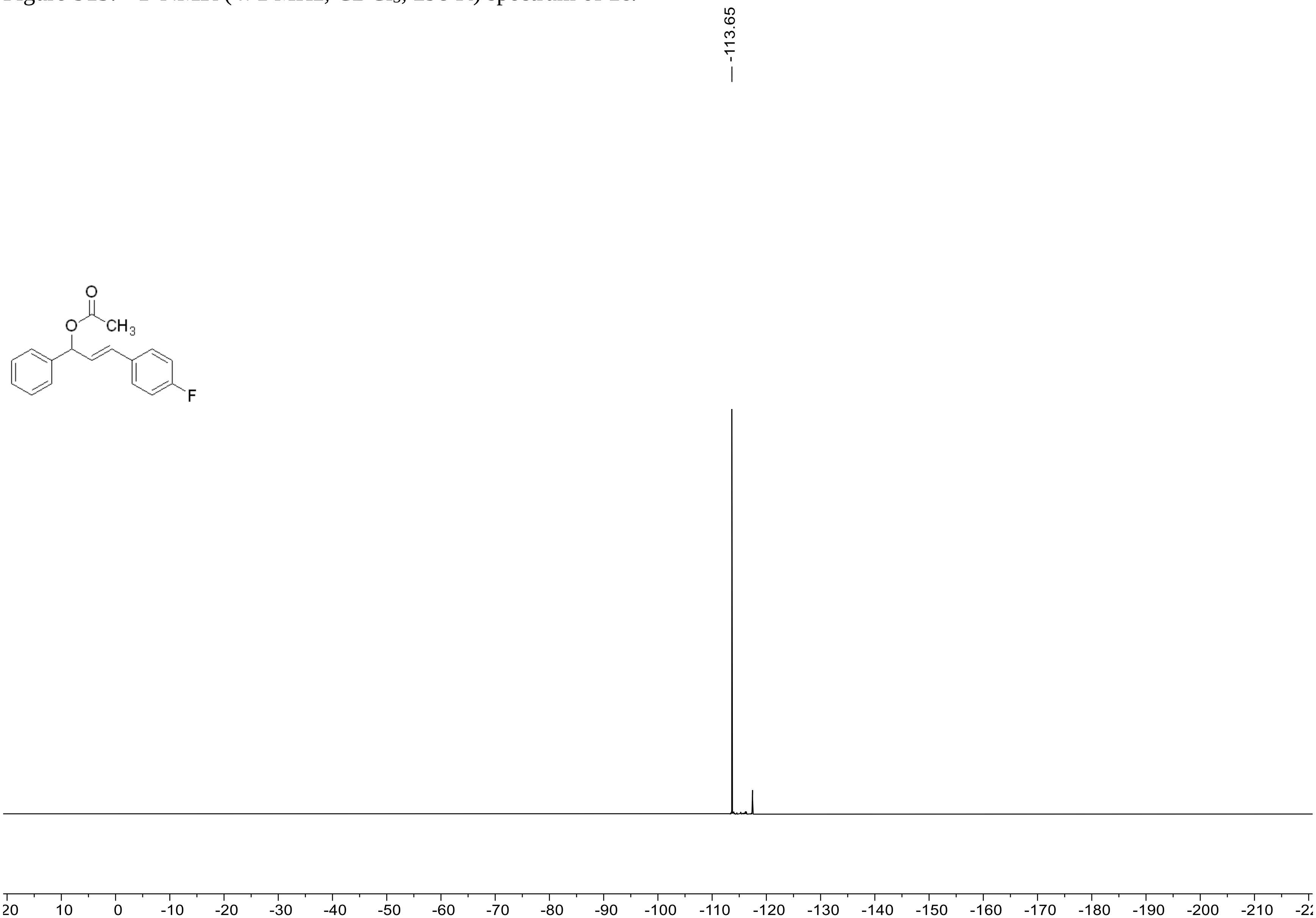


Figure S14: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **1f**.

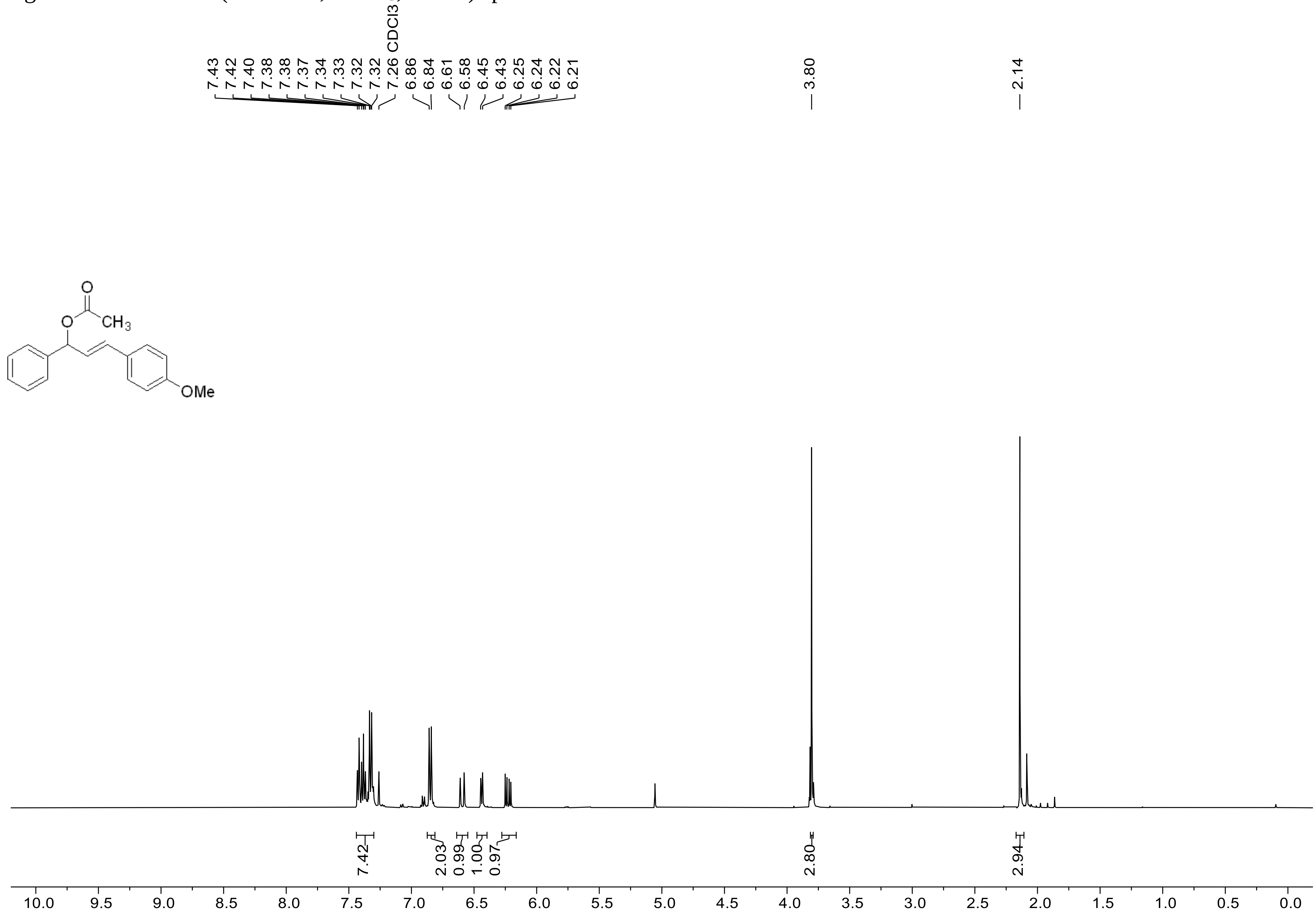


Figure S15: ^{13}**C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **1f**.

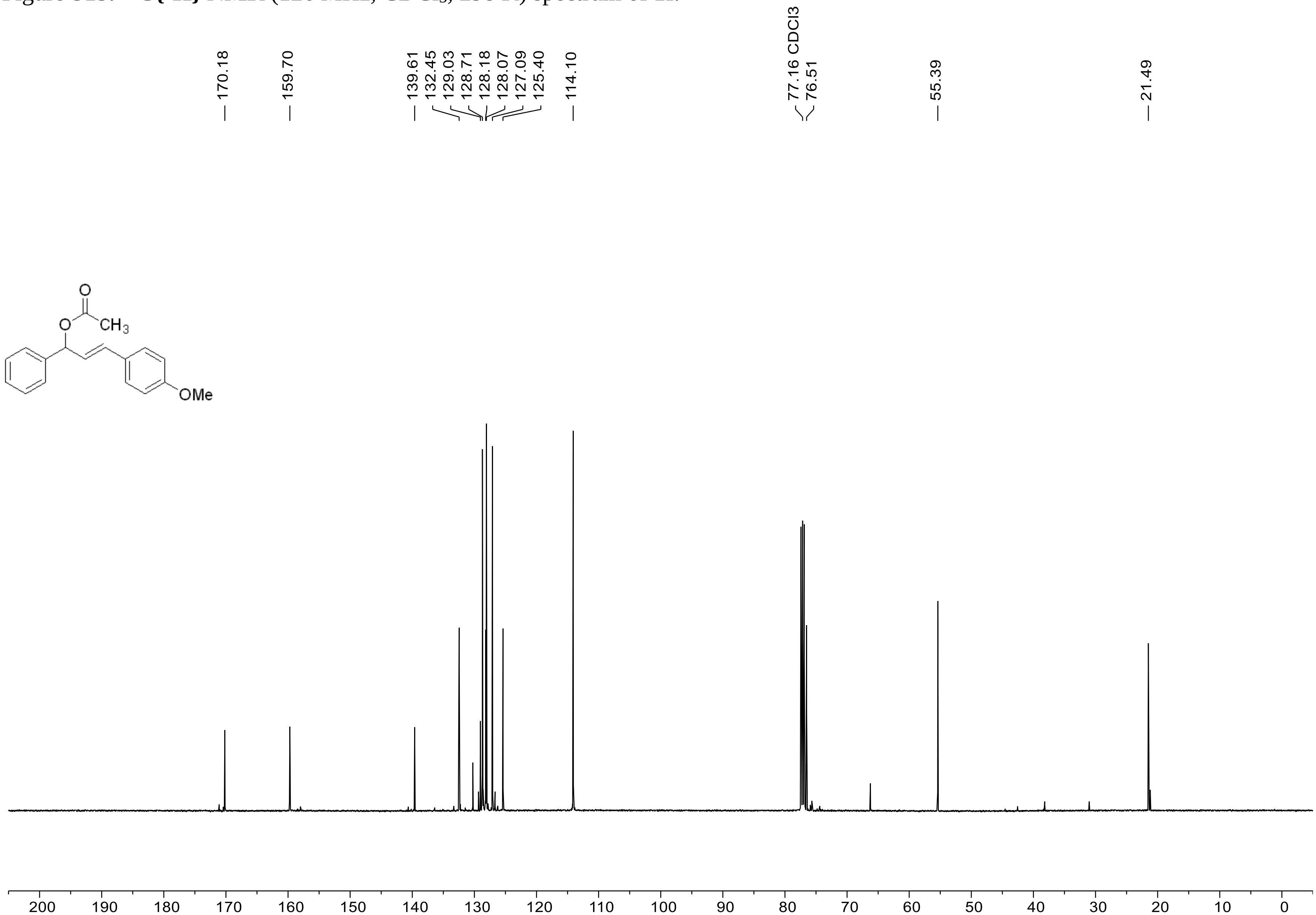


Figure S16: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3a**.

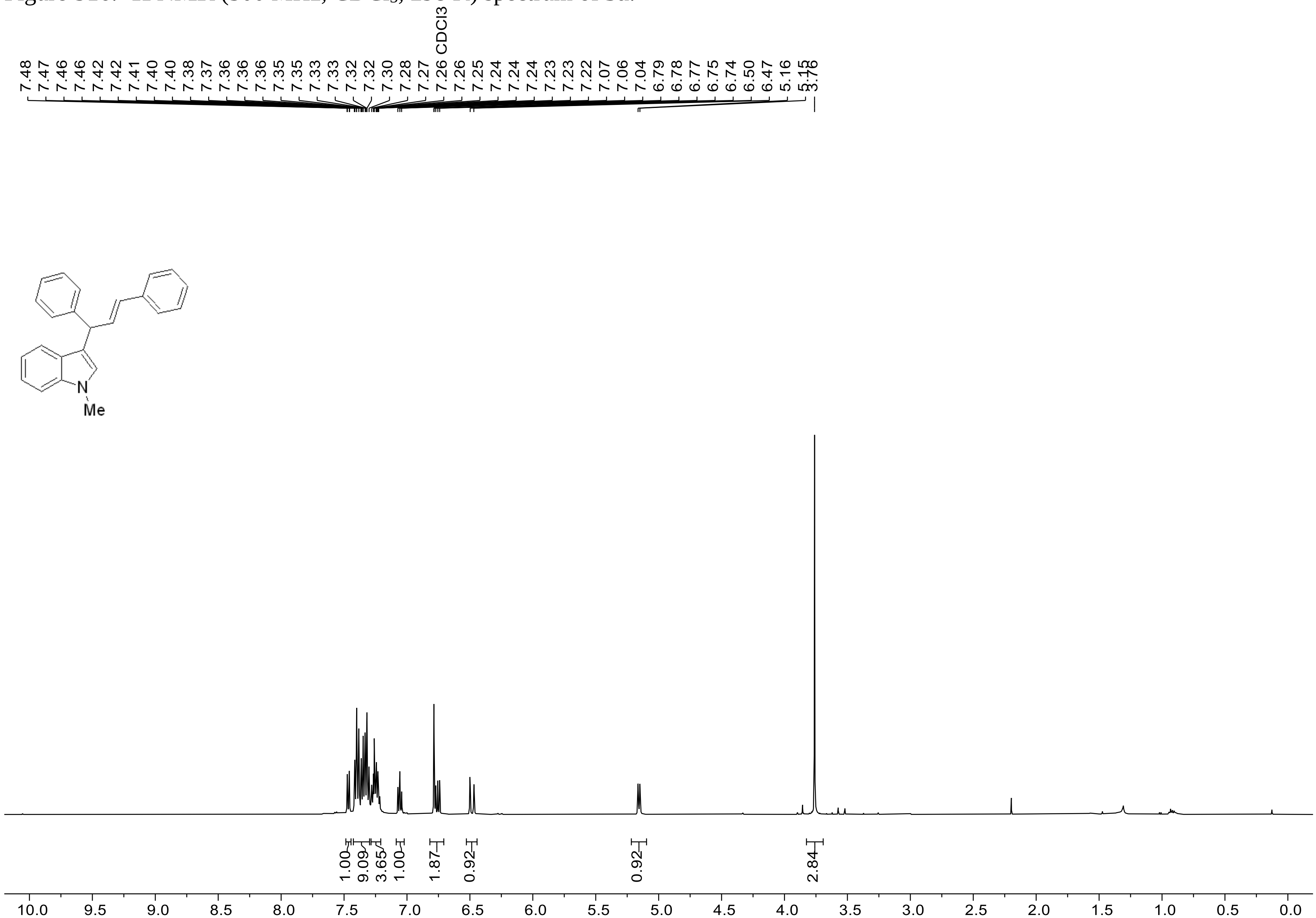


Figure S17: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3a**.

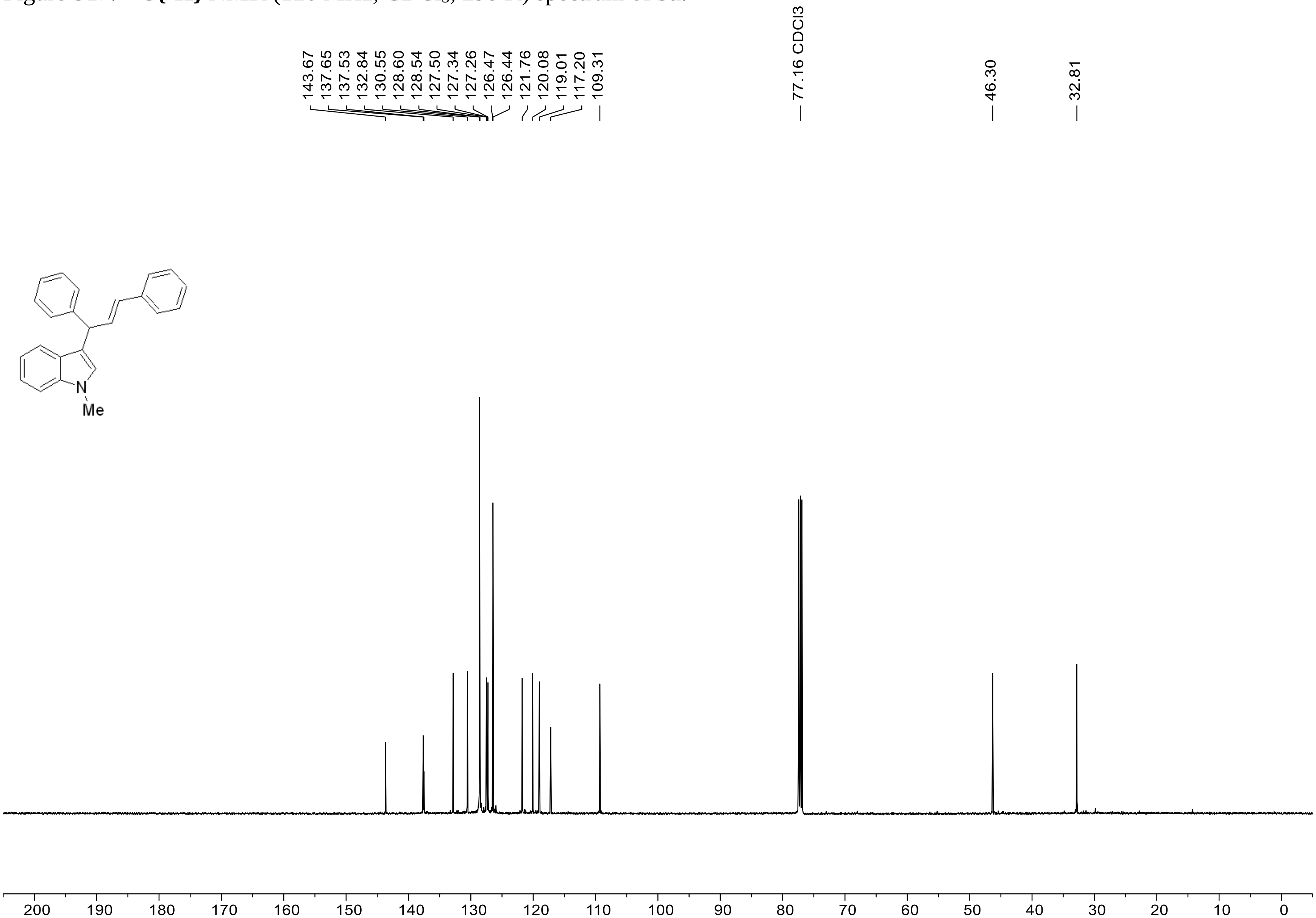


Figure S18: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3b**.

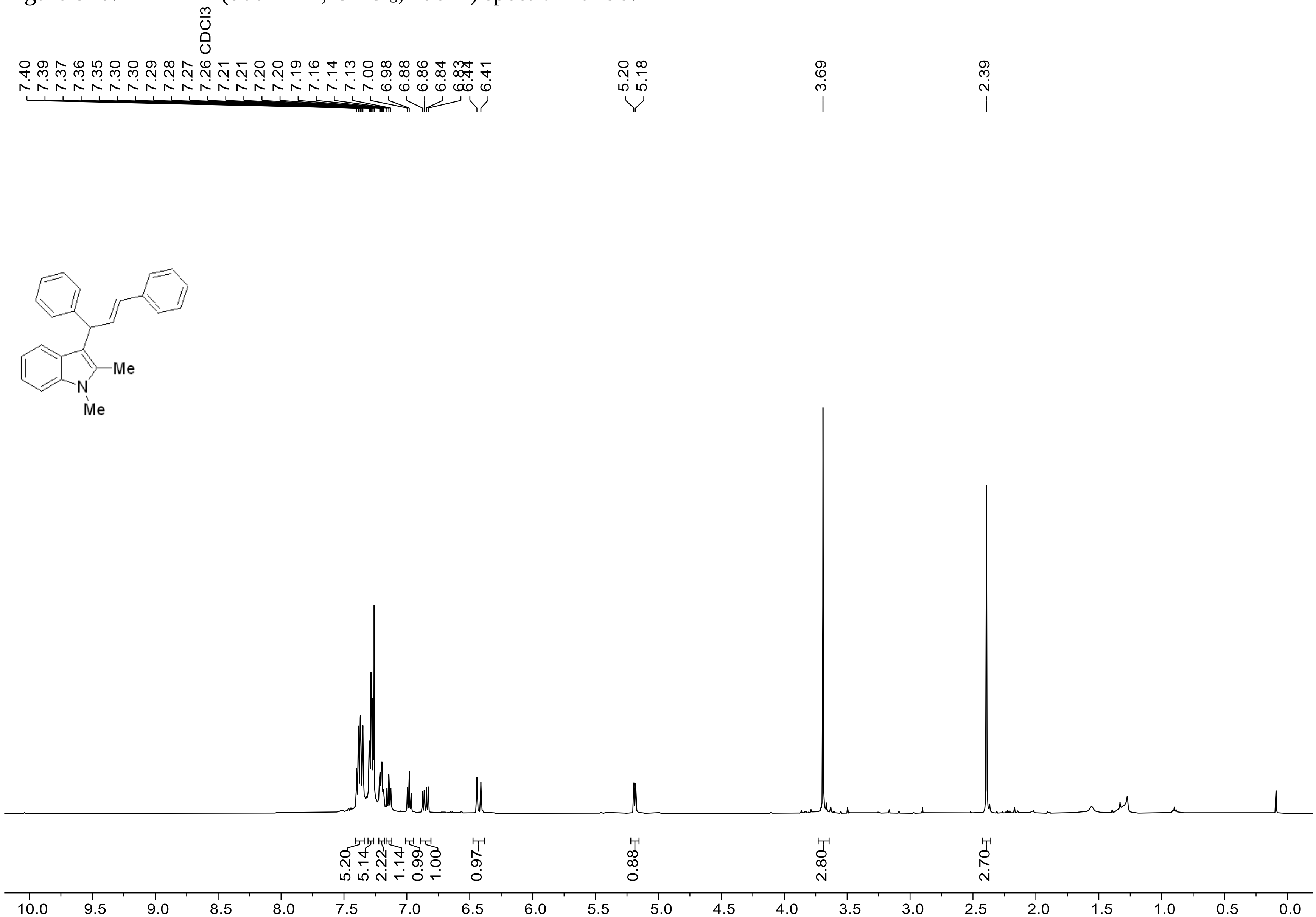


Figure S19: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3b**.

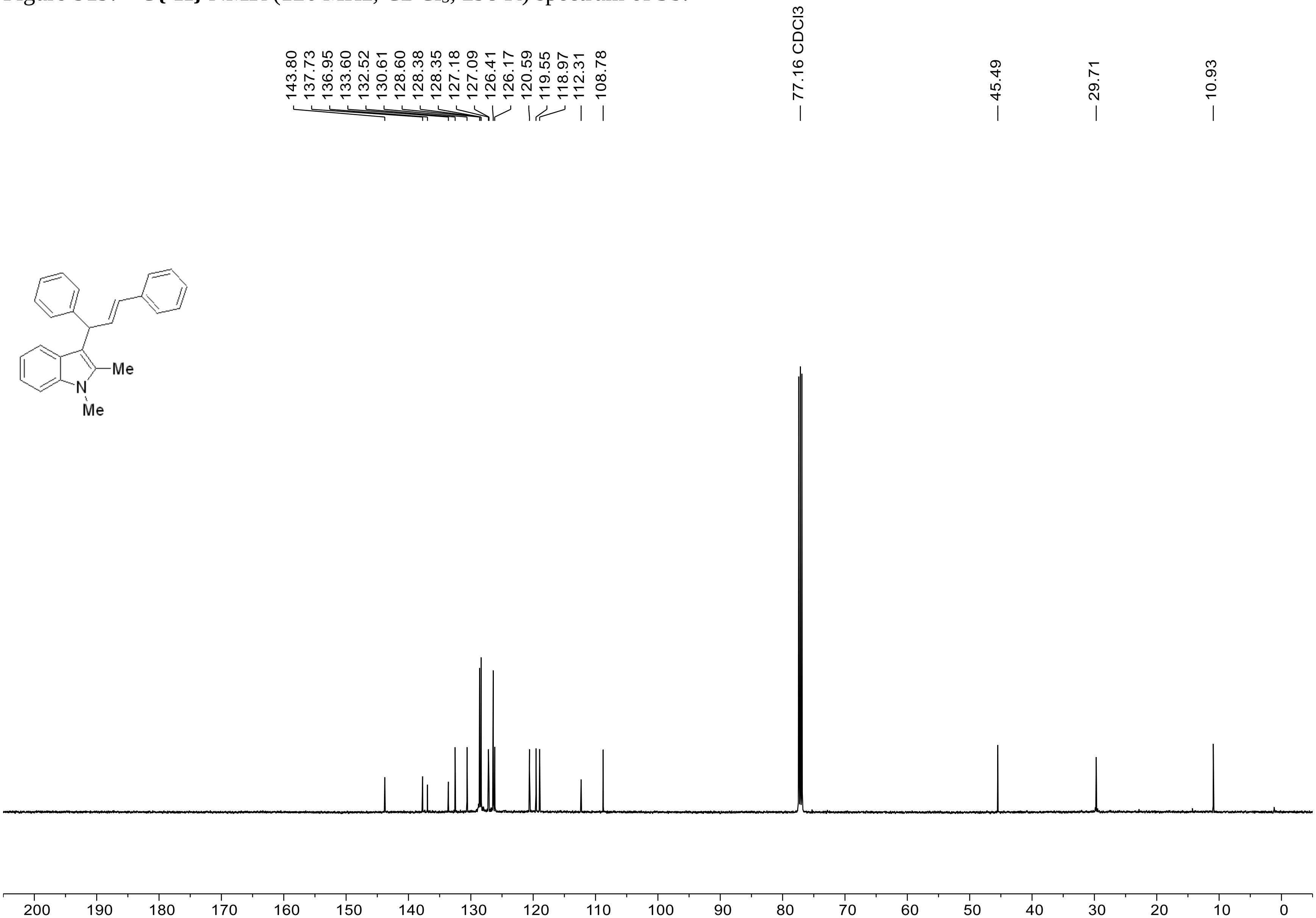


Figure S20: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3c**.

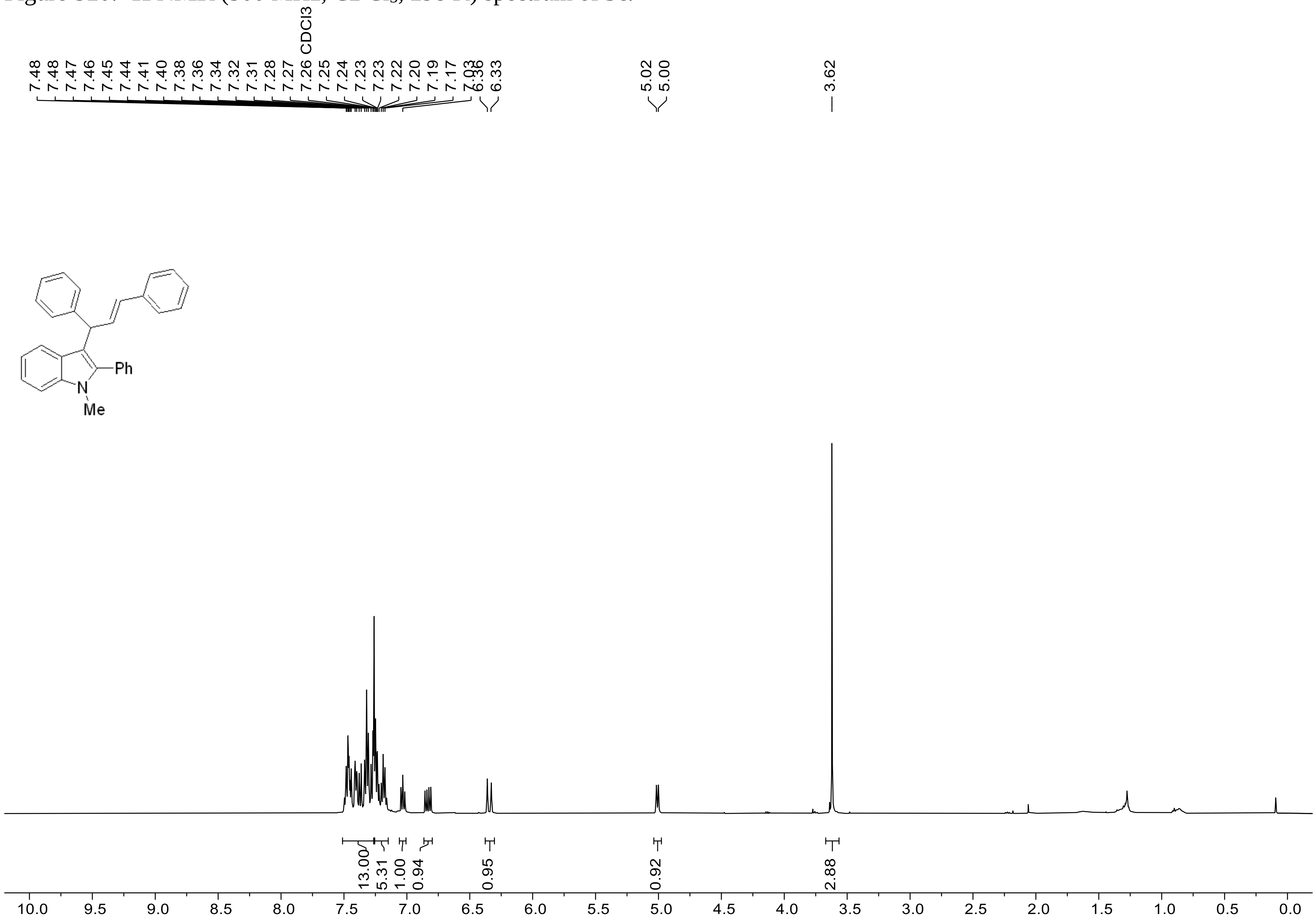


Figure S21: **$^{13}C\{^1H\}$ NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3c**.

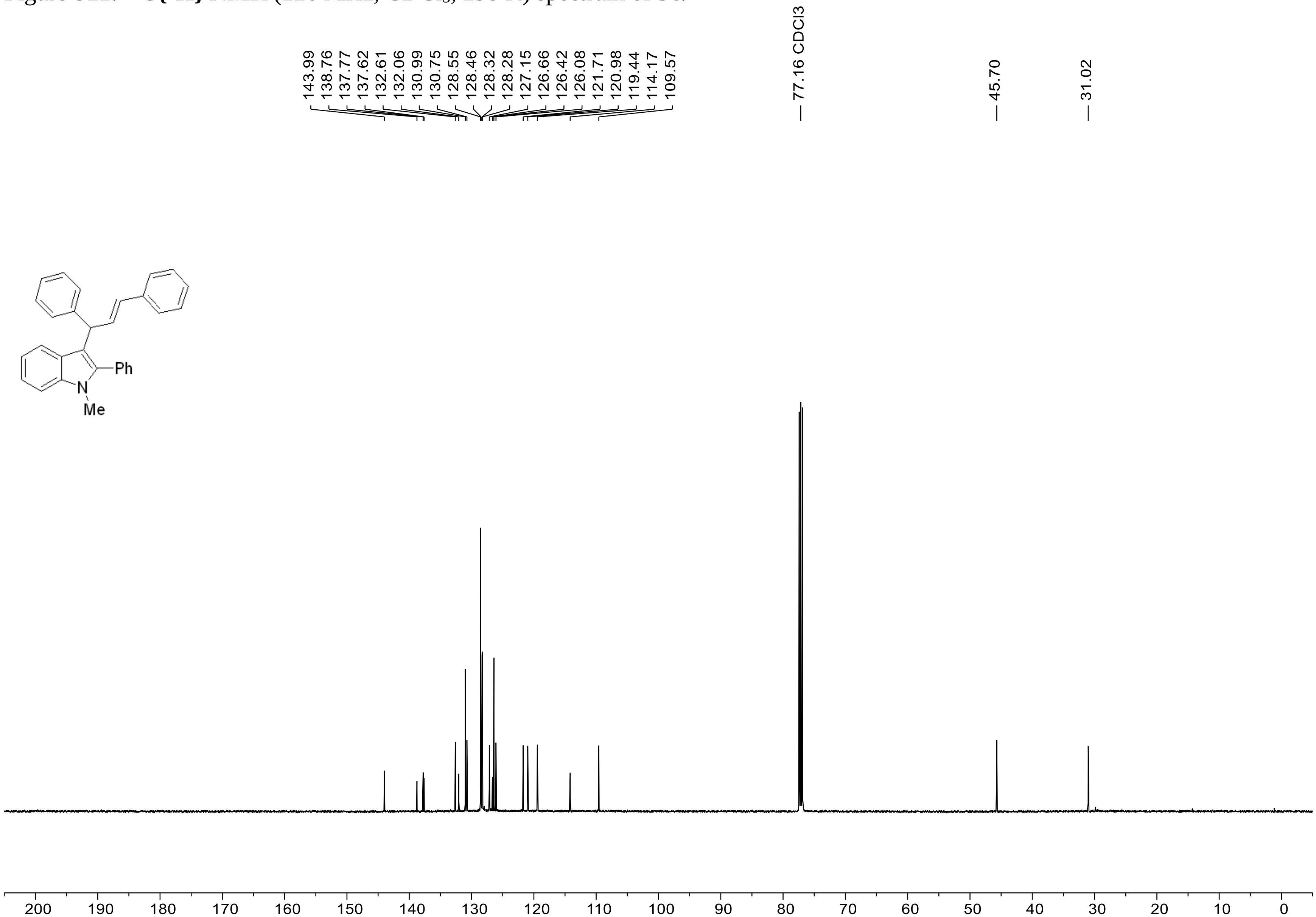


Figure S22: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3d**.

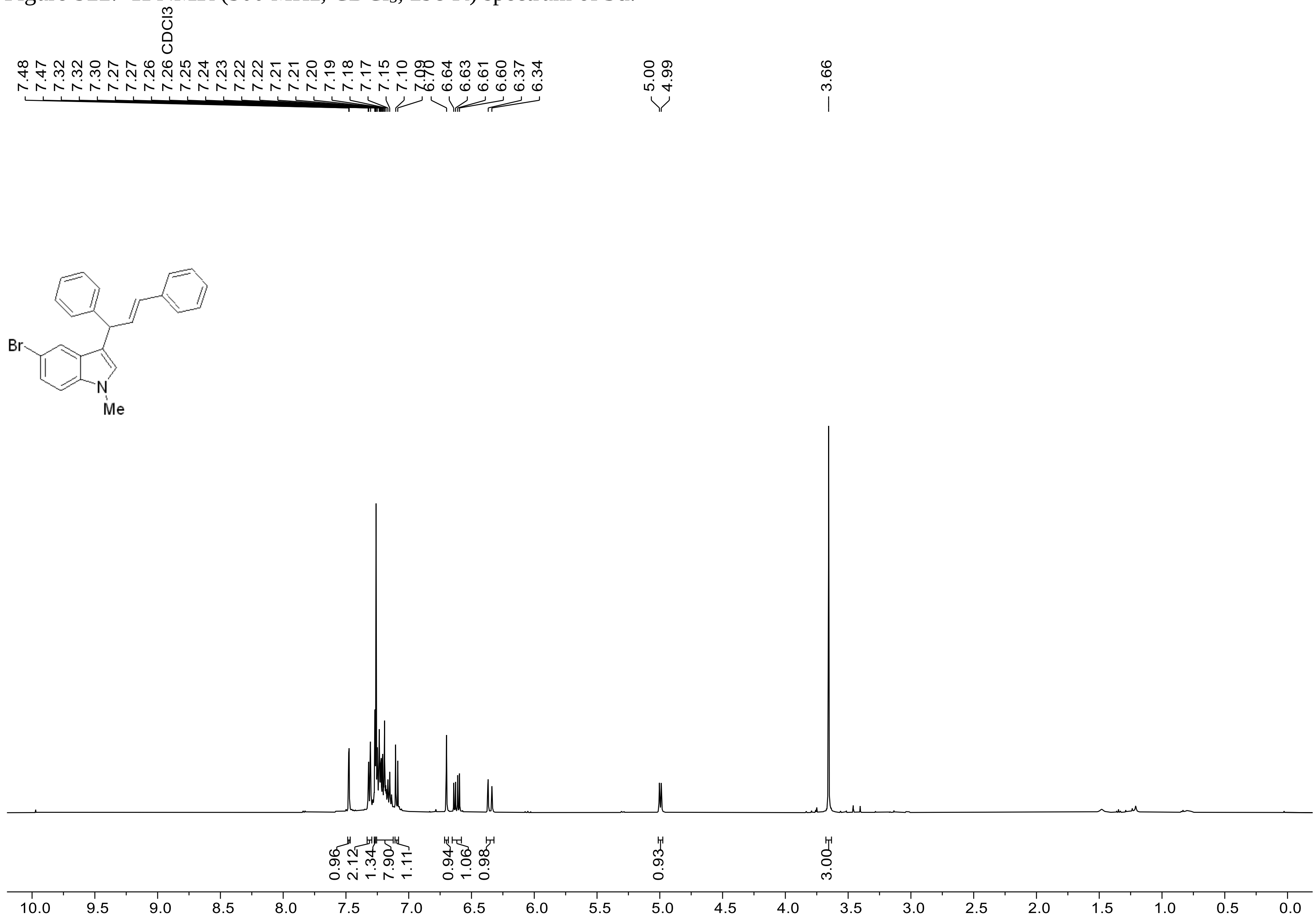
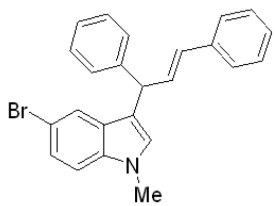


Figure S23: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3d**.



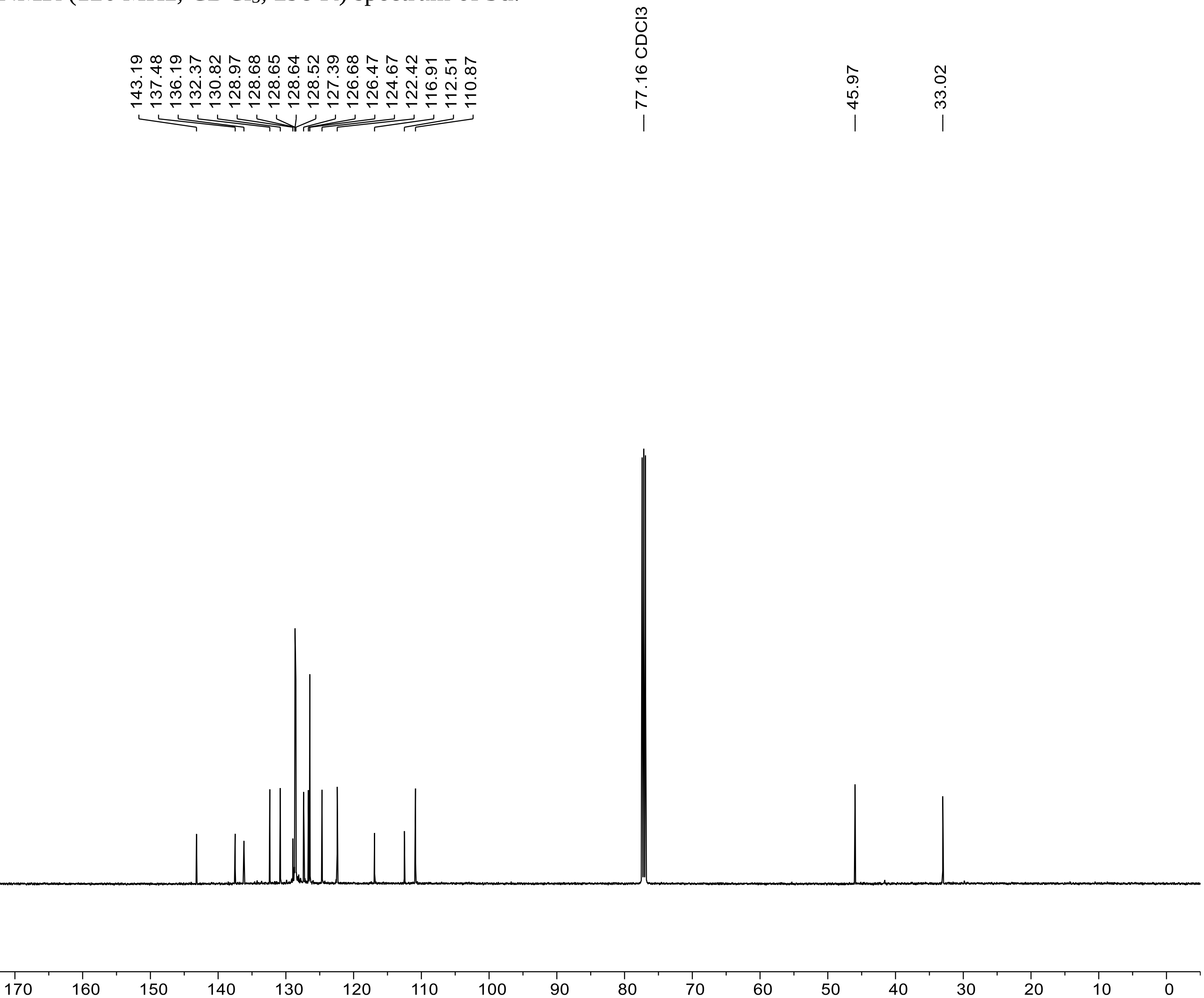


Figure S24: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3e**.

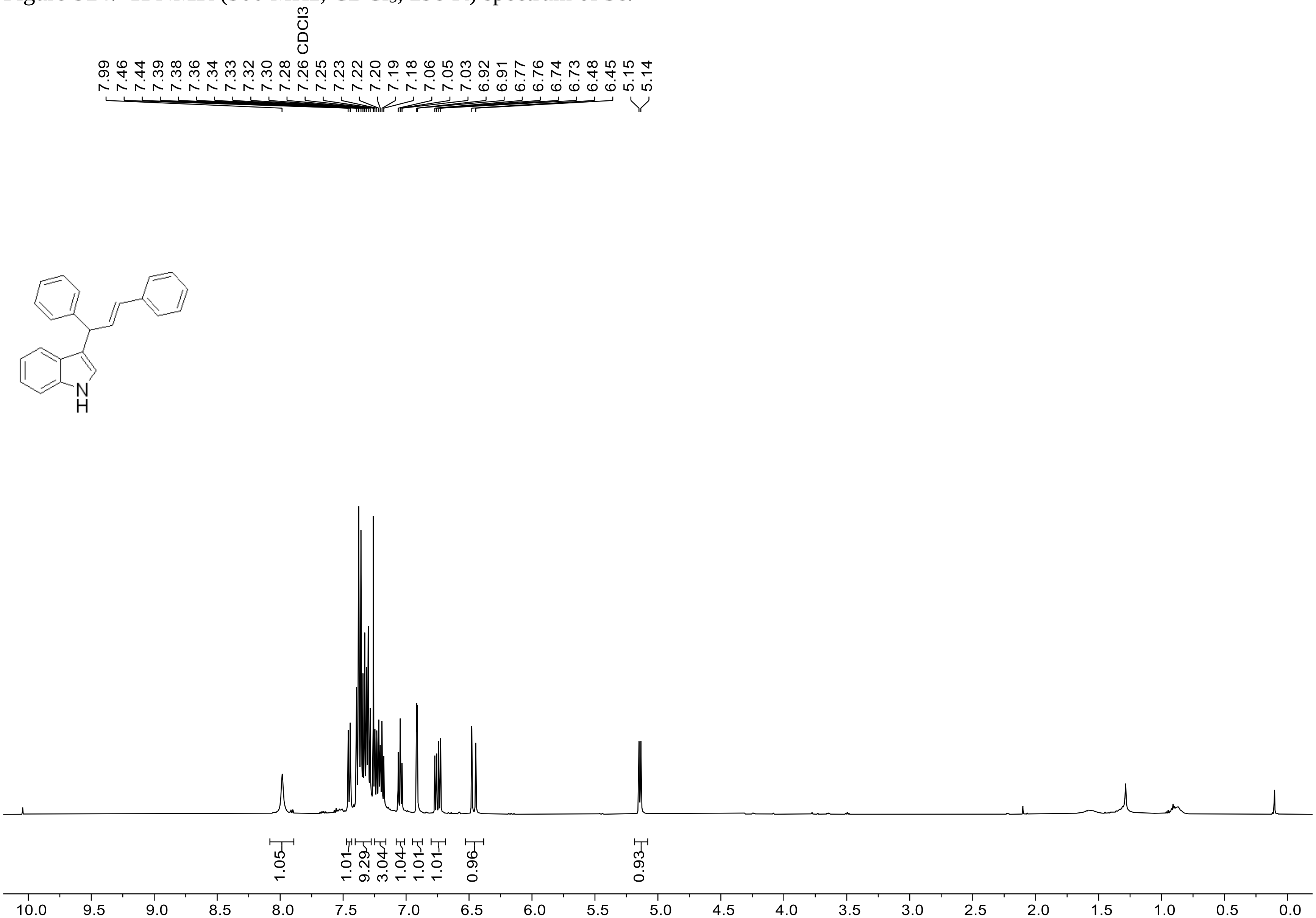


Figure S25: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3e**.

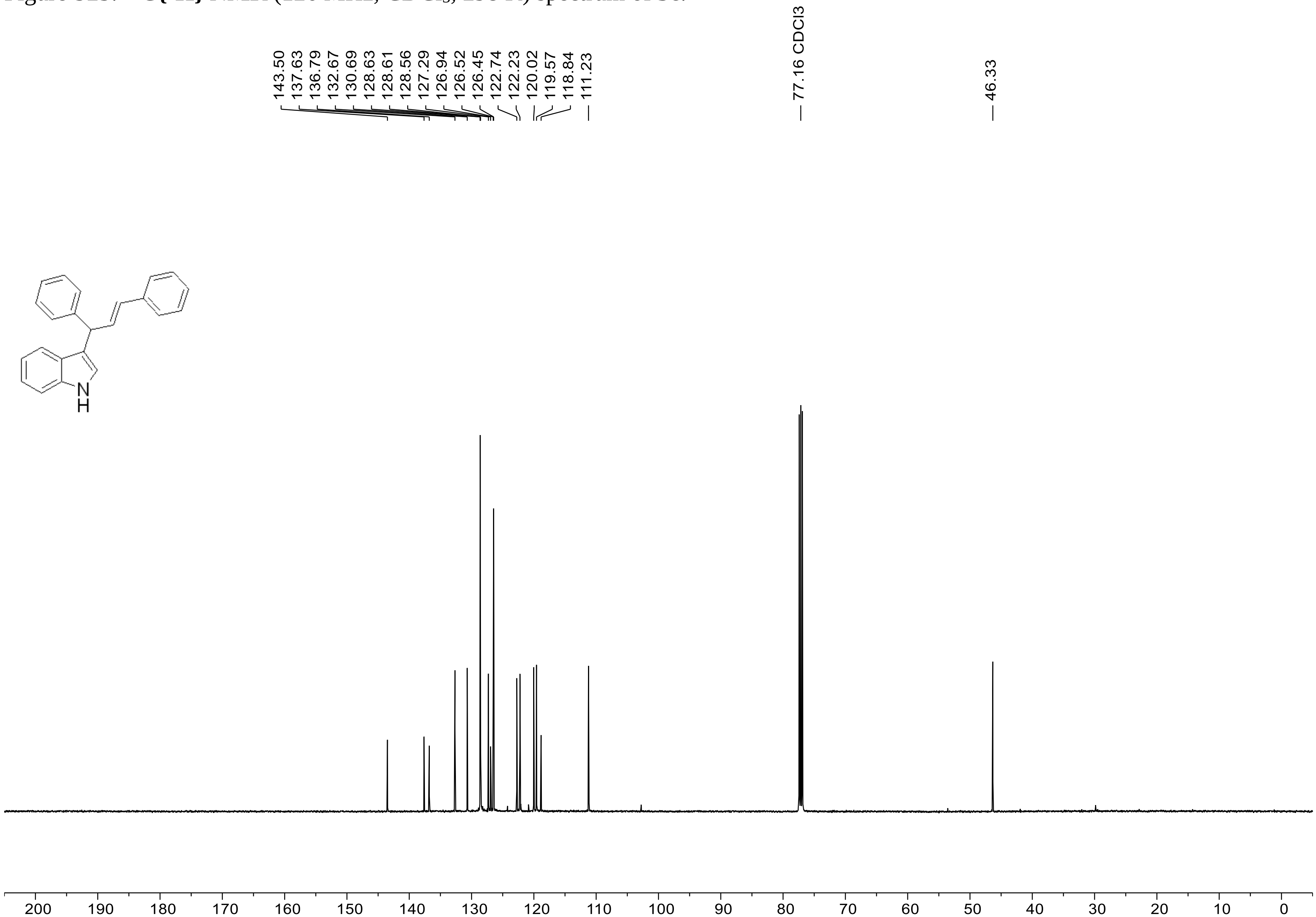


Figure S26: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3f**.

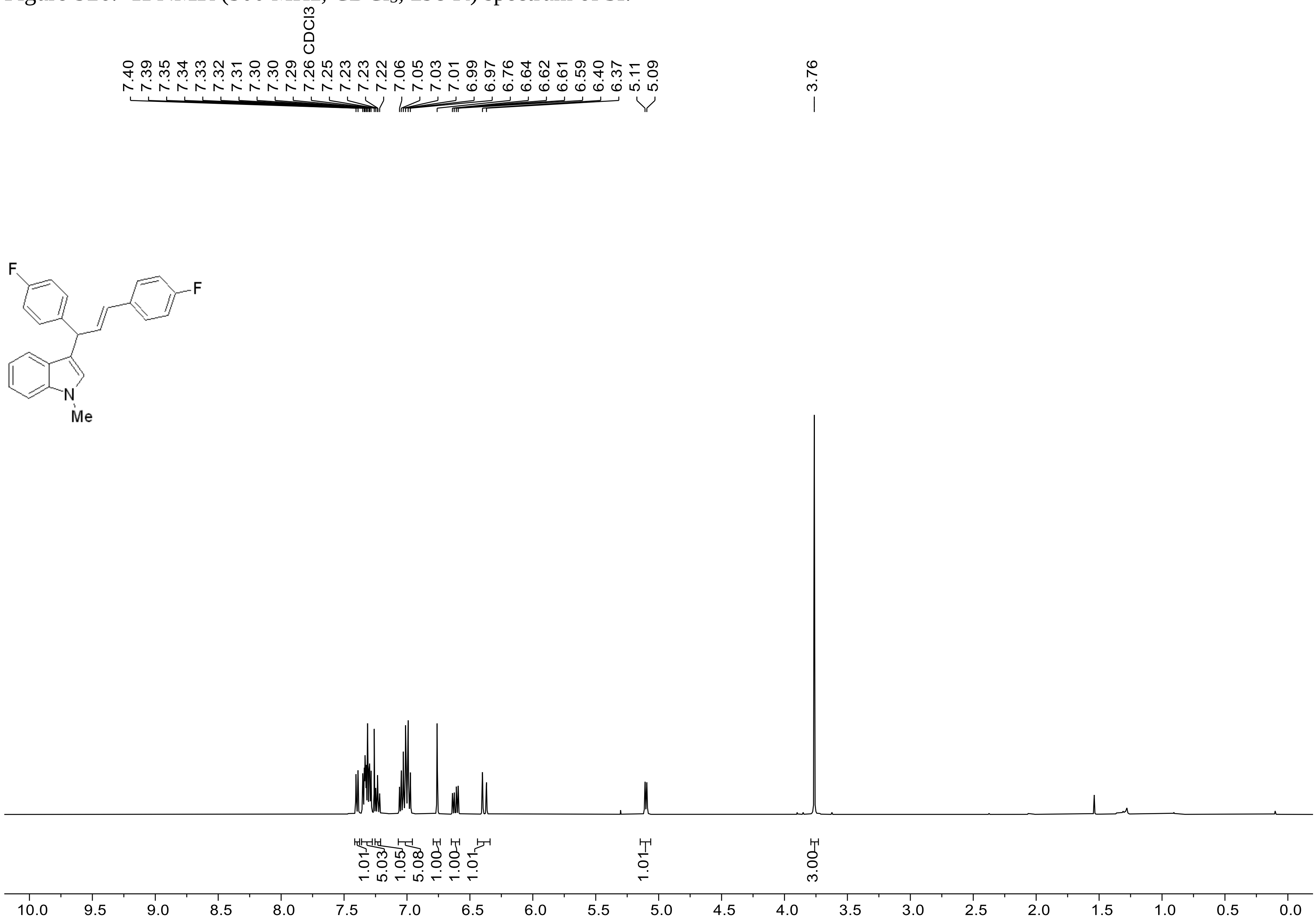


Figure S27: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3f**.

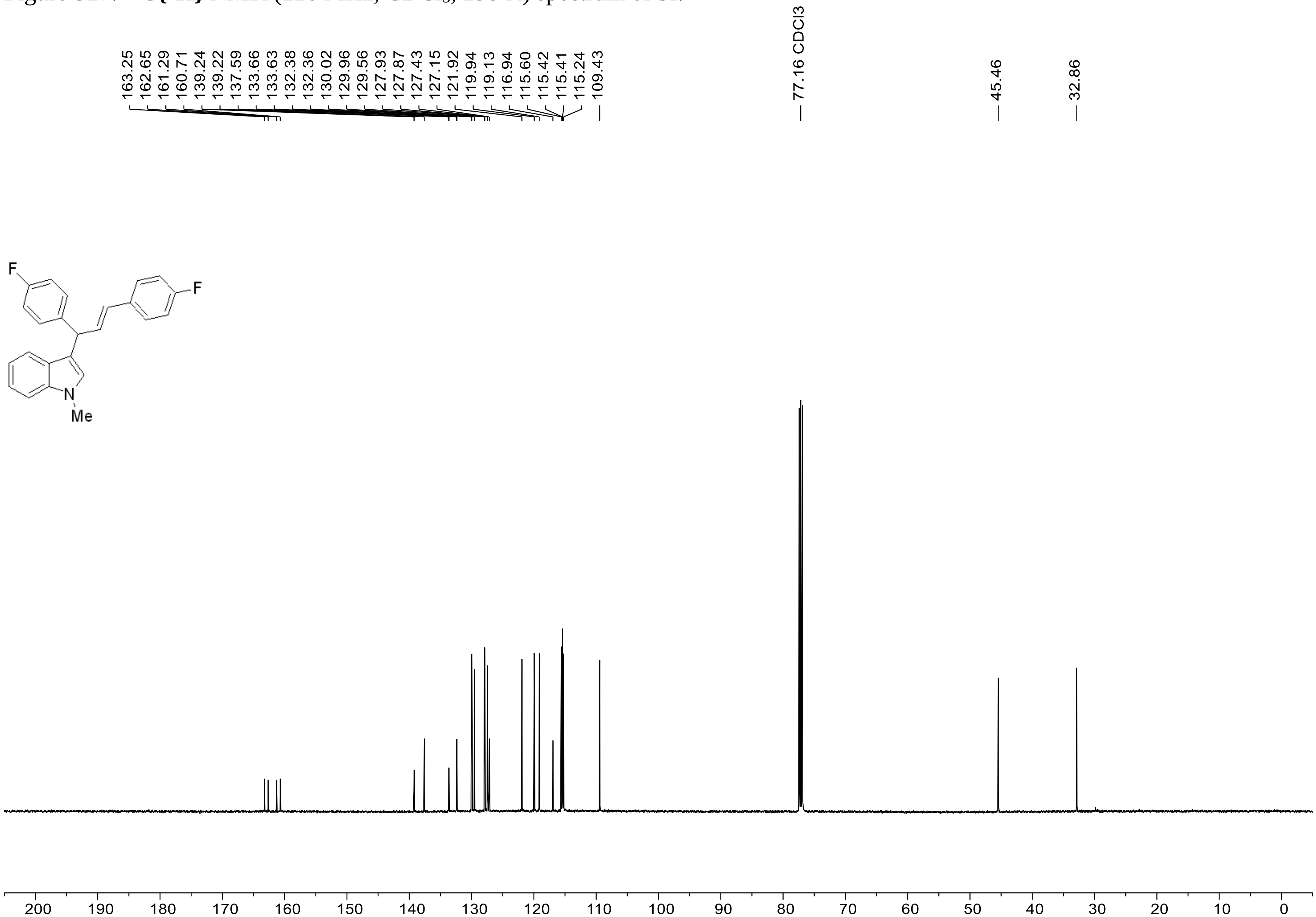


Figure S28: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3f**.

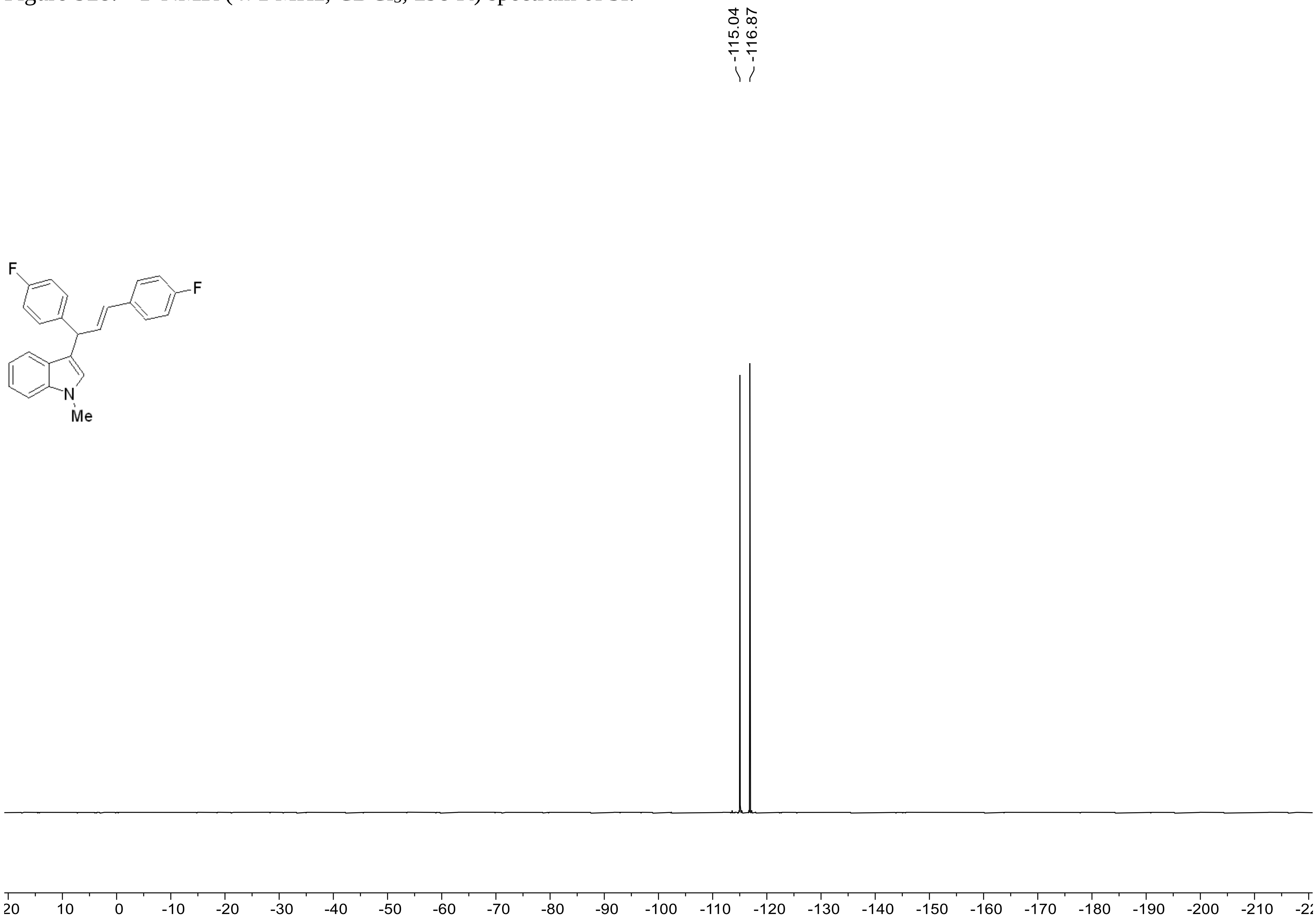
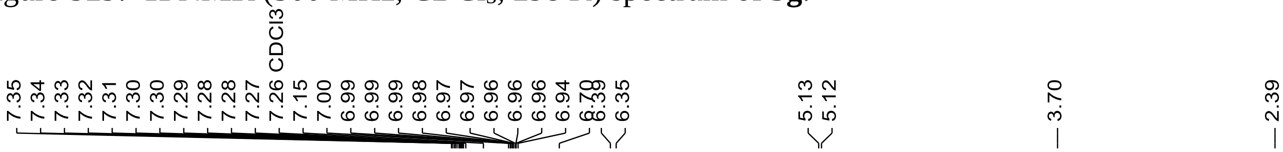
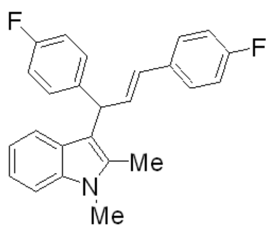


Figure S29: ^{1}**H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3g**.





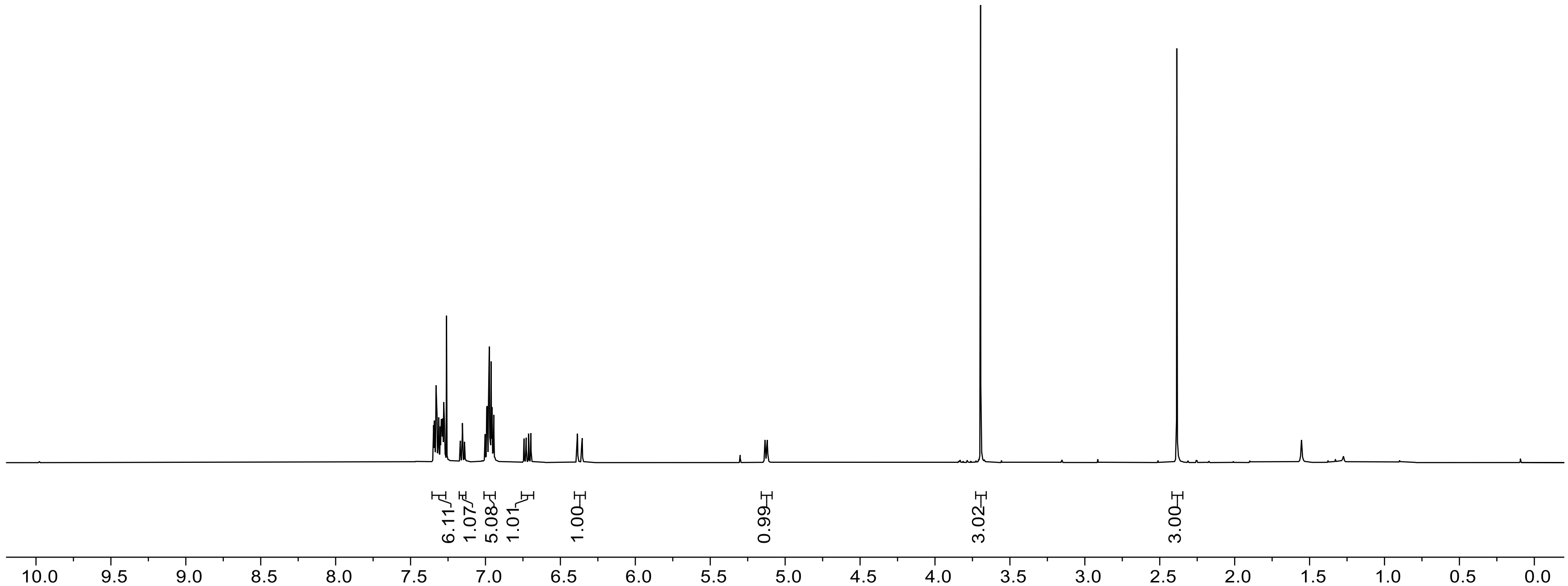


Figure S30: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3g**.

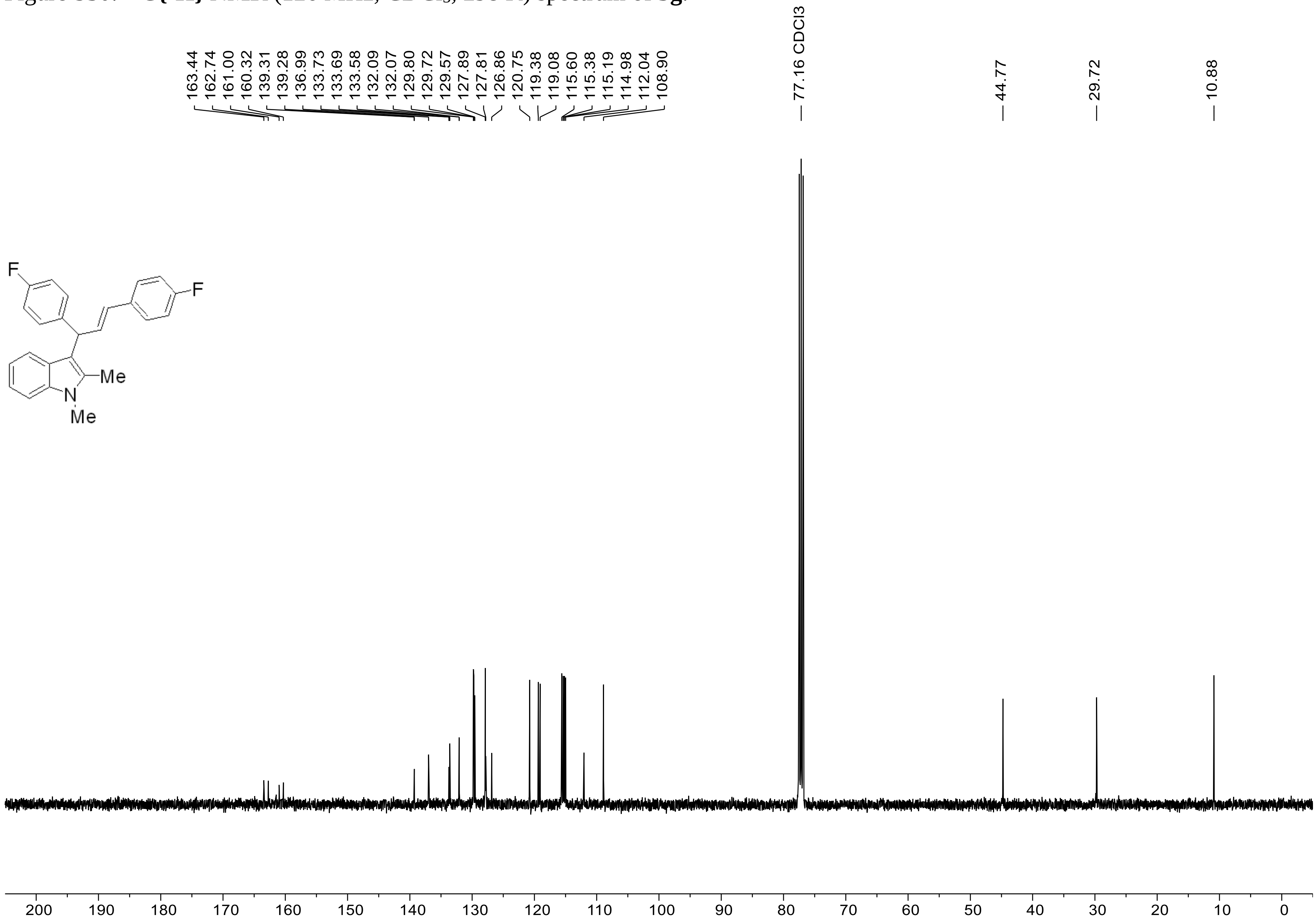


Figure S31: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3g**.

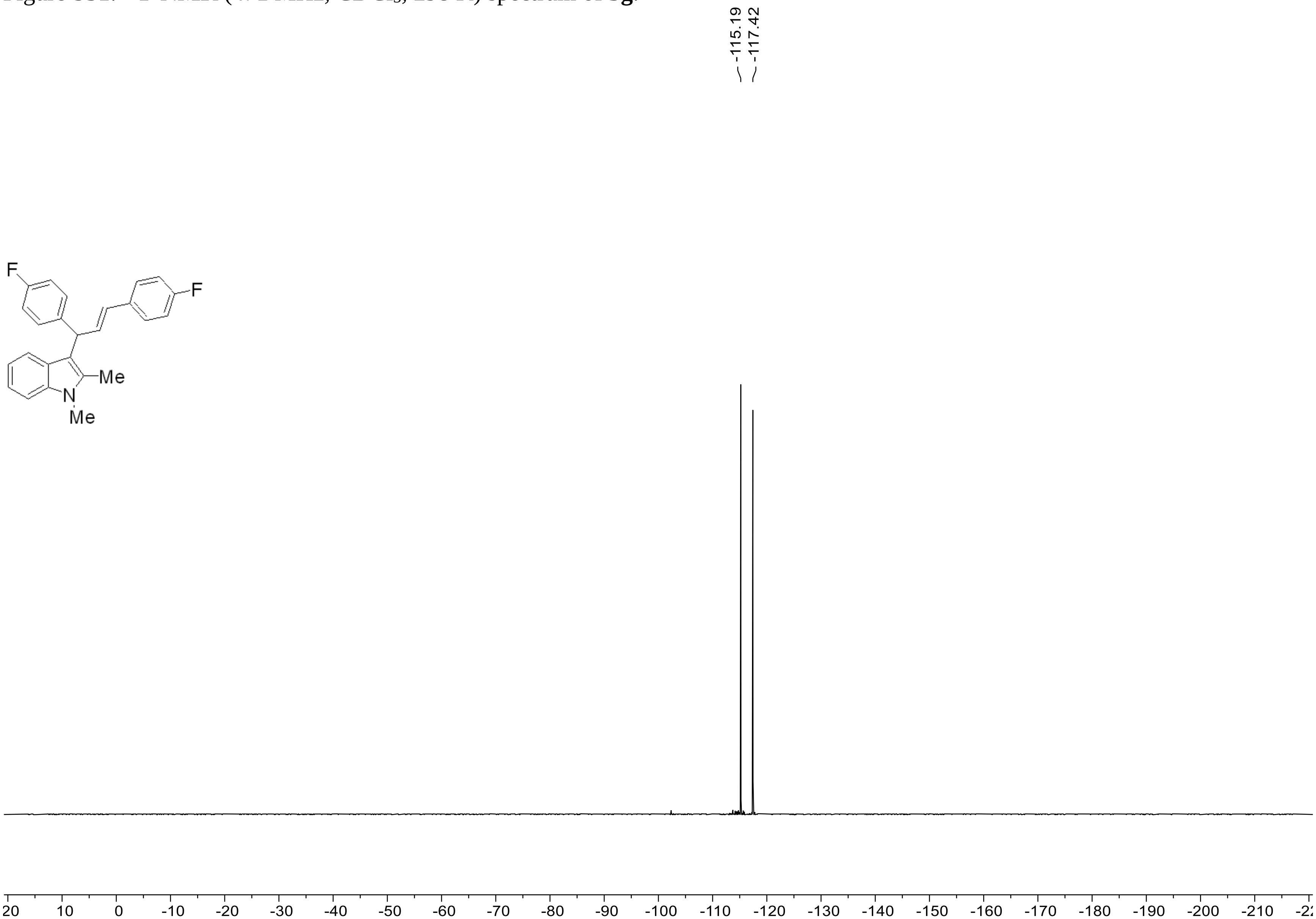
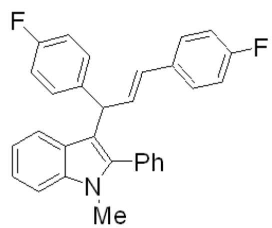


Figure S32: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3h**.



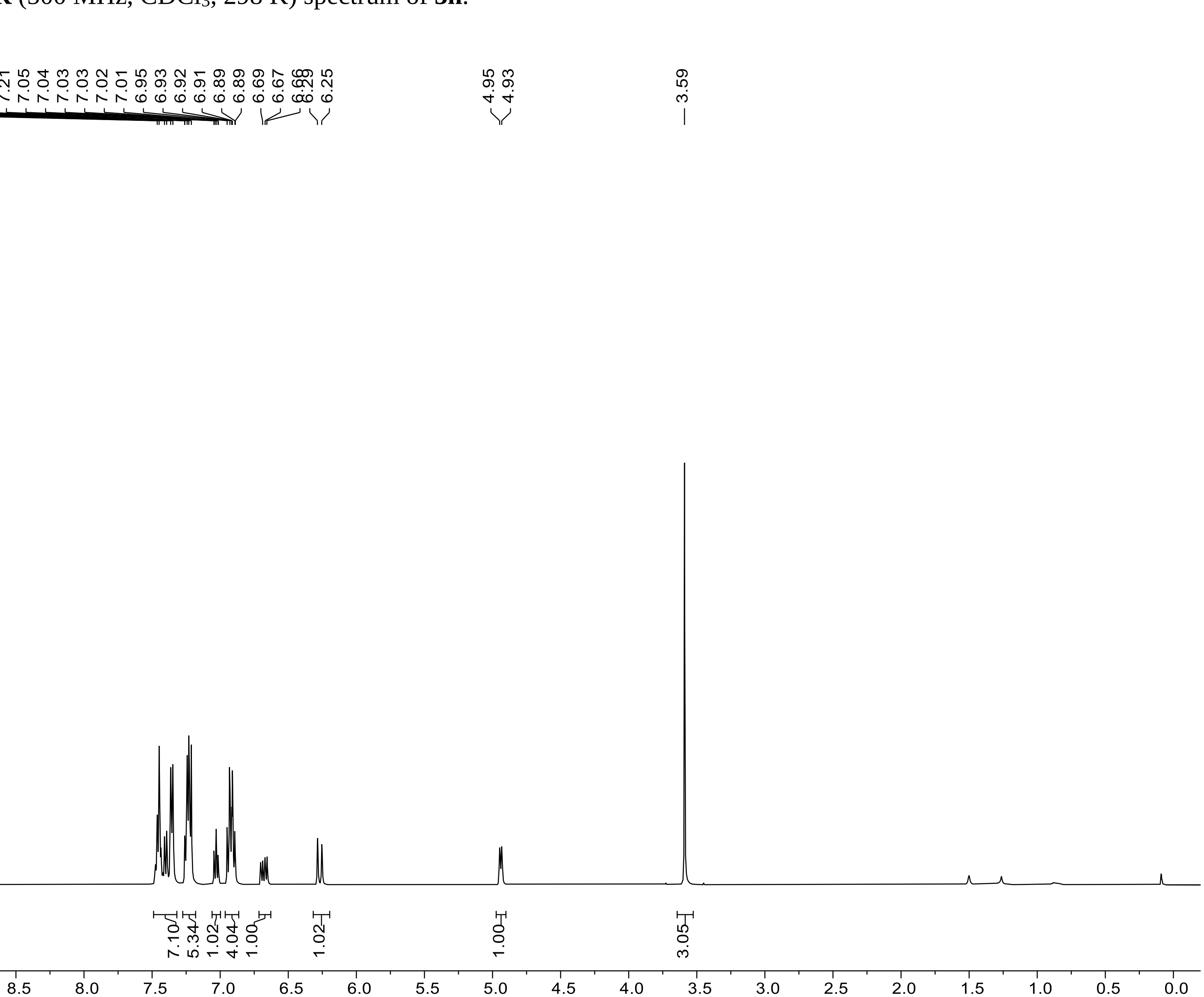


Figure S33: ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$, 298 K) spectrum of **3h**.

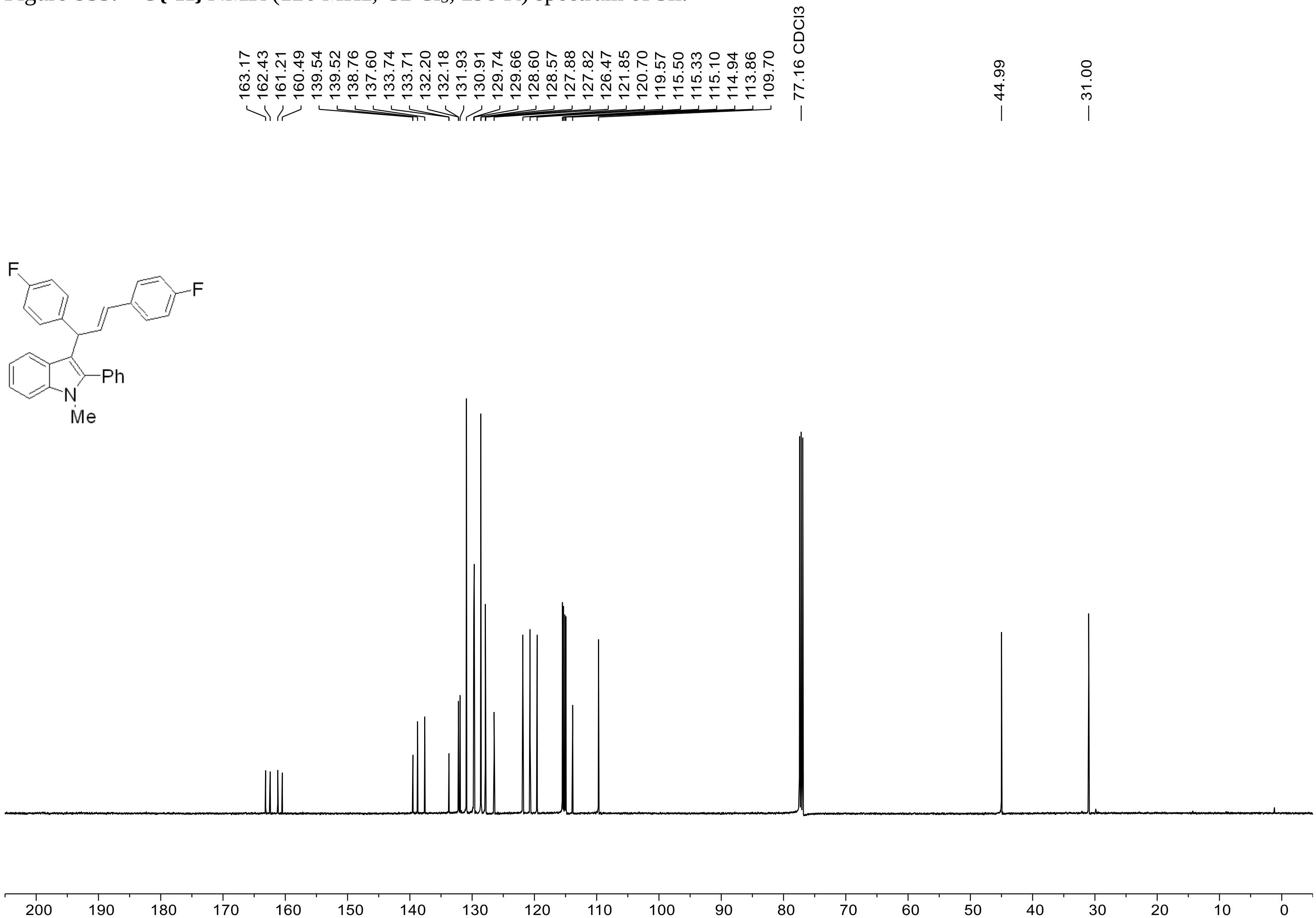


Figure S34: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3h**.

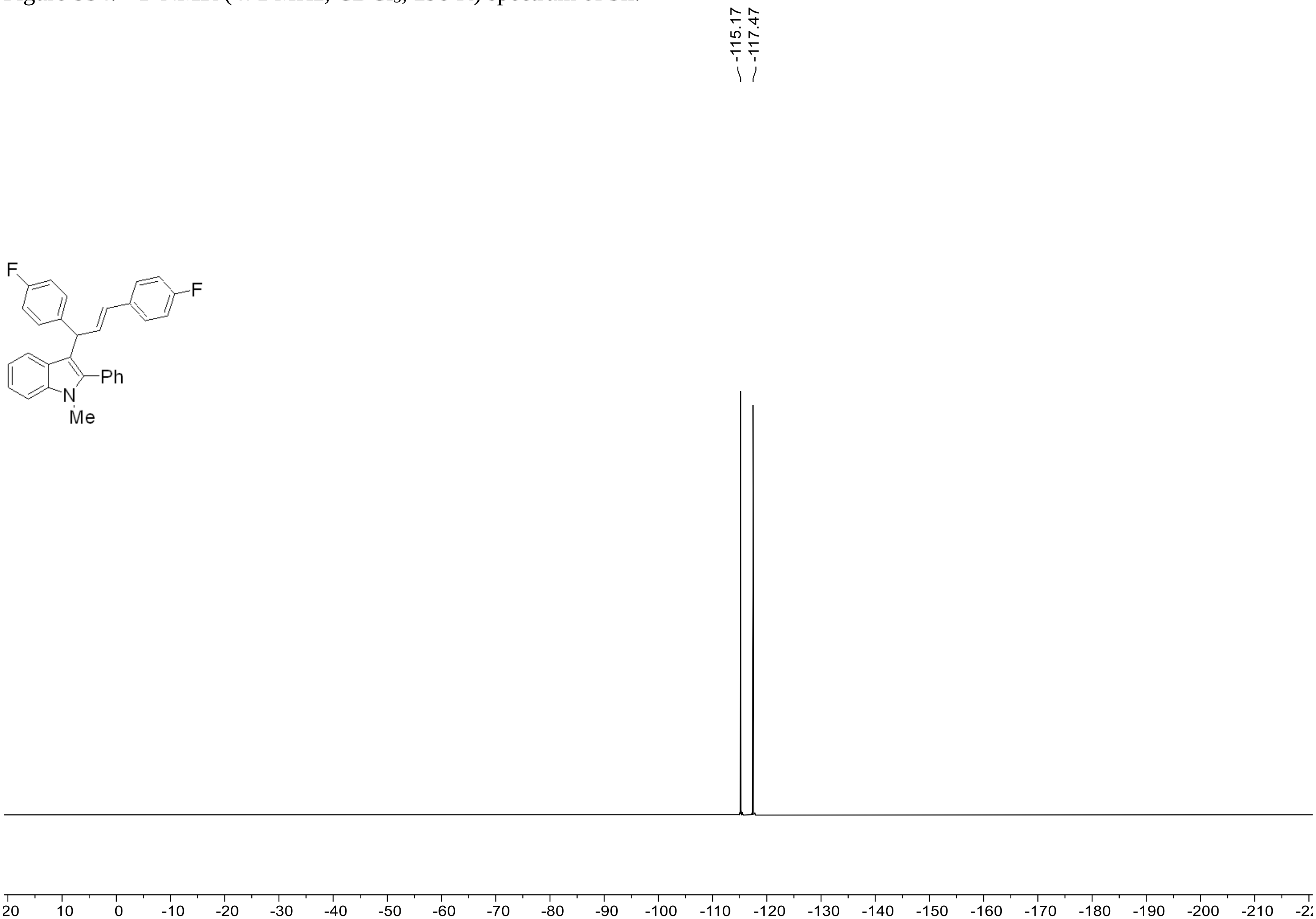


Figure S35: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3i**.

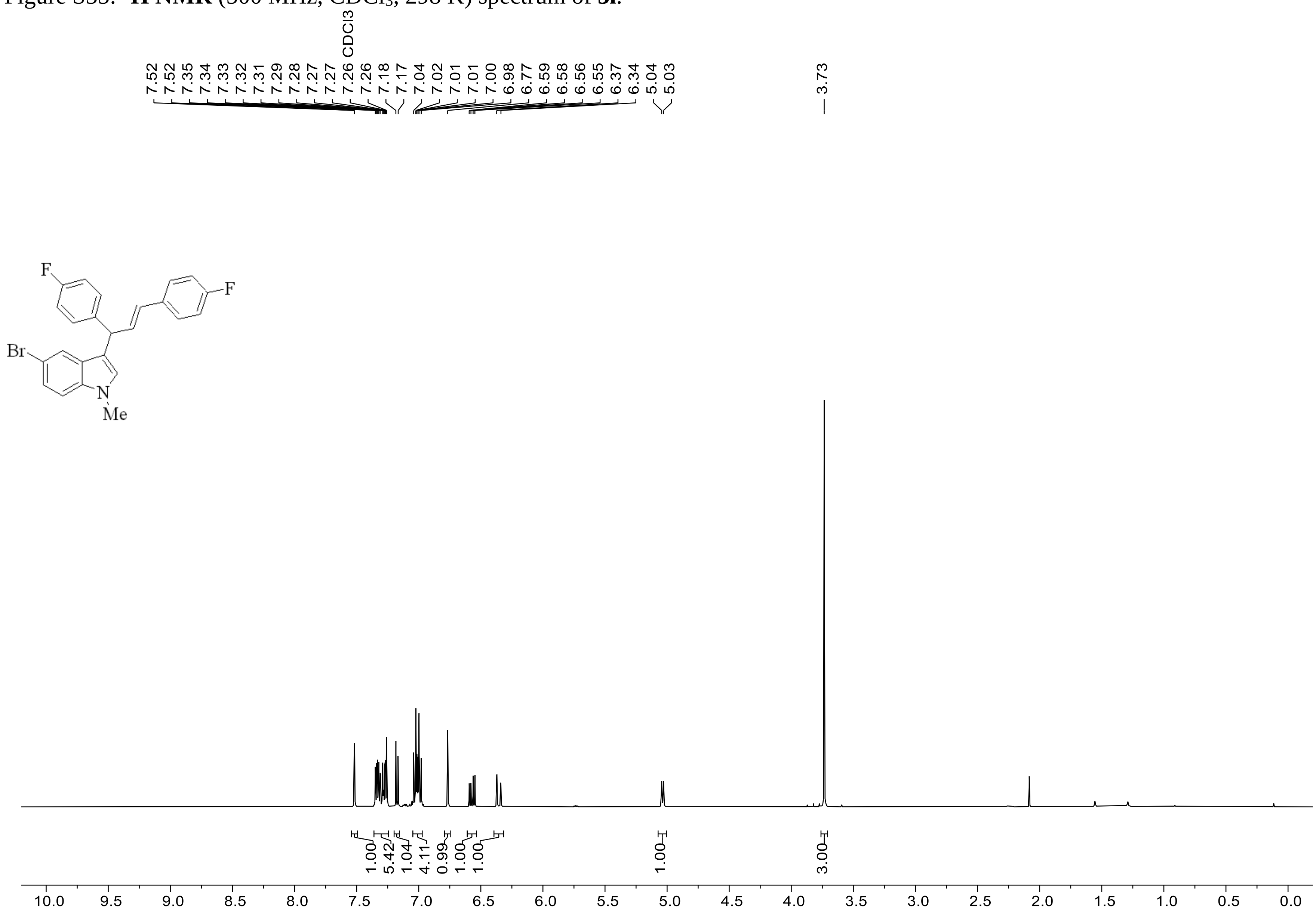


Figure S36: ^{13}**C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3i**.

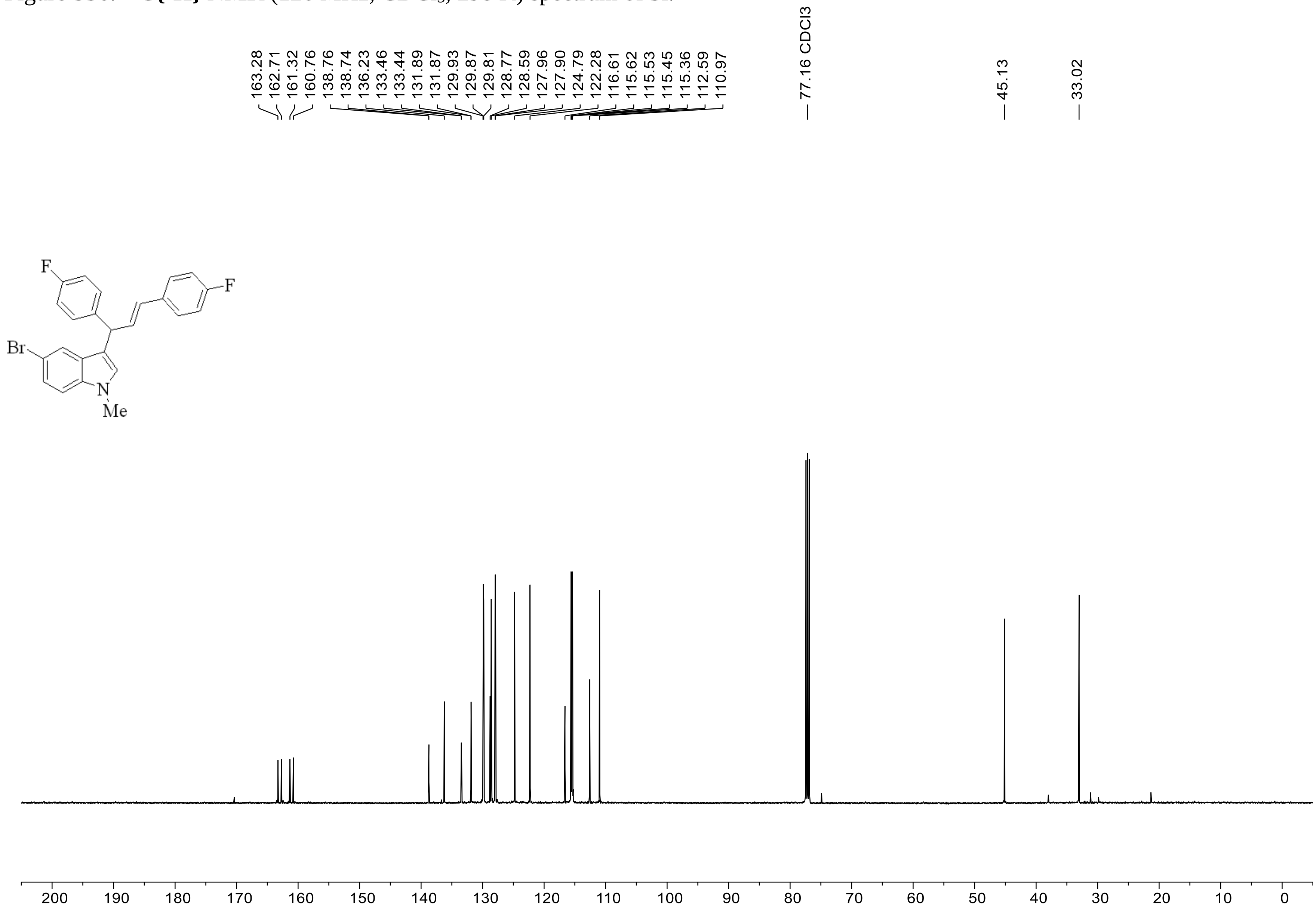


Figure S37: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3i**.

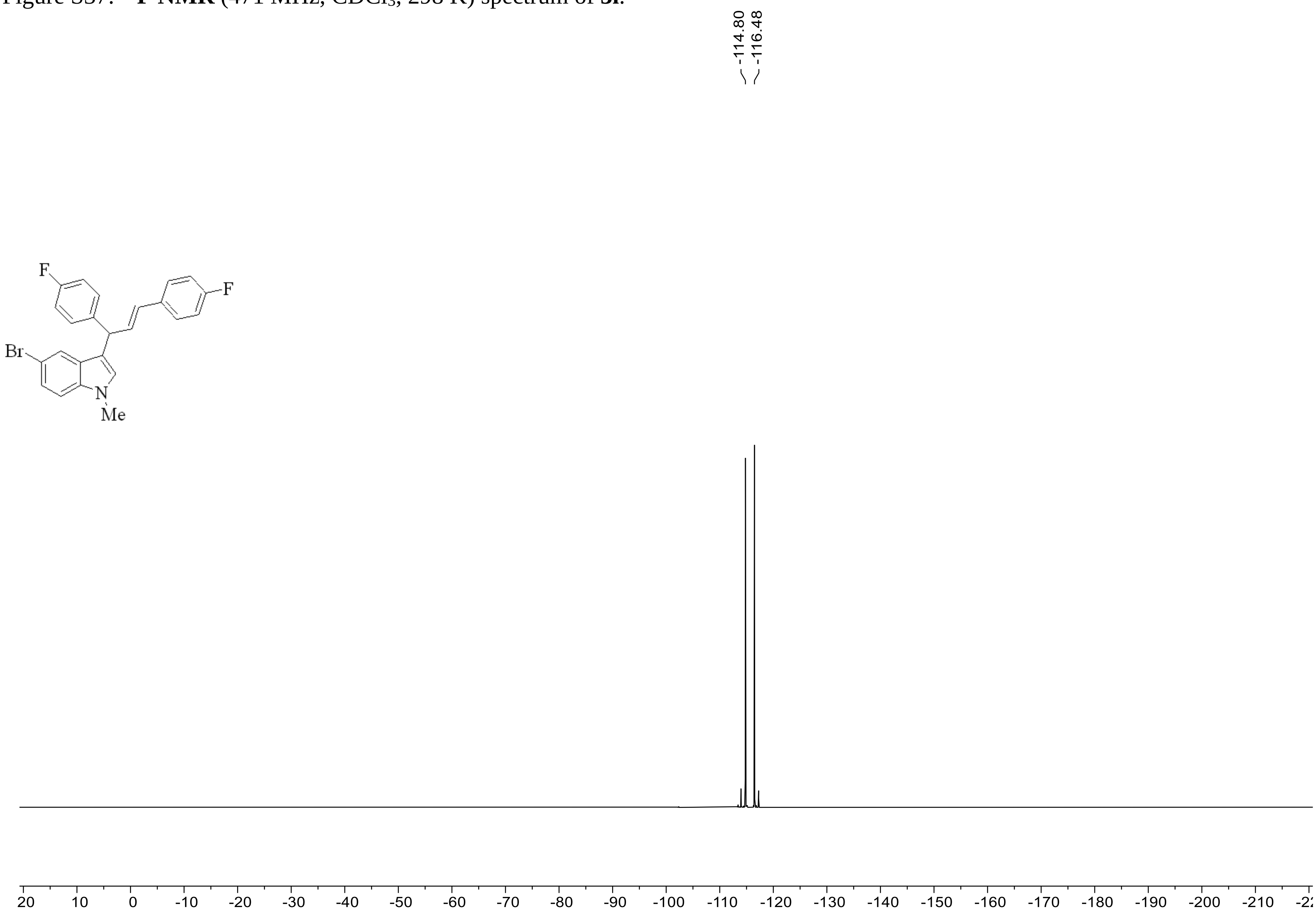
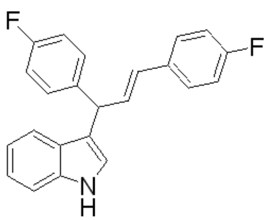


Figure S38: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3j**.



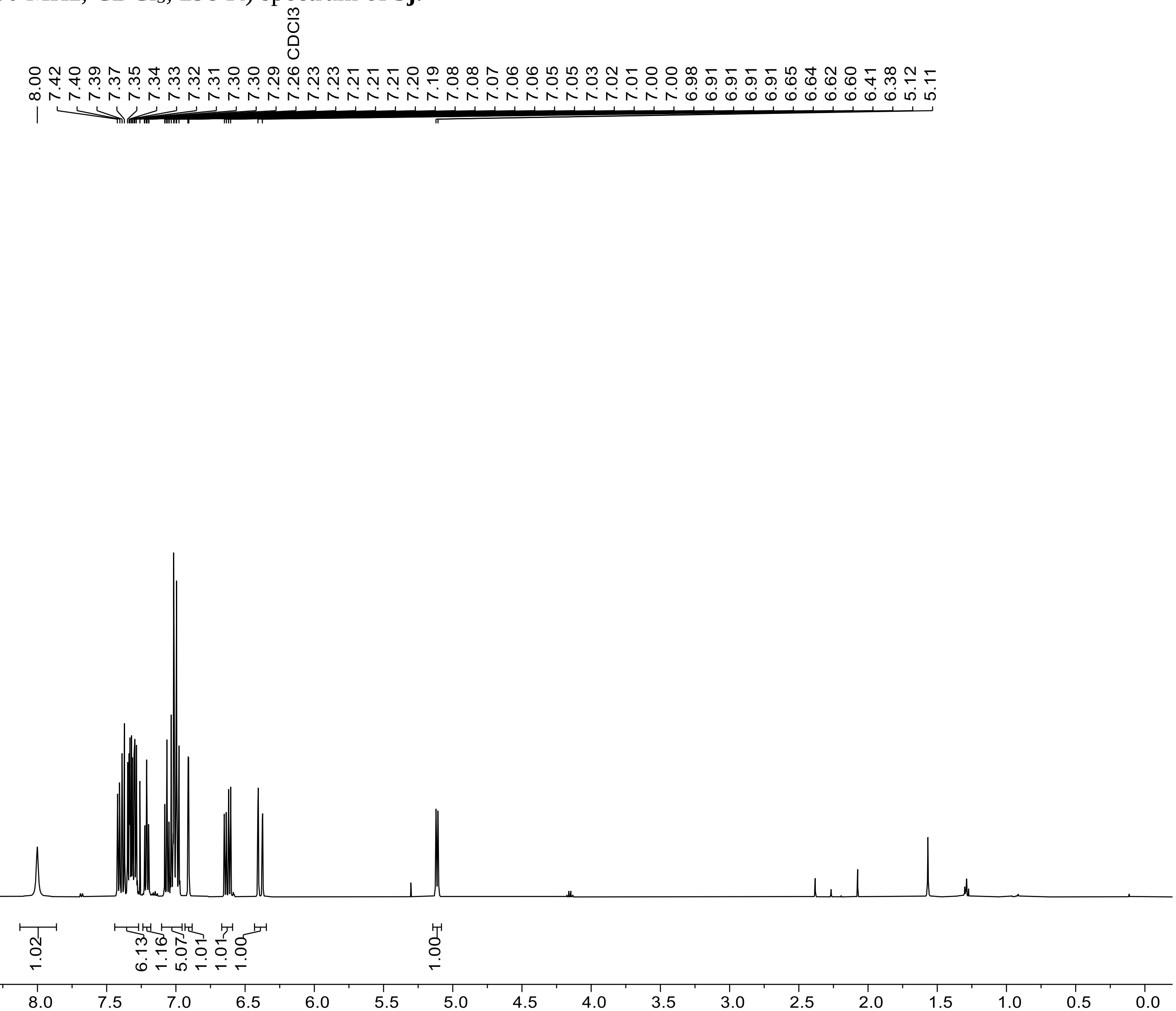


Figure S39: ^{13}**C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3j**.

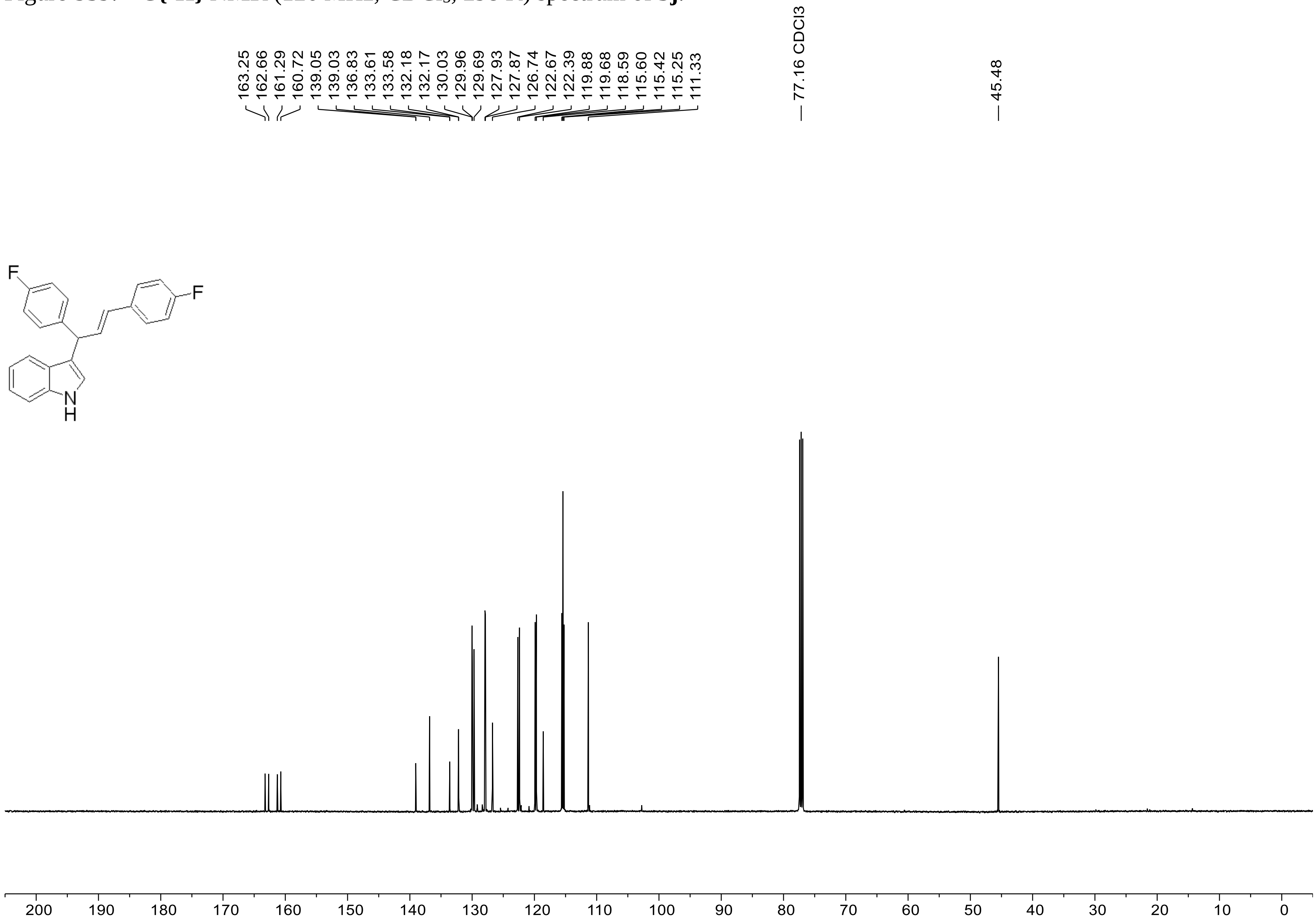


Figure S40: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3j**.

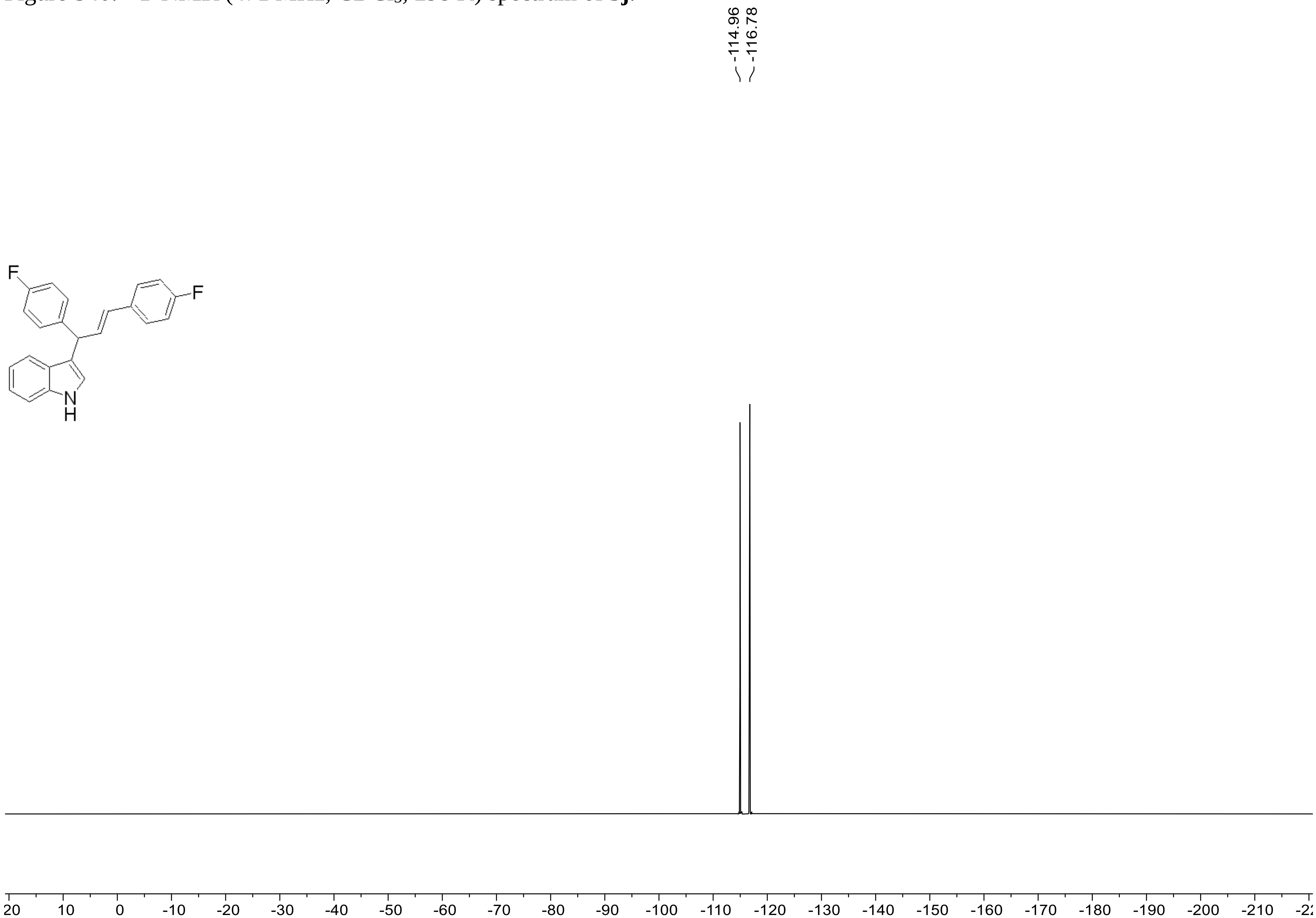


Figure S41: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3k**.

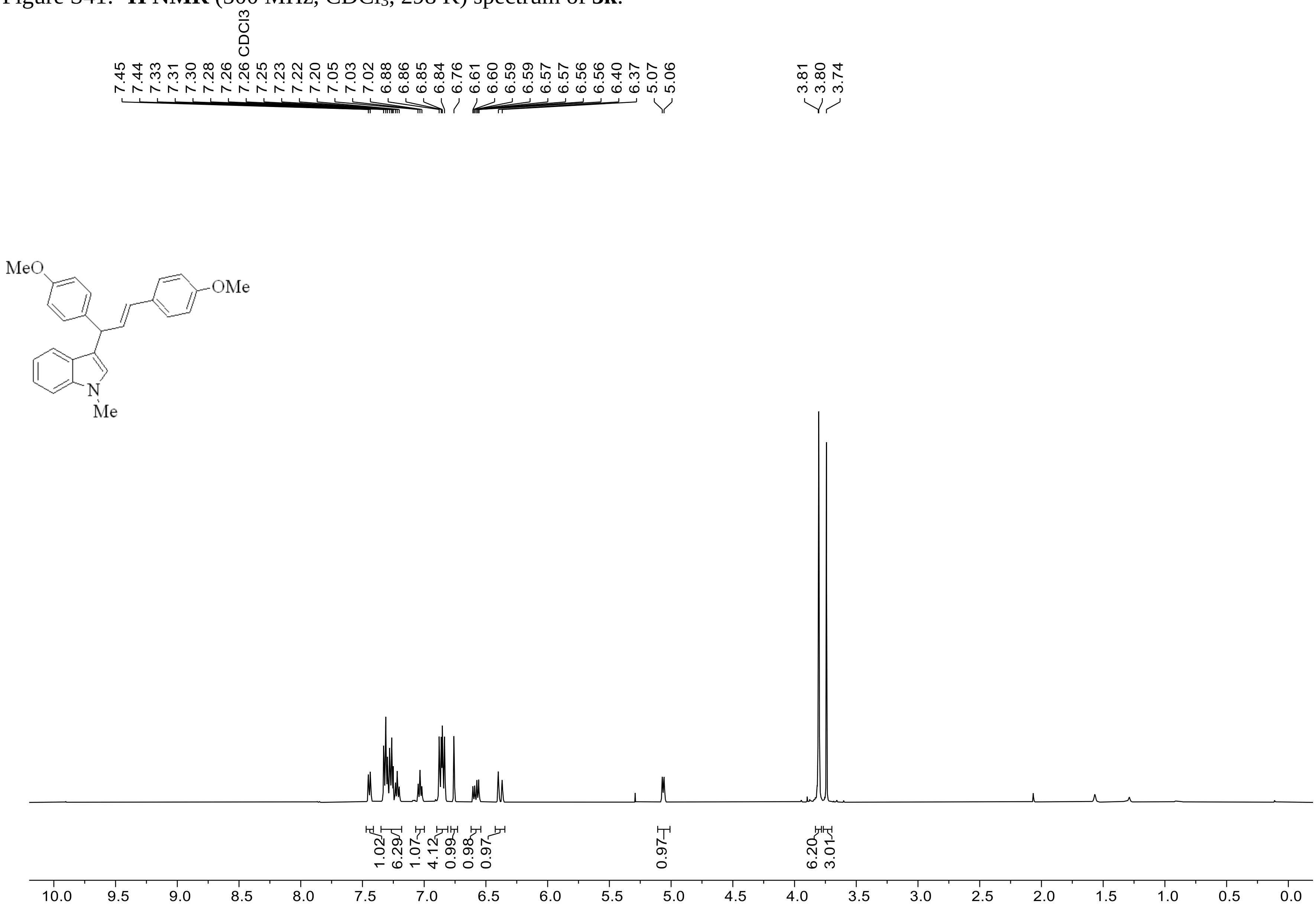


Figure S42: **$^{13}C\{^1H\}$ NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3k**.

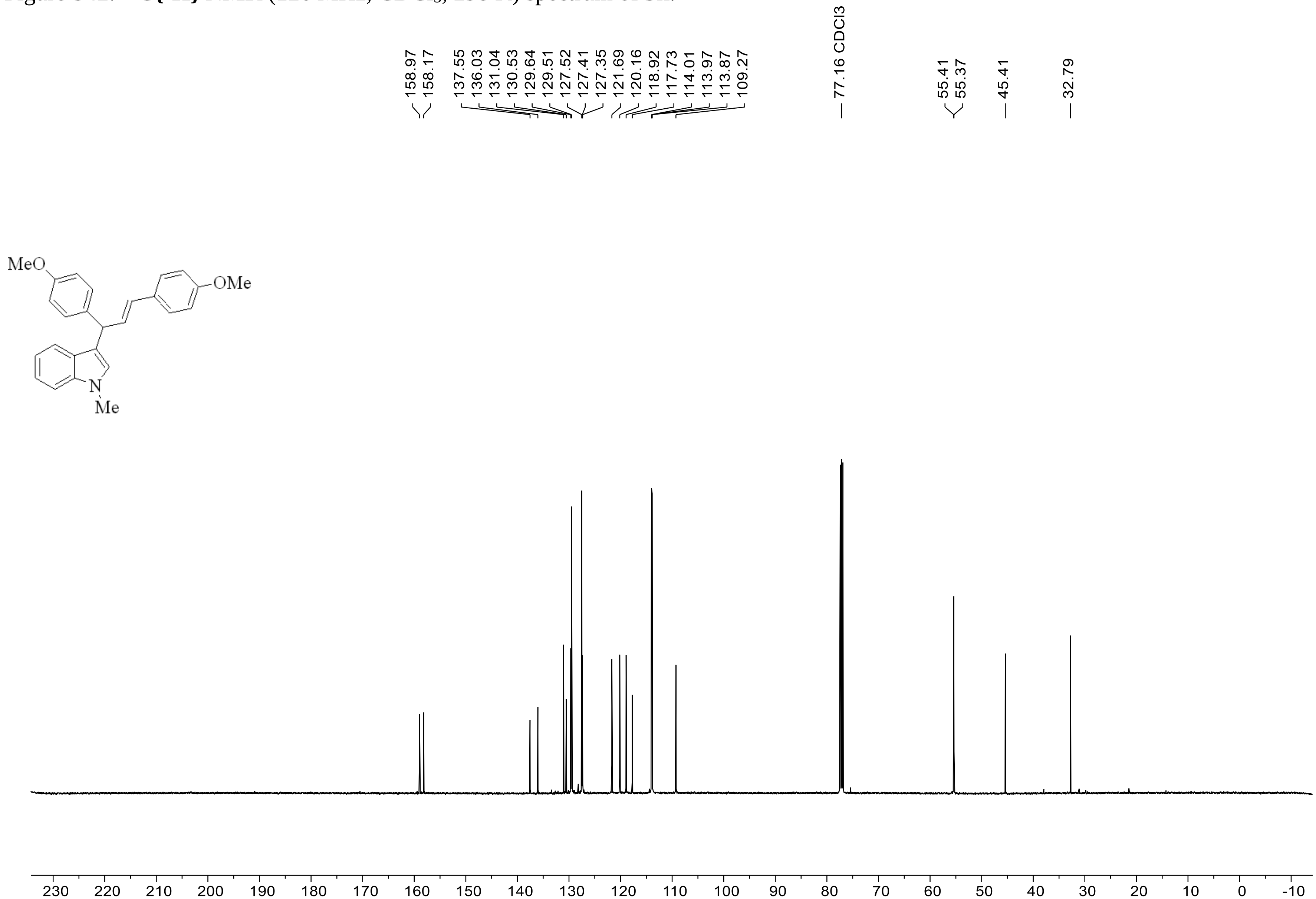


Figure S43: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3l**.

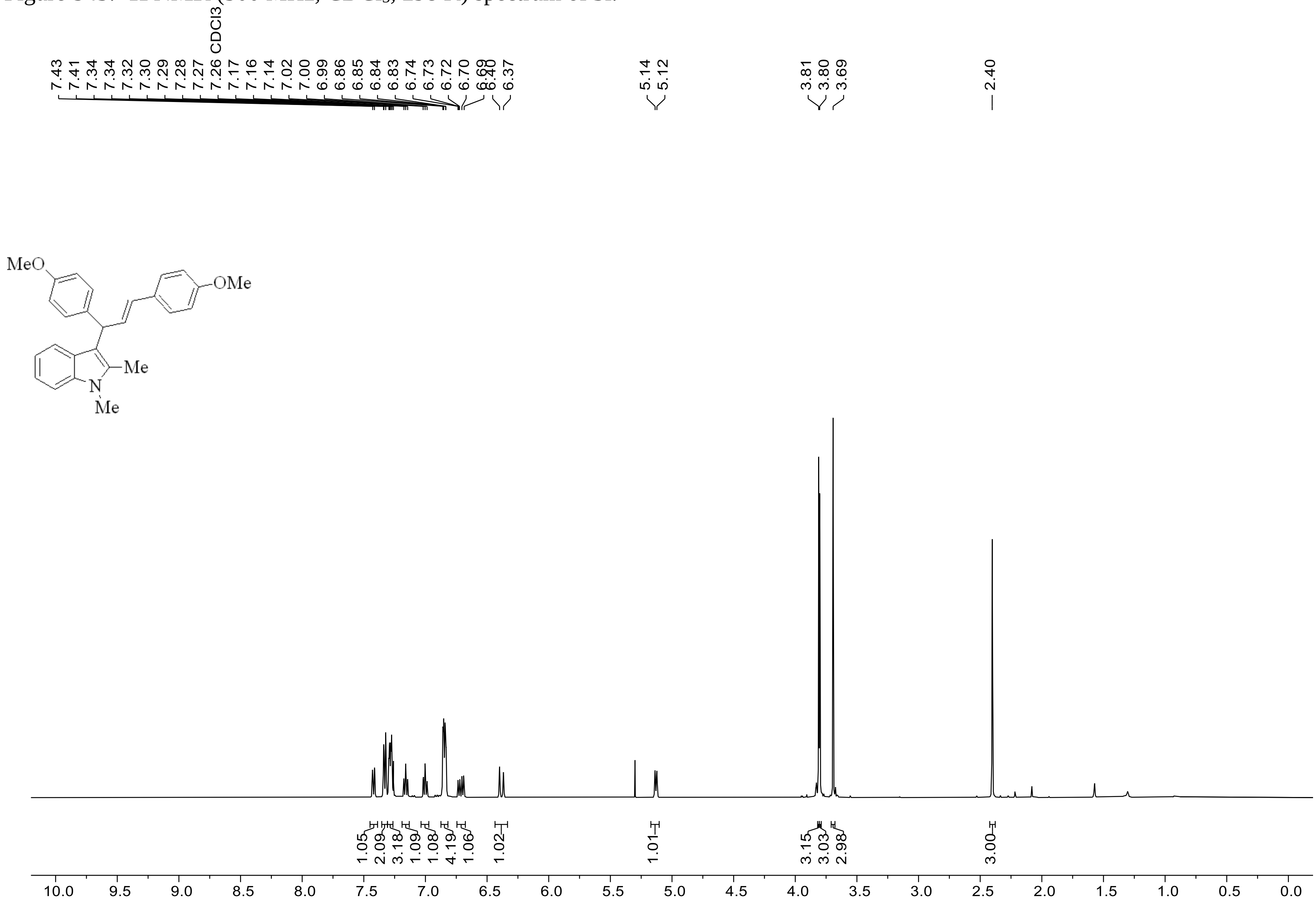


Figure S44: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3l**.

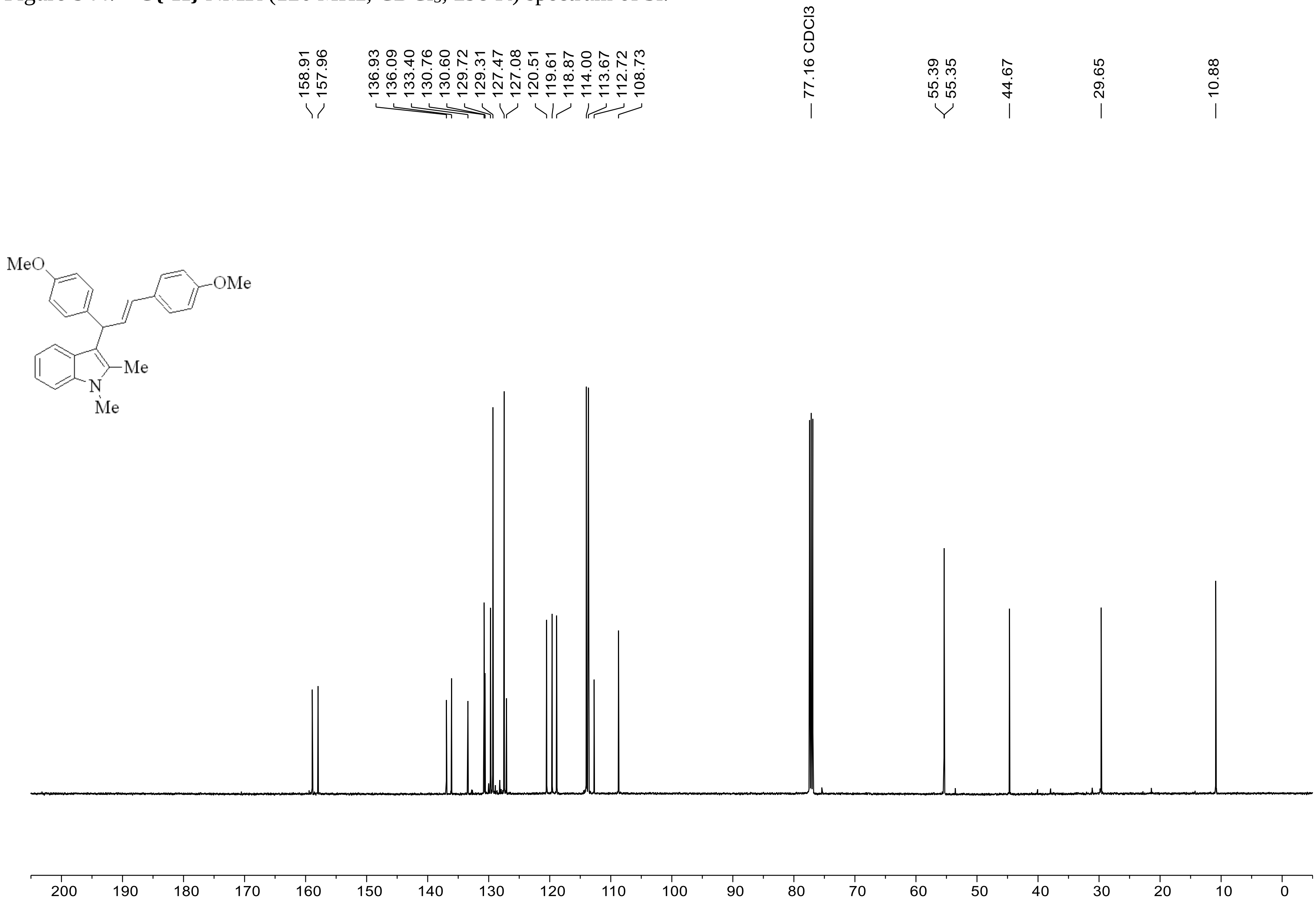


Figure S45: ^{1}**H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3m**.

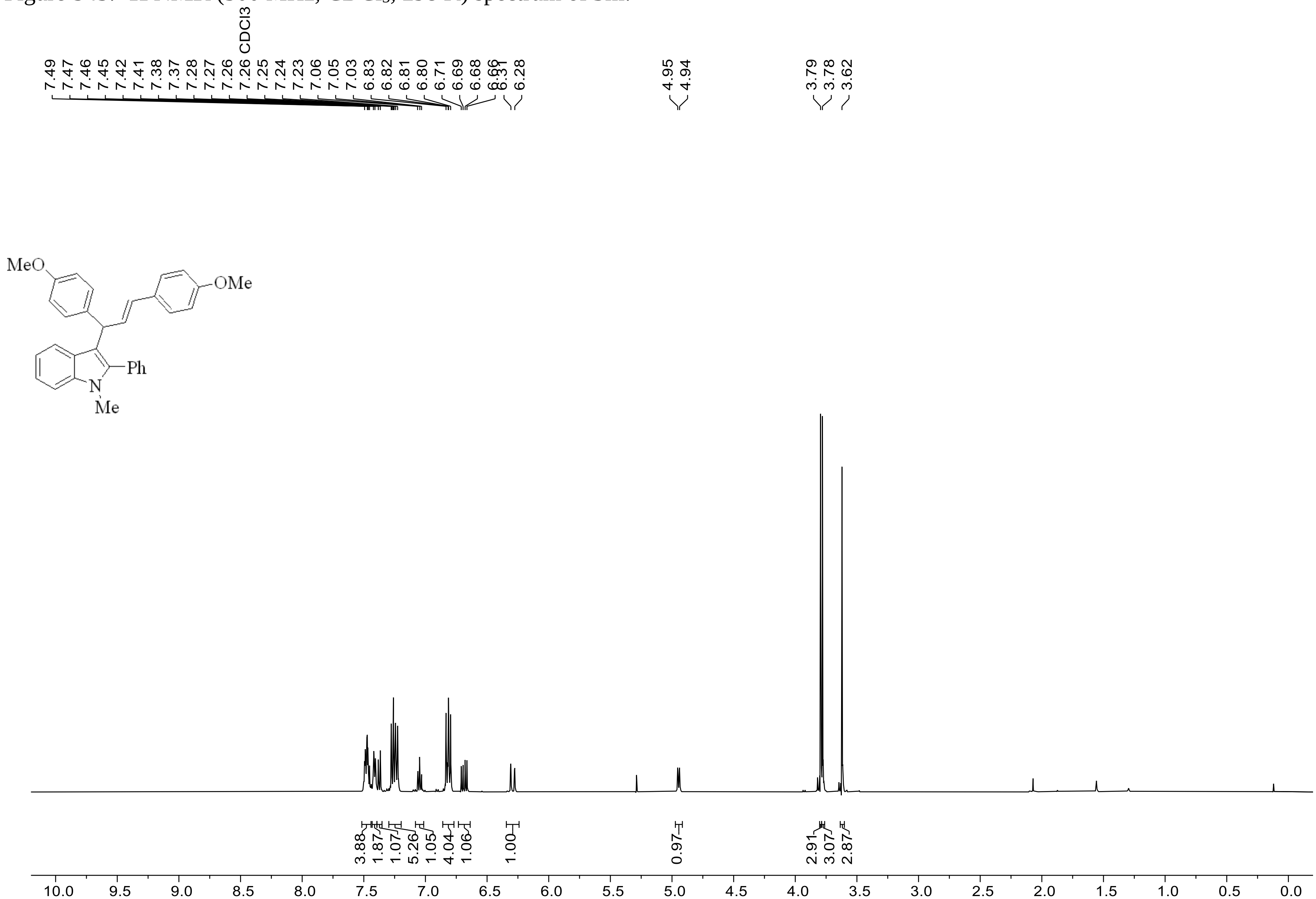


Figure S46: ^{13}**C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3m**.

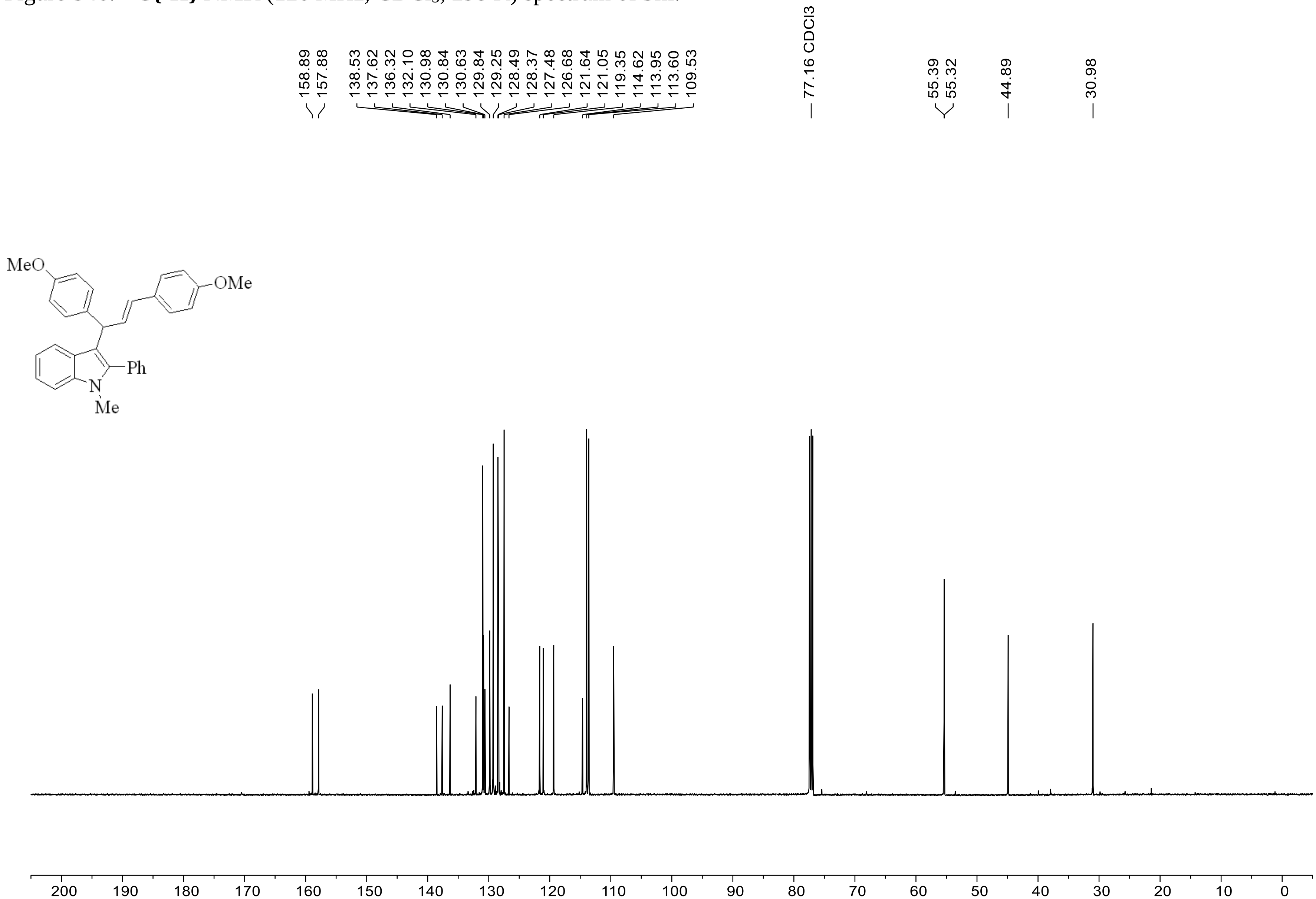


Figure S47: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3n**.

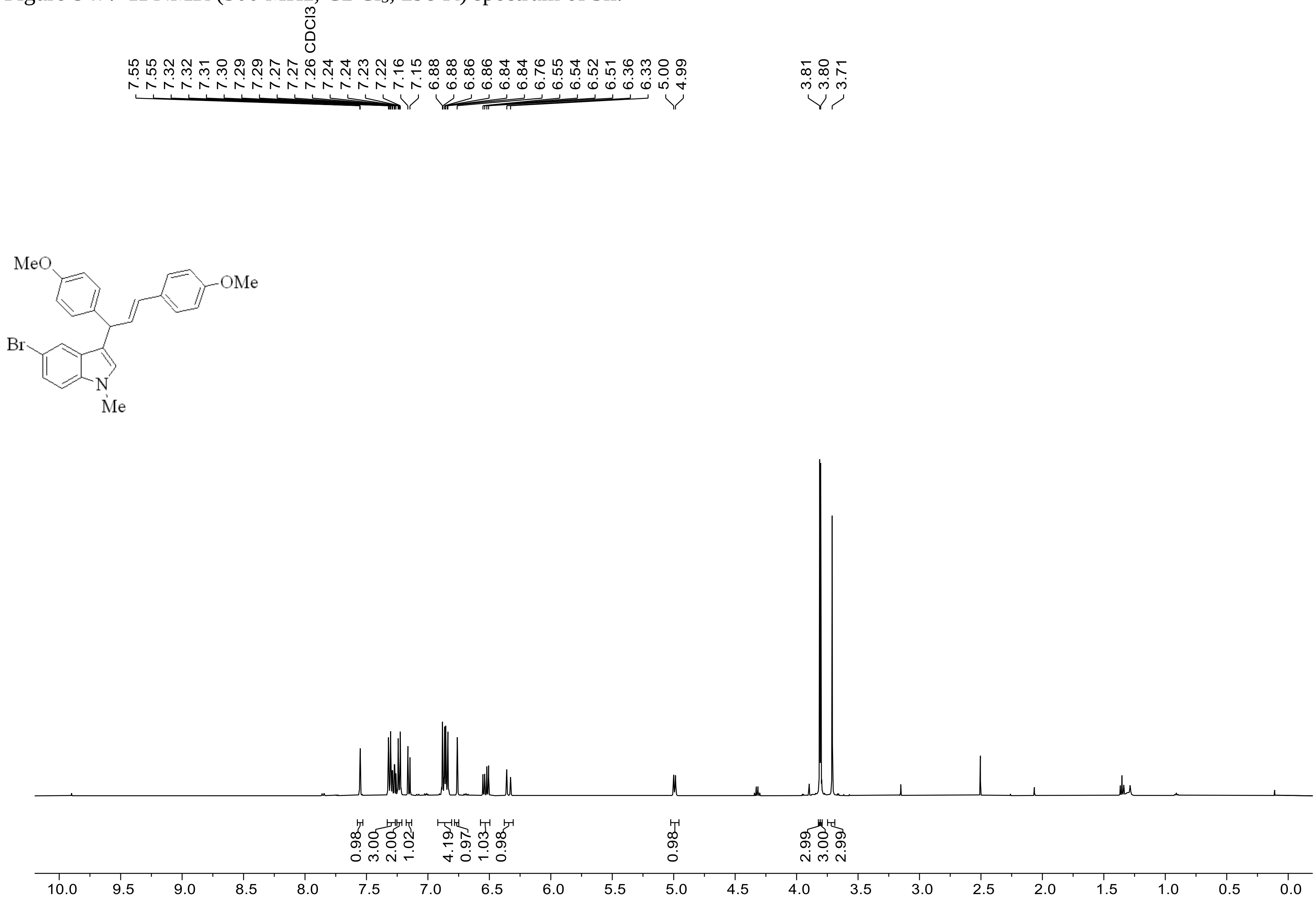


Figure S48: **$^{13}C\{^{1}H\}$ NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3n**.

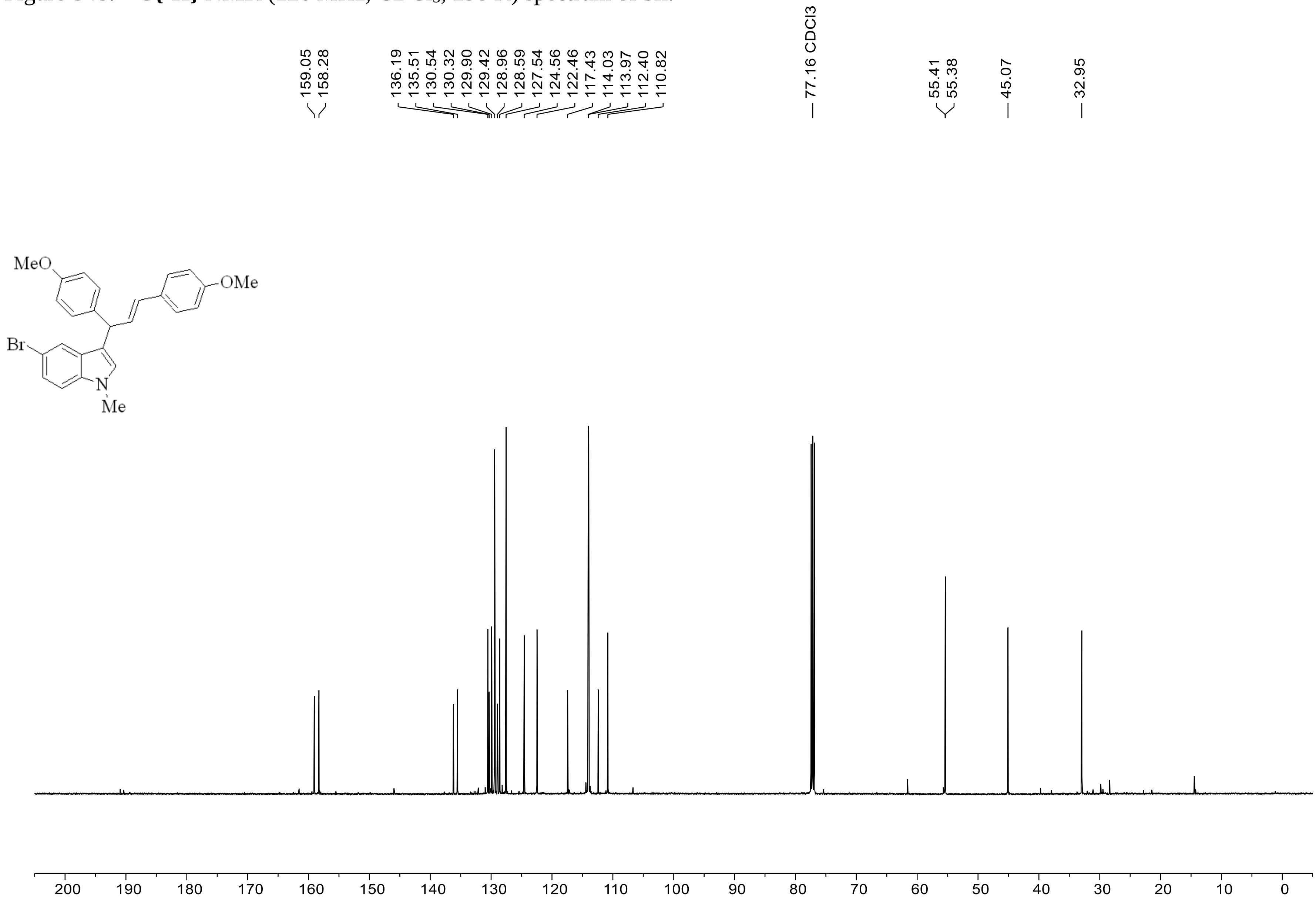


Figure S49: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3o**.

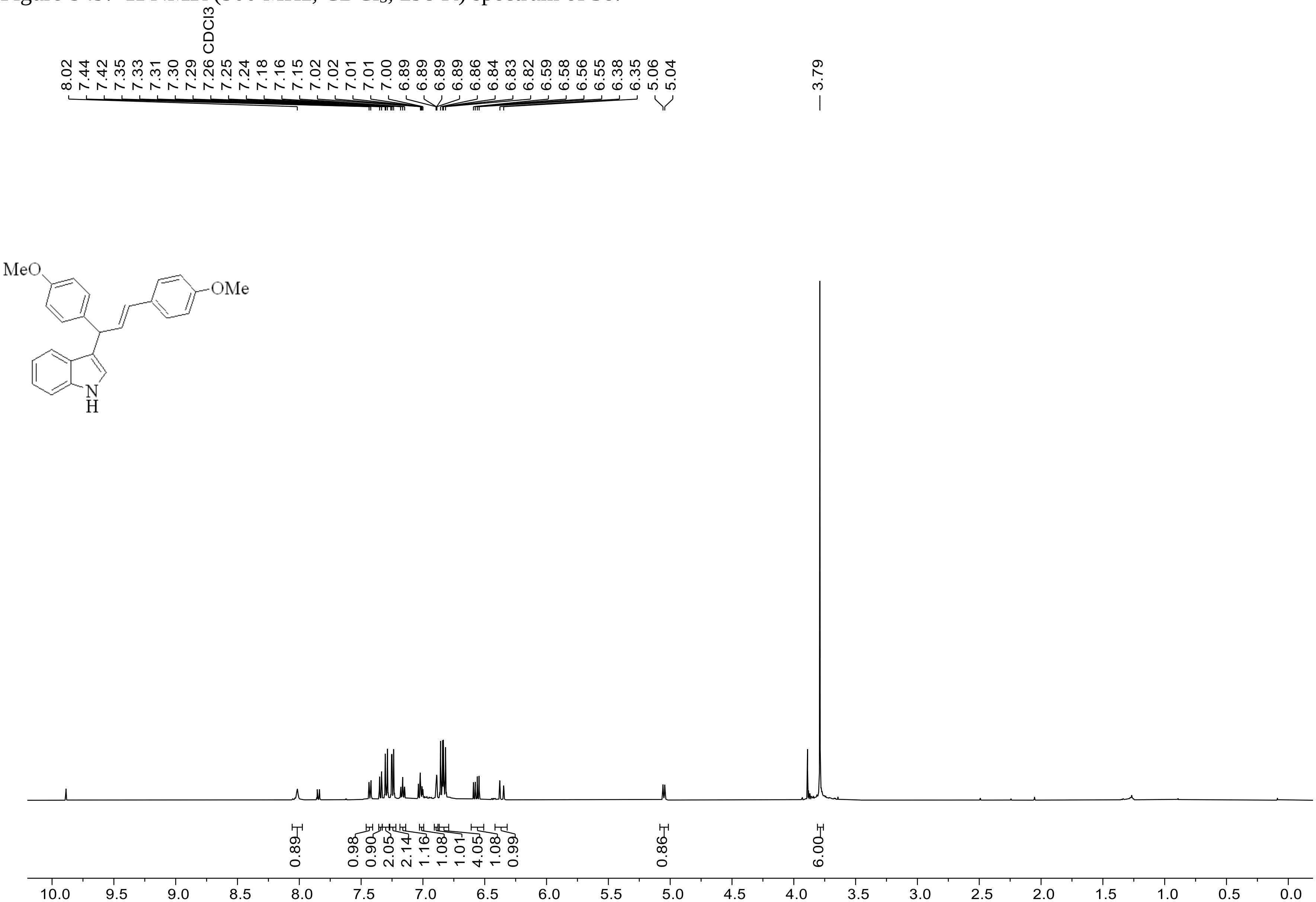


Figure S50: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3o**.

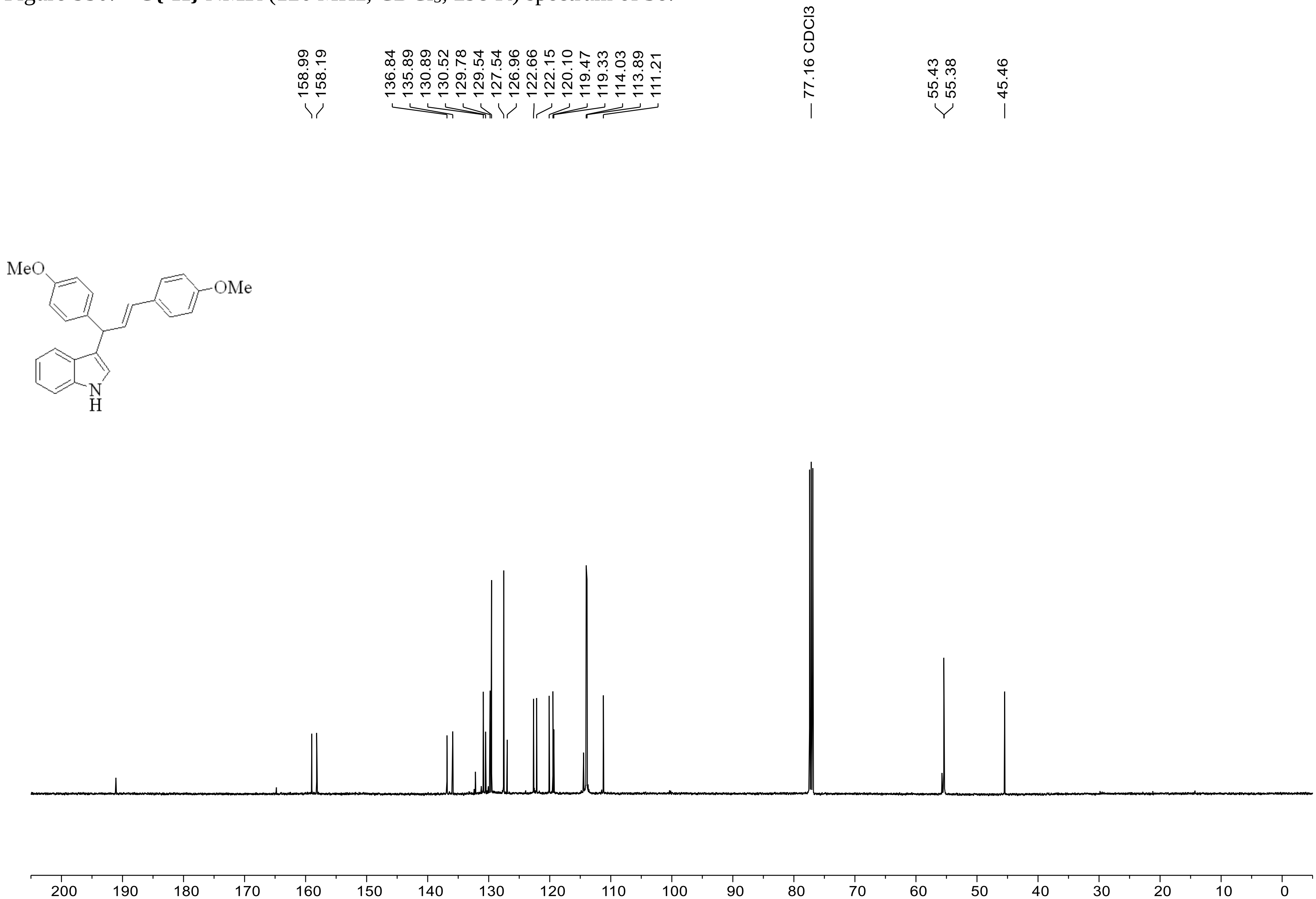


Figure S51: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3p** and **3p′**.

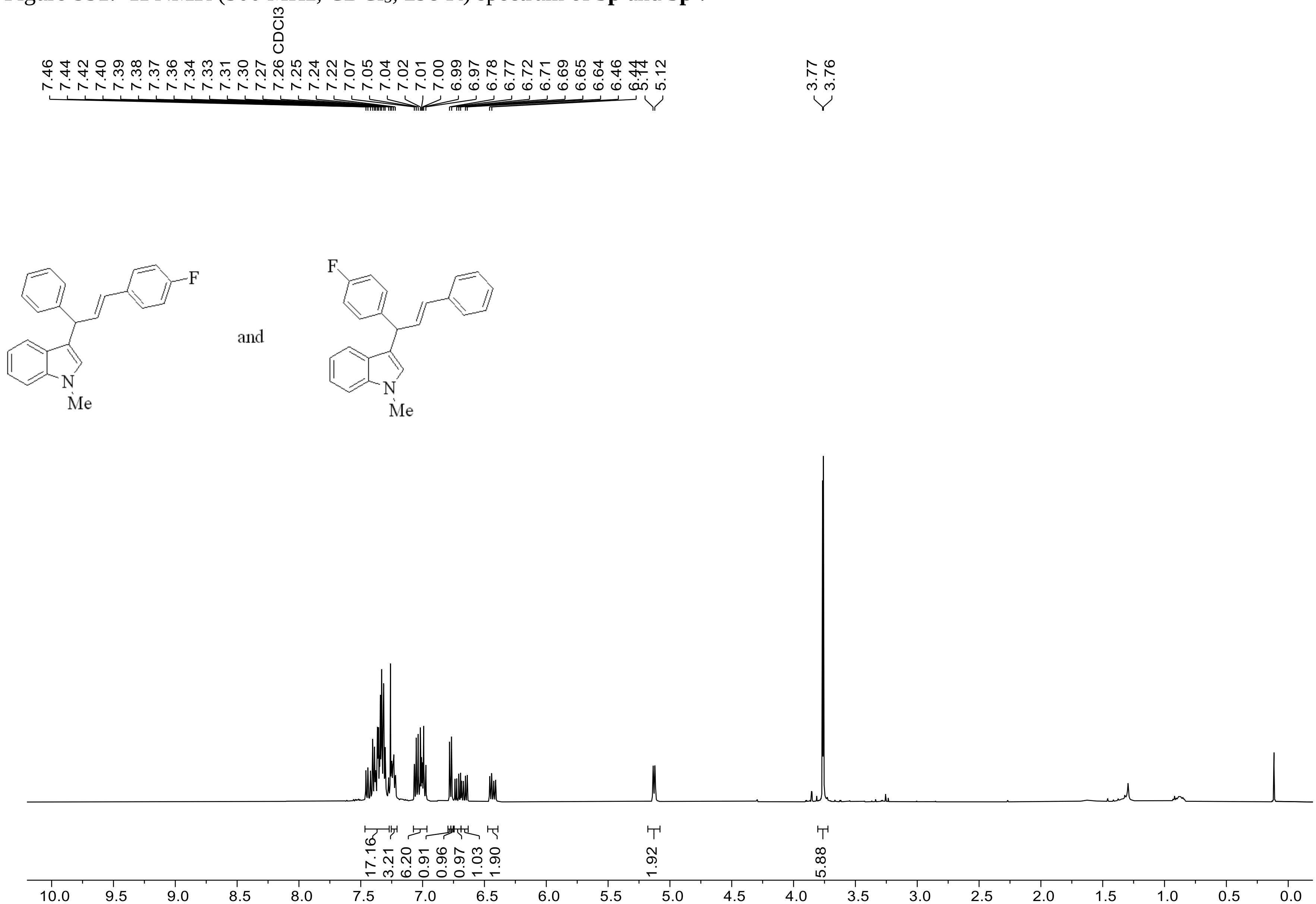


Figure S52: **$^{13}C\{^1H\}$ NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3p** and **3p′**.

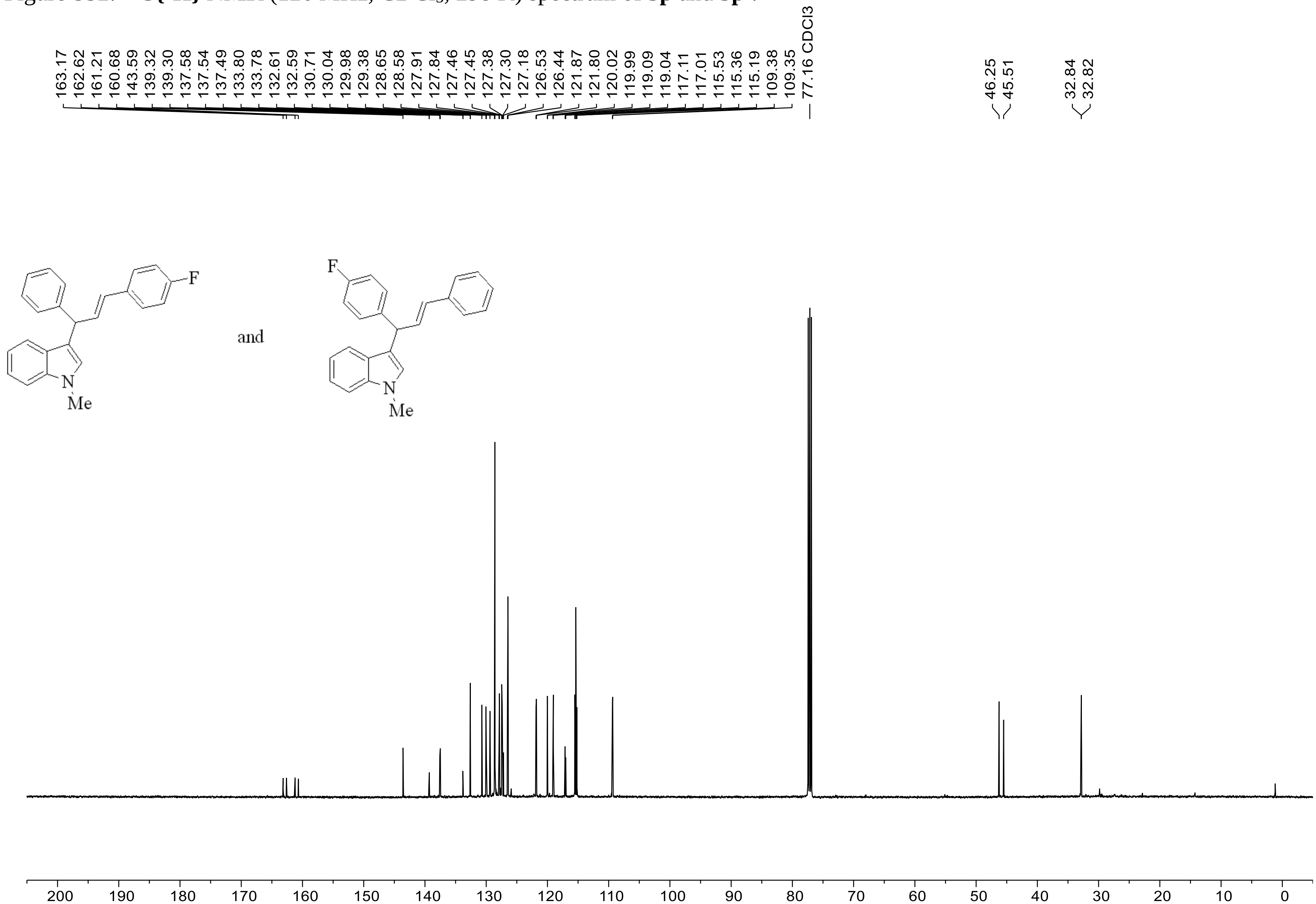


Figure S53: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3p** and **3p′**.

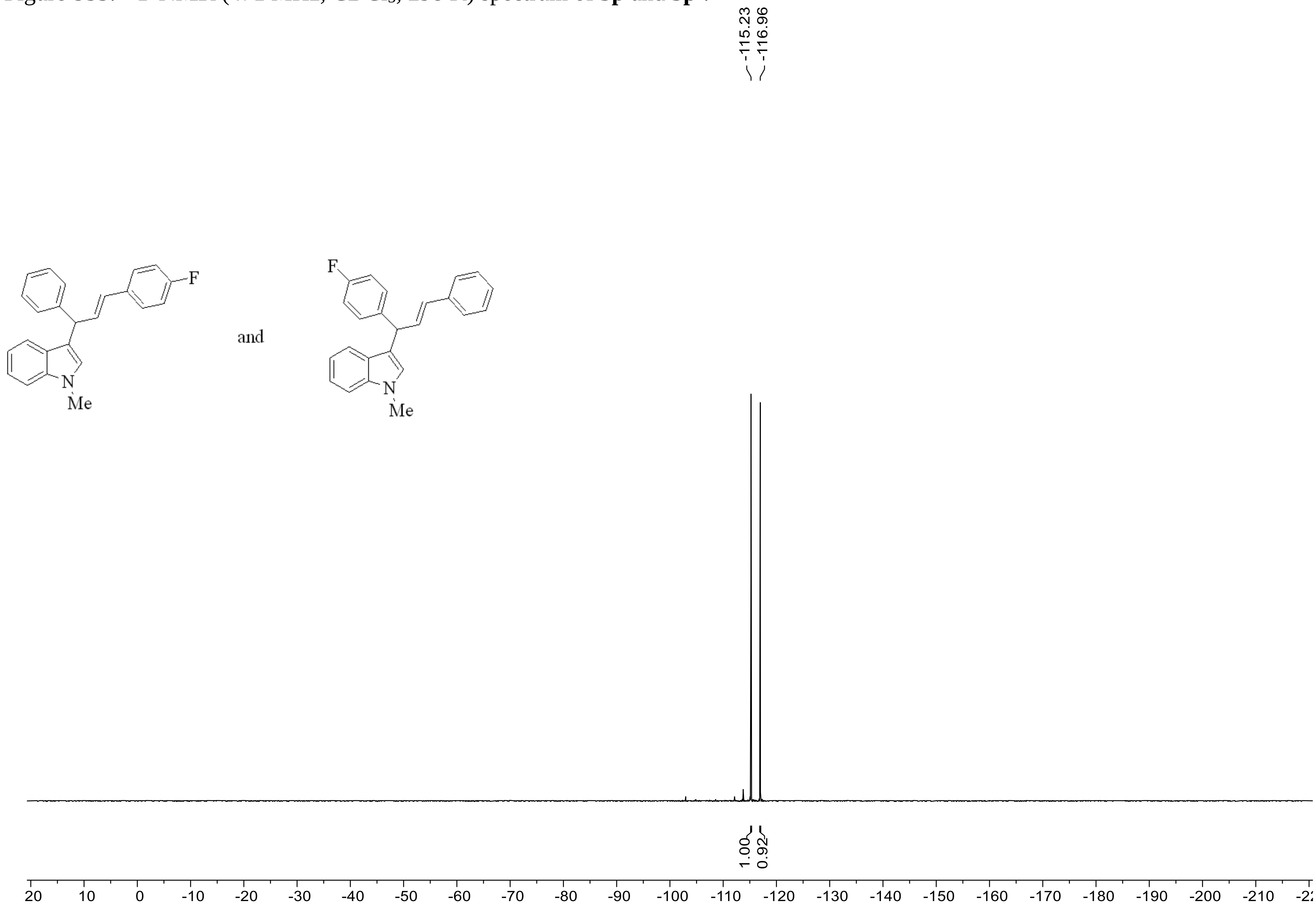


Figure S54: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3q** and **3q′**.

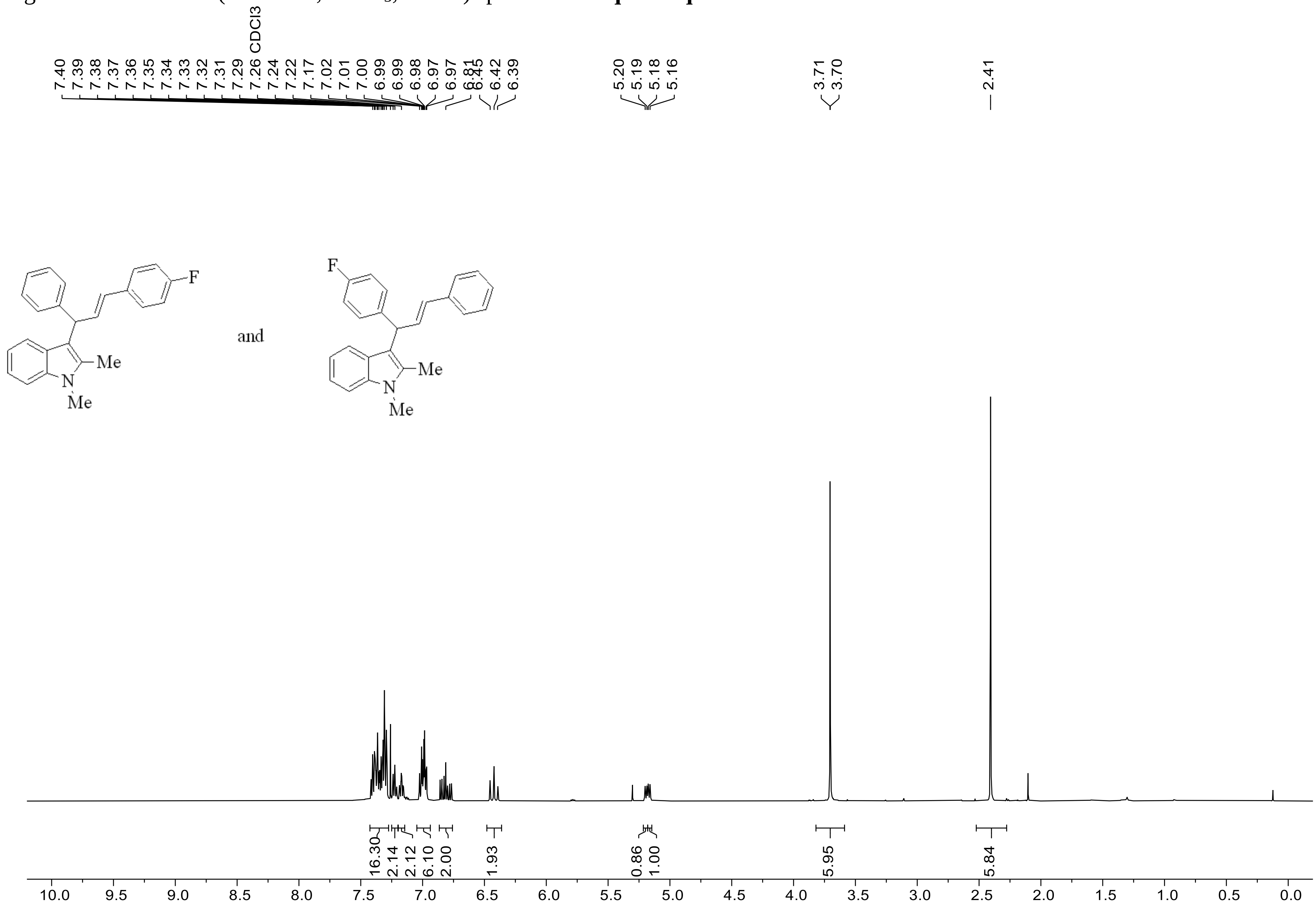


Figure S55: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3q** and **3q′**.

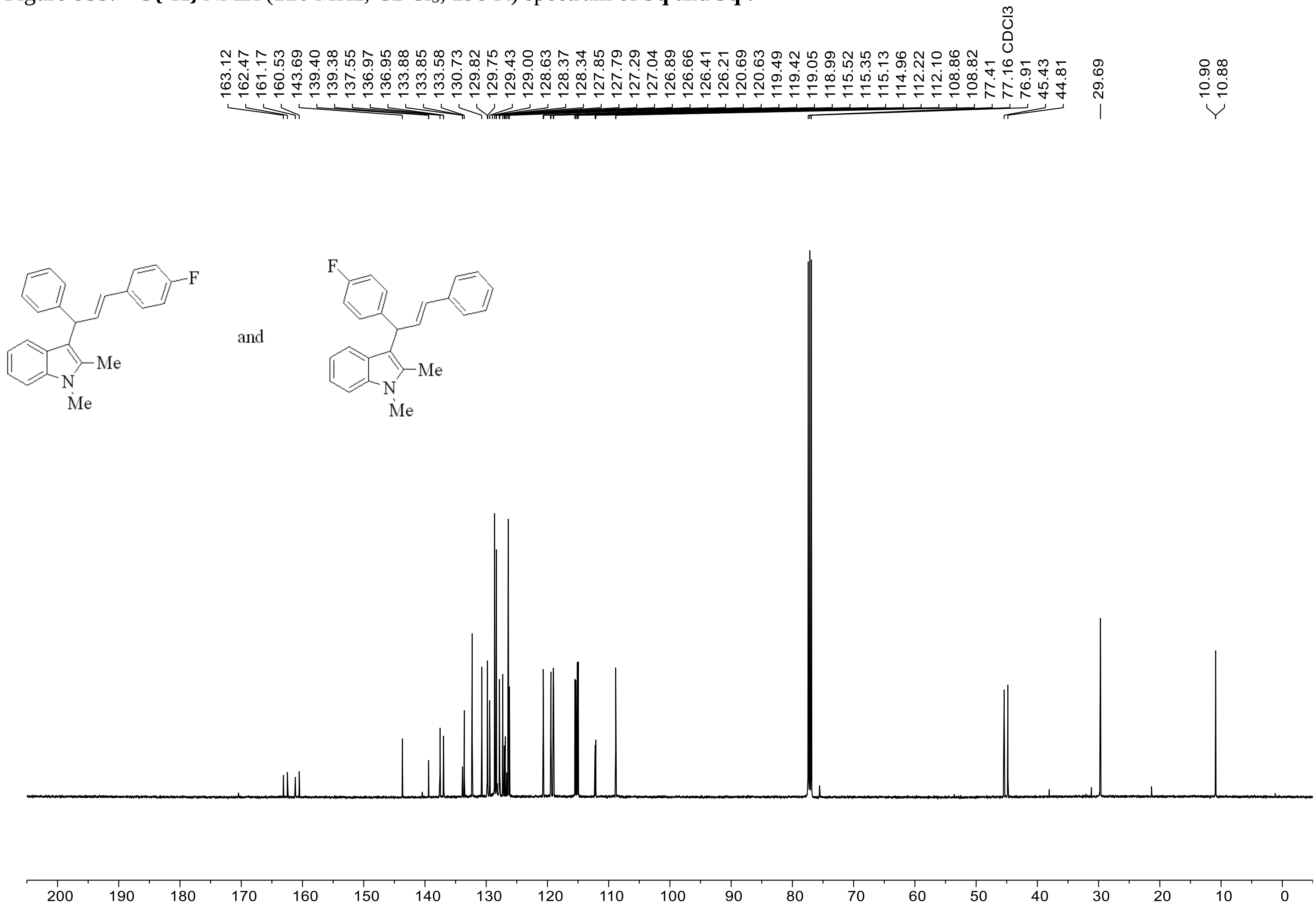
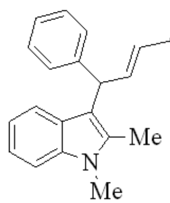
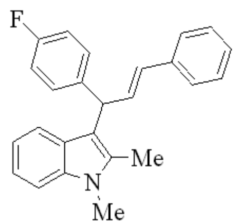


Figure S56: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3q** and **3q′**.



and



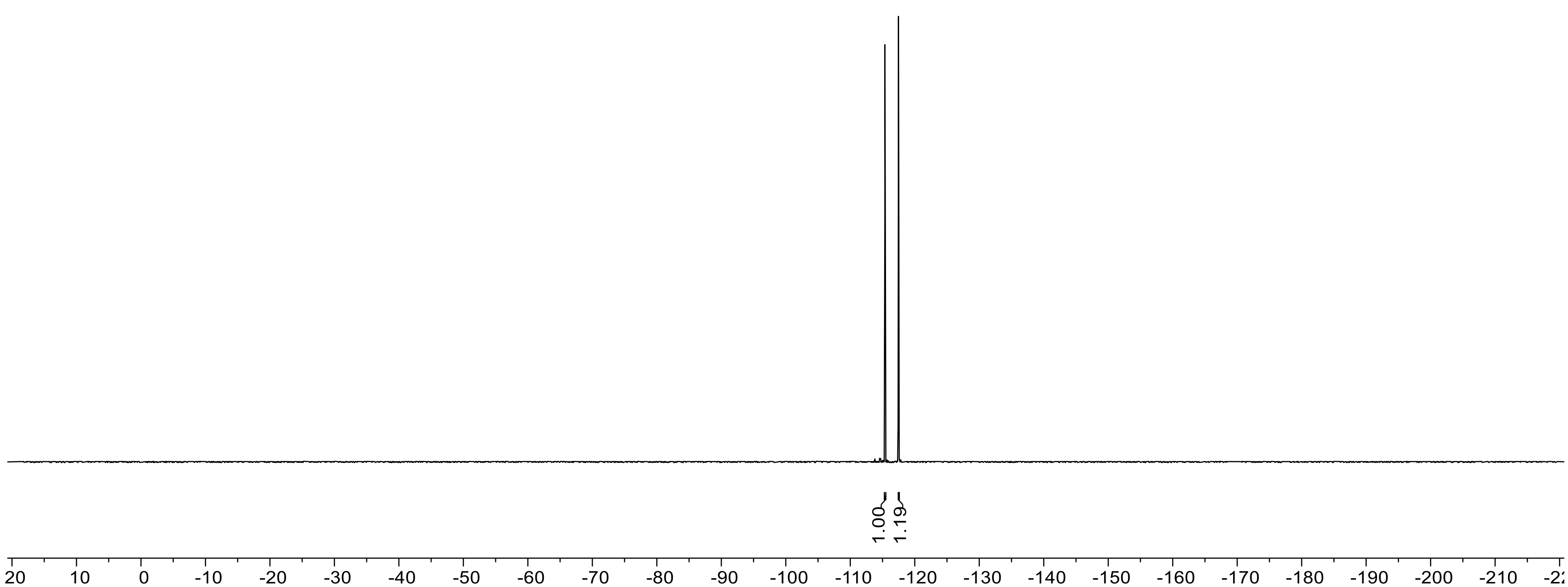


Figure S57: ^{1}**H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3r** and **3r′**.

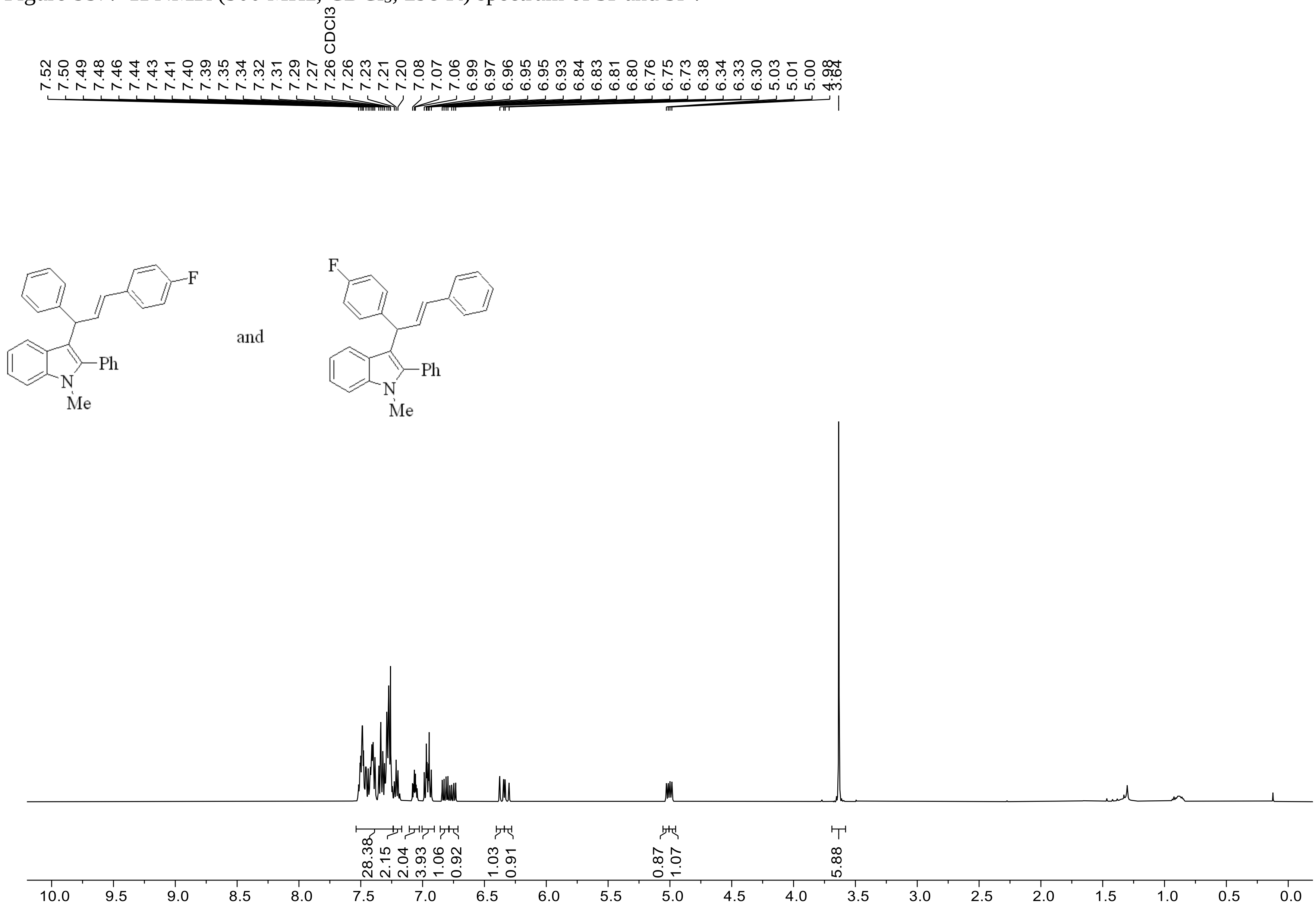


Figure S58: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3r** and **3r′**.

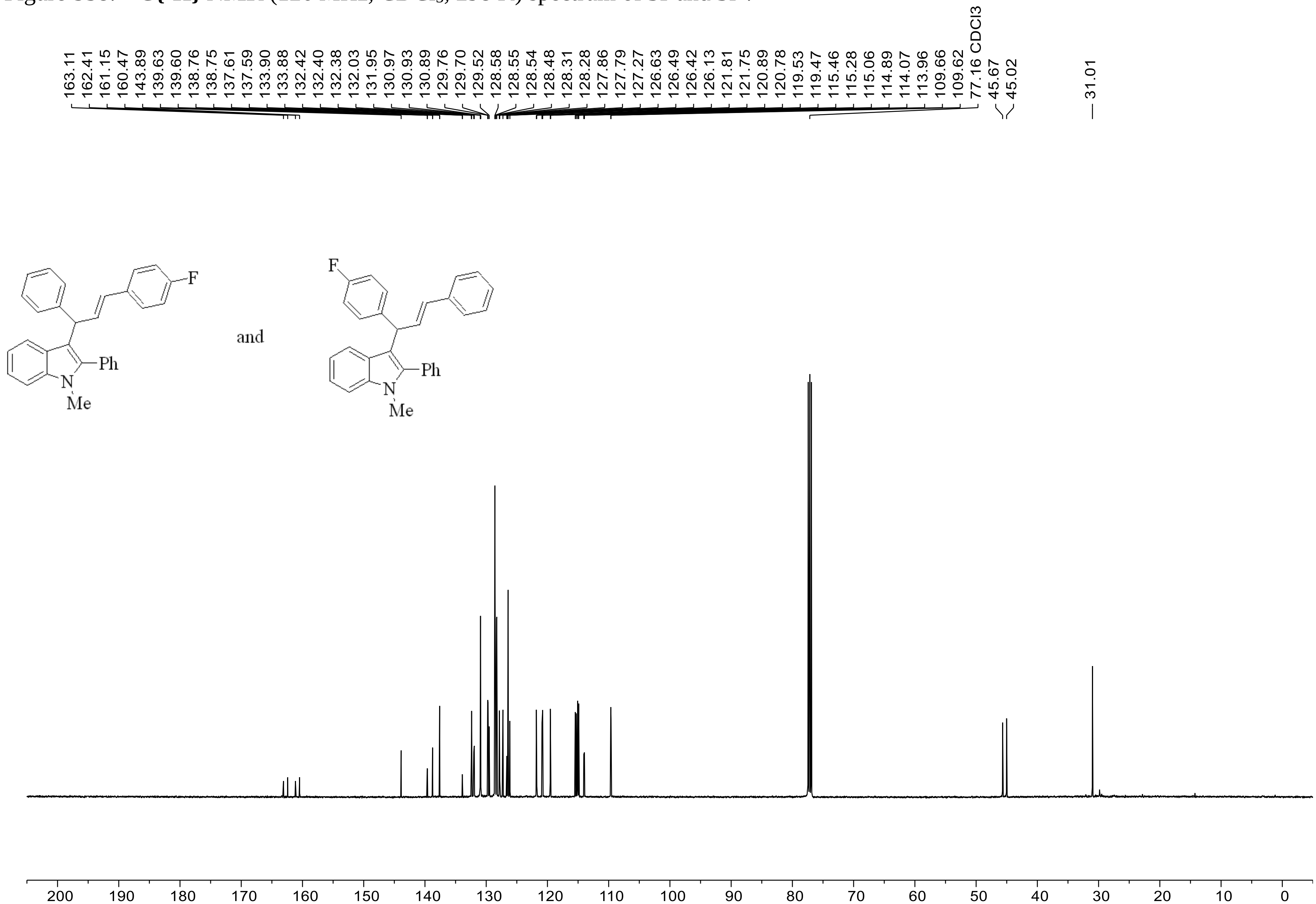


Figure S59: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3r** and **3r′**.

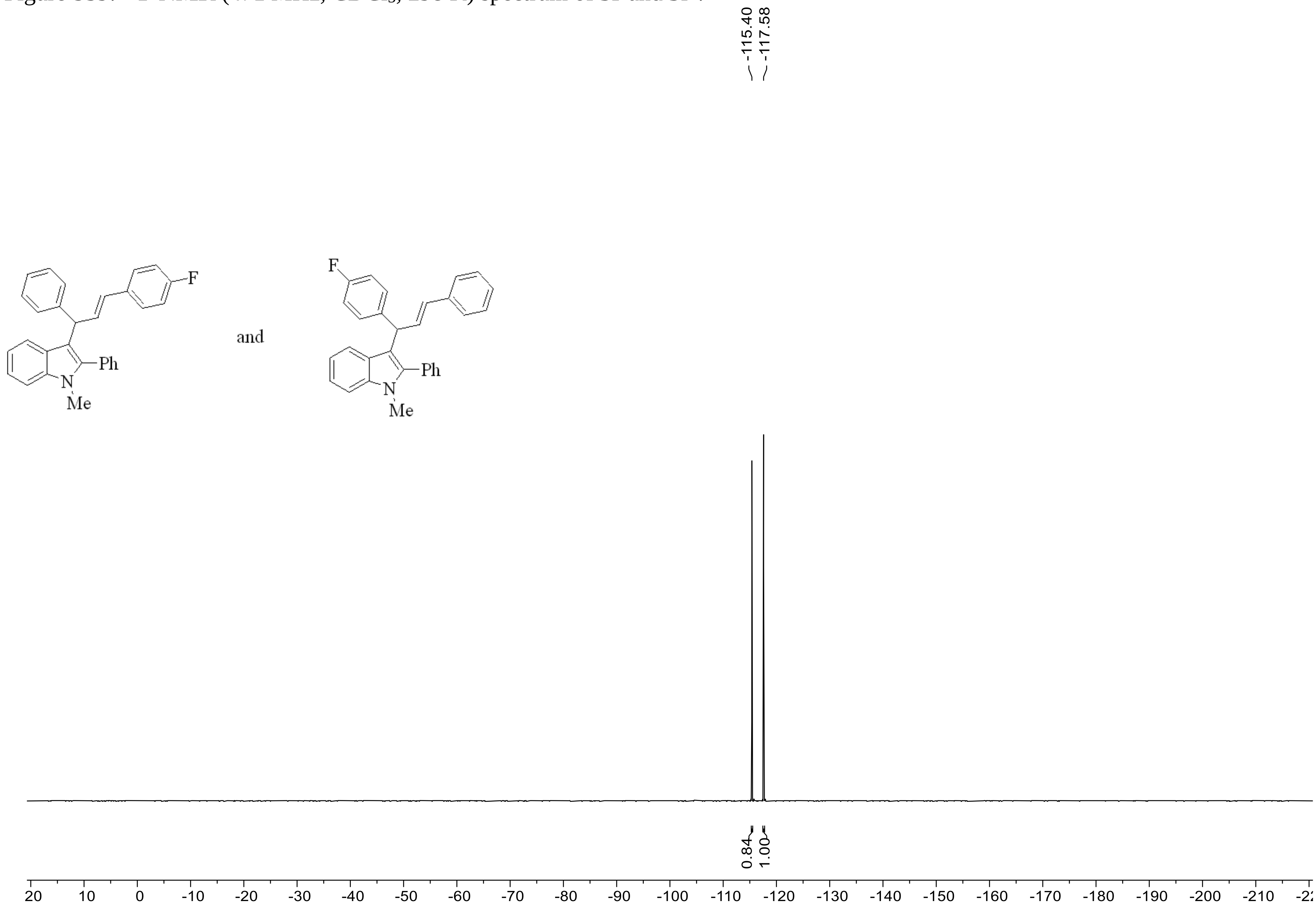


Figure S60: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3s** and **3s′**.

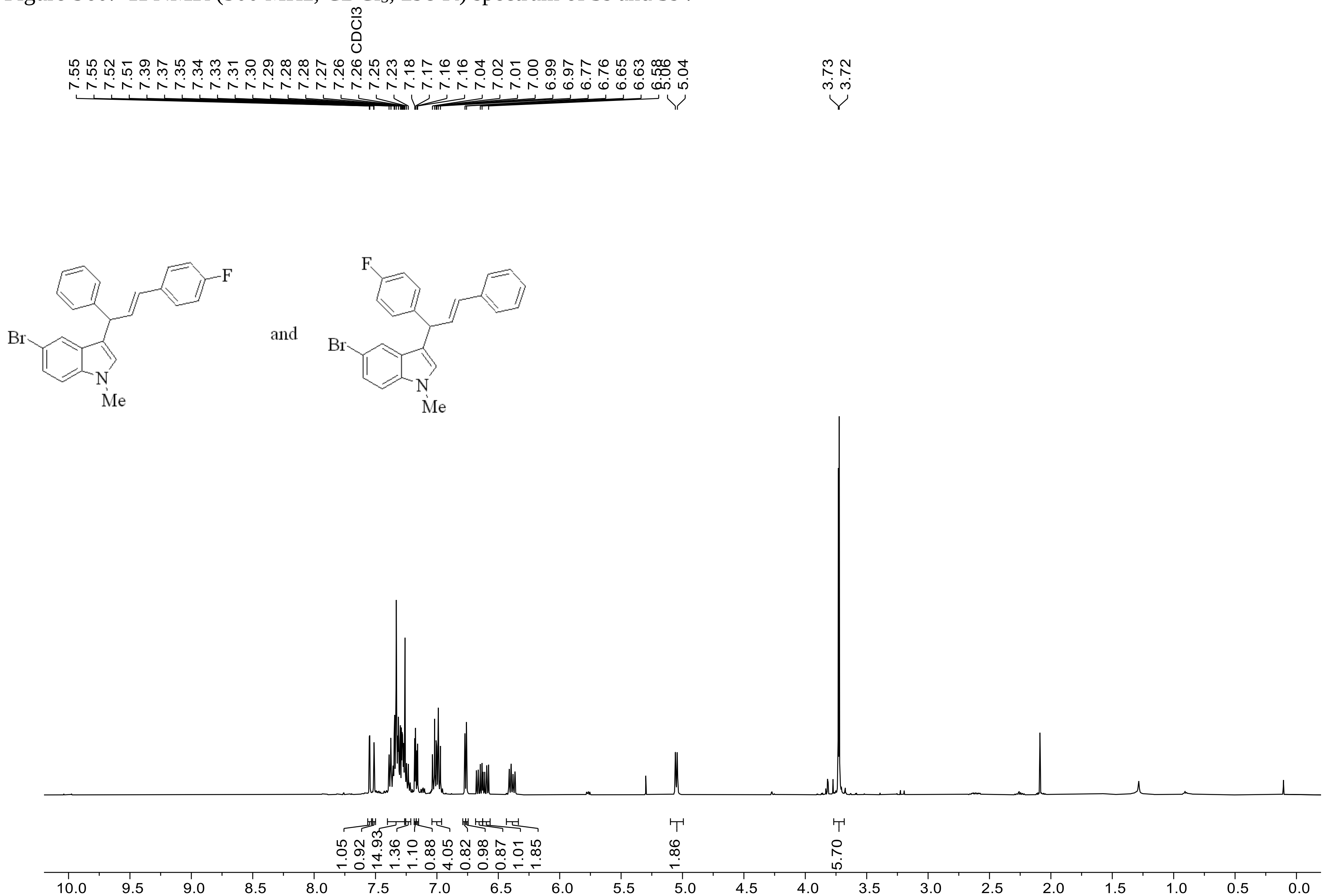


Figure S61: **$^{13}C\{^1H\}$ NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3s** and **3s′**.

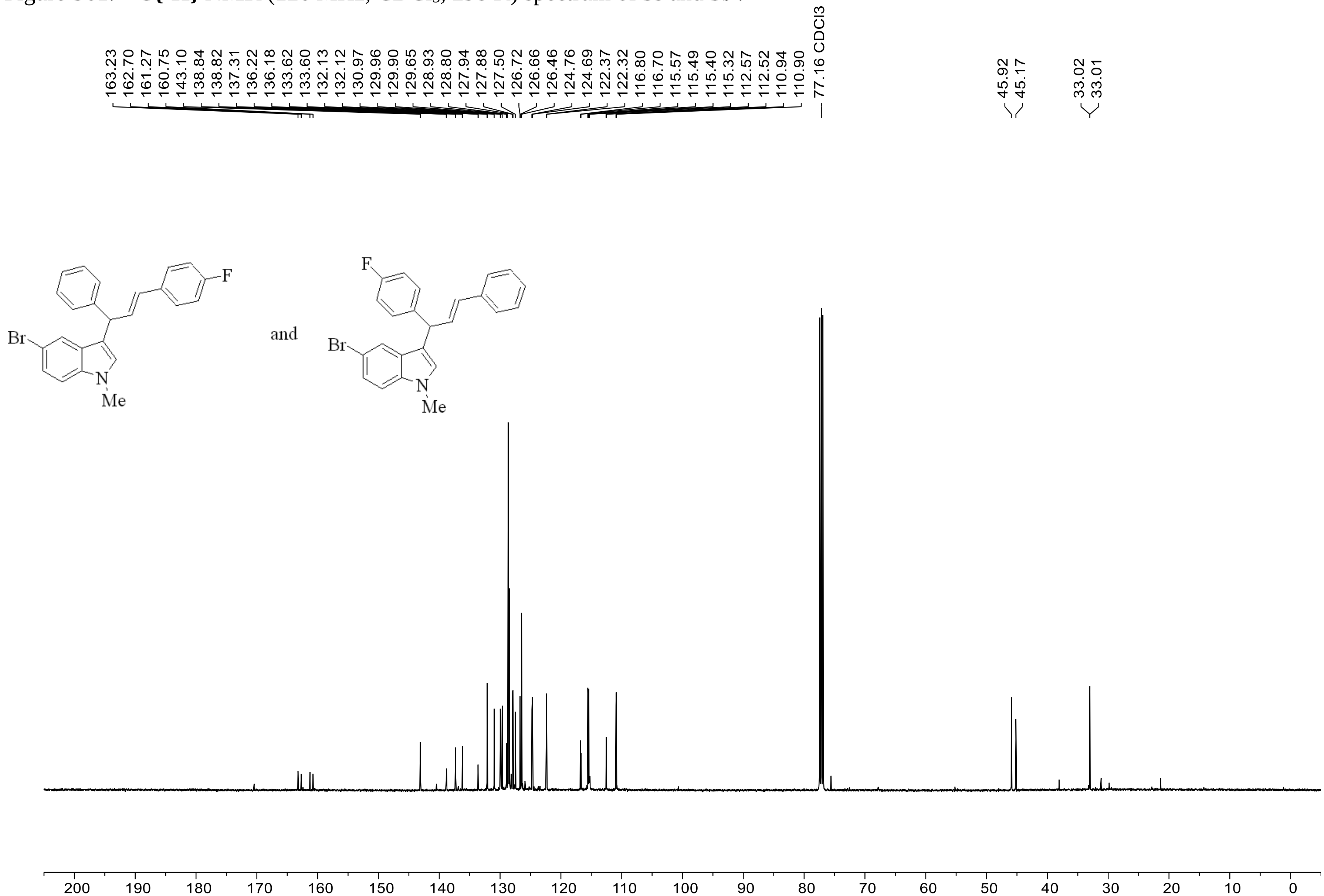


Figure S62: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3s** and **3s′**.

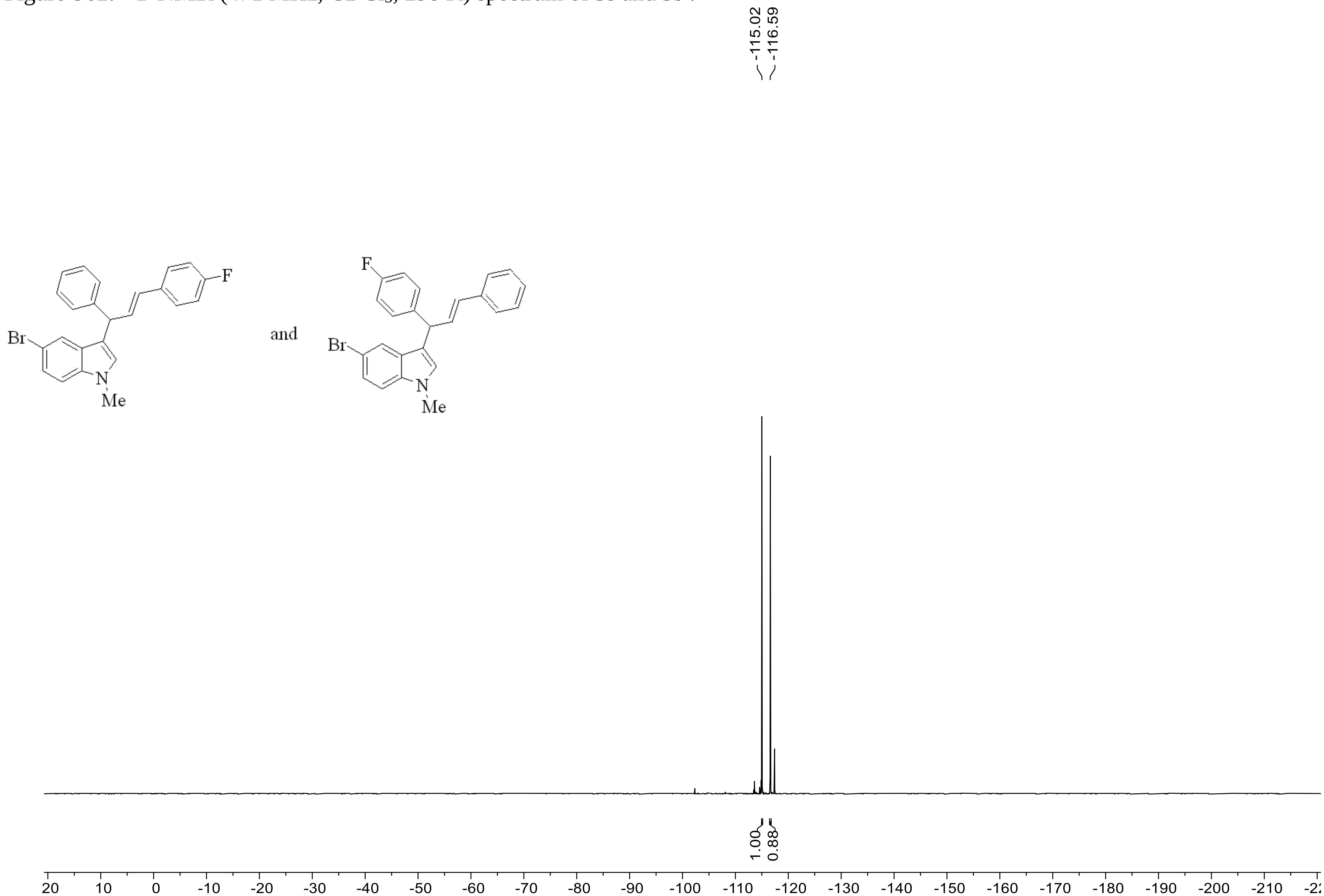


Figure S63: **[1]H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3t** and **3t′**.

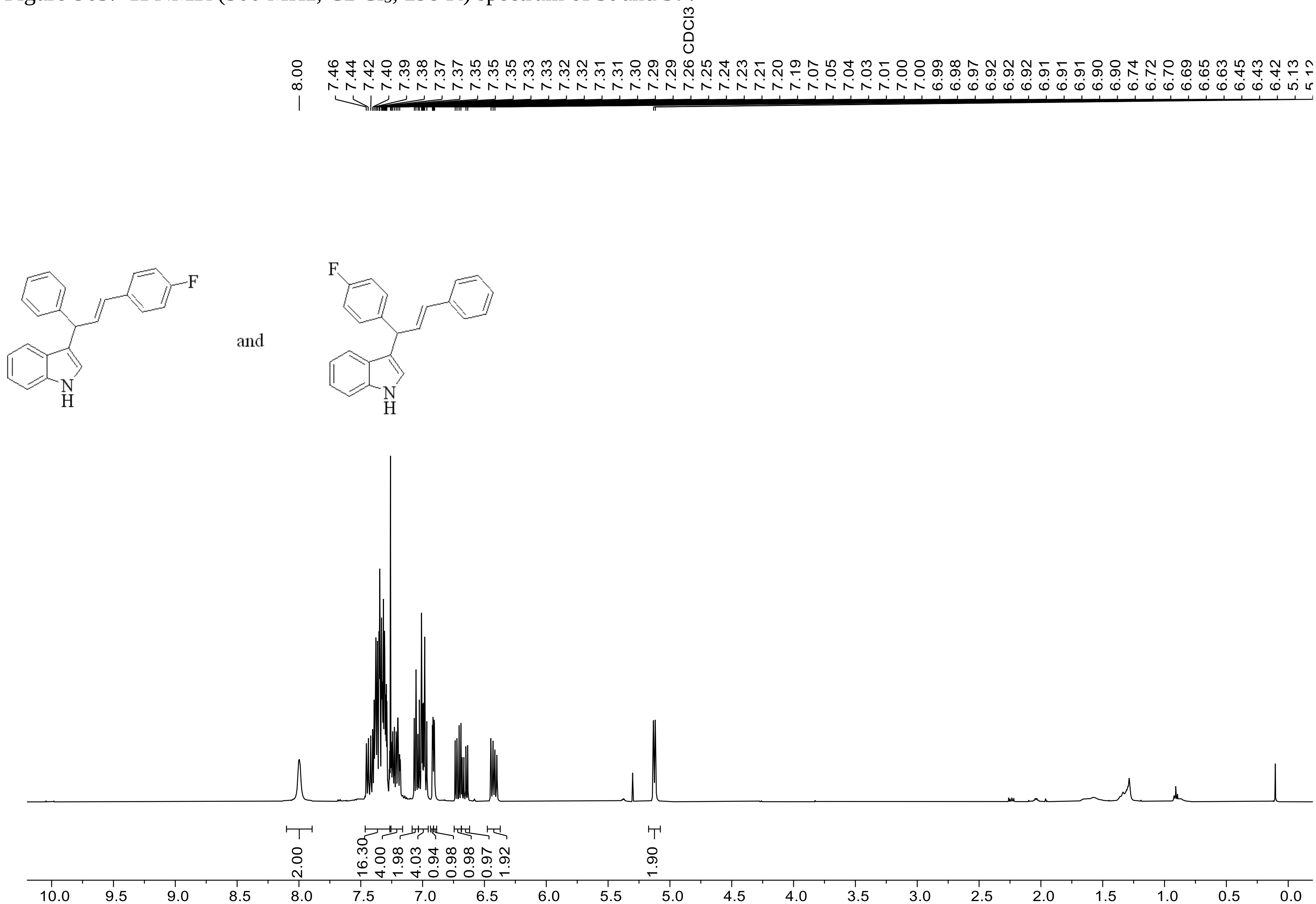


Figure S64: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3t** and **3t′**.

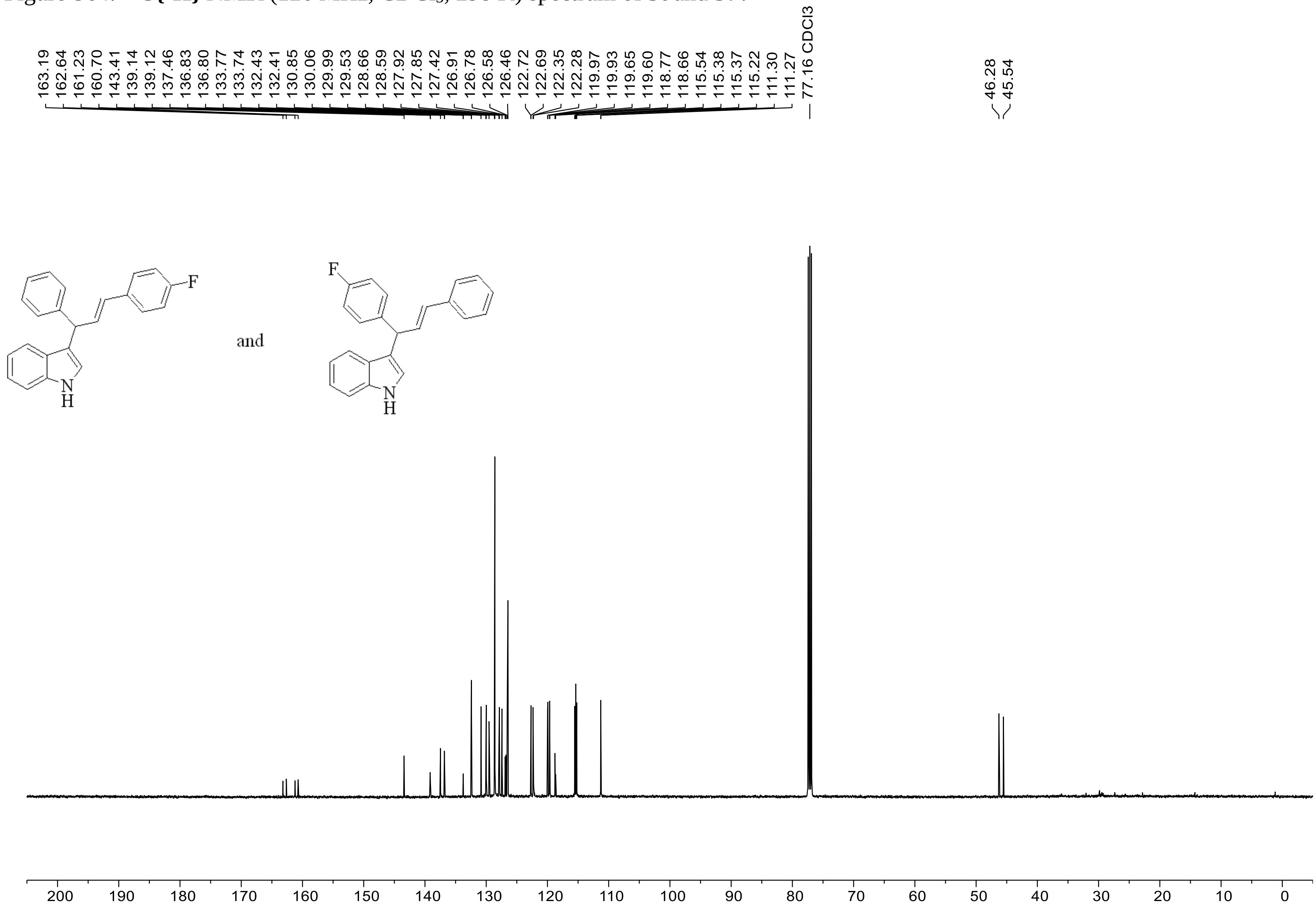
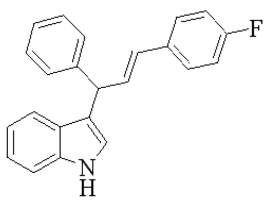
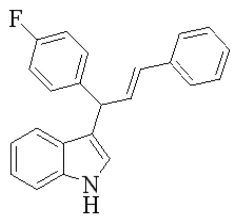


Figure S65: **^{19}F NMR** (471 MHz, $CDCl_3$, 298 K) spectrum of **3t** and **3t′**.



and



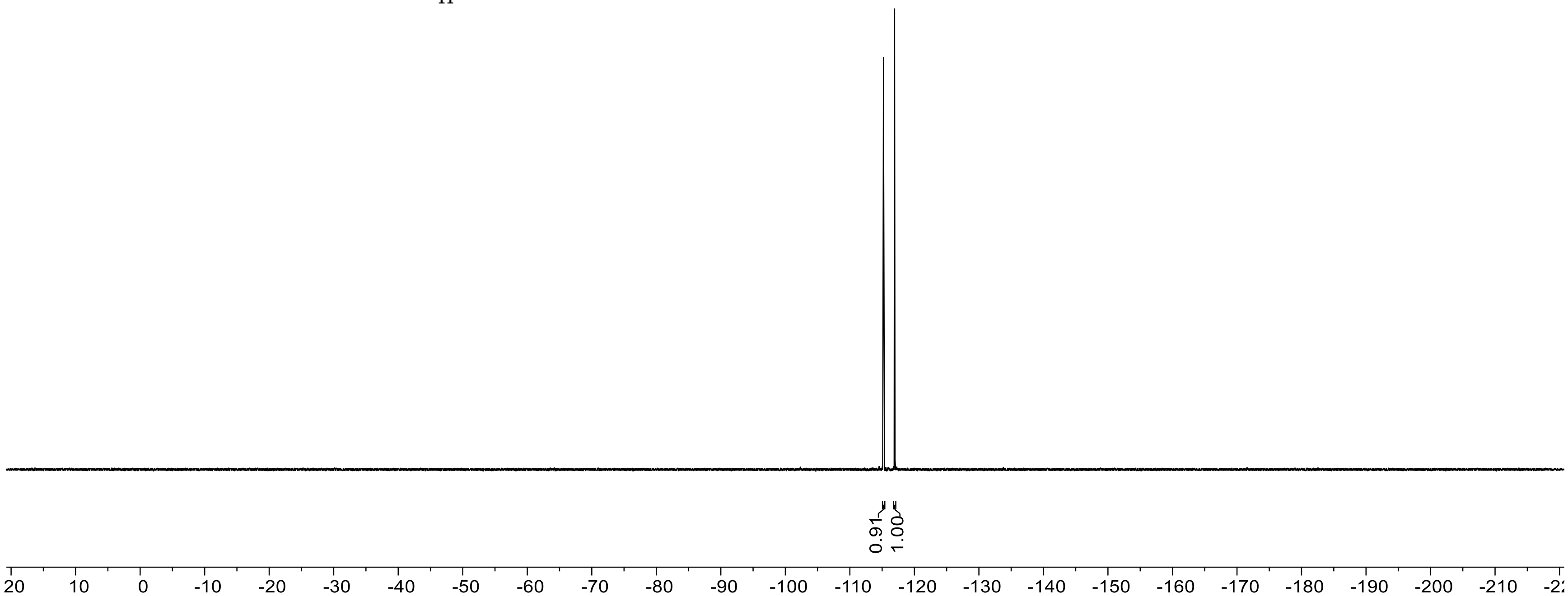


Figure S66: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3u** and **3u′**.

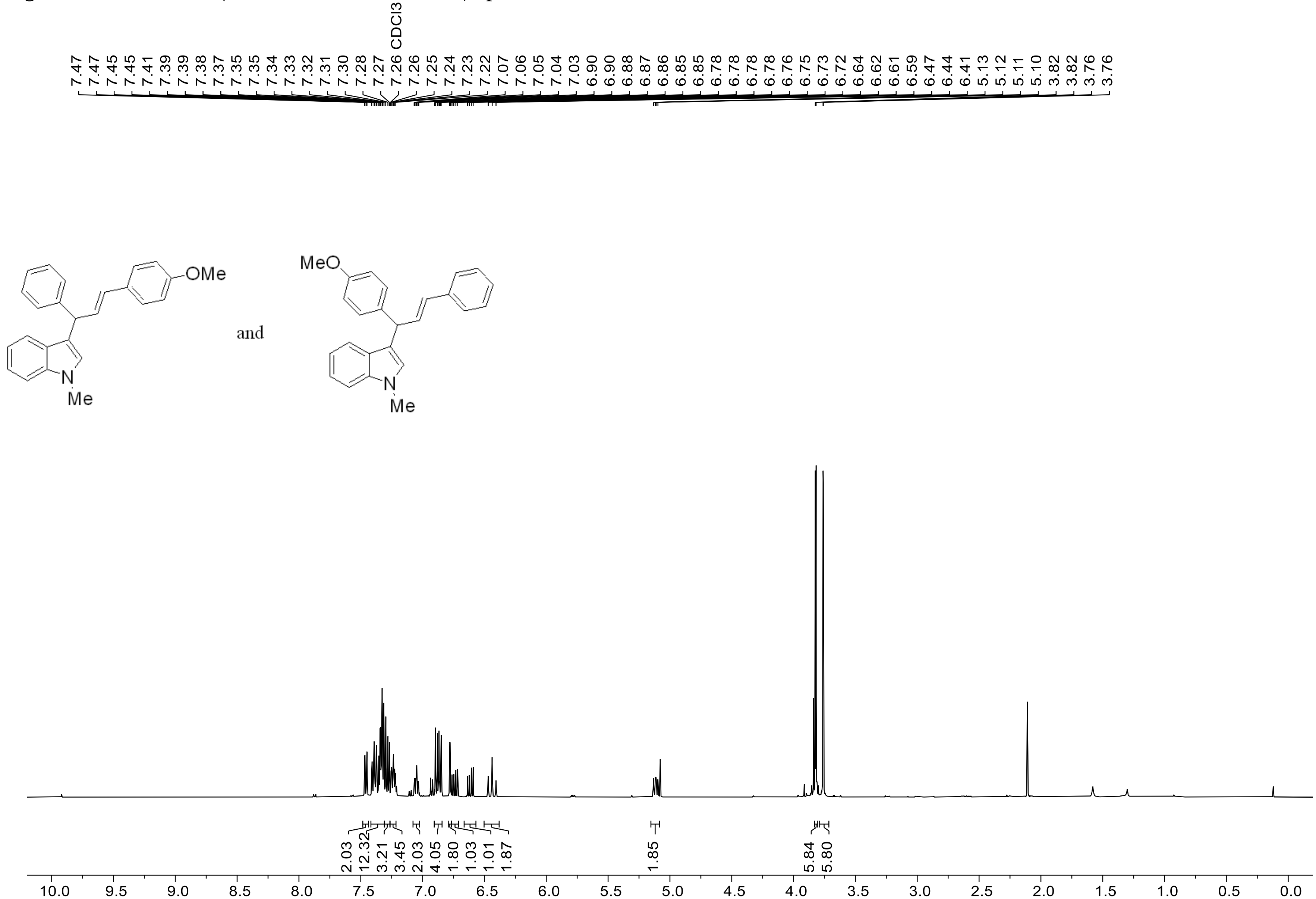


Figure S67: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3u** and **3u′**.

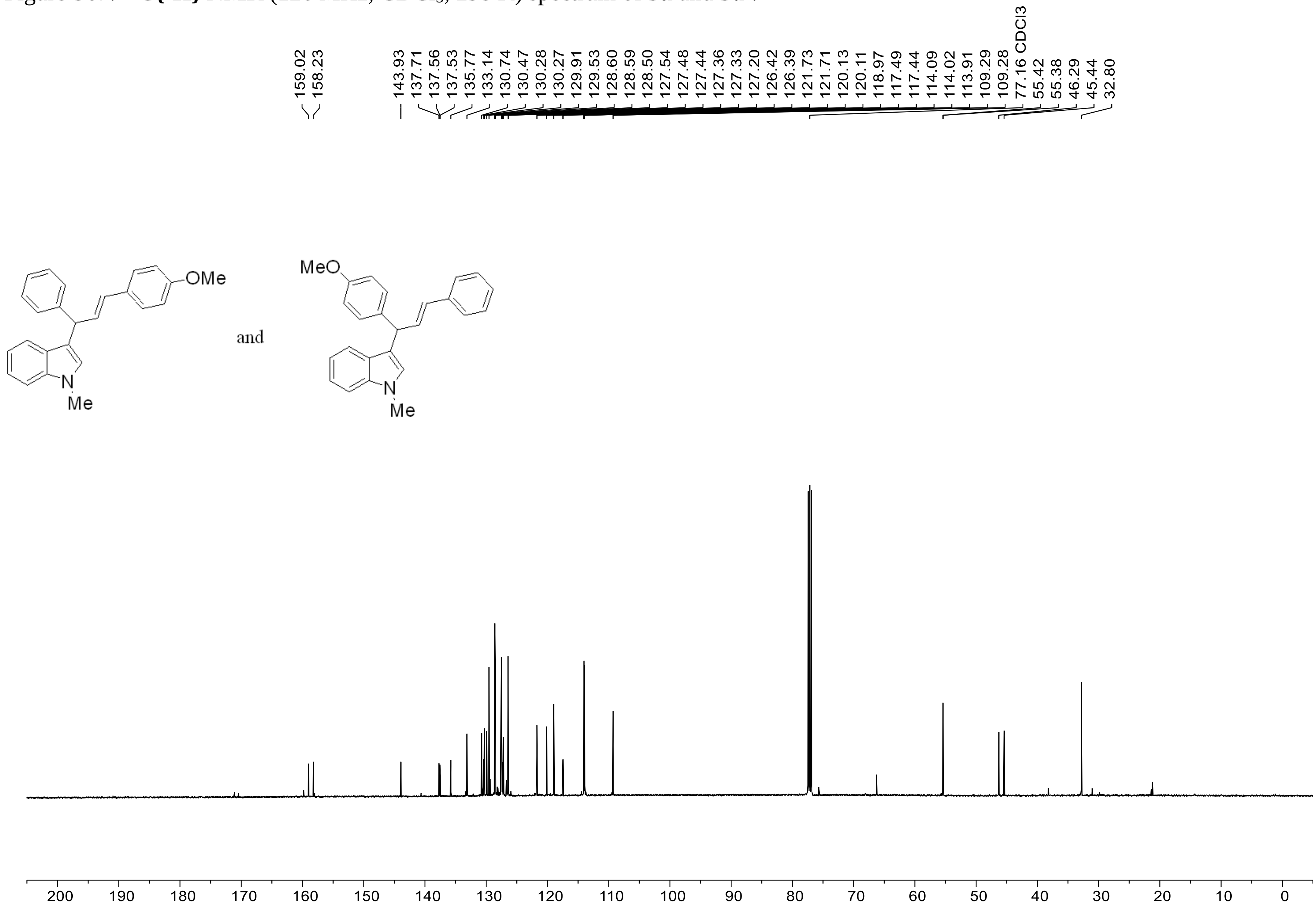


Figure S68: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3v** and **3v′**.

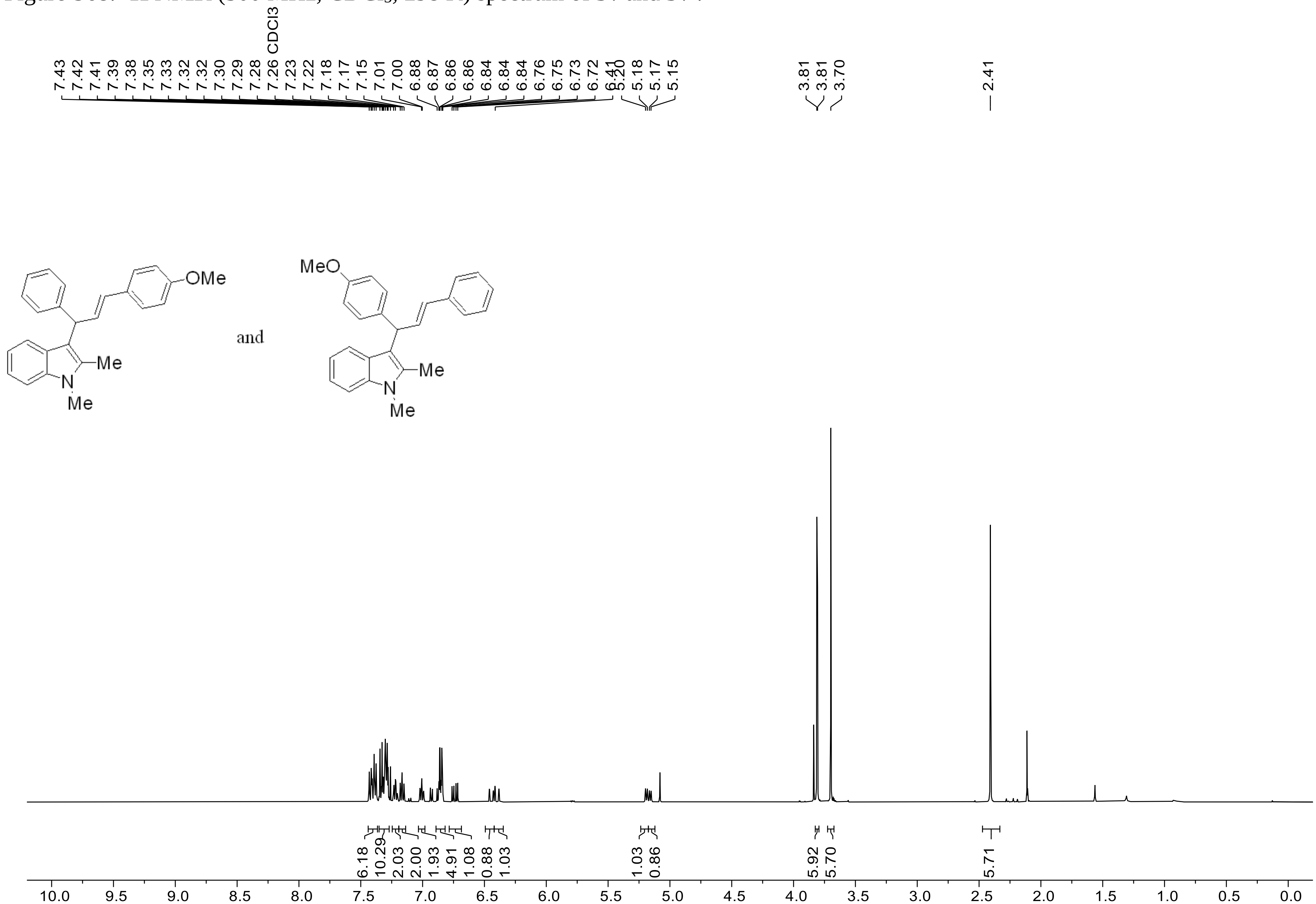
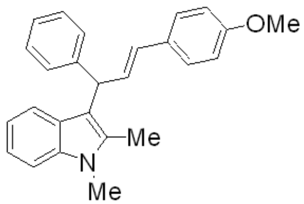
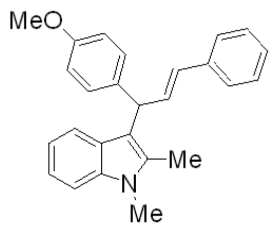


Figure S69: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3v** and **3v′**.



and



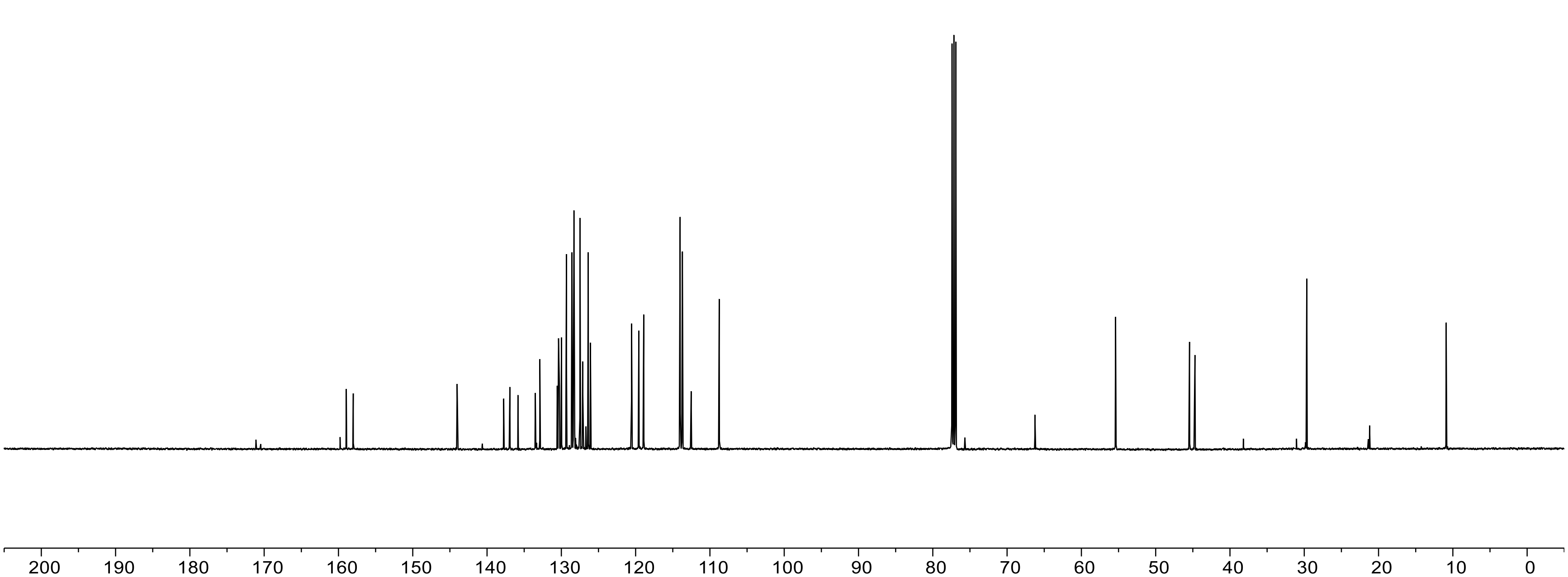


Figure S70: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **2w** and **2w′**.

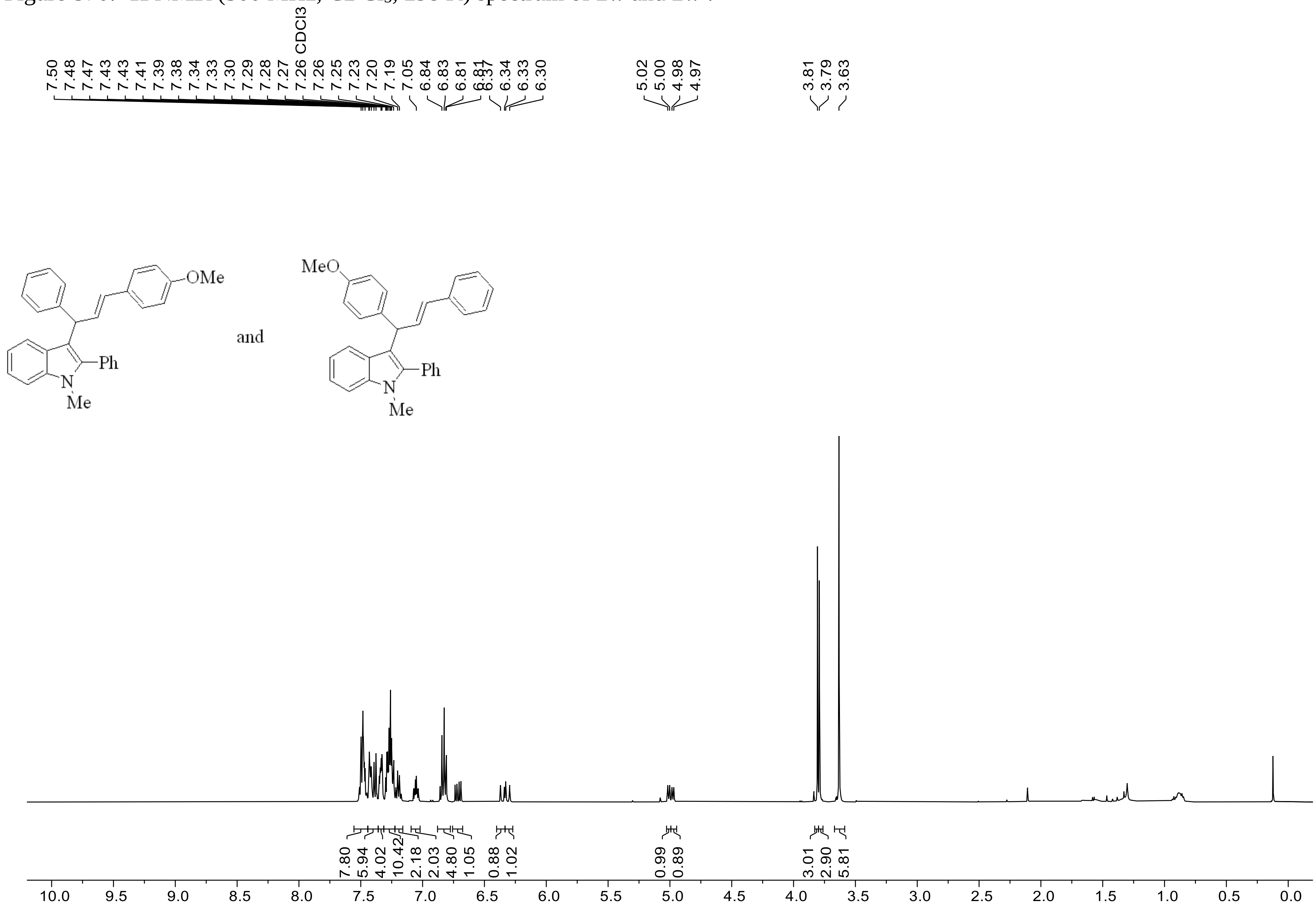


Figure S71: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3w** and **3w′**.

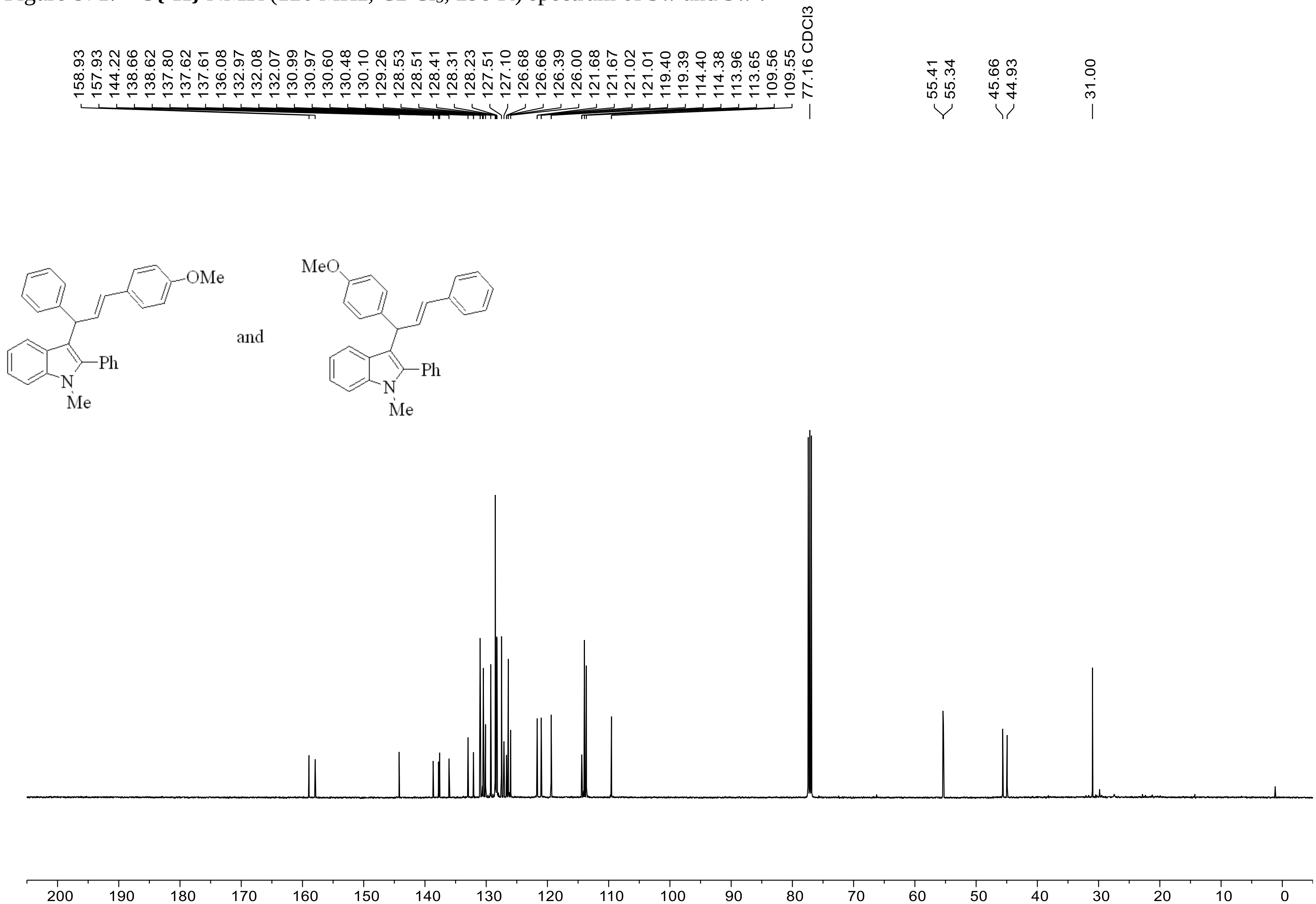


Figure S72: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3x** and **3x′**.

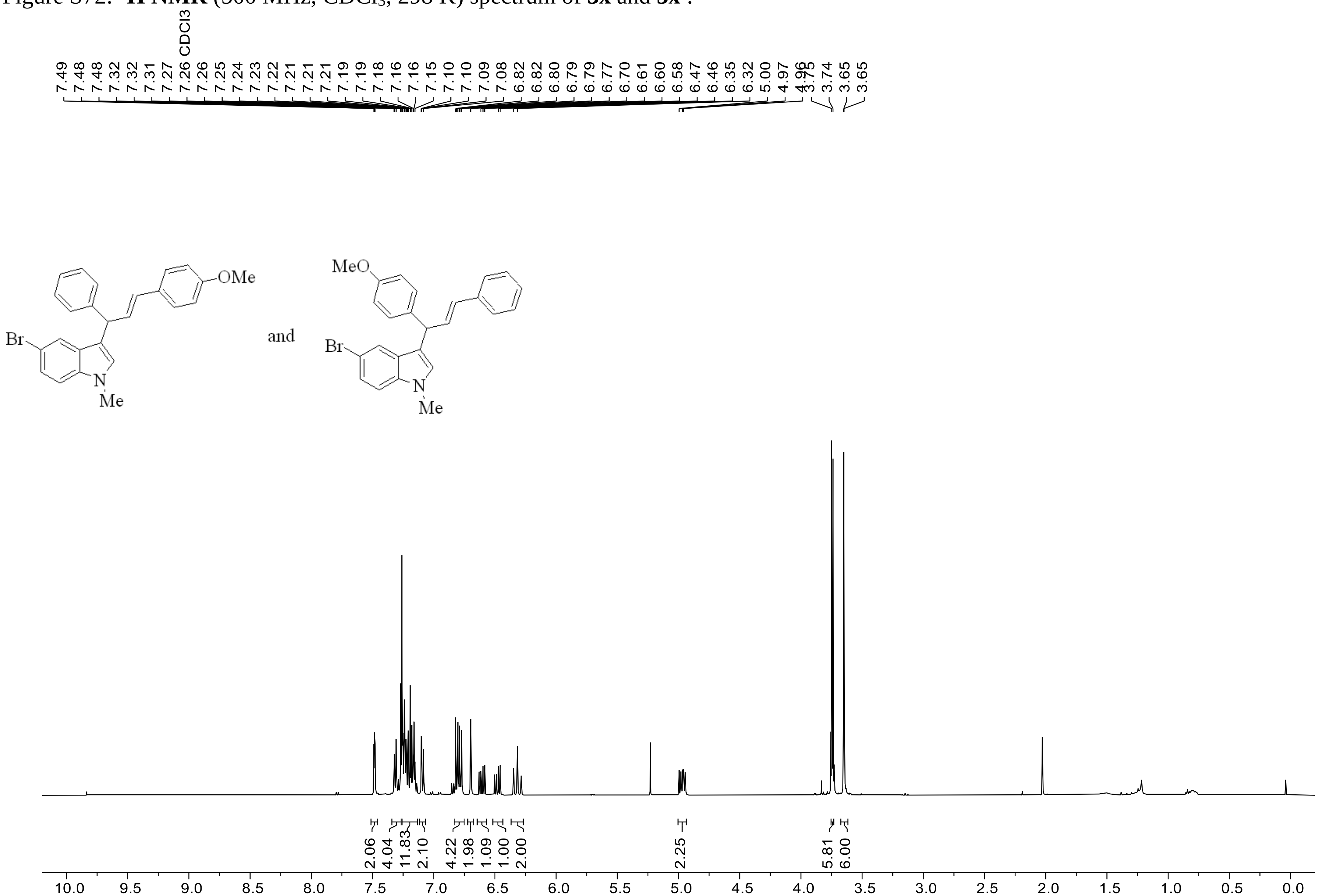


Figure S73: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3x** and **3x′**.

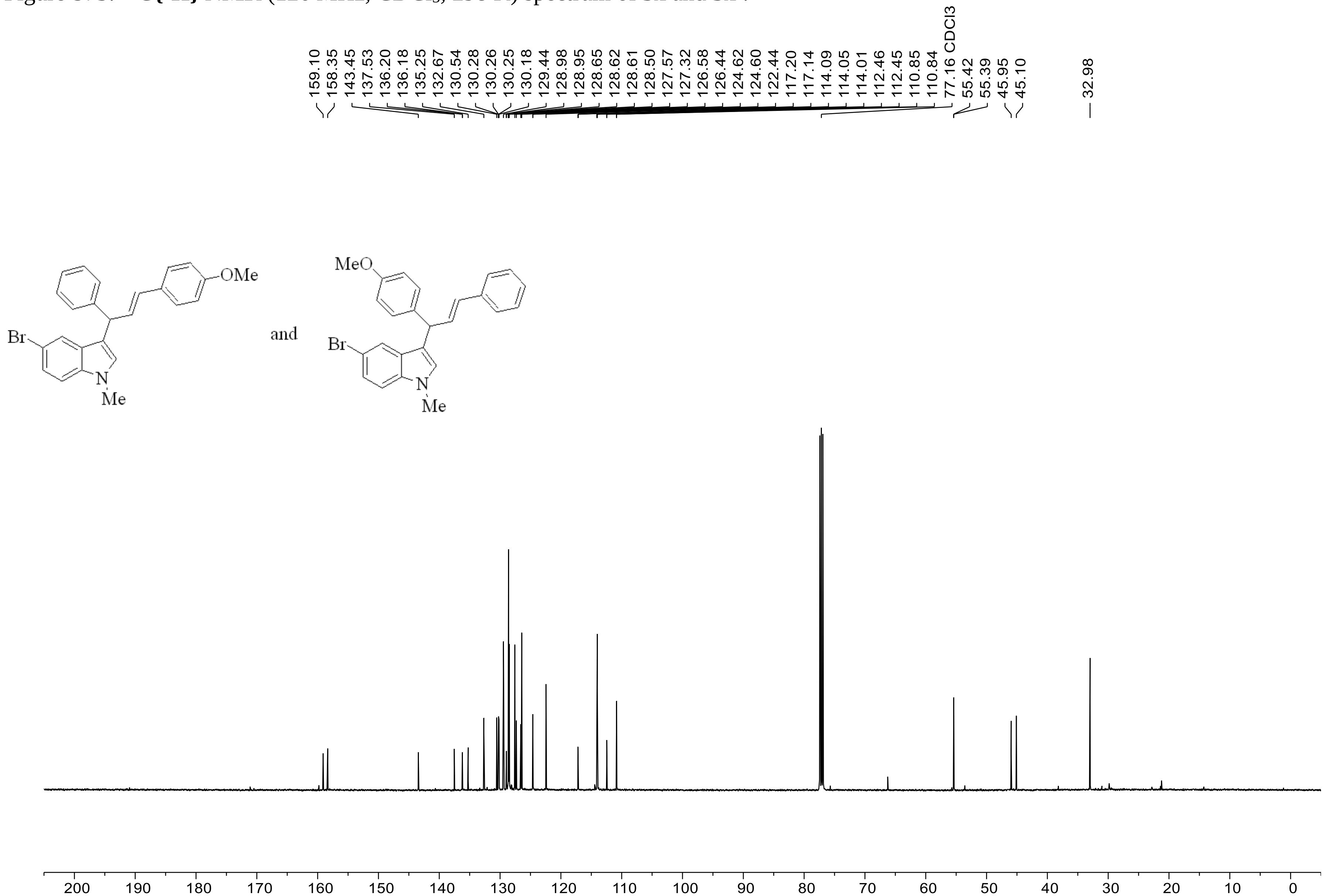


Figure S74: **¹H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of **3y** and **3y′**.

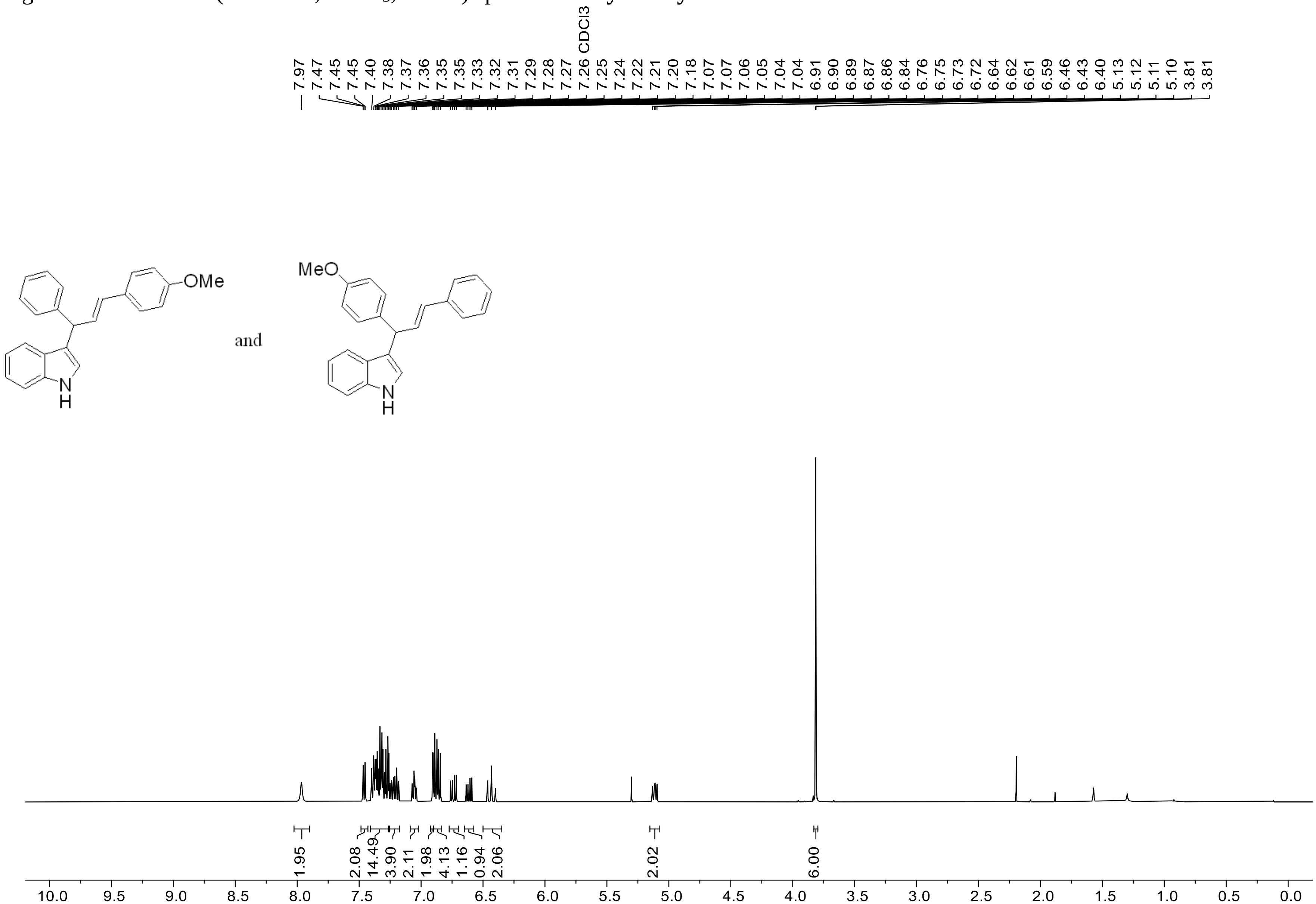


Figure S75: **^{13}C{^{1}H} NMR** (126 MHz, $CDCl_3$, 298 K) spectrum of **3y** and **3y′**.

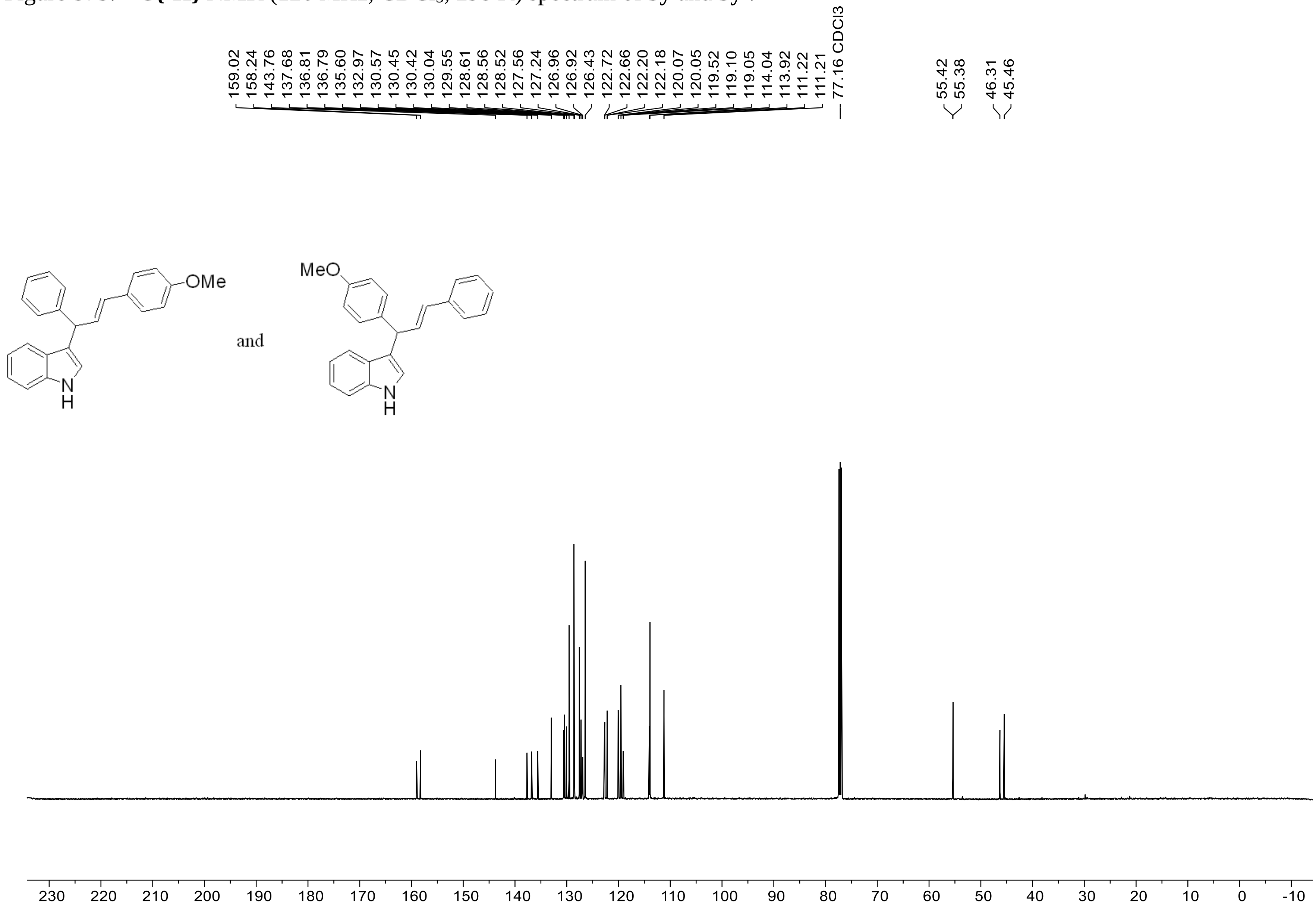
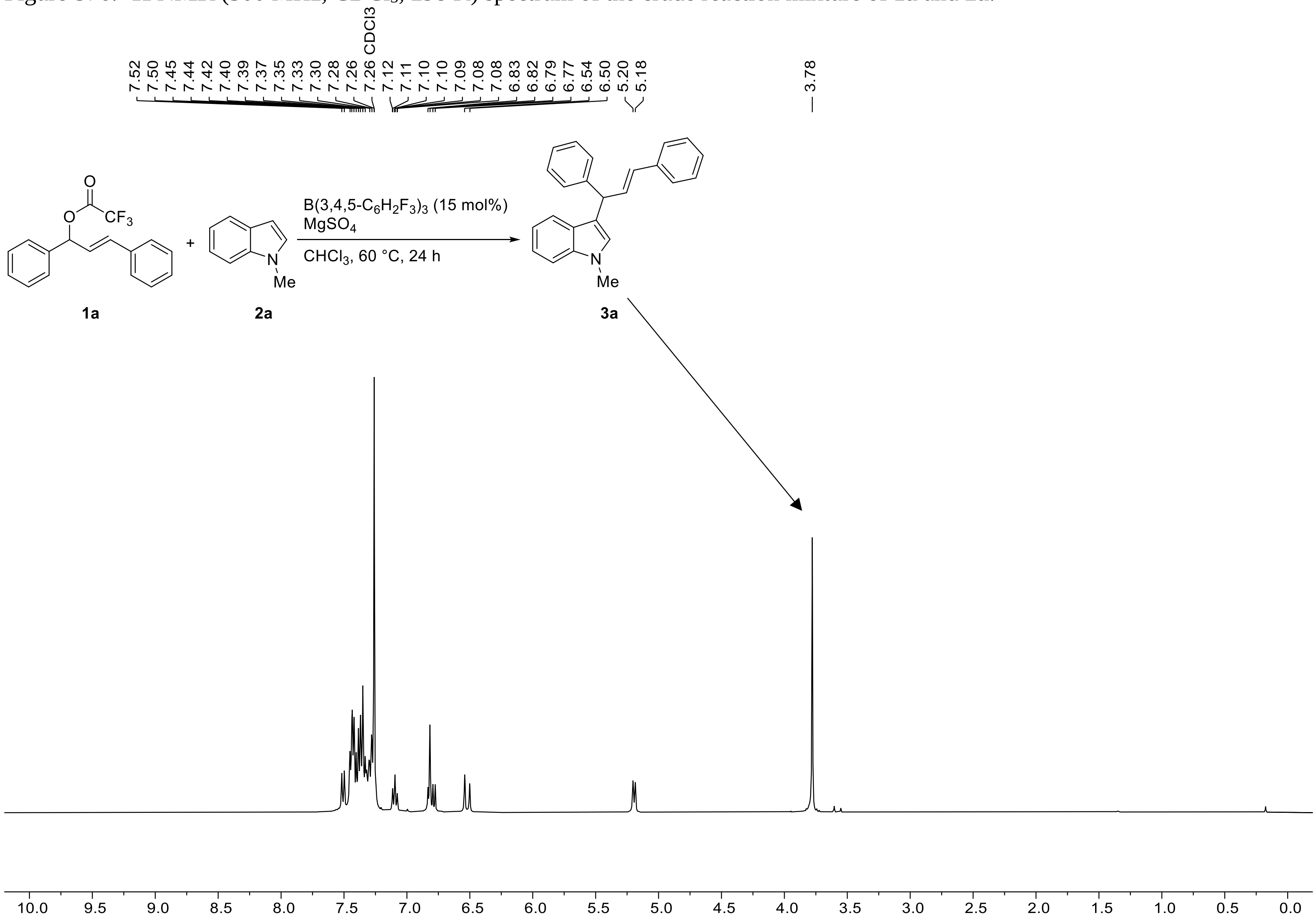


Figure S76: **^{1}H NMR** (500 MHz, $CDCl_3$, 298 K) spectrum of the crude reaction mixture of **1a** and **2a**.



6. Computational Data

6.1 Computational details

Gaussian 16[11] was used to fully optimize all the structures at the M06-2X level[12] of theory using the SMD solvation model[13] in Chloroform. The 6-31G(d) basis set[14] was chosen for all atoms. Frequency calculations were carried out at the same level of theory as those for thestructural optimization. Transition structures were located using the Berny algorithm and intrinsic reaction coordinate (IRC) calculations[15,16] were employed to confirm the connectivity between transition structures and minima. To further refine the energies obtained from the SMD/M06-2X/6-31G(d) calculations, single-point energy calculations using the M06-2X functional method were carried out for all of the structures with a larger basis set def2-TZVP[17] and the SMD solvation model in dichloromethane. Furthermore, the B3LYP[18–22] and B3LYP-D3[23] functional methods were utilized to perform single-point energy calculations for **TS3**, with the aim of investigating the impact of dispersive interactions. All thermodynamic data were calculated in the standard state (298.15 K and 1 atm). An additional correction for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state (1.89 kcal/mol) was applied.[24]

6.2 Cartesian coordinates and total energies for the calculated structures in Chloroform

1a·B($C_6F_3H_2$)$_3$

E(SMD/ M06-2X /6-31G(d)) = -2717.538913 au

H(SMD/M06-2X/6-31G(d)) = -2717.020889 au

G(SMD/M06-2X/6-31G(d)) = -2717.145445 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2718.668489 au

C	-8.00127900	2.70430800	0.60223800
C	-6.64406200	2.46233200	0.41060200
C	-6.08625900	1.21421600	0.71421800
C	-6.92899300	0.20299100	1.19701500
C	-8.28425200	0.44363700	1.38784400
C	-8.82565900	1.69571300	1.09428300
H	-8.41442900	3.67993900	0.36453900
H	-6.00156300	3.24994500	0.02453400
H	-6.52649700	-0.78355200	1.40832600
H	-8.92389700	-0.35139000	1.75933800
H	-9.88557500	1.87934400	1.24153900
C	-4.64087500	1.01674000	0.50557400
C	-3.91810500	0.00622000	0.99477900
C	-2.45432700	-0.21070600	0.75888500
C	-2.15678600	-1.49961400	0.02048300
C	-2.64236100	-1.66878300	-1.28036500

C	-1.40372100	-2.50653900	0.62098300
C	-2.36414100	-2.83789500	-1.97839100
H	-3.23252200	-0.88082000	-1.74234400
C	-1.14391800	-3.68882000	-0.07460500
H	-1.00929500	-2.36592700	1.62489400
C	-1.61766900	-3.85131000	-1.37338900
H	-2.72697800	-2.96093900	-2.99381900
H	-0.55321500	-4.47178800	0.39215700
H	-1.40150200	-4.76423600	-1.91984300
H	-4.36524000	-0.76838300	1.61419800
H	-4.14743000	1.78541500	-0.08596300
O	-1.99118500	0.91255100	-0.07541900
C	-0.72490900	1.09044100	-0.22179100
O	0.12945600	0.50002700	0.43305900
C	-0.43813000	2.12662600	-1.33175900
F	-0.51396300	1.53138700	-2.51807500
F	-1.35118600	3.09047700	-1.27818300
F	0.76339100	2.65853200	-1.17967600
H	-1.89162200	-0.17350600	1.69739000
B	1.75850000	0.04448500	0.14732300
C	2.67549600	1.22412100	0.73104700
C	4.06738100	1.07225300	0.62643500
C	2.18463800	2.34808600	1.40450400
C	4.92041200	2.02161000	1.15975200
H	4.50743300	0.20972500	0.13217200
C	3.05689400	3.28452800	1.93760000
H	1.12140900	2.52539800	1.53409500
C	4.42947600	3.13879000	1.82160800
C	1.80341300	-1.26701900	1.08667000
C	2.10528800	-2.54485100	0.60647500
C	1.50848100	-1.12463600	2.45288900
C	2.07624700	-3.63834200	1.45942200
H	2.34487100	-2.72263400	-0.43727300
C	1.48528200	-2.22591500	3.28707000
H	1.28873900	-0.15142700	2.88480800
C	1.76021200	-3.49889500	2.80059900
C	1.78297300	-0.20458500	-1.44287500
C	2.58350800	0.54887300	-2.31014900
C	0.90993800	-1.15325400	-2.00321900
C	2.50970200	0.35363400	-3.67971800

H	3.26154700	1.31221300	-1.94064700
C	0.84623700	-1.32868300	-3.37373900
H	0.26689400	-1.76931000	-1.37909600
C	1.64172000	-0.57806800	-4.22844700
F	2.32400000	-4.87305800	0.99995900
F	1.72749000	-4.55974200	3.61124600
F	1.19808100	-2.10373500	4.59004400
F	6.24899300	1.88875300	1.05837300
F	5.26109800	4.04895800	2.33634600
F	2.59180500	4.36278900	2.58298500
F	0.01615800	-2.22731700	-3.91979000
F	1.57365800	-0.75140300	-5.55004300
F	3.26704100	1.07165400	-4.51895100

1a

E(SMD/ M06-2X /6-31G(d)) = -1105.191193 au
H(SMD/M06-2X/6-31G(d)) = -1104.904906 au
G(SMD/M06-2X/6-31G(d)) = -1104.977169 au
E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -1105.639887 au

C	-5.28226500	-1.10323300	0.70738500
C	-3.89799400	-1.15160400	0.56816400
C	-3.20342400	-0.13910100	-0.10599100
C	-3.93799800	0.92940400	-0.64142500
C	-5.31967300	0.97866500	-0.50340400
C	-5.99871000	-0.03668700	0.17166400
H	-5.79964600	-1.89933900	1.23440700
H	-3.34054900	-1.98564400	0.98733900
H	-3.42916100	1.72931700	-1.17137200
H	-5.87149500	1.81361300	-0.92501000
H	-7.07848000	0.00567800	0.27742600
C	-1.73786100	-0.24947700	-0.21833200
C	-0.92277500	0.62883300	-0.80757100
C	0.56792900	0.49048000	-0.90628500
C	1.31492100	1.64666500	-0.27101600
C	0.99976600	2.04687200	1.02989800
C	2.33092200	2.29832000	-0.96880300
C	1.69568100	3.09355700	1.62548700
H	0.20627000	1.53638200	1.57009200
C	3.02141400	3.35345500	-0.37534400
H	2.58522900	1.97344200	-1.97421800
C	2.70496200	3.75067000	0.92127100

H	1.44859900	3.40087000	2.63712600
H	3.80935500	3.86000600	-0.92432300
H	3.24425500	4.57117700	1.38503900
H	-1.30052800	1.53988100	-1.26702500
H	-1.30675900	-1.14366000	0.22731900
O	0.93913000	-0.74464700	-0.24001700
C	2.09741800	-1.27891200	-0.58549000
O	2.87701800	-0.88172800	-1.40609300
C	2.33428300	-2.54752100	0.25118900
F	3.42871900	-3.17442600	-0.15972400
F	2.47958000	-2.22967600	1.53965700
F	1.29564500	-3.37984800	0.14451400
H	0.86867300	0.40250100	-1.95633500

2a

E(SMD/ M06-2X /6-31G(d)) = -402.9666165 au

H(SMD/M06-2X/6-31G(d)) = -402.797992 au

G(SMD/M06-2X/6-31G(d)) = -402.839699 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -403.116407 au

C	0.38628600	0.98631200	0.00000400
C	-0.15278800	-0.32622300	-0.00006100
C	0.65476600	-1.47036700	-0.00002800
C	2.02680400	-1.28032200	-0.00000700
C	2.58621000	0.01445600	0.00002900
C	1.78307500	1.14243100	0.00003100
C	-0.72986600	1.88807900	0.00004200
C	-1.85784400	1.11387600	-0.00003500
H	0.22244800	-2.46688500	-0.00001200
H	2.68482500	-2.14418500	-0.00001500
H	3.66658400	0.12405900	-0.00000200
H	2.22372200	2.13571200	0.00009100
H	-0.69732800	2.96849300	0.00001900
H	-2.90115900	1.40125800	-0.00001100
N	-1.52273600	-0.22026700	-0.00014000
C	-2.44320600	-1.33719700	0.00010600
H	-2.29819000	-1.95592800	-0.89075500
H	-2.29868800	-1.95524100	0.89153100
H	-3.46368600	-0.95168000	-0.00035900

3a

E(SMD/ M06-2X /6-31G(d)) = -981.5522314 au

H(SMD/M06-2X/6-31G(d)) = -981.144385 au

G(SMD/M06-2X/6-31G(d)) = -981.218499 au
E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -981.9093043 au

C	5.70913000	-1.13440100	0.20669900
C	4.61573400	-0.31852600	-0.07031800
C	3.30491100	-0.79827300	0.05223500
C	3.12017000	-2.12069100	0.48293700
C	4.21112100	-2.93624500	0.76039200
C	5.51105700	-2.44892100	0.62128900
H	6.71601400	-0.74132100	0.10049200
H	4.77372000	0.70781400	-0.39284800
H	2.11533600	-2.51072700	0.61739900
H	4.04666800	-3.95629000	1.09537300
H	6.36080500	-3.08779200	0.84223100
C	2.18456200	0.10623400	-0.26831100
C	0.91628600	-0.26233800	-0.47143700
C	-0.23674500	0.65876600	-0.83553800
C	0.02109800	2.12362500	-0.53564500
C	0.37367000	2.54032900	0.75432700
C	-0.12177000	3.08843300	-1.53342300
C	0.57122600	3.88865300	1.03651900
H	0.49898200	1.79688300	1.53789600
C	0.07861200	4.44034500	-1.25538600
H	-0.39450700	2.77829000	-2.53932100
C	0.42424300	4.84432000	0.03079700
H	0.84446700	4.19438100	2.04236200
H	-0.03520800	5.17589500	-2.04638700
H	0.58192800	5.89616300	0.24998400
H	0.64775700	-1.31669500	-0.41478400
H	2.45284000	1.15846900	-0.35520900
H	-0.37486400	0.56859000	-1.92474600
C	-2.17242000	-1.08187100	-0.49876000
C	-3.32785400	-1.15278300	0.31928000
C	-4.20828400	-2.24040900	0.28116900
C	-3.91464000	-3.26627300	-0.60280000
C	-2.77643100	-3.21407100	-1.43301200
C	-1.90722200	-2.13582900	-1.38983400
C	-1.51876400	0.16621300	-0.19618800
C	-2.29323400	0.77604300	0.75573200
H	-5.08807900	-2.27642300	0.91727200
H	-4.57547800	-4.12605400	-0.65975700

H	-2.58173100	-4.03406200	-2.11763700
H	-1.03499700	-2.10463900	-2.03839200
H	-2.16676900	1.73420100	1.24231800
N	-3.37880900	-0.00840300	1.07498500
C	-4.41432500	0.31109800	2.03405300
H	-5.39325100	0.34725600	1.54611100
H	-4.44196100	-0.43414500	2.83508400
H	-4.20078800	1.28845000	2.46899800

$B(C_6F_3H_2)_3$

E(SMD/ M06-2X /6-31G(d)) = -1612.333093 au

H(SMD/M06-2X/6-31G(d)) = -1612.102882 au

G(SMD/M06-2X/6-31G(d)) = -1612.1813 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -1613.023787 au

B	-0.00223000	0.00194000	-0.00223600
C	0.36852200	-1.52059000	-0.00307800
C	-0.44851500	-2.45887400	-0.65722600
C	-0.10407100	-3.79816500	-0.66077400
C	1.02988400	-4.24744300	0.00264800
C	1.83136500	-3.32570600	0.66282100
C	1.52352400	-1.97749200	0.65450200
C	-1.50626400	0.44333400	-0.00122200
C	-1.90776000	1.62583400	-0.64695400
C	-3.23963400	1.99788900	-0.65173400
C	-4.19807300	1.23478400	0.00134500
C	-3.80377500	0.07359800	0.65249600
C	-2.48251000	-0.33414800	0.64538100
C	1.13330200	1.08205000	-0.00321800
C	0.95614100	2.31263700	0.65280700
C	1.97298900	3.24987900	0.65925800
C	3.17075300	3.01121700	-0.00109700
C	3.34393100	1.80344300	-0.66399000
C	2.35264700	0.83907500	-0.65921100
F	-0.85699000	-4.70355400	-1.29377600
F	1.34262100	-5.54091300	0.00563000
F	2.91385700	-3.78298300	1.30045000
F	-3.64548300	3.10679100	-1.27830100
F	-5.47444400	1.61077800	0.00455200
F	-4.74425200	-0.64213600	1.27757800
F	4.50326000	1.59913700	-1.29792000
F	4.13702000	3.92595100	0.00100600

F	1.83183700	4.41745200	1.29485800
H	-1.35114400	-2.15881400	-1.17968200
H	2.18645200	-1.29631900	1.17808700
H	2.53982700	-0.09343100	-1.18232200
H	0.03623100	2.55082100	1.17693100
H	-1.19556000	2.26005700	-1.16499300
H	-2.22624000	-1.25466000	1.15993400

I

E(SMD/ M06-2X /6-31G(d)) = -578.9737561 au

H(SMD/M06-2X/6-31G(d)) = -578.724834 au

G(SMD/M06-2X/6-31G(d)) = -578.778087 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -579.1808252 au

C	4.89921900	-0.78721900	0.00042300
C	3.58623500	-1.22770900	0.00044200
C	2.51951700	-0.30181400	0.00002800
C	2.80582400	1.08303000	-0.00047300
C	4.11888900	1.51516700	-0.00053300
C	5.16350700	0.58315900	-0.00008800
H	5.71564000	-1.50124700	0.00075500
H	3.36104900	-2.29064800	0.00082400
H	2.00305800	1.81286700	-0.00085200
H	4.34082000	2.57689500	-0.00091900
H	6.19147200	0.93225900	-0.00017500
C	1.19005000	-0.82509800	0.00000200
C	-0.00000400	-0.11339000	-0.00010000
C	-1.19005800	-0.82510500	-0.00004900
C	-2.51954600	-0.30184100	0.00012000
C	-2.80580900	1.08300800	0.00063700
C	-3.58625600	-1.22772400	-0.00035700
C	-4.11886400	1.51519000	0.00051800
H	-2.00300100	1.81279800	0.00119700
C	-4.89922200	-0.78720100	-0.00046600
H	-3.36108700	-2.29066900	-0.00065300
C	-5.16347900	0.58318700	-0.00007400
H	-4.34079200	2.57691600	0.00090700
H	-5.71567100	-1.50120000	-0.00085300
H	-6.19144800	0.93228100	-0.00023000
H	-0.00001900	0.97151100	-0.00009900
H	1.11539600	-1.91280100	0.00011400
H	-1.11543500	-1.91280400	-0.00018600

II

E(SMD/ M06-2X /6-31G(d)) = -2138.536235 au

H(SMD/M06-2X/6-31G(d)) = -2138.270746 au

G(SMD/M06-2X/6-31G(d)) = -2138.36283 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2139.471387 au

C	-0.20560700	-1.45390400	2.16547000
O	-0.65603400	-2.43564800	1.62295900
O	0.07110400	-0.28606500	1.67852000
C	0.18841900	-1.49830900	3.65393500
F	-0.22195800	-2.62334900	4.23520900
F	-0.32393700	-0.46612900	4.33308000
F	1.52498600	-1.43439200	3.77139200
B	-0.06018600	0.03856300	0.18258200
C	0.92508100	-0.95245100	-0.65633300
C	0.75704200	-1.16990100	-2.03140400
C	2.04419400	-1.52989800	-0.03799900
C	1.66608500	-1.93444900	-2.74405400
H	-0.09038600	-0.75578400	-2.57128800
C	2.93931200	-2.29376600	-0.76527900
H	2.23856500	-1.38999800	1.02236600
C	2.76596100	-2.50695100	-2.12495500
C	-1.63270500	-0.05007900	-0.25092000
C	-2.47724400	1.05779300	-0.08407800
C	-2.20672500	-1.23535800	-0.73636800
C	-3.82542200	0.97820700	-0.39112900
H	-2.09668900	2.00471100	0.28847600
C	-3.55449700	-1.29535000	-1.04414700
H	-1.61124400	-2.13380300	-0.86335500
C	-4.38126500	-0.19376400	-0.87869500
C	0.52266700	1.55576800	0.05261900
C	0.44324500	2.24418700	-1.16856300
C	1.15480800	2.19836900	1.12455100
C	0.97481000	3.51358200	-1.30031900
H	-0.04011300	1.80152800	-2.03615700
C	1.68274000	3.47097700	0.97226800
H	1.24119600	1.71656400	2.09314800
C	1.60233900	4.14523800	-0.23493700
F	4.01063700	-2.85219300	-0.17811200
F	3.63794700	-3.24943900	-2.82058000
F	1.50623800	-2.14946100	-4.06036600

F	-4.10926400	-2.42563400	-1.51306200
F	-5.68388100	-0.26177700	-1.18274300
F	-4.63662800	2.03755900	-0.23181300
F	0.89929600	4.18045700	-2.46392900
F	2.11227600	5.37694500	-0.37241200
F	2.28869100	4.09386100	1.99712200

III

E(SMD/ M06-2X /6-31G(d)) = -981.9765869 au

H(SMD/M06-2X/6-31G(d)) = -981.555644 au

G(SMD/M06-2X/6-31G(d)) = -981.627955 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.3291514 au

C	6.08276100	0.65895300	0.25993200
C	4.72579600	0.93256600	0.11382500
C	3.81789100	-0.07808500	-0.22745900
C	4.30680000	-1.38090700	-0.40587900
C	5.66103400	-1.65534900	-0.25929000
C	6.55547100	-0.63701200	0.07268300
H	6.76926500	1.45856500	0.52101800
H	4.35860500	1.94541800	0.25976300
H	3.62639000	-2.19087500	-0.65263500
H	6.02203300	-2.66986100	-0.39978100
H	7.61258900	-0.85596000	0.18786300
C	2.39440200	0.27807500	-0.37240500
C	1.43127700	-0.50782600	-0.86397600
C	-0.01865600	-0.12898900	-1.04891500
C	-0.46982500	1.15802600	-0.38578000
C	-0.27969600	1.38188900	0.98322600
C	-1.14920400	2.12159200	-1.13372500
C	-0.76313300	2.53872000	1.58837300
H	0.27217600	0.65847000	1.58046500
C	-1.63115100	3.28240000	-0.53216200
H	-1.30361100	1.95826600	-2.19767000
C	-1.44229200	3.49187900	0.83106400
H	-0.60135000	2.70022100	2.64991900
H	-2.15465700	4.02188400	-1.13033300
H	-1.81727600	4.39526800	1.30208700
H	1.67850200	-1.50825600	-1.21966700
H	2.14113600	1.28877500	-0.05598700
H	-0.20845500	-0.03662800	-2.12710900
C	-2.40517000	-1.08095400	-0.81533400

C	-3.03445900	-1.15865800	0.42424900
C	-4.38938300	-0.95574900	0.62244300
C	-5.13280000	-0.65006500	-0.51687700
C	-4.52656600	-0.55905000	-1.77334800
C	-3.15610200	-0.77152400	-1.93885200
C	-0.93543300	-1.32820600	-0.61652800
C	-0.87558800	-1.58757800	0.84988400
H	-4.84896300	-1.02762400	1.60238800
H	-6.19983400	-0.47846300	-0.42377200
H	-5.13505600	-0.31690200	-2.63855900
H	-2.69628700	-0.69628800	-2.91944800
H	-0.58369800	-2.22356100	-1.14842100
H	0.00572000	-1.82545400	1.43754400
N	-2.03836000	-1.47573800	1.40080400
C	-2.33776800	-1.59709600	2.82461900
H	-2.71959500	-0.63598800	3.17506400
H	-3.09451100	-2.37199500	2.95822100
H	-1.42382700	-1.86116600	3.35482500

IV

E(SMD/ M06-2X /6-31G(d)) = -2138.954116 au

H(SMD/M06-2X/6-31G(d)) = -2138.674906 au

G(SMD/M06-2X/6-31G(d)) = -2138.771202 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2139.884572 au

C	-0.75968500	-1.13150700	2.16574200
O	-1.58202600	-1.93753900	1.59316800
O	-0.07201000	-0.25000200	1.65083000
C	-0.61116300	-1.38383200	3.67567600
F	-1.78754400	-1.67388100	4.21154500
F	-0.09854900	-0.31564500	4.26085000
F	0.20872600	-2.41881900	3.84488000
B	0.04823300	0.10915900	0.04811200
C	1.01173200	-1.03391700	-0.56235400
C	1.29997000	-0.96794100	-1.93610500
C	1.60952100	-2.05375800	0.18633900
C	2.13826300	-1.89630000	-2.52424000
H	0.88075900	-0.18716700	-2.56573400
C	2.45093600	-2.97370000	-0.42336900
H	1.46941200	-2.15792300	1.25871700
C	2.72360700	-2.91217800	-1.77859100
C	-1.47298900	0.11583800	-0.51552700

C	-2.38305000	1.05539800	0.00119700
C	-1.93936900	-0.79787400	-1.47427700
C	-3.69486700	1.07411400	-0.43335200
H	-2.07448500	1.79416500	0.73627400
C	-3.26214700	-0.75873000	-1.89908300
H	-1.28552200	-1.54177900	-1.92054000
C	-4.15174600	0.16928300	-1.38546300
C	0.75252200	1.55590000	0.06072000
C	0.42800500	2.52286400	-0.89774200
C	1.77039700	1.84555400	0.98149600
C	1.10397300	3.73287200	-0.92879900
H	-0.35644300	2.35913200	-1.63133700
C	2.42313400	3.06402700	0.94098800
H	2.06769500	1.13191900	1.74429400
C	2.10257000	4.02099300	-0.01274700
F	3.02622600	-3.94861700	0.29098700
F	3.53156500	-3.80385300	-2.35640100
F	2.41332200	-1.84491000	-3.83256800
F	-3.71015200	-1.61953000	-2.81662000
F	-5.41837500	0.20036100	-1.79591400
F	-4.56844700	1.96326300	0.04614100
F	0.80128700	4.66513000	-1.84160000
F	2.73986700	5.19441600	-0.04180100
F	3.38841800	3.35968100	1.82119700
H	-1.68508800	-1.74479200	0.62646700

TFA

E(SMD/ M06-2X /6-31G(d)) = -526.6105371 au

H(SMD/M06-2X/6-31G(d)) = -526.564447 au

G(SMD/M06-2X/6-31G(d)) = -526.600194 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -526.8568165 au

C	-0.93463900	0.15668800	-0.00245600
O	-1.50640900	-1.03938000	-0.00115000
O	-1.48270500	1.22184800	-0.00090900
C	0.59421400	-0.00099300	-0.00063400
F	0.99067700	-0.70442400	-1.06303400
F	0.99000500	-0.64760400	1.09793500
F	1.17860500	1.18874800	-0.03136800
H	-2.47812100	-0.92440700	0.00321500

TS1

E(SMD/ M06-2X /6-31G(d)) = -2717.537557 au

H(SMD/M06-2X/6-31G(d)) = -2717.020517 au
G(SMD/M06-2X/6-31G(d)) = -2717.144114 au
E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2718.667579 au

C	-7.95082900	-2.66002100	-1.30020800
C	-6.60336300	-2.44011100	-1.02923200
C	-6.06978400	-1.14521100	-1.03563900
C	-6.92843800	-0.06888700	-1.30104300
C	-8.27393900	-0.28749000	-1.57124800
C	-8.79048300	-1.58370500	-1.57496300
H	-8.34430600	-3.67207300	-1.29422400
H	-5.94888300	-3.28116400	-0.81363200
H	-6.54625100	0.94761300	-1.27937300
H	-8.92567400	0.55759300	-1.77217700
H	-9.84289000	-1.75065400	-1.78336400
C	-4.63287800	-0.97189200	-0.75761100
C	-3.92482300	0.13673800	-0.98674000
C	-2.46710300	0.31216300	-0.68292400
C	-2.20550600	1.41911500	0.31869300
C	-2.70197300	1.28995500	1.61990000
C	-1.48111800	2.55345300	-0.04113700
C	-2.46733700	2.28977200	2.55599900
H	-3.26758700	0.40233100	1.89341200
C	-1.26343400	3.56587500	0.89569500
H	-1.07641600	2.64372700	-1.04714700
C	-1.75084900	3.43195300	2.19249800
H	-2.84096900	2.18094000	3.56915700
H	-0.69540200	4.44885200	0.61724500
H	-1.57061000	4.21414700	2.92356700
H	-4.37974500	1.02522600	-1.41984100
H	-4.12948700	-1.84604900	-0.34922200
O	-1.99414100	-0.94844800	-0.10861200
C	-0.71204200	-1.15813400	-0.08854000
O	0.12864500	-0.46586300	-0.62986600
C	-0.38351900	-2.41822000	0.73635000
F	-0.46034400	-2.13506000	2.03566300
F	-1.25656800	-3.38382800	0.46119400
F	0.83851100	-2.84680700	0.45452100
H	-1.89532000	0.49378500	-1.59946000
B	1.97855200	0.11863100	-0.09909300
C	2.91156600	-0.87792600	-0.91569400

C	4.29556300	-0.71925000	-0.73632400
C	2.46599900	-1.83596500	-1.83257400
C	5.18806200	-1.50458600	-1.44438600
H	4.69936000	0.01810900	-0.04707900
C	3.37900700	-2.60704600	-2.53435400
H	1.41143900	-2.00606600	-2.01839900
C	4.74425700	-2.45643500	-2.35142300
C	1.82802400	1.56975200	-0.73617300
C	1.97511900	2.73809500	0.01936400
C	1.55278100	1.69105800	-2.10854400
C	1.82015500	3.97901500	-0.57921900
H	2.19531400	2.71066200	1.08187800
C	1.39704900	2.93677800	-2.68413400
H	1.44955300	0.81461200	-2.74239400
C	1.52119500	4.09659900	-1.92639600
C	1.82830300	-0.07282700	1.47205200
C	2.58175200	-1.03568400	2.15748700
C	0.87951400	0.67228000	2.19482500
C	2.39560600	-1.23371400	3.51487300
H	3.31179700	-1.65536100	1.64599400
C	0.70459900	0.45267200	3.54914200
H	0.25762700	1.42311000	1.71302500
C	1.45683200	-0.49959900	4.22399400
F	1.91843700	5.10509700	0.14080000
F	1.36504600	5.29580000	-2.48933500
F	1.12467600	3.06985800	-3.98812700
F	6.50886000	-1.36653900	-1.27740800
F	5.61292200	-3.20838700	-3.03186500
F	2.96187300	-3.52681500	-3.41392100
F	-0.19397900	1.14890700	4.25592100
F	1.27929300	-0.70309900	5.52948400
F	3.10814900	-2.14906700	4.18208900

TS2

E(SMD/ M06-2X /6-31G(d)) = -2717.522813 au

H(SMD/M06-2X/6-31G(d)) = -2717.007117 au

G(SMD/M06-2X/6-31G(d)) = -2717.13123 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2718.655148 au

C	-7.87107800	-2.74512100	0.36101400
C	-6.56738200	-2.37804500	0.05278600
C	-6.12453500	-1.06244300	0.26866900

C	-7.02097500	-0.11731700	0.80033000
C	-8.32190400	-0.48661100	1.10511100
C	-8.74876900	-1.79915500	0.88681600
H	-8.20264600	-3.76448000	0.19234000
H	-5.87574100	-3.10908100	-0.35737700
H	-6.70065300	0.90521900	0.97380100
H	-9.00963500	0.24620800	1.51461700
H	-9.76887300	-2.08183000	1.12825600
C	-4.74992800	-0.74025700	-0.06617700
C	-4.12741900	0.46072300	0.07090200
C	-2.78067400	0.59092700	-0.36318800
C	-2.15230000	1.88115200	-0.59640500
C	-2.39209400	2.97427900	0.25544300
C	-1.31030900	2.03222900	-1.70830500
C	-1.79243600	4.19587700	-0.00521700
H	-3.01344900	2.84523600	1.13713100
C	-0.74945000	3.27524800	-1.99017600
H	-1.10851500	1.18066000	-2.35320700
C	-0.98151700	4.34939700	-1.13498300
H	-1.94964000	5.03217100	0.66794000
H	-0.10617600	3.39638100	-2.85624700
H	-0.51899500	5.31049600	-1.33791100
H	-4.63439700	1.33287100	0.47176900
H	-4.16420000	-1.56226200	-0.47902900
O	-1.84411000	0.10759100	1.43242200
C	-0.65350200	-0.21219700	1.38124900
O	-0.03425400	-0.48900700	0.30651600
C	0.03214100	-0.30054500	2.77095300
F	0.27999500	0.92147900	3.24439900
F	-0.80026300	-0.90926700	3.61805500
F	1.16826700	-0.98883300	2.74684700
H	-2.34100700	-0.25913500	-0.88218900
B	1.49662600	-0.37059500	-0.10497500
C	2.21311000	-1.80475500	0.10263600
C	3.54034100	-1.96838500	-0.32573400
C	1.54961400	-2.92570400	0.61491000
C	4.17168600	-3.19456500	-0.21773500
H	4.09947000	-1.14237700	-0.75870900
C	2.19527000	-4.14866600	0.70582800
H	0.51949000	-2.87323800	0.95416700

C	3.51025700	-4.30088000	0.29738100
C	1.35775900	-0.07085900	-1.70177700
C	1.85390500	1.07787900	-2.32437500
C	0.65659500	-0.99676300	-2.49378500
C	1.62310300	1.30254500	-3.67400500
H	2.39873000	1.83667300	-1.77040800
C	0.43999100	-0.75844800	-3.83770900
H	0.26669100	-1.91787100	-2.06746500
C	0.91014300	0.40052500	-4.44554500
C	2.11228200	0.87641800	0.73138000
C	3.28188300	0.80018800	1.49655100
C	1.41685400	2.09714900	0.71965800
C	3.72901300	1.90064800	2.21022600
H	3.85362000	-0.11998000	1.57121600
C	1.87457900	3.18397000	1.44200800
H	0.49884000	2.21744800	0.14955500
C	3.03672900	3.10211500	2.19509500
F	2.05223300	2.42986600	-4.26410000
F	0.68762100	0.62971000	-5.74377500
F	-0.23259500	-1.63365700	-4.59979900
F	5.44151200	-3.35592900	-0.61703300
F	4.12593000	-5.48483700	0.39127200
F	1.56095600	-5.22560500	1.19397000
F	1.20886500	4.34891500	1.43502100
F	3.47687300	4.15493400	2.89156200
F	4.84560300	1.83409800	2.94937600

TS3

E(SMD/ M06-2X /6-31G(d)) = -981.946285 au

H(SMD/M06-2X/6-31G(d)) = -981.527699 au

G(SMD/M06-2X/6-31G(d)) = -981.599414 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.2989694 au

E(SMD/B3LYP/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.7266612 au

E(SMD/B3LYP-D3/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.7826158 au

C	5.99993700	1.03936200	0.34468300
C	4.64270300	1.21577000	0.10651500
C	3.83467300	0.13089400	-0.27312500
C	4.41945100	-1.14263700	-0.39834600
C	5.77372400	-1.31605800	-0.15708700
C	6.56694700	-0.22664500	0.21221400
H	6.61437600	1.88579500	0.63396200

H	4.19365200	2.20011000	0.20998400
H	3.81261600	-1.99963700	-0.67458500
H	6.21699300	-2.30194500	-0.25382900
H	7.62684500	-0.36879300	0.39948100
C	2.42170000	0.37904300	-0.50537600
C	1.53009900	-0.49670200	-1.04514800
C	0.16703400	-0.17730400	-1.31711800
C	-0.60499700	0.90136600	-0.77337900
C	-0.37803300	1.43832300	0.51295200
C	-1.69817800	1.37568800	-1.53196000
C	-1.19196200	2.45220900	0.99649300
H	0.40731300	1.02519100	1.13936100
C	-2.50637100	2.38776300	-1.04415600
H	-1.88693900	0.94229700	-2.50977200
C	-2.25416900	2.92392400	0.22142100
H	-1.01680700	2.86443300	1.98505500
H	-3.34089800	2.75093800	-1.63452600
H	-2.89684900	3.70755300	0.61123800
H	1.87343400	-1.45978600	-1.41359300
H	2.08640500	1.38776100	-0.27340900
H	-0.26314400	-0.65540400	-2.19510000
C	-2.44460700	-1.57783300	-0.46166300
C	-2.67777000	-0.92338000	0.76944800
C	-3.84601200	-0.21278100	1.04079100
C	-4.79731100	-0.16005700	0.03023800
C	-4.58636400	-0.79472300	-1.20726900
C	-3.41988000	-1.50161500	-1.46566800
C	-1.12315600	-2.13836500	-0.38413700
C	-0.65364700	-1.85237300	0.89357900
H	-4.00460800	0.27931100	1.99568700
H	-5.72328500	0.38058800	0.19922000
H	-5.35493500	-0.73227300	-1.97132500
H	-3.26754200	-1.99082800	-2.42365600
H	-0.64768300	-2.80157800	-1.09351100
H	0.28955700	-2.11616300	1.35461600
N	-1.55954100	-1.11693300	1.57289800
C	-1.43846300	-0.65241100	2.94291000
H	-1.63477500	0.42169600	2.98893400
H	-2.15384200	-1.17763100	3.58154300
H	-0.42518300	-0.85186500	3.29307000

TS3’

E(SMD/ M06-2X /6-31G(d)) = -981.9344145 au

H(SMD/M06-2X/6-31G(d)) = -981.515841 au

G(SMD/M06-2X/6-31G(d)) = -981.588169 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.2865278 au

C	6.20270800	0.06546800	-0.15640000
C	4.89081500	0.51483800	-0.25425100
C	3.81558500	-0.38110200	-0.15317100
C	4.08671100	-1.74315800	0.06047700
C	5.39652800	-2.18987400	0.15991700
C	6.45761200	-1.28839200	0.04955000
H	7.02411300	0.77013000	-0.23863300
H	4.68575400	1.57047600	-0.41255000
H	3.27207800	-2.45407200	0.15976700
H	5.59543800	-3.24368400	0.32775000
H	7.48041600	-1.64362500	0.12870700
C	2.46170600	0.15588600	-0.26268900
C	1.32290300	-0.56867200	-0.34640600
C	-0.00119900	-0.00340600	-0.51906800
C	-0.29497600	1.43031300	-0.44018100
C	0.27315800	2.27401200	0.53036400
C	-1.21952100	1.96069700	-1.35351000
C	-0.04925900	3.62345000	0.55547400
H	0.94424600	1.86390500	1.28049600
C	-1.53301900	3.31615800	-1.33084400
H	-1.67723400	1.30425500	-2.08888100
C	-0.94701200	4.14741300	-0.37826300
H	0.38960000	4.26983400	1.30866800
H	-2.23726200	3.72066600	-2.05066600
H	-1.19601600	5.20378700	-0.35394900
H	1.37646700	-1.65333600	-0.37701000
H	2.40499500	1.23986800	-0.32949500
H	-0.63303000	-0.52934600	-1.23210800
C	-2.53524000	-2.02028200	0.13289500
C	-3.17897200	-0.79586000	0.48059200
C	-4.50961600	-0.52782400	0.11616100
C	-5.17164500	-1.51235500	-0.58623000
C	-4.55126700	-2.74128000	-0.94137800
C	-3.24773100	-3.00284100	-0.59744200
C	-1.22552000	-1.94070400	0.63657000

C	-1.07402700	-0.65962800	1.21140200
H	-4.99141100	0.40880200	0.37611000
H	-6.20272100	-1.34562000	-0.88245900
H	-5.12459600	-3.47692300	-1.49533900
H	-2.76796100	-3.93815900	-0.86792200
H	-0.44385300	-2.68532900	0.56125200
H	-0.32344500	-0.33019100	1.91923600
N	-2.29941900	-0.02010900	1.17498500
C	-2.60729400	1.27182300	1.76506700
H	-2.69403300	2.04408300	0.99409500
H	-3.54577700	1.19769400	2.31964600
H	-1.80841600	1.53946400	2.45657200

TS4

E(SMD/ M06-2X /6-31G(d)) = -3120.521855 au
H(SMD/M06-2X/6-31G(d)) = -3119.837982 au
G(SMD/M06-2X/6-31G(d)) = -3119.981429 au
E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -3121.798433 au

C	7.29050500	4.47754600	0.42298000
C	6.84876400	3.15850300	0.47482000
C	5.48325200	2.85186700	0.41607400
C	4.56821600	3.90674300	0.28260200
C	5.00828300	5.22401400	0.23117300
C	6.37071900	5.51615000	0.30356000
H	8.35360400	4.69300600	0.47511300
H	7.56829200	2.34884200	0.56927500
H	3.50567000	3.69565200	0.20561400
H	4.28541800	6.02783300	0.12694700
H	6.71099700	6.54628800	0.26060300
C	5.07002700	1.43813900	0.49070400
C	3.82981000	0.99767300	0.72203900
C	3.40386200	-0.45463300	0.77446100
C	4.57515300	-1.41921300	0.89197600
C	5.15663000	-2.02755200	-0.22119000
C	5.11647400	-1.67082200	2.15617200
C	6.25834000	-2.86944100	-0.07480200
H	4.74456500	-1.85220800	-1.21239000
C	6.21435800	-2.51242800	2.30648700
H	4.67072000	-1.19800400	3.02856700
C	6.78978800	-3.11481100	1.18852900
H	6.69736100	-3.33794300	-0.95070400

H	6.61852200	-2.70085700	3.29671700
H	7.64399500	-3.77528000	1.30276600
H	3.02341100	1.70938900	0.89040900
H	5.87342700	0.71293000	0.36555000
H	2.79770100	-0.57428300	1.68456900
C	1.78856000	-2.05593400	-0.55548100
C	1.46740500	-2.18808900	-1.91738700
C	0.72966400	-3.26015100	-2.42120400
C	0.31493400	-4.21674800	-1.50518600
C	0.62276300	-4.10214900	-0.13711900
C	1.35509800	-3.02869300	0.35131900
C	2.49345300	-0.78380300	-0.40088400
C	2.63629000	-0.29752200	-1.71609400
H	0.47707900	-3.33580300	-3.47485700
H	-0.26952700	-5.06301100	-1.85074800
H	0.27190900	-4.86418100	0.55177400
H	1.57804300	-2.94334500	1.41103100
H	1.29688500	-0.00790700	-0.09764400
H	3.14307600	0.59954600	-2.05236300
N	2.00193700	-1.08803700	-2.59113000
C	1.90138500	-0.87925600	-4.02821700
H	2.48082100	-1.64566800	-4.54900500
H	0.85986300	-0.93694800	-4.34745900
H	2.29780200	0.10757600	-4.26782200
C	-0.38018300	1.34532500	0.26752700
O	0.20748800	0.24135700	0.32565700
O	-1.60915100	1.52195500	0.41522200
C	0.42652400	2.62781400	-0.01189000
F	1.37245900	2.36755600	-0.92049100
F	1.02338400	3.05035500	1.10293500
F	-0.35661000	3.58996600	-0.47406300
B	-2.68691000	0.33411700	0.32836000
C	-2.36318000	-0.40765300	-1.08388900
C	-2.61327100	-1.77087800	-1.28746000
C	-1.86889500	0.33571400	-2.16855100
C	-2.34173100	-2.36349700	-2.51045500
H	-2.99556400	-2.40510200	-0.49311200
C	-1.60413800	-0.27482300	-3.37942000
H	-1.68392600	1.40539600	-2.09644500
C	-1.82660100	-1.63019800	-3.56618400

C	-2.53219500	-0.57816200	1.66056200
C	-3.26712400	-0.28267300	2.81777700
C	-1.62849600	-1.65036800	1.71818900
C	-3.09963800	-1.03003600	3.97224200
H	-3.98426200	0.53276600	2.84046500
C	-1.47703000	-2.38799300	2.87806000
H	-1.02243200	-1.92260600	0.86049000
C	-2.20741600	-2.09060300	4.01946000
C	-4.09487300	1.12250300	0.22794800
C	-5.28938200	0.38605500	0.25305500
C	-4.17883000	2.50924900	0.05348800
C	-6.50982300	1.02028700	0.11127500
H	-5.28595100	-0.69279800	0.38697600
C	-5.41303900	3.12532500	-0.08629200
H	-3.29149900	3.13351000	0.02233700
C	-6.59003300	2.39597700	-0.06024600
F	-1.09637100	0.42309800	-4.40925200
F	-1.49869400	-2.22153300	-4.72312600
F	-2.52537000	-3.67752700	-2.69614400
F	-0.61134800	-3.41470700	2.93514400
F	-2.05588000	-2.80877200	5.13622700
F	-3.79841800	-0.75134500	5.08236800
F	-7.65685700	0.32663200	0.13608900
F	-7.77587800	3.00011000	-0.19454900
F	-5.50241600	4.45370400	-0.25077400

1a·B($C_6F_3H_2$)$_3$_(al)

E(SMD/ M06-2X /6-31G(d)) = -2267.317761 au

H(SMD/M06-2X/6-31G(d)) = -2266.820045 au

G(SMD/M06-2X/6-31G(d)) = -2266.933423 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2268.255705 au

C	-6.87105500	-0.82289800	-0.91166000
C	-5.51087600	-0.55338200	-0.79166400
C	-4.63117800	-1.50967700	-0.26919400
C	-5.14651300	-2.75621200	0.11373000
C	-6.50440100	-3.02596200	-0.00663700
C	-7.37266200	-2.06038700	-0.51707600
H	-7.53751100	-0.06643800	-1.31482600
H	-5.12112100	0.41397300	-1.09951000
H	-4.48186800	-3.52603600	0.49496100
H	-6.88723000	-3.99703900	0.29269600

H	-8.43255000	-2.27593500	-0.61171300
C	-3.20417700	-1.16206900	-0.14700200
C	-2.29092600	-1.83913300	0.55466400
C	-0.83289900	-1.48885700	0.66393000
C	0.05548400	-2.68279900	0.37013500
C	0.25040000	-3.14352900	-0.93248300
C	0.66152000	-3.34901000	1.43510900
C	1.08241900	-4.23486800	-1.16812000
H	-0.23868300	-2.65577600	-1.77443200
C	1.47758700	-4.45333400	1.20180500
H	0.51050300	-2.98722600	2.44954300
C	1.69890600	-4.88996600	-0.10222800
H	1.24791600	-4.57541500	-2.18579900
H	1.95458000	-4.95845200	2.03592200
H	2.34963400	-5.73835700	-0.29039800
H	-2.55872200	-2.73177300	1.11618300
H	-2.90910800	-0.25518800	-0.67256900
O	-0.55329100	-0.34052600	-0.19309300
H	-0.60772500	-1.12143700	1.66949700
B	0.73834900	0.68585800	-0.02815600
C	0.39628400	1.85443600	-1.09240800
C	1.43515700	2.60119300	-1.66722100
C	-0.92230400	2.23405800	-1.38244300
C	1.15670800	3.66923800	-2.50292900
H	2.47773900	2.36466800	-1.47418800
C	-1.18008000	3.29975900	-2.22863400
H	-1.77601500	1.72796700	-0.94075900
C	-0.14961700	4.02907000	-2.80113800
C	0.62470800	1.26166200	1.47194100
C	1.76539700	1.74540700	2.12677000
C	-0.61844400	1.43049900	2.10132600
C	1.65908000	2.35975100	3.36391200
H	2.75384900	1.65872000	1.68430200
C	-0.70199800	2.03886900	3.34180600
H	-1.54500700	1.09670000	1.63926700
C	0.43083600	2.51010000	3.98940700
C	2.02534500	-0.21978600	-0.38696300
C	2.37023200	-0.45860200	-1.72678300
C	2.69545800	-0.95480500	0.60001800
C	3.32700400	-1.40392100	-2.05388900

H	1.88692900	0.07261800	-2.54191500
C	3.63631400	-1.90935800	0.25435700
H	2.46221300	-0.83541700	1.65414800
C	3.96393400	-2.14761700	-1.07205900
F	2.74453000	2.82304900	3.99669400
F	0.33958400	3.09466200	5.18705300
F	-1.88330800	2.19366400	3.95399800
F	2.14381700	4.38438300	-3.05717600
F	-0.40803700	5.05468200	-3.61681600
F	-2.43865500	3.65986300	-2.51449000
F	4.23826000	-2.65280200	1.19175700
F	4.85983300	-3.08289600	-1.39552900
F	3.64960600	-1.64622700	-3.33220300
H	-0.67776000	-0.57785300	-1.13475200

1a_(al)

E(SMD/ M06-2X /6-31G(d)) = -654.9603465 au

H(SMD/M06-2X/6-31G(d)) = -654.69513 au

G(SMD/M06-2X/6-31G(d)) = -654.752487 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -655.2136466 au

C	4.75489000	0.26438100	0.60727900
C	3.50513400	0.87396900	0.54005000
C	2.40309200	0.20646300	-0.01039900
C	2.58667600	-1.10358900	-0.47766200
C	3.83383400	-1.71344800	-0.41162600
C	4.92495300	-1.03226400	0.12907000
H	5.59529400	0.80279200	1.03553100
H	3.37561000	1.88653700	0.91439100
H	1.74405100	-1.65625900	-0.88338200
H	3.95456200	-2.72926800	-0.77671200
H	5.89714900	-1.51283300	0.18243500
C	1.10600900	0.90456200	-0.06869600
C	0.03750300	0.51585900	-0.76860800
C	-1.27651100	1.24990200	-0.78192100
C	-2.38235700	0.33593300	-0.27152600
C	-2.51481100	0.11577000	1.10194300
C	-3.24731400	-0.30750900	-1.15519400
C	-3.50538200	-0.73386100	1.58351400
H	-1.83603800	0.61967200	1.78512000
C	-4.23606400	-1.16549300	-0.67452800
H	-3.15014400	-0.13247500	-2.22440800

C	-4.36755000	-1.37827700	0.69525700
H	-3.60487500	-0.89795400	2.65257100
H	-4.90741900	-1.66042700	-1.37013100
H	-5.14001700	-2.04226000	1.07165100
H	0.05488700	-0.38599300	-1.37828900
H	1.03950000	1.82850300	0.50191300
O	-1.15251400	2.41612100	0.00714500
H	-1.51130600	1.51499100	-1.82598000
H	-2.02376300	2.84159800	0.03640500

H_2O

E(SMD/ M06-2X /6-31G(d)) = -76.38034807 au

H(SMD/M06-2X/6-31G(d)) = -76.355217 au

G(SMD/M06-2X/6-31G(d)) = -76.376661 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -76.43310411 au

O	0.00000000	0.00000000	0.11955600
H	0.00000000	-0.76140300	-0.47822400
H	0.00000000	0.76140300	-0.47822400

II_(al)

E(SMD/ M06-2X /6-31G(d)) = -1688.28613 au

H(SMD/M06-2X/6-31G(d)) = -1688.041308 au

G(SMD/M06-2X/6-31G(d)) = -1688.124258 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -1689.027399 au

O	0.01967700	0.07942400	-2.48195500
B	-0.04660400	-0.00062000	-1.00851200
C	0.87776300	-1.24655100	-0.45094000
C	0.83068500	-1.71221700	0.87379400
C	1.80753800	-1.84454600	-1.31243600
C	1.67612400	-2.72026600	1.30223400
H	0.12587400	-1.30184300	1.59338500
C	2.64610900	-2.85334400	-0.86798900
H	1.88286300	-1.51315300	-2.34422500
C	2.59435000	-3.30527100	0.44108900
C	0.60518800	1.38686500	-0.43444000
C	0.48712400	1.77948400	0.90828800
C	1.35472300	2.20920600	-1.28678300
C	1.09496800	2.93517400	1.36549200
H	-0.09236400	1.19583200	1.61966000
C	1.95686100	3.36253900	-0.81187900
H	1.46741100	1.95027000	-2.33497400
C	1.83836000	3.74218500	0.51596800

C	-1.61509000	-0.16558100	-0.52429000
C	-2.20248400	-1.42226500	-0.31144800
C	-2.45728700	0.95627300	-0.44459800
C	-3.55464300	-1.54304800	-0.03286600
H	-1.61245600	-2.33403400	-0.35758800
C	-3.80507500	0.81996200	-0.16373100
H	-2.06847600	1.95888600	-0.60354300
C	-4.37345000	-0.42839200	0.04728000
F	0.98020700	3.32021000	2.64936800
F	2.42001800	4.86350000	0.96904600
F	2.67582100	4.15703300	-1.62599300
F	1.63304400	-3.17328200	2.56799100
F	3.40692600	-4.28493900	0.86559100
F	3.53960100	-3.43009900	-1.69226700
F	-4.61210100	1.89251100	-0.08350400
F	-5.67982300	-0.55174500	0.32331800
F	-4.11670000	-2.74781800	0.17110000
H	-0.42077900	-0.69783300	-2.85284100

III_(al)

E(SMD/ M06-2X /6-31G(d)) = -2670.301229 au

H(SMD/M06-2X/6-31G(d)) = -2669.634594 au

G(SMD/M06-2X/6-31G(d)) = -2669.765655 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2671.386557 au

C	-1.83266000	6.35366100	0.12254100
C	-2.51695100	5.16390400	-0.10826500
C	-1.94710200	4.14459700	-0.88079600
C	-0.68450400	4.36379800	-1.45083100
C	-0.00004800	5.55164600	-1.22037700
C	-0.56784800	6.54871400	-0.42711000
H	-2.28691600	7.12797400	0.73370300
H	-3.50140600	5.01088000	0.32762700
H	-0.23840700	3.60377200	-2.08690800
H	0.97835600	5.70302300	-1.66669900
H	-0.03062300	7.47507000	-0.24775400
C	-2.67686500	2.87236700	-1.03348000
C	-2.10909500	1.71278600	-1.37786600
C	-2.79124800	0.37359700	-1.52467600
C	-4.26112900	0.31295100	-1.16084300
C	-4.71323900	0.64035500	0.12314000
C	-5.19448900	-0.11487200	-2.10687900

C	-6.06236800	0.53949100	0.45086500
H	-4.01085900	1.00212400	0.87149700
C	-6.54638200	-0.21635600	-1.78338400
H	-4.85878100	-0.37220200	-3.10854600
C	-6.98362200	0.10874500	-0.50265800
H	-6.39490100	0.80271300	1.45056700
H	-7.25606400	-0.55135200	-2.53381200
H	-8.03609300	0.03056400	-0.24773200
H	-1.03665000	1.66727100	-1.57317300
H	-3.74144500	2.90949900	-0.80658100
H	-2.69331500	0.07083600	-2.57663700
C	-2.35600600	-2.11980600	-0.85660900
C	-2.42906300	-2.65256200	0.42905700
C	-2.71386100	-3.98003700	0.70351400
C	-2.95036100	-4.79653000	-0.40150000
C	-2.89748600	-4.28638600	-1.70225600
C	-2.59733200	-2.94521500	-1.94609000
C	-1.95302200	-0.67837900	-0.74466500
C	-1.90285400	-0.49478200	0.72586300
H	-2.75040700	-4.36655000	1.71674100
H	-3.17721000	-5.84607800	-0.24692900
H	-3.08634700	-4.95056300	-2.53943100
H	-2.54694900	-2.56268100	-2.96126000
H	-0.89758200	-0.54221000	-1.08243600
H	-1.67352100	0.41905000	1.26630300
N	-2.14812200	-1.60156600	1.35330600
C	-2.12519600	-1.80015600	2.79849800
H	-3.06066300	-2.27816500	3.09494300
H	-1.27901200	-2.44225400	3.05346200
H	-2.02526100	-0.83261300	3.28797500
O	0.91021100	0.08894600	-1.60117300
B	1.80783400	-0.25177900	-0.46265700
C	1.12425500	0.43770200	0.86143900
C	0.93796200	-0.20967900	2.09098800
C	0.70688200	1.77763600	0.76369800
C	0.35930300	0.45656200	3.16260000
H	1.23362600	-1.24527500	2.23816700
C	0.12472500	2.42588300	1.83883000
H	0.84306300	2.33477800	-0.15943100
C	-0.06790000	1.77021200	3.05208600

C	1.92569300	-1.88442200	-0.29166600
C	2.85232300	-2.49625800	0.57007800
C	1.05756400	-2.72977000	-0.99709600
C	2.88417600	-3.87120100	0.72272500
H	3.57447000	-1.91179200	1.13406700
C	1.10290000	-4.10620100	-0.83624100
H	0.33204300	-2.32969100	-1.69868100
C	2.01030300	-4.69659100	0.02751600
C	3.30036500	0.40504900	-0.67248700
C	4.18025500	0.62031900	0.40049000
C	3.74554400	0.76956200	-1.95030500
C	5.44398300	1.14519500	0.19194800
H	3.88789700	0.40080900	1.42466300
C	5.01228100	1.29585300	-2.14276800
H	3.10859000	0.66439900	-2.82408000
C	5.88027300	1.48780300	-1.07957600
F	-0.26540700	3.70439600	1.75778600
F	-0.63220400	2.39915300	4.08956000
F	0.15460200	-0.17062400	4.33487200
F	0.26698400	-4.90879100	-1.51561400
F	2.05179500	-6.02623700	0.18280200
F	3.76524300	-4.45527900	1.55045100
F	6.28535600	1.35281100	1.21795100
F	7.10168800	2.00328600	-1.27142400
F	5.43684800	1.64457400	-3.36878100
H	1.24730500	-0.31774500	-2.41325800

III_(al)'

E(SMD/ M06-2X /6-31G(d)) = -2670.316109 au

H(SMD/M06-2X/6-31G(d)) = -2669.647829 au

G(SMD/M06-2X/6-31G(d)) = -2669.783655 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2671.400647 au

C	-7.79699300	2.22535500	0.22900400
C	-6.87916700	1.37936700	-0.38722600
C	-5.58395000	1.22284900	0.12310300
C	-5.23672800	1.92827700	1.28484000
C	-6.15247600	2.77321300	1.90081100
C	-7.43588600	2.92782300	1.37571800
H	-8.79458400	2.33364400	-0.18639100
H	-7.16334300	0.83143900	-1.28230800
H	-4.24785500	1.80964900	1.71736000

H	-5.86547300	3.31021500	2.80021300
H	-8.14904800	3.58698000	1.86143300
C	-4.65316300	0.31899100	-0.57818400
C	-3.33708600	0.22577400	-0.36814200
C	-2.38963100	-0.70909800	-1.09209800
C	-3.07199100	-1.53075800	-2.17514600
C	-3.73561500	-2.72172200	-1.86891100
C	-3.07572600	-1.07726100	-3.49576400
C	-4.38671700	-3.44526700	-2.86457700
H	-3.73671500	-3.08226000	-0.84317100
C	-3.72413200	-1.80030200	-4.49547500
H	-2.56702900	-0.14727900	-3.74099400
C	-4.38129200	-2.98758100	-4.18156800
H	-4.89678100	-4.37035900	-2.61224200
H	-3.71373500	-1.43614700	-5.51862100
H	-4.88487600	-3.55478300	-4.95864100
H	-2.85815000	0.86316600	0.37607200
H	-5.11117700	-0.30696200	-1.34285700
H	-1.65312600	-0.06661300	-1.60345100
C	-0.63075700	-2.55907200	-0.41689900
C	-0.22925300	-3.14359900	0.81344700
C	0.72952800	-4.16316000	0.87917000
C	1.29507400	-4.58448400	-0.31307600
C	0.92010300	-4.01133700	-1.54710600
C	-0.03615700	-3.01110300	-1.61281000
C	-1.64240000	-1.57690300	-0.10426800
C	-1.80168000	-1.62767000	1.25933800
H	1.01457600	-4.60737500	1.82815000
H	2.04647400	-5.36722000	-0.29829200
H	1.38159100	-4.37375200	-2.46047200
H	-0.34337300	-2.59620700	-2.57032700
H	0.42944000	-0.68263500	-0.71069000
H	-2.47540600	-1.06666200	1.89550100
N	-0.95531900	-2.55314900	1.81623400
C	-0.88536100	-2.91000300	3.22010900
H	-1.33887600	-3.89092600	3.39268500
H	0.15584300	-2.93048200	3.55002400
H	-1.42215400	-2.15843200	3.80253400
O	1.01569300	-0.04831600	-1.18715000
B	2.03553900	0.70474000	-0.12941600

C	1.17333000	0.66783800	1.23808400
C	1.54377300	-0.09418600	2.35272500
C	-0.02493600	1.39961300	1.30116800
C	0.73928800	-0.12143100	3.48098300
H	2.46180000	-0.67391100	2.36628100
C	-0.82072600	1.34192400	2.42933900
H	-0.35237100	2.02021200	0.47017200
C	-0.45666700	0.57636200	3.52847200
C	3.37194900	-0.20125800	-0.13099000
C	4.65241700	0.35846000	-0.21748800
C	3.26582500	-1.59922900	-0.03749300
C	5.77547300	-0.45284900	-0.20202700
H	4.79919200	1.43099100	-0.30338700
C	4.39965100	-2.39326500	-0.02951700
H	2.30139000	-2.09658900	0.04629000
C	5.66635300	-1.83228800	-0.11229500
C	2.23301000	2.19132600	-0.71164600
C	2.71480400	3.19676500	0.14062600
C	1.98368800	2.52368800	-2.04857700
C	2.94369700	4.47477300	-0.33859100
H	2.91336900	3.00020600	1.19111400
C	2.21107100	3.81173400	-2.50691200
H	1.60023200	1.79849800	-2.75979100
C	2.69407100	4.80049600	-1.66447100
F	-1.99149800	1.99747100	2.48576300
F	-1.25288700	0.49401100	4.59849600
F	1.07926800	-0.85288900	4.55236700
F	4.31180400	-3.72709700	0.06045100
F	6.75554100	-2.60504200	-0.10655400
F	7.00462800	0.07205900	-0.28515800
F	3.40475800	5.44116500	0.46627900
F	2.90858800	6.03980000	-2.11580000
F	1.96788000	4.13929700	-3.78351000
H	1.49370100	-0.57535300	-1.86064400

IV_(al)

E(SMD/ M06-2X /6-31G(d)) = -1688.738139 au

H(SMD/M06-2X/6-31G(d)) = -1688.479598 au

G(SMD/M06-2X/6-31G(d)) = -1688.562628 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -1689.473372 au

O	0.00181800	0.00370900	-2.42031500

B	-0.06217500	-0.00297500	-0.76654200
C	0.78540400	-1.31043100	-0.35767000
C	0.63258900	-1.85890300	0.92453900
C	1.74850700	-1.87358400	-1.20577100
C	1.41049600	-2.92979900	1.32791000
H	-0.09448300	-1.46294700	1.62842100
C	2.51138800	-2.95117000	-0.78489000
H	1.93623900	-1.48385200	-2.20200200
C	2.35489100	-3.49298000	0.48089300
C	0.70431100	1.35325500	-0.35482900
C	0.46214600	1.94065400	0.89548500
C	1.69189100	1.92191700	-1.17143500
C	1.18005300	3.05281200	1.30005400
H	-0.28900200	1.54455300	1.57326400
C	2.39200800	3.04097500	-0.75138200
H	1.94631700	1.50336800	-2.14103300
C	2.14840800	3.62021100	0.48424800
C	-1.64192000	-0.04966400	-0.42296700
C	-2.32022500	-1.26985300	-0.27796400
C	-2.40029000	1.13091200	-0.37256800
C	-3.69061200	-1.29705500	-0.07927300
H	-1.79398500	-2.21950200	-0.30864300
C	-3.76971400	1.08385400	-0.17395200
H	-1.93728200	2.10822100	-0.47627500
C	-4.43170000	-0.12598000	-0.02369500
F	0.95468400	3.62133900	2.49129200
F	2.82930600	4.69895600	0.88034700
F	3.33036500	3.59577800	-1.53007700
F	1.27047300	-3.46148400	2.54881100
F	3.09445000	-4.53245900	0.87684200
F	3.42765500	-3.50009300	-1.59363100
F	-4.49773700	2.20632200	-0.12158400
F	-5.75114200	-0.16207500	0.17095900
F	-4.34334600	-2.45737600	0.06313600
H	-0.44916500	-0.78353700	-2.79041900
H	-0.46047200	0.78770200	-2.78333500

TS2_(al)

E(SMD/ M06-2X /6-31G(d)) = -981.946285 au

H(SMD/M06-2X/6-31G(d)) = -981.527699 au

G(SMD/M06-2X/6-31G(d)) = -981.599414 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -982.2989694 au

C	5.45628900	-1.36774800	-0.17288700
C	4.60067900	-0.38167700	-0.64051200
C	3.66222400	0.21916400	0.21918600
C	3.59696800	-0.19789500	1.56183000
C	4.45023100	-1.18989000	2.02407900
C	5.37704600	-1.77575400	1.15940900
H	6.16974600	-1.83272800	-0.84522300
H	4.63189300	-0.07764300	-1.68343900
H	2.86450100	0.23363800	2.23765600
H	4.38397400	-1.52163500	3.05518600
H	6.03127300	-2.56208400	1.52335800
C	2.73814600	1.17688400	-0.34886800
C	1.78481600	1.88126600	0.33441500
C	0.78566700	2.64512200	-0.30083600
C	0.89120800	3.37987900	-1.54465600
C	2.12693500	3.70411800	-2.13299600
C	-0.29398200	3.85950600	-2.13589100
C	2.16707600	4.43666200	-3.31267500
H	3.05225200	3.43216200	-1.63729400
C	-0.25013800	4.57959400	-3.31767500
H	-1.24710900	3.65069300	-1.65692400
C	0.98276200	4.86128100	-3.91209900
H	3.12390900	4.69152300	-3.75619400
H	-1.16895100	4.93209300	-3.77434000
H	1.01879500	5.43460100	-4.83330900
H	1.65939700	1.72547100	1.40036100
H	2.77435300	1.26636700	-1.43323500
O	-0.60691700	0.97913000	-1.08915800
H	-0.08153100	2.88226100	0.31077400
B	-0.97958400	-0.10086700	-0.10633100
C	-2.29835200	-0.89978700	-0.66477600
C	-3.12863300	-1.64744500	0.18431600
C	-2.59093600	-0.90994000	-2.03581300
C	-4.19549200	-2.36725400	-0.32398600
H	-2.96015200	-1.67475300	1.25799600
C	-3.66675200	-1.63194900	-2.52658800
H	-1.97674400	-0.35920900	-2.74328900
C	-4.48202100	-2.36883700	-1.68229200
C	0.26082700	-1.16199100	-0.09646400

C	0.53411800	-2.03935800	0.96319100
C	1.06283500	-1.26614400	-1.24476400
C	1.59329200	-2.93162200	0.89005500
H	-0.06387600	-2.04235900	1.87045100
C	2.10260400	-2.17573500	-1.30604200
H	0.89049000	-0.61368000	-2.09567200
C	2.39490300	-3.01010200	-0.23795800
C	-1.31629600	0.60189400	1.34594500
C	-2.50341900	1.34814400	1.46213500
C	-0.45065000	0.61494000	2.44898900
C	-2.79305100	2.06560500	2.60935300
H	-3.23203600	1.37199500	0.65479100
C	-0.75534000	1.33508400	3.59471100
H	0.48583300	0.06417400	2.44023200
C	-1.92482500	2.07046700	3.69286200
F	1.89042200	-3.73513600	1.92343300
F	3.43388300	-3.85371500	-0.28685400
F	2.90139700	-2.24194500	-2.38560800
F	-4.99652700	-3.08130700	0.48257600
F	-5.52237700	-3.06163800	-2.16288400
F	-3.95458700	-1.63879500	-3.83848800
F	0.08401300	1.34492300	4.64289700
F	-2.21214100	2.76410300	4.80003900
F	-3.92403600	2.78005400	2.71318500
H	-1.41561500	1.44263000	-1.35780400

TS4_(al)

E(SMD/ M06-2X /6-31G(d)) = -2670.295984 au

H(SMD/M06-2X/6-31G(d)) = -2669.633613 au

G(SMD/M06-2X/6-31G(d)) = -2669.763916 au

E(SMD/M06-2X/def2-TZVP//SMD/M06-2X /6-31G(d)) = -2671.380302 au

C	-4.21384700	4.70102700	1.33295400
C	-4.30791700	3.39314300	0.86662600
C	-3.42385600	2.91118400	-0.10635600
C	-2.46176800	3.78810400	-0.62849200
C	-2.36788900	5.09495100	-0.16399600
C	-3.23918600	5.55532100	0.82296200
H	-4.90275300	5.05313600	2.09513900
H	-5.06796900	2.72713200	1.26812900
H	-1.79213500	3.44970600	-1.41482300
H	-1.61667200	5.76022000	-0.57944000

H	-3.16414200	6.57662800	1.18387100
C	-3.52334700	1.50220200	-0.52865800
C	-2.53884200	0.80831900	-1.10740500
C	-2.59491700	-0.65223600	-1.50125300
C	-4.00404700	-1.21993800	-1.55631700
C	-4.51783000	-2.08074600	-0.58707800
C	-4.83228600	-0.83624300	-2.61798900
C	-5.83076200	-2.54667100	-0.67194400
H	-3.89556200	-2.40737600	0.24245800
C	-6.14025300	-1.29829500	-2.70664400
H	-4.44232300	-0.16092300	-3.37644900
C	-6.64520200	-2.15723000	-1.72985900
H	-6.21194200	-3.21892900	0.09100600
H	-6.76651900	-0.99010700	-3.53859300
H	-7.66574200	-2.52167000	-1.79726800
H	-1.57173100	1.27545700	-1.28920000
H	-4.47154000	1.00931400	-0.31418800
H	-2.17688100	-0.72001800	-2.51624300
C	-1.27075600	-2.85053100	-0.85952500
C	-0.98751700	-3.43605300	0.38185600
C	-0.47473800	-4.72137000	0.52468600
C	-0.27071800	-5.43893200	-0.64762400
C	-0.56994800	-4.88466200	-1.90227500
C	-1.06441100	-3.59042300	-2.02438500
C	-1.63764900	-1.44329100	-0.60585000
C	-1.68206500	-1.36090400	0.82550500
H	-0.23607000	-5.13888300	1.49771500
H	0.13251900	-6.44469700	-0.59218200
H	-0.40433700	-5.47914500	-2.79511400
H	-1.28386900	-3.16710900	-3.00030600
H	-0.52737300	-0.83788400	-0.82336400
H	-1.94547000	-0.50394600	1.43862000
N	-1.27180400	-2.48706000	1.38021900
C	-1.09061600	-2.74115800	2.80237100
H	-1.61880200	-3.66091000	3.06303100
H	-0.02688800	-2.84792600	3.02757600
H	-1.50667900	-1.90696400	3.36584200
O	0.56454100	-0.13574000	-1.32299400
B	1.67015800	0.26324500	-0.34383300
C	0.90383000	0.60809800	1.06001000

C	1.04376800	-0.17392600	2.21345500
C	0.03977800	1.71590200	1.12414500
C	0.34209800	0.13666100	3.36887000
H	1.70319900	-1.03762900	2.23476100
C	-0.65446100	2.01193400	2.28489400
H	-0.08815400	2.38023000	0.27291000
C	-0.52100000	1.21921600	3.41984300
C	2.70903300	-0.98825300	-0.17146100
C	4.00606000	-0.80854000	0.33445400
C	2.31198400	-2.29967600	-0.47417200
C	4.84936100	-1.88837800	0.52788600
H	4.38698800	0.17853200	0.58061600
C	3.17180100	-3.36978000	-0.28013500
H	1.32523100	-2.52293400	-0.87193500
C	4.44793100	-3.18223800	0.22463900
C	2.41823500	1.59252800	-0.92279300
C	3.14408200	2.44841600	-0.07906100
C	2.37627000	1.91092000	-2.28670400
C	3.80876900	3.55109200	-0.58777700
H	3.19098700	2.27738400	0.99369300
C	3.04279500	3.02120900	-2.77849200
H	1.81497700	1.30643800	-2.99317200
C	3.76931700	3.85327300	-1.94130800
F	-1.46561200	3.07377700	2.36338300
F	-1.18971500	1.51018100	4.54084500
F	0.46051900	-0.62247300	4.47187200
F	2.79139100	-4.62287700	-0.57472600
F	5.27389400	-4.21838900	0.41025300
F	6.08851300	-1.71888200	1.01214100
F	4.50295500	4.37135300	0.21569400
F	4.40674900	4.92670000	-2.42383900
F	3.00016000	3.32917800	-4.08453700
H	0.92976500	-0.62928700	-2.07690700

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