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Electronic Supplementary Information

Gold(I)-Catalyzed Nucleophilic Cyclization of *β*-Monosubstituted *o*-(Alkynyl)styrenes: A Combined Experimental and Computational Study

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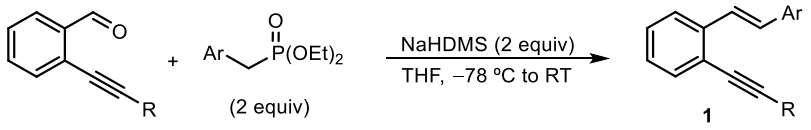
Contents:

General information:

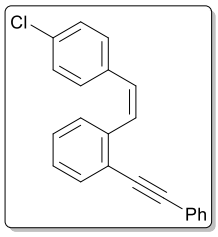
All reactions involving air-sensitive compounds were carried out under a N_2 atmosphere in oven-dried glassware with magnetic stirring. Temperatures are reported as bath temperatures. Solvents used for extraction and purification were distilled prior to use. TLC was performed on alumina-backed plates coated with silica gel 60 with F254 indicator; the chromatograms were visualized by UV light (254 nm) and/or by staining with a Ce/Mo reagent solution and subsequent heating. R_f values refer to silica gel. Flash column chromatography was carried out on silica gel 60, 230-400 mesh. ^{1}H NMR spectra were recorded at 300 or 400 MHz. Chemical shifts are reported in ppm with the residual solvent resonance as the internal standard ($CHCl_3$: δ 7.26). Data are reported as follows: chemical shift, multiplicity (s: singlet, bs: broad singlet, d: doublet, dd: doublet of doublets, ddd: doublet of doublet of doublets, td: triplet of doublets, t: triplet, dq: doublet of quartets, sex: sextet, sep: septet, m: multiplet), coupling constants (J in Hz) and integration. ^{13}C NMR spectra were recorded at 75.4 or 100.6 MHz using broadband proton decoupling. Chemical shifts are reported in ppm with the solvent resonance as internal standard ($CDCl_3$: δ 77.16). Carbon multiplicities were assigned by DEPT techniques. Gas chromatography–mass spectra (GC-MS) were recorded on an instrument equipped with a 30 m × 0.25 mm capillary apolar column (stationary phase: 5% diphenyldimethylpolysiloxane film, 0.25 μm). Low-resolution electron impact mass spectra (EI-LRMS) were obtained at 70 eV and only the molecular ions and/or base peaks as well as significant peaks in MS are given. High-resolution mass spectra (HRMS) were recorded on an instrument equipped with a magnetic sector ion analyzer using EI at 70 eV or on an instrument equipped with a QTOF analyzer using ESI (+). Melting points were measured on a Gallenkamp apparatus using open capillary tubes and are uncorrected. All commercially available reagents were used without purification unless otherwise indicated and were purchased from standard chemical suppliers.

Synthesis and characterization data of *o*-(alkynyl)styrenes 1:

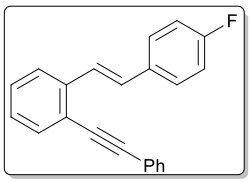


NaHMDS (10 mmol, 10 mL, 1 M in hexanes) was added to a solution of the appropriate diethyl phosphonate (10 mmol, 2.0 mL) in THF (20 mL) at −78 ºC and the resulting mixture was stirred for

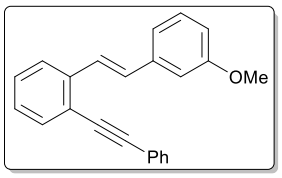
30 min at RT.[1] After cooling to −50 ºC, the corresponding 2-alkynylbenzaldehyde derivative[2] (5 mmol) was added to the solution, and the reaction was stirred at RT until the aldehyde was consumed as determined by GC-MS (overnight). The crude is partitioned between aqueous NH_4Cl / CH_2Cl_2 and the aqueous layer further extracted with CH_2Cl_2 (2 × 20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solvents were removed under reduce pressure. The residue was purified by flash column chromatography using a mixture of hexane/EtOAc as eluent to obtain the corresponding *o*-(alkynyl)styrene **1** as almost pure *E*-isomers. For the synthesis of mixtures of *E*/*Z* isomers and selected *Z*-isomers of *o*-(alkynyl)styrenes **1**, standard Wittig reactions were carried out and the obtained crudes were carefully purified by column chromatography (yields not reported). Characterization data for **1a,b,c,g,h,i,j,l,n,o,p** has been reported in our previous communication: *Org*. *Biomol*. *Chem*. **2018**, *16*, 2623−2628. The data of novel compounds are reported below:



(*Z*)-1-(4-Chlorostyryl)-2-(phenylethynyl)benzene (*Z*-1d): yellow oil; R_f = 0.22 (hex/EtOAc, 100/1); isolated as a ~1/8 mixture of *E*/*Z*; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79–7.19 (m, 15H) ppm; $^{13}C\{^1H\}$ RMN (75.4 MHz, $CDCl_3$) δ 139.2 (C), 135.5 (C), 132.9 (C), 132.6 (C), 132.5 (CH), 131.7 (2 x CH), 130.4 (2 x CH), 130.0 (CH), 129.7 (CH), 129.02 (CH), 128.99 (CH), 128.55 (2 x CH), 128.51 (2 x CH), 128.1 (CH), 127.4 (CH), 123.4 (C), 123.0 (C), 94.3 (C), 88.2 (C) ppm; LRMS (EI) *m/z* (%) 314 (M^+, 32), 279 (100); HRMS (EI) calcd. for $C_{22}H_{15}Cl$ 314.0862, found 314.0864.



(*E*)-1-(4-Fluorostyryl)-2-(phenylethynyl)benzene (1e): white solid; mp 100−102 ºC; 69% yield; isolated as a >20/1 mixture of *E*/*Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72–7.52 (m, 7H), 7.41−7.16 (m, 6H), 7.11−7.06 (m, 2H) ppm; $^{13}C\{^1H\}$ NMR (75.4 MHz, $CDCl_3$) δ 162.6 (d, J = 247.6 Hz, C), 138.7 (C), 133.7 (d, J = 3.2 Hz, C), 132.9 (CH), 131.6 (2 x CH), 129.3 (CH), 128.7 (CH), 128.64 (2 x CH), 128.61 (CH), 128.3 (d, J = 8.0 Hz, 2 x CH), 127.4 (CH), 126.7 (d, J = 2.0 Hz, CH), 124.9 (CH), 123.5 (C), 122.3 (C), 115.8 (d, J = 21.7 Hz, 2 x CH), 94.6 (C), 88.1 (C) ppm; LRMS (EI) *m/z* (%) 298 (M^+, 100), 283 (20), 276 (22), 220 (45); HRMS (ESI) calcd for $C_{22}H_{16}F^+$ [$(M+H)^+$] 299.1231, found 299.1234.

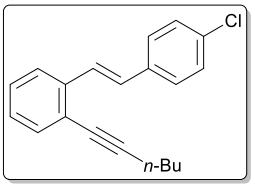


(*E*)-1-(3-Methoxystyryl)-2-(phenylethynyl)benzene (*E*-1f): yellow oil; R_f = 0.18 (hex/AcOEt, 50/1); 79% yield; isolated as a 6/1 mixture of *E*/*Z*. Data for *E*-isomer: ^{1}H NMR (400 MHz, C_6D_6) δ 7.97 (d, J = 16.3 Hz, 1H),

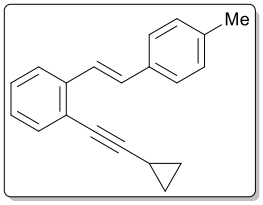
[1] K. Bera, C. Schneider, *Chem. Eur. J.* **2016**, *22*, 7074−7078.

[2] A. M. Sanjuán, M. A. Rashid, P. García-García, A. Martínez-Cuezva, M. A. Fernández-Rodríguez, F. Rodríguez, R. Sanz, *Chem. Eur. J.* **2015**, *21*, 3042−3052.

7.49–7.42 (m, 4H), 7.11–6.90 (m, 10H), 3.31 (s, 3H) ppm; $^{13}C\{^{1}H\}$ RMN (75.4 MHz, $CDCl_3$) δ 159.9 (C), 138.8 (C), 138.7 (C), 132.7 (CH), 131.5 (2 x CH), 130.3 (CH), 129.8 (CH), 128.6 (CH), 128.5 (CH), 128.4 (2 x CH), 127.3 (CH), 127.0 (CH), 124.8 (CH), 123.4 (C), 122.2 (C), 119.5 (CH), 113.8 (CH), 111.8 (CH), 94.6 (C), 88.1 (C), 55.1 (OCH_3) ppm; LRMS (EI) *m/z* (%) 310 (M^+, 100), 265 (42), 207 (13); HRMS (ESI) calcd for $C_{23}H_{16}Na$ [$(M+Na)^+(-H_2O)$] 315.1144, found 315.1166.

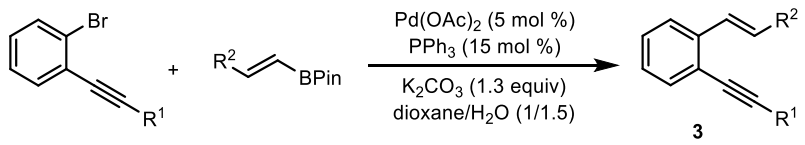


(*E*)-1-(4-Chlorostyryl)-2-(hex-1-yn-1-yl)benzene (*E*-1k): yellow oil; R_f = 0.45 (hex/EtOAc, 10/1); 80% yield; isolated as a >20/1 mixture of *E*/*Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64–7.59 (m, 2H), 7.46–7.17 (m, 7H), 7.07 (d, J = 164 Hz, 1H), 2.51 (t, J = 6.9Hz, 2H), 1.66–1.53 (m, 4H), 0.97 (t, J = 7.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 138.2 (C), 136.1 (C), 133.3 (C), 132.7 (CH), 128.9 (2 x CH), 128.4 (CH), 127.9 (2 x CH), 127.82 (CH), 127.78 (CH), 127.5 (CH), 124.6 (CH), 123.3 (C), 95.9 (C), 79.1 (C), 31.9 (CH_2), 22.2 (CH_2), 19.5 (CH_2), 13.8 (CH_3) ppm; LRMS (EI) *m/z* (%) 294 (M^+, 32), 215 (100); HRMS (EI) calcd. for $C_{20}H_{19}Cl$ 294.1175, found 294.1177.



(*E*)-1-(Cyclopropylethynyl)-2-(4-methylstyryl)benzene (1m): yellow oil; R_f = 0.25 (hex/EtOAc, 50/1); 65% yield; isolated as a >20/1 mixture of *E*/*Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, J = 7.4 Hz, 1H), 7.57 (d, J = 16.4 Hz, 1H), 7.46–7.39 (m, 3H), 7.21–7.10 (m, 5H), 2.39 (s, 3H), 158–1.54 (m, 1H), 0.95–0.86 (m, 4H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.0 (C), 137.7 (C), 134.9 (C), 132.8 (CH), 129.9 (CH), 129.5 (2 x CH), 127.8 (CH), 127.0 (CH), 126.7 (2 x CH), 126.2 (CH), 124.6 (CH), 122.9 (C), 98.8 (C), 74.4 (C), 21.4 (CH_3), 9.0 (2 x CH_2), 0.6 (CH) ppm; LRMS (EI) *m/z* (%) 258 (M^+, 21), 243 (73), 225 (59), 215 (100); HRMS (ESI) calcd for $C_{20}H_{19}^+$ [$(M+H)^+$] 259.1481, found 259.1485.

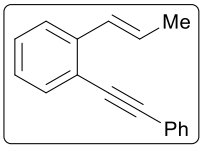
Synthesis and characterization data of *o*-(alkynyl)styrenes 3:



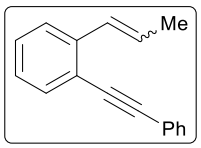
$Pd(OAc)_2$ (0.07 mmol, 17 mg), PPh_3 (60 mg, 0.22 mmol) and K_2CO_3 (270 mg, 1.95 mmol) were place in a two-necked flask under nitrogen atmosphere, and dioxane (10 mL) and H_2O (15 mL) were added.[3]

[3] C. C. Lin, T. M. Teng, C. C. Tsai, H. Y. Liao, R. S. Liu. *J. Am. Chem. Soc.* **2008**, *130*, 16417–16423.

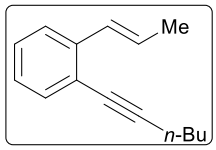
The corresponding 2-(bromo)ethynylbenzene[4] (1.5 mmol) and (*E*)-boronic acid pinacol ester (1.8 mmol) were added to the reaction mixture and it was stirred at 90 ºC for 24 h. The resulting mixture was partitioned between Et_2O/H_2O and the aqueo layer further extracted with Et_2O (2 × 20 mL). The organic phase was dried over anhydrous Na_2SO_4 and the solvents were removed under reduce pressure. The residue was purified by flash chromatography using a mixture of hexane/EtOAc as eluent to obtain the corresponding *o*-(alkynyl)styrenes as almost pure *E*-isomers. For the synthesis of selected mixtures of *E*/*Z* isomers of *o*-(alkynyl)styrenes **3** standard Wittig reactions were carried out. The characterization data of novel compounds are reported below:



(*E*)-1-(Phenylethynyl)-2-(prop-1-en-1-yl)benzene (*E*-3a): yellow oil; R_f = 0.21 (hex/EtOAc, 100/1); 88% yield; isolated as a >20/1 mixture of *E/Z* isomers. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.77–7.68 (m, 3H), 7.52–7.19 (m, 7H), 6.52 (dq, *J* = 13.6, 6.7 Hz, 1H), 2.13 (d, *J*= 6.7 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.4 (C), 133.3 (CH), 132.6 (2 × CH), 131.6 (2 × CH), 129.2 (CH), 128.5 (CH), 128.4 (CH), 127.8 (CH), 126.5 (CH), 124.7 (CH), 123.6 (C), 121.1 (C), 93.8 (C), 88.3 (C), 19.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 218 (M^+, 80), 202 (100); HRMS (EI) calcd for $C_{17}H_{14}$ 218.1096, found 218.1099.



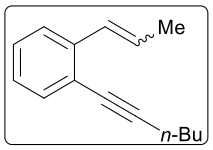
1-(Phenylethynyl)-2-(prop-1-en-1-yl)benzene (3a): yellow oil; R_f = 0.21 (hex/EtOAc, 100/1); 88% yield; isolated as a ~ 1/2 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65–7.31 (m, 13.5H), 7.05 (d, *J* = 15.8 Hz, 1H, min), 6.87 (d, *J* = 11.6 Hz, 1H, may), 6.43 (dq, *J* = 15.8, 6.7 Hz, 1H, min), 6.00 (dq, *J* = 11.6, 7.1 Hz, 1H, may), 2.02 (d, *J* = 6.7 Hz, 3H, min), 1.95 (d, *J* = 7.2 Hz, 4H, may) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.5 (C, min), 139.4 (C, may), 132.6 (CH, min), 132.4 (CH, may), 131.7 (2 x CH, may), 131.6 (2 x CH, min), 129.2 (CH, min), 129.1 (CH, may), 128.63 (CH, may), 128.60 (CH, min), 128.5 (2 x CH, min), 128.44 (2 x CH, may), 128.41 (CH, min), 128.3 (CH, may), 128.1, (CH, may), 127.94 (CH, min), 127.92 (CH, may), 126.59 (CH, may), 126.57 (CH, min), 124.7 (CH, min), 123.61 (C, min), 123.58 (C, may), 122.8 (C, may), 121.1 (C, min), 93.8 (C, may), 93.7 (C, min), 88.5 (C, may), 88.2 (C, min), 19.0 (CH_3, min), 14.9 (CH_3, may) ppm; LRMS (EI) *m/z* (%) 218 (M^+, 80), 202 (100); HRMS (ESI) calcd for $C_{17}H_{14}^+$ [$(M+H)^+$] 219.1096, found 219.1099.



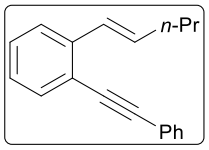
(*E*)-1-(Hex-1-yn-1-yl)-2-(prop-1-en-1-yl)benzene (*E*-3b): yellow oil; R_f = 0.27 (hex/EtOAc, 100/1); 84% yield; isolated as a >20/1 mixture of *E/Z* isomers. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55–7.44 (m, 2H), 7.30–7.16 (m, 2H), 6.99 (d,

[4] A. M. Sanjuán, A. Martínez, P. García-García, M. A. Fernández-Rodríguez, R. Sanz. *Beilstein J. Org. Chem.* **2013**, *9*, 2242–2249.

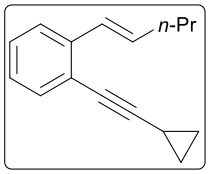
J = 15.7 Hz, 1H), 6.36 (dq, *J* = 15.7, 6.7 Hz, 1H), 2.56 (t, *J* = 6.7 Hz, 2H), 2.00 (d, *J* = 6.6 Hz, 3H), 1.71–1.62 (m, 4H), 1.06 (t, *J* = 7.1 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.3 (C), 132.5 (CH), 129.5 (CH), 127.7 (CH), 127.2 (CH), 126.4 (CH), 124.5 (CH), 122.1 (C), 94.9 (C), 79.3 (C), 31.0 (CH_2), 22.1 (CH_2), 19.4 (CH_2), 18.9 (CH_3), 13.8 (CH_3) ppm; LRMS (EI) *m/z* (%) 198 (M^+, 4), 141 (100); HRMS (EI) calcd for $C_{15}H_{18}$ 198.1409, found 198.1406.



1-(Hex-1-yn-1-yl)-2-(prop-1-en-1-yl)benzene (3b): yellow oil; R_f = 0.27 (hex/AcOEt, 100/1); 77% yield; obtained as a ~ 1/1 mixture of *E/Z* isomers; isolated as 1/1 mixture of *E/Z* isomers; ^1H NMR (300 MHz, $CDCl_3$) δ 7.55–7.39 (m, 4H), 7.27–7.17 (m, 4H), 6.98 (d, *J* = 15.8 Hz, 1H), 6.79 (d, *J* = 11.6 Hz, 1H), 6.36 (dq, *J* = 15.8, 6.7 Hz, 1H), 5.94 (dq, *J* = 11.6, 7.1 Hz, 1H), 2.54 (dt, *J* = 9.2, 6.9 Hz, 4H), 2.00 (dd, *J* = 6.7, 1.8 Hz, 3H), 1.93 (dd, *J* = 7.1, 1.9 Hz, 3H), 1.70–1.53 (m, 8H), 1.04 (td, *J* = 7.2, 6.1 Hz, 6H) ppm; $^{13}C\{^1H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.2 (C), 139.1 (C), 132.5 (CH), 132.4 (CH), 129.5 (CH), 128.9 (CH), 128.8 (CH), 127.7 (CH), 127.4 (CH), 127.2 (CH), 127.0 (CH), 126.4 (CH), 126.4 (CH), 124.5 (CH), 123.7 (C), 122.1 (C), 95.0 (C), 94.9 (C), 79.5 (C), 79.3 (C), 31.03 (CH_2), 30.99 (CH_2), 22.12 (CH_2), 22.11 (CH_2), 19.41 (CH_2), 19.39 (CH_2), 18.9 (CH_2), 14.8 (CH_2), 13.76 (CH_3), 13.75 (CH_3) ppm; LRMS (EI) *m/z* (%) 198 (M^+, 10), 169 (35), 155 (38), 141 (100); HRMS (ESI) calcd. para $C_{15}H_{19}$ [$(M+H)^+$] 199.1481, encontrada 199.1479.

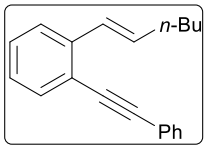


(*E*)-1-(Pent-1-en-1-yl)-2-(phenylethynyl)benzene (*E*-3c): red oil. R_f = 0.25 (hex/EtOAc, 100/1); 70% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^1H NMR (300 MHz, $CDCl_3$) δ 7.67–7.59 (m, 4H), 7.45–7.26 (m, 5H), 7.07 (d, *J* = 15.9 Hz, 1H), 6.44 (dt, *J* = 15.9, 6.9 Hz, 1H), 2.36 (q, *J* = 6.9 Hz, 2H), 1.78–1.54 (m, 2H), 1.08 (t, *J* = 7.4 Hz, 3H) ppm; $^{13}C\{^1H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.5 (C), 133.1 (CH), 132.6(CH), 131.6 (2 × CH), 128.54 (2 × CH), 128.51 (CH), 128.3 (CH), 128.1 (CH), 126.6 (CH), 124.8 (CH), 123.6 (C), 121.3 (C), 93.8(C), 88.3 (C), 35.5 (CH_2), 22.6 (CH_2), 13.9 (CH_3) ppm; LRMS (EI) *m/z* (%) 246 (M^+, 26), 215 (78), 128 (100); HRMS (EI) calcd for $C_{19}H_{18}$ 246.3462, found 246.3466.

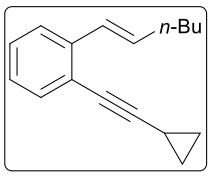


(*E*)-1-(Cyclopropylethynyl)-2-(pent-1-en-1-yl)benzene (*E*-3d): incolourless oil. R_f = 0.38 (hexane); 60% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^1H NMR (300 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.4 Hz, 1H), 7.35 (d, *J* = 7.4 Hz, 1H), 7.22–7.17 (m, 1H), 7.13–7.07 (m, 1H), 6.84 (d, *J* = 15.9 Hz, 1H), 6.28 (dt, *J* = 15.9, 6.9 Hz, 1H), 2.25 (q, *J* = 6.9 Hz, 2H), 1.57–1.50 (m, 3H), 0.99 (t, *J* = 7.3 Hz, 3H), 0.91–0.82 (m, 4H) ppm; $^{13}C\{^1H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.5 (C), 132.6 (CH), 132.5 (CH), 128.3 (CH), 127.7 (CH), 126.5 (CH), 124.7 (CH), 122.0 (C), 98.1 (C), 74.5 (C), 35.5 (CH_2), 22.6 (CH_2), 13.9

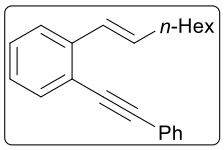
(CH_3), 8.9 (2 x CH_2), 0.5 (CH) ppm; LRMS (EI) *m/z* (%) 210 (M^+, 6), 181 (54), 165 (78), 153 (100); HRMS (ESI) calcd for $C_{16}H_{19}$ [$(M+H)^+$] 211.1481, found 211.1480.



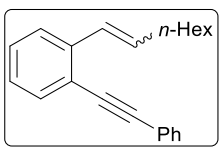
(*E*)-1-(Hex-1-en-1-yl)-2-(phenylethynyl)benzene (*E*-3e): uncolourless oil; R_f = 0.25 (hexane); 70% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61–7.53 (m, 4H), 7.41–7.38 (m, 5H), 7.00 (d, J = 15.8 Hz, 1H), 6.41 (dt, J = 15.8, 7.0Hz, 1H), 2.33 (q, J = 7.0 Hz, 2H), 1.56–1.43 (m, 4H), 0.98 (t, J = 7.1 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.6 (C), 133.4 (CH), 132.6 (CH), 131.6 (2 × CH), 128.53 (2 × CH), 128.50 (CH), 128.3 (CH), 128.0 (CH), 126.6 (CH), 124.8 (CH), 123.7 (C), 121.3 (C), 93.8(C), 88.3 (C), 33.1 (CH_2), 31.6 (CH_2), 22.4 (CH_2), 14.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 260 (M^+, 6), 215 (100), 202 (88), 128 (88); HRMS (ESI) calcd for $C_{20}H_{21}$ [$(M+H)^+$] 261.1638, found 261.1635.



(*E*)-1-(Cyclopropylethynyl)-2-(hex-1-en-1-yl)benzene (*E*-3f): uncolourless oil; R_f = 0.20 (hexane); 81% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (d, J = 7.1 Hz, 1H), 7.35 (d, J = 7.1 Hz, 1H), 7.22–7.16 (m, 1H), 7.12–7.07 (m, 1H), 6.83 (d, J = 15.9 Hz, 1H), 6.28 (dt, J = 15.9, 6.9 Hz, 1H), 2.27 (q, J = 6.9 Hz, 2H), 1.54–1.39 (m, 5H), 0.98–0.82 (m, 7H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.4 (C), 132.7 (CH), 132.6 (CH), 128.1 (CH), 127.6 (CH), 126.4 (CH), 124.6 (CH), 122.0 (C), 98.0 (C), 74.5 (C), 33.0 (CH_2), 31.6 (CH_2), 22.4 (CH_2), 14.1 (CH_3), 8.9 (2 x CH_2), 0.5 (CH) ppm; LRMS (EI) *m/z* (%) 224 (M^+, 4), 181 (64), 165 (68) (100); HRMS (ESI) calcd for $C_{17}H_{21}$ [$(M+H)^+$] 225.1638, found 225.1634.

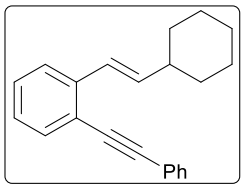


(*E*)-1-(Oct-1-en-1-yl)-2-(phenylethynyl)benzene (*E*-3g): yellow oil; R_f = 0.22 (hex/EtOAc, 100/1); 55% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59–6.96 (m, 9H), 6.99 (d, J = 15.8 Hz, 1H), 6.37 (dt, J = 15.8, 6.9 Hz, 1H), 2.30 (q, J = 6.9 Hz, 2H), 1.55–1.30 (m, 8H), 0.93–0.89 (m, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.6 (C), 133.4 (CH), 132.6 (CH), 131.6 (2 × CH), 128.51 (CH), 128.53 (2 × CH), 128.3 (CH), 127.9 (CH), 126.6(CH), 124.8 (CH), 123.7 (C), 121.3 (C), 93.8 (C), 88.3 (C), 33.5 (CH_2), 31.9 (CH_2), 29.4 (CH_2), 29.1 (CH_2), 22.8 (CH_2), 14.2 (CH_3) ppm; LRMS (EI) *m/z* (%) 288 (M^+, 6), 215 (100), 128 (63); HRMS (EI) calcd for $C_{22}H_{24}$ 288.1878, found 288.1879.

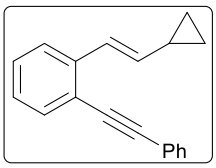


1-(Oct-1-en-1-yl)-2-(phenylethynyl)benzene (3g): yellow oil; R_f = 0.22 (hex/EtOAc, 100/1); 64% yield; isolated as a 1/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62–7.59 (m, 8H), 7.42–7.38 (m, 10H), 7.06 (d, J = 15.9 Hz, 1H), 6.86 (d, J = 11.6 Hz, 1H), 6.42 (dt, J = 15.9, 6.9 Hz, 1H), 5.88

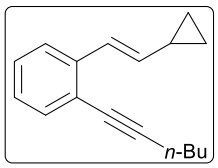
(dt, J = 11.6, 7.3 Hz, 1H), 2.37–2.32 (m, 5H), 1.59–1.36 (m, 15H) 0.99–0.94 (m, 6H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.7 (C), 139.5 (C), 134.3 (CH), 133.4 (CH), 132.6 (CH), 132.3 (CH), 131.63 (2 x CH), 131.59 (2 x CH), 128.9 (CH), 128.5 (CH), 128.45 (2 x CH), 128.41 (2 x CH), 128.30 (CH), 128.28 (CH), 127.9 (CH), 127.8 (CH), 127.4 (CH), 126.6 (CH), 126.5 (CH), 124.8 (CH), 123.6 (C), 122.7 (C), 121.2 (C), 93.8 (C), 93.8 (C), 88.5 (C), 88.3 (C), 33.4 2 (CH_2), 31.7 (CH_2), 31.6 (CH_2), 29.7 (CH_2), 29.1 (CH_2), 28.8 (CH_2), 22.71 (CH_2), 22.67 (CH_2), 14.2 (CH_3) ppm, two CH_2 and one CH_3 do not appear due to overlapping; LRMS (EI) *m/z* (%) 288 (M^+, <1), 215 (100); HRMS (EI) calcd for $C_{22}H_{24}$ 288.1878, found 288.1879.



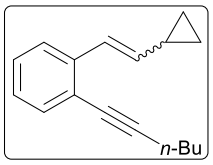
(*E*)-1-(2-Cyclohexylvinyl)-2-(phenylethynyl)benzene (*E*-3h): yellow oil; R_f = 0.20 (hex/EtOAc, 100/1); 84% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58–6.49 (m, 4H), 7.40–7.15 (m, 5H), 6.94 (d, J = 16.0 Hz, 1H), 6.30 (dd, J = 16.0, 6.9 Hz, 1H), 2.22–2.20 (m, 1H), 1.88–1.71 (m, 5H), 1.38–1.20 (m, 5H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 138.5 (C), 134.7 (CH), 132.3 (2 × CH), 129.8 (C), 129.3 (CH), 128.8 (CH), 128.3 (2 × CH), 127.5 (CH), 127.4 (C), 126.0 (CH), 125.8 (CH), 124.2 (CH), 99.3 (C), 93.3 (C), 33.7 (2 × CH_2), 32 4 (CH), 26.1 (CH_2), 25.9 (2 × CH_2) ppm; LRMS (EI) *m/z* (%) 286 (M^+, 16), 204 (100); HRMS (EI) calcd for $C_{22}H_{22}$ 286.1722, found 286.1726.



(*E*)-1-(2-Cyclopropylvinyl)-2-(phenylethynyl)benzene (*E*-3i): red oil; R_f = 0.31 (hex/EtOAc, 100/1); 70% yield; isolated as a >20/1 mixture of *E/Z* isomers. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69–7.17(m, 10H), 5.96 (dd, J = 15.8, 9.0 Hz, 1H), 1.78–1.72 (m, 1H), 0.98–0.94 (m, 2H), 0.67–0.65 (m, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.2 (C), 137.1 (CH), 132.6 (CH), 131.6 (2 × CH), 128.5 (2 × CH), 128.4 (CH), 128.3 (CH), 126.3 (CH), 125.4 (CH), 124.4 (CH), 123.6 (C), 120.8 (C), 93.8 (C), 88.4 (C), 15.1 (CH), 7.7 (2 × CH_2) ppm; LRMS (EI) *m/z* (%) 244 (M^+, 76), 228 (100); HRMS (ESI) calcd for $C_{19}H_{17}^+$ [$(M+H)^+$] 245.1252, found 245.1252.

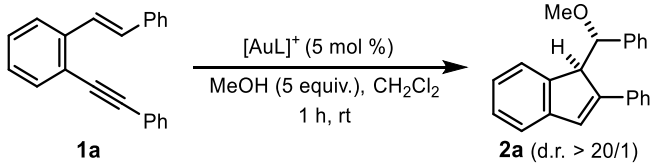


(*E*)-1-(2-Cyclopropylvinyl)-2-(hex-1-yn-1-yl)benzene (*E*-3j): red oil; R_f = 0.28 (hex/EtOAc, 100/1); 77% yield; isolated as a >20/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.48–6.99 (m, 6H), 5.84 (dd, J = 15.8, 9.0 Hz, 1H), 2.53 (t, J = 6.9 Hz, 2H), 1.68–1.58 (m, 5H), 1.02 (t, J = 7.2 Hz, 2H), 0.90–0.88 (m, 2H), 0.59–0.57 (m, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 139.1 (C), 136.5 (CH), 132.6 (CH), 127.7 (CH), 126.2 (CH), 125.8 (CH), 124.2 (CH), 121.8 (C), 95.0 (C), 79.3 (C), 31.0 (CH_2), 22.2 (CH_2), 19.5 (CH_2), 15.0 (CH), 13.8 (CH_3), 7.6 (2 × CH_2) ppm; LRMS (EI) *m/z* (%) 224 (M^+, 12), 167 (100); HRMS (ESI) calcd for $C_{17}H_{21}^+$ [$(M+H)^+$] 225.1638, found 225.1640.



1-(2-Cyclopropylvinyl)-2-(hex-1-yn-1-yl)benzene (3j): uncolourless oil; R_f= 0.28 (hexane); 81% yield; isolated as 1.6/1 mixture of *E/Z* isomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.61 (d, J = 7.7 Hz, 1H), 7.44–7.35 (m, 4H), 7.25□7.07 (m 5H), 6.98 (d, J = 15.8 Hz, 1H), 6.62 (d, J = 11.5 Hz, 1H), 5.81 (dd, J = 15.8, 8.9 Hz, 1H), 5.14 (dd, J = 11.5, 10.0 Hz, 1H), 2.52–2.44 (m, 4H), 1.65–1.53 (m, 10H), 1.01–0.94 (m, 6H), 0.87–0.82 (m, 4H), 0.56–0.49 (m, 4H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 139.6 (C), 139.0 (C), 137.3 (CH), 136.3 (CH), 132.6 (CH), 132.4 (CH), 128.7 (CH), 127.6 (CH), 127.0 (CH), 126.3 (CH), 126.2 (CH), 125.8 (CH), 124.2 (CH), 123.6 (C), 121.8 (C), 95.1 (C), 94.9 (C), 79.5 (C), 79.4 (C), 31.1 (CH_2), 31.0 (CH_2), 22.11 (CH_2), 22.08 (CH_2), 19.4 (CH_2), 14.9 (CH_2), 13.7 (CH), 11.3 (CH), 8.2 (2 x CH_2), 7.6 (2 x CH_2) ppm; LRMS (EI) *m/z* (%) 224 (M^+, 12), 167 (100); HRMS (ESI) calcd. para $C_{17}H_{20}$ [$(M+H)^+$] 225.1638, found 225.1640.

Effect of gold catalyst on methoxycyclization of 1a

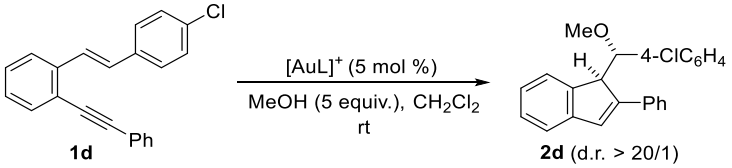


1a **2a** (d.r. > 20/1)

[AuL]$^+$	Conversion (%)^b	Yield (%)^c
$Ph_3PAuNTf_2$	76	51
$Ph_3PAuCl/AgSbF_6$	66	54
$[(3,5\text{-}t\text{-}Bu)_2C_6H_3O_3]_3PAuCl/AgNTf_2$	97	65
$XPhosAuNTf_2$	100	76
$BrettPhosAuNTf_2$	100	62
$JohnPhosAuNTf_2$	100	84
$IPrAuNTf_2$	100	89
$IPrAuNTf_2$	100	84
$IPrAuCl/AgNTf_2$	100	63
$IPrAuCl/AgSbF_6$	100	79
$IPrAuCl/AgBF_4$	100	86

^{a}Reactions conducted using 0.1 mmol of **1a** in CH_2Cl_2 (0.8 mL). ^{b}Determined by ^{1}H NMR analysis of the crude reaction mixture. ^{c}Determined by ^{1}H NMR using CH_2Br_2 as internal standard. ^{d}Carried out with 2.5 mol % of catalyst.

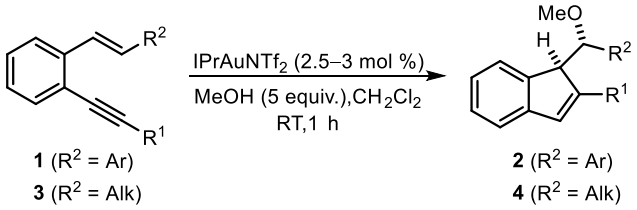
Effect of gold catalyst on methoxycyclization of 1d



[AuL]$^+$	Time (h)	Conversion (%)^b	NMR yield (%)^c
$Ph_3PAuNTf_2$	16	65	55
$[(3,5\text{-}t\text{-}Bu)_2C_6H_3O_3]_3PAuCl/AgNTf_2$	1	33	27
$[(3,5\text{-}t\text{-}Bu)_2C_6H_3O_3]_3PAuCl/AgNTf_2$	16	100	78
$IPrAuNTf_2$	1	100	82

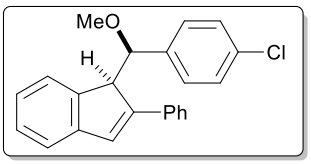
[a]Reactions conducted using 0.1 mmol of **1a** in CH_2Cl_2 (0.8 mL). [b]Determined by ^1H NMR analysis of the crude reaction mixture. [c]Determined by ^1H NMR using CH_2Br_2 as internal standard.

Synthesis and characterization data of methoxy-functionalized indenes 2 and 4:



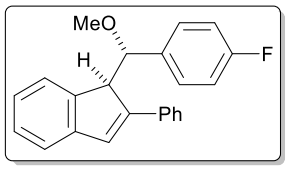
MeOH (1.5 mmol, 0.06 mL) was added to a solution of $IPrAuNTf_2$ (0.009 mmol, 7.8 mg) in CH_2Cl_2 (0.6 mL) and the solution mixture was stirred 5 min. A solution of the corresponding starting *o*-(alkynyl)styrene **1** or **3** (0.3 mmol) in CH_2Cl_2 (0.4 mL) was subsequently added. The resulting reaction mixture was stirred at RT until complete consumption of the styrene derivative was observed by GC-MS (1−6 h). The mixture was filtered through a short pad of silica gel using a 100/1 mixture of hexane/EtOAc as eluent, the solvent was removed under reduced pressure, and the crude mixture was purified by flash column chromatography on silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding 1-(α-methoxybenzyl)-1*H*-indenes **2** and 1-(α-methoxyalkyl)-1*H*-indenes **4**, in the yields reported in Tables 1 and 2.

Characterization data for **2a,b,c,g,h,i,j,l,n,o,p** has been reported in our previous communication: *Org. Biomol. Chem.* **2018**, *16*, 2623−2628. The data of novel compounds are reported below:

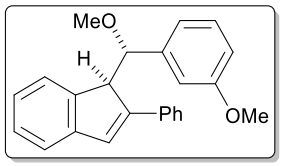


(*R)-1-[(*R**)-(4-Chlorophenyl)(methoxy)methyl]-2-phenyl-1*H*-indene (diast-2d):** yellow oil; R_f = 0.20 (hexane); 80% yield (83 mg); obtained with d.r. = 8/1 starting from a ~ 1/8 mixture of *E*/*Z* diastereoisomers of **1d**; isolated with d.r. = 10/1. Data for the *(R*,R*)*

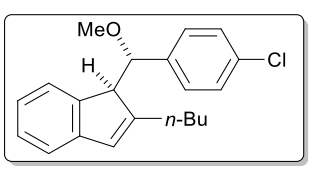
diastereoisomer: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96–7.93 (m, 1H), 7.57–7.21 (m, 8H), 6.93 (d, J = 8.3 Hz, 2H), 6.85 (s, 1H), 6.53 (d, J = 8.3 Hz, 2H), 4.83 (d, J = 4.7 Hz, 1H), 4.65 (d, J = 4.7 Hz, 1H), 3.42 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 146.8 (C), 144.8 (C), 143.6 (C), 136.0 (C), 135.1 (C), 133.0 (C), 129.4 (CH), 129.1 (2 × CH), 128.5 (2 × CH), 127.7 (CH), 127.3 (CH), 127.04 (2 x CH), 127.02 (2 x CH), 126.3 (CH), 124.6 (CH), 121.0 (CH), 83.8 (CH), 57.3 (CH_3), 54.1 (CH) ppm; LRMS (EI) *m/z* (%) 346 (M^+, 7), 189 (11), 155 (100); HRMS (ESI) calcd. for $C_{23}H_{20}ClO^+$ [$(M+H)^+$] 347.1124, found 347.1123.



(*R)-1-((*S**)-(4-Fluorophenyl)(methoxy)methyl)-2-phenyl-1*H*-indene (2e):** yellow solid; mp 91–93 ºC; 92% yield (87 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54–7.51 (m, 2H), 7.39–7.33 (m, 5H), 7.12–7.07 (m, 7H), 4.70 (d, J = 4.3 Hz, 1H), 4.37 (d, J = 4.3 Hz, 1H), 3.13 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 162.2 (d, J = 245.0 Hz, C), 149.2 (C), 144.7 (C), 144.0 (C), 136.6 (C), 135.3 (d, J = 3.0 Hz, C), 129.5 (CH), 128.5 (d, J = 8.0 Hz, 2 × CH), 128.4 (2 × CH), 127.42 (2 × CH), 127.37 (CH), 127.2 (CH), 124.7 (CH), 124.6 (CH), 121.2 (CH), 114.7 (d, J = 21.3 Hz, 2 x CH), 83.8 (CH), 57.7 (CH), 56.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 330 (M^+, 7), 139 (100); HRMS (ESI) calcd for $C_{22}H_{16}F^+$ [$(M+H)^+(-CH_3O)$] 299.1231, found 299.1236.

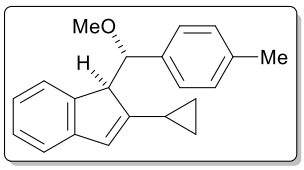


(*R)-1-((*S**)-Methoxy(3-methoxyphenyl)methyl)-2-phenyl-1*H*-indene (2f):** yellow oil; R_f = 0.18 (hex/EtOAc, 50/1); 71% yield (73 mg); obtained with d.r. = 5.5/1 starting from a ~ 6/1 mixture of *E*/*Z* diastereoisomers of **1f** and isolated as a single diastereoisomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54 (d, J = 7.1 Hz, 2H), 7.38–7.19 (m, 6H), 7.08 (dt, J = 7.4, 1.2 Hz, 1H), 7.01 (s, 1H), 6.96 (d, J = 7.4 Hz, 1H), 6.78 (d, J = 8.1 Hz, 2H), 6.71 (s, 1H), 4.71 (d, J = 4.0 Hz, 1H), 4.35 (d, J = 3.9 Hz, 1H), 3.72 (s, 3H), 3.09 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.4 (C), 149.3 (C), 144.8 (C), 143.9 (C), 141.7 (C), 136.5 (C), 129.2 (CH), 129.0 (CH), 128.5 (2 x CH), 127.33 (2 x CH), 127.30 (CH), 127.2 (CH), 124.9 (CH), 124.4 (CH), 121.2 (CH), 119.3 (CH), 113.3 (CH), 112.1 (CH), 83.7 (CH), 58.0 (CH_3), 56.2 (CH_3), 55.3 (CH) ppm; LRMS (EI) *m/z* (%) 342 (M^+, 33), 189 (14), 151 (100); HRMS (ESI) calcd for $C_{24}H_{22}NaO_2^+$ [$(M+Na)^+$] 365.1512, found 365.1515.

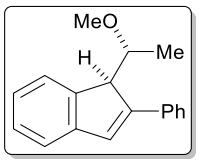


(*S)-2-Butyl-1-[(*S**)-(4-chlorophenyl)(methoxy)methyl]-1*H*-indene (2k):** colourless oil; mp 78–80 ºC; 74% yield (72 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1k**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23–7.04 (m, 8H), 6.41 (s, 1H), 4.67 (d, J = 4.9 Hz, 1H), 3.77 (d, J = 4.9 Hz, 1H), 3.32 (s, 3H), 2.44–2.34 (m, 2H), 1.54–1.34 (m, 4H), 0.41 (t, J = 7.3 Hz, 3H) ppm;

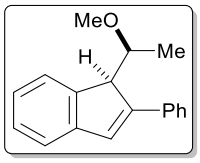
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 151.5 (C), 145.2 (C), 143.6 (C), 137.8 (C), 130.2 (C), 128.4 (2 × CH), 128.0 (2 x CH), 127.9 (CH), 127.0 (CH), 124.1 (CH), 123.6 (CH), 120.1 (CH), 84.2 (CH), 57.5 (CH_3), 56.7 (CH), 31.3 (CH_2), 30.5 (CH_2), 22.7 (CH_2), 14.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 326 (M^+, 2), 157 (32), 155 (100); HRMS (ESI) calcd. for $C_{21}H_{24}ClO^+$ [$(M+H)^+$] 327.1510, found 327.1509.



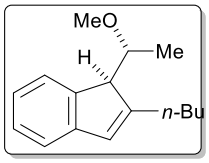
(*S)-2-Cyclopropyl-1-((*S**)-methoxy(p-tolyl)methyl)-1H-indene (2m):** yellow solid; mp 71–73ºC; 90% yield (85 mg), obtained and isolated with d.r. > 20/1 starting from (*E*)-**1m**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28–7.17 (m, 7H), 7.09–7.06 (m, 1H), 6.24 (s, 1H), 4.74 (d, *J* = 5.4 Hz, 1H), 3.92 (d, *J* = 5.3 Hz, 1H), 3.37 (s, 3H), 2.41 (s, 3H), 1.57–1.54 (m, 1H), 0.89–0.86 (m, 2H), 0.69–0.65 (m, 2H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 154.3 (C), 145.0 (C), 144.0 (C), 137.1 (C), 136.7 (C), 128.7 (2 x CH), 127.4 (2 x CH), 126.9 (CH), 124.4 (CH), 123.4 (CH), 123.2 (CH), 120.0 (CH), 84.5 (CH), 58.7 (CH), 57.2 (CH_3), 21.3 (CH_3), 11.1 (CH), 9.6 (CH_2), 9.4 (CH_2) ppm; LRMS (EI) *m/z* (%) 290 (M^+, 100), 207 (8), 135 (98); HRMS (ESI) calcd for $C_{21}H_{22}NaO^+$ [$(M+Na)^+$] 313.1563, found 313.1564.



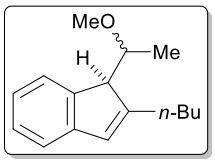
(*R)-1-((*R**)-1-Methoxyethyl)-2-phenyl-1*H*-indene (4a):** red oil; R_f = 0.31 (hexane/EtOAc, 100/1); 85% yield (64 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.61–7.56 (m, 1H), 7.50–7.23 (m, 6H), 7.15 (s, 1H), 4.34 (d, *J* = 2.9 Hz, 1H), 4.02 (dq, *J* = 6.4, 3.1 Hz, 1H),3.38 (s, 3H), 1.08 (d, *J* = 6.4 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (75 MHz, $CDCl_3$) δ 150.2 (C), 145.0 (C), 144.7 (C), 136.9 (C), 129.3 (CH), 128.4 (2 × CH), 127.5 (2 × CH), 127.4 (CH), 127.2 (CH), 124.8 (CH), 123.7 (CH), 121.2 (CH), 78.9 (CH), 56.9 (OCH_3), 54.1 (CH), 16.4 (CH_3) ppm; LRMS (EI) *m/z* (%) 250 (M^+, 19), 189 (17), 59 (100); HRMS (ESI) calcd for $C_{18}H_{18}O$ [$(M+H)^+$] 251.1432, found 251.1430.



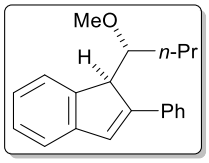
(*R)-1-((*S**)-1-(Methoxyethyl)-2-phenyl-1*H*-indene (diast-4a):** red oil; R_f = 0.31 (hexane/EtOAc, 100/1); 88% yield (66 mg); obtained and isolated with d.r. ~ 2/1 starting from a ~ 1/2 mixture of *E*/*Z* diastereoisomers of **3a**. Data for the *(R*,S*)* diastereoisomer: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.72 (d, *J* = 7.4 Hz, 1H), 7.62–7.25 (m, 8H), 7.14 (s, 1H), 4.53 (d, *J* = 3.8 Hz, 1H), 4.01–3.98 (m, 1H), 3.66 (s, 3H), 0.57 (d, *J* = 6.2 Hz, 3H) ppm; $^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$) δ 148.3 (C), 145.0 (C), 144.6 (C), 135.7 (C), 128.9 (2 × CH), 128.7 (CH), 127.7 (CH), 127.1 (CH), 126.9 (2 × CH), 125.6 (CH), 125.0 (CH), 121.1 (CH), 77.8 (CH), 56.6 (CH_3), 52.2 (CH), 13.2 (CH_3) ppm; LRMS (EI) *m/z* (%) 250 (M^+, 19), 189 (17), 59 (100); HRMS (ESI) calcd. para $C_{18}H_{19}O^+$ [$(M+H)^+$] 251.1432, encontrada 251.1430.



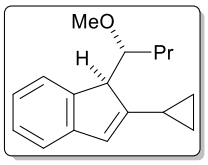
(*S)-2-Butyl-1-((*R**)-1-methoxyethyl)-1*H*-indene (4b):** yellow oil; R_f 0.34 = (hexane/EtOAc, 100/1); 87% yield (64 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3b**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37–7.24 (m, 3H), 7.19–7.09 (m, 1H), 6.58 (s, 1H), 4.06 (dq, J = 6.3, 3.6 Hz, 1H), 3.82–3.77 (m, 1H), 3.55 (s, 3H), 2.68–2.50 (m, 2H), 1.75–1.59 (m, 2H), 1.51–1.38 (m, 2H), 1.00 (t, J = 7.2 Hz, 3H), 0.79 (d, J = 6.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 153.3 (C), 145.4 (C), 144.5 (C), 127.2 (CH), 126.8 (CH), 123.7 (CH), 122.6 (CH), 120.0 (CH), 79.1 (CH), 56.7 (OCH_3), 53.9 (CH), 31.0 (CH_2), 30.8 (CH_2), 22.8 (CH_2),14.3 (CH_3), 14.2 (CH_3) ppm; LRMS (EI) *m/z* (%) 230 (M^+, 21), 128 (26), 59 (100); HRMS (ESI) calcd for $C_{16}H_{23}O^+$ [$(M+H)^+$] 231.1743, found 231.1743.



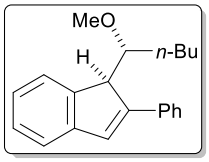
2-Butyl-1-(1-methoxyethyl)-1*H*-indene (diast-4b): yellow oil; R_f 0.34 = (hexane/EtOAc, 100/1); 81% yield (61 mg); obtained and isolated with d.r. = 1.5/1 starting from a ~ 1/1 mixture of *E*/*Z* diastereoisomers of **3b**. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (d, J = 7.3 Hz, 1H, may), 7.29 (d, J = 7.3 Hz, 1H, min), 7.24–7.22 (m, 4H, may + min), 7.13–7.08 (m, 2H, may + min), 6.53 (s, 1H, min), 6.51 (s, 1H, may), 4.01 (dq, J = 6.3, 3.6 Hz, 1H, min), 3.92 (dq, J = 6.3, 3.6 Hz, 1H, may), 3.79 (d, J = 3.6 Hz, 1H, may), 3.75 (d, J = 3.6 Hz, 1H, min), 3.56 (s, 3H, may), 3.50 (s, 3H, min), 2.58–2.50 (m, 2H, min), 2.40–2.31 (m, 2H, may), 1.66–1.58 (m, 4H, may + min), 1.46–1.38 (m, 4H, may + min), 0.99–0.95 (m, 6H, may + min), 0.75 (d, J = 6.3 Hz, 3H, min), 0.65 (d, J = 6.3 Hz, 3H, may) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 153.3 (C), 151.0 (C), 145.52 (C), 145.48 (C), 144.5 (C), 144.1 (C), 127.3 (CH), 127.2 (CH), 126.8 (CH), 126.7 (CH), 125.1 (CH), 123.9 (CH), 123.7 (CH), 122.6 (CH), 120.1 (CH), 119.9 (CH), 79.1 (CH), 77.4 (CH), 56.7 (CH_3), 56.6 (CH_3), 54.0 (CH), 53.9 (CH), 31.1 (CH_2), 31.0 (CH_2), 30.8 (CH_2), 29.5 (CH_2), 22.8 (CH_2),22.7 (CH_2), 14.3 (CH_3), 14.2 (CH_3), 14.1 (CH_3), 13.7 (CH_3) ppm; LRMS (EI) *m/z* (%) 230 (M^+, 21), 128 (26), 59 (100); HRMS (ESI) calcd for $C_{16}H_{23}O^+$ [$(M+H)^+$] 231.1743, found 231.1743.



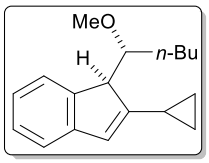
(*R)-1-((*R**)-1-Methoxybutyl)-2-phenyl-1*H*-indene (4c):** yellow oil; R_f = 0.31 (hexane/EtOAc, 100/1); 73% yield (60 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3c**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65–7.26 (m, 10H), 7.15 (s, 1H), 4.35 (s, 1H), 3.84 (d, J = 8.5 Hz, 1H), 3.40 (s, 3H), 1.62–1.45 (m, 2H), 1.36–1.24 (m, 2H), 0.89 (t,J = 7.1 Hz,3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 150.5 (C), 144.9 (C), 144.8 (C), 136.8 (C), 129.0 (CH), 128.5 (2 x CH), 127.5 (CH), 127.3 (2 x CH), 127.1 (CH), 124.8 (CH), 123.6 (CH), 121.2 (CH), 83.2(CH), 58.2 (OCH_3), 52.5 (CH), 34.1 (CH_2), 19.9 (CH_2), 14.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 278 (M^+, 19), 189 (25), 87 (100); HRMS (ESI) calcd for $C_{20}H_{22}O^+$ [$(M+H)^+$] 279.1671, found 279.1671.



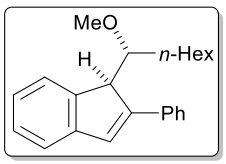
(*S)-2-Cyclopropyl-1-((*R**)-1-methoxybutyl)-1*H*-indene (4d):** yellow oil; R_f = 0.20 (hex/EtOAc, 40/1); 84% yield (61 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3j**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.7.29 (d, J = 7.3 Hz, 1H), 7.21–7.19 (m, 2H), 7.11–7.06 (m, 1H), 6.24 (s, 1H), 3.86–3.82 (m, 2H), 3.59 (s, 3H), 1.92–1.87 (m, 1H), 1.44–1.39 (m, 2H), 1.20–1.16 (m, 1H), 0.95–0.91 (m, 2H), 0.80–0.76 (m, 5H), 0.60–0.55 (m, 1H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 156.3 (C), 145.4 (C), 144.3 (C), 126.8 (CH), 123.6 (CH), 122.5 (CH), 122.4 (CH), 120.1 (CH), 83.8 (CH), 57.5 (CH_3), 53.7 (CH), 32.4 (CH_2), 19.9 (CH_2), 14.0 (CH_3), 11.1 (CH_2), 10.1 (CH_2), 9.1 (CH); LRMS (EI) *m/z* (%) 242 (M^+, 21), 87 (100), 45 (51); HRMS (ESI) calcd for $C_{17}H_{23}O^+$ [(M+H)$^+$] 243.1743, found, 243.1744.



(*R)-1-((*R**)-1-Methoxypentyl)-2-phenyl-1*H*-indene (4e):** yellow solid; mp 66–68 ºC; 72% yield (81 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (d, J = 7.0 Hz, 2H), 7.52 (d, J = 7.0 Hz, 1H), 7.46–7.22 (m, 6H), 7.12 (s, 1H), 4.31 (d, J = 2.2 Hz, 1H), 3.77 (dt, J = 8.8, 2.2 Hz, 1H), 3.36 (s, 3H), 1.58–1.25 (m, 6H), 0.86 (t, J = 7.1 Hz, 3H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 150.5 (C), 144.9 (C), 144.8 (C), 136.8 (C), 129.0 (CH), 128.5 (2 x CH), 127.5 (CH), 127.3 (2 x CH), 127.1 (CH), 124.8 (CH), 123.7 (CH), 121.3 (CH), 83.4 (CH), 58.2 (CH_3), 52.5 (CH), 31.8 (CH_2), 29.0 (CH_2), 22.7 (CH_2), 14.2 (CH_3) ppm; LRMS (EI) *m/z* (%) 292 (M^+, 7), 215 (100), 202 (82), 128 (87); HRMS (ESI) calcd for $C_{21}H_{24}NaO^+$ [(M+Na)$^+$] 315.1719, found 315.1727.

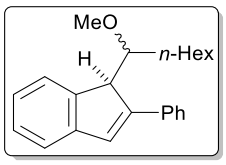


(*S)-2-Cyclopropyl-1-((*R**)-1-methoxypentyl)-1*H*-indene (4f):** yellow oil; R_f = 0.28 (hex/EtOAc, 40/1); 87% yield (76 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3f**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.29 (d, J = 7.3 Hz, 1H), 7.20–7.19 (m, 2H), 7.11–7.07 (m, 1H), 6.24 (s, 1H), 3.86–3.80 (m, 2H), 3.59 (s, 3H), 1.91–1.86 (m, 1H), 1.42–1.39 (m, 2H), 1.18–1.16 (m, 3H), 0.90–0.7 (m, 7H), 0.60–0.57 (m, 1H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 156.3 (C), 145.4 (C), 144.3 (C), 126.8 (CH), 123.6 (CH), 122.5 (CH), 122.4 (CH), 120.1 (CH), 83.8 (CH), 57.5 (CH_3), 53.7 (CH), 30.0 (CH_2), 29.1 (CH_2), 22.6 (CH_2), 14.1 (CH_3), 11.1 (CH_2), 10.1 (CH_2), 9.1 (CH); LRMS (EI) *m/z* (%) 256 (M^+, 20), 101 (100), 69 (61); HRMS (ESI) calcd for $C_{18}H_{25}O^+$ [(M+H)$^+$] 257.1900, found, 257.1903.

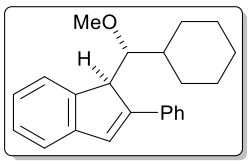


(*R)-1-((*R**)-1-Methoxyheptyl)-2-phenyl-1*H*-indene (4g):** yellow oil; R_f = 0.11 (hexane); 84% yield (81 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3g**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57–7.20 (m, 9H), 7.07 (s, 1H), 4.27 (s, 1H), 3.77–3.73 (m, 1H), 3.32 (s, 3H), 1.48–1.19 (m, 10H), 0.84 (t, J = 6.8 Hz, 3H); ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 150.5 (C), 144.9 (C), 144.8 (C), 136.8 (C), 129.0 (CH), 128.9 (2 x CH), 127.5 (CH), 127.3 (2 x CH), 127.1 (CH), 124.8 (CH), 123.7 (CH), 121.3 (CH),

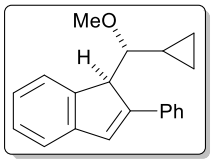
83.4 (CH), 58.3 (OCH_3), 52.5 (CH), 32.1 (CH_2), 31.9 (CH_2), 29.3 (CH_2), 26.8 (CH_2), 22.7 (CH_2), 14.2 (CH_3); LRMS (EI) *m/z* (%) 320 (M^+, 29), 235 (100), 129 (61); HRMS (ESI) calcd for $C_{23}H_{28}O^+$ [$(M+H)^+$] 321.2140, found, 321.2142.



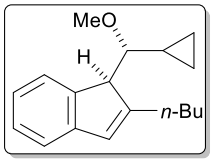
1-(Methoxyheptyl)-2-phenyl-1*H*-indene (4g): yellow oil; R_f = 0.11 (hexane); 89% yield (87 mg), obtained and isolated with d.r. ~ 1/1 starting from a ~ 1/1 mixture of *E*:*Z* diastereoisomers of **3g**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 7.5 Hz, 1H), 7.62–7.22 (m, 17H), 7.14–7.12 (m, 2H), 4.56 (d, *J* = 4.5 Hz, 1H), 4.32 (s, 1H), 3.81–3.74 (m, 5H), 3.37 (s, 3H), 1.56–0.80 (m, 23H), 0.73 (t, *J* = 7.0 Hz, 3H)) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 150.5 (C), 148.3 (C), 145.1 (C), 144.9 (C), 144.84, (C), 144.80 (C), 136.8 (C), 135.7 (C), 129.0 (CH), 128.9 (2 × CH), 128.7 (CH), 128.5 (2 x CH), 127.6 (CH), 127.5 (CH), 127.3 (2 × CH), 127.1 (CH), 127.0 (CH), 126.8 (2 x CH), 125.3 (CH), 124.9 (CH), 124.8 (CH), 123.7 (CH), 121.3 (CH), 121.1 (CH), 83.4 (CH), 82.6 (CH), 58.2 (CH_3), 57.3 (CH_3), 52.5 (CH), 50.6 (CH), 32.0 (CH_2), 31.8 (CH_2), 31.6 (CH_2), 28.7 (CH_2), 26.5 (CH_2), 26.0 (CH_2), 22.7 (CH_2), 22.5 (CH_2), 14.2 (CH_3), 14.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 320 (M^+, 29), 235 (100), 129 (61); HRMS (ESI) calcd. para $C_{23}H_{29}O^+$ [$(M+H)^+$] 321.2140, encontrada 321.2142.



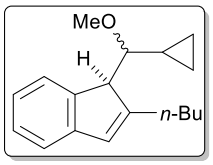
(*R)-1-((*R**)-1-(Cyclohexyl(methoxy)methyl)-2-phenyl-1*H*-indene (4h):** yellow oil; R_f 0.34 (hexane/EtOAc, 100/1); 90% yield (88 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3h**; ^{1}H NMR (300 MHz, $CDCl_3$,) δ 7.55–7.12 (m, 10H), 4.31 (s, 1H), 3.41 (dd, *J* = 9.5, 1.9 Hz, 1H), 3.01 (s, 3H), 2.14–1.85 (m, 6H), 1.25–1.17 (m, 3H), 0.96–0.89 (m, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 150.2 (C), 145.3 (C), 144.4 (C), 136.4 (C), 128.9 (2 x CH), 128.8 (CH), 127.4 (CH), 127.1 (CH), 127.0 (2 x CH), 124.8 (CH), 124.1 (CH), 121.4 (CH), 86.9(CH), 61.0 (OCH_3), 51.3 (CH), 42.3 (CH), 30.7 (CH_2), 30.3 (CH_2), 26.6 (CH_2), 26.4 (CH_2), 26.1 (CH_2) ppm; LRMS (EI) *m/z* (%) 318 (M^+,<1), 243 (26), 204 (100); HRMS (ESI) calcd for $C_{23}H_{26}O^+$ [$(M+H)^+$] 318.1984, found 482.0537.



(*R)-1-((*R**)-1-(Cyclopropyl(methoxy)methyl)-2-phenyl-1*H*-indene (4i):** red oil; R_f = 0.10 (hexane); 85% yield (70 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3i**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67–7.58 (m, 3H), 7.47–7.23 (m, 6H), 7.13 (s, 1H), 4.35 (d, *J* = 2.9 Hz, 1H), 3.28 (s, 3H), 3.10 (dd, *J* = 8.7, 2.9 Hz, 1H), 1.21–1.08 (m, 1H), 0.72–0.58 (m, 1H), 0.49–0.32 (m, 2H), 0.10–0.04 (m, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 150.1 (C), 145.2 (C), 144.9 (C), 136.7 (C), 128.8 (CH), 128.6 (2 x CH), 127.34 (CH), 127.29 (2 x CH), 127.1(CH), 124.7 (CH), 124.1 (CH), 121.3 (CH), 86.6 (CH), 57.9 (OCH_3), 54.6 (CH), 13.6 (CH), 5.6 (CH_2), 1.2 (CH_2) ppm; LRMS (EI) *m/z* (%) 276 (M^+, 10), 189 (20), 85 (100); HRMS (ESI) calcd for $C_{20}H_{20}O^+$ [$(M+H)^+$] 277.1587, found 277.1592.

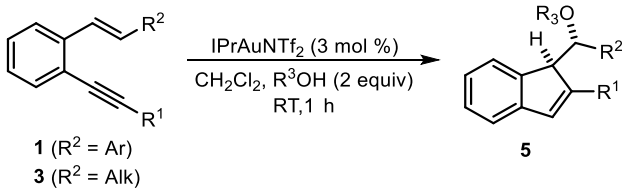


(*S)-2-Butyl-1-((*R**)-(cyclopropyl(methoxy)methyl)-1*H*-indene (4j):** orange oil; R_f = 0.33 (hexane/EtOAc, 100/1); 88% yield (77 mg), obtained and isolated with d.r. >20/1 starting from (*E*)-**3j**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 (d, J = 7.4 Hz, 1H), 7.32–7.23 (m, 2H), 7.15–7.07 (m, 1H), 6.58 (s, 1H), 3.77 (s, 1H), 3.52 (s, 3H), 3.19 (dd, J = 8.6, 3.2 Hz, 1H), 2.70–2.50 (m, 2H), 1.78–1.56 (m, 2H),1.57–1.38 (m, 2H), 1.00 (t, J = 7.3 Hz, 3H), 0.92–0.73 (m, 1H), 0.63–0.44 (m, 1H), 0.41–0.29 (m, 1H), 0.26–0.17 (m, 1H), -0.20–-0.25 (m, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 153.3 (C), 145.6 (C), 144.6 (C), 126.9 (CH), 126.7 (CH), 123.5 (CH), 123.2 (CH), 120.1 (CH), 86.9 (CH), 57.4 (CH_3), 54.7 (CH), 31.2 (CH_2), 30.4 (CH_2), 22.8 (CH_2), 14.2 (CH_3), 11.5 (CH), 4.0 (CH_2), 1.4 (CH_2) ppm; LRMS (EI) *m/z* (%) 256 (M^+, <1), 128 (16), 85 (100); HRMS (ESI) calcd for $C_{18}H_{24}O^+$ [(M+Na)$^+$] 279.1719, found 279.1720.



2-Butyl-1-(cyclopropyl(methoxy)methyl)-1*H*-indene (4j): yellow oil; R_f = 0.25 (hexane/EtOAc, 40/1); 83% yield (77 mg), obtained and isolated with d.r. 1.6/1 starting from a ~ 1.6/1 mixture of *E*:*Z* diastereoisomers of **3j**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, J = 7.4 Hz, 1H, min), 7.35 (d, J = 7.4 Hz, 1H, may), 7.24–7.22 (m, 4H, may + min), 7.12–7.04 (m, 2H, may + min), 6.53 (s, 2H, may + min), 3.79 (d, J = 2.3 Hz, 1H, min), 3.73 (d, J = 2.8 Hz, 1H, may), 3.55 (s, 3H, min), 348 (s, 3H, may), 3.15 (dd, J = 8.6, 2.8 Hz, 1H, may), 3.11 (dd, J = 8.3, 2.3 Hz, 1H, min), 2.58–2.44 (m, 4H, may + min), 1.65–1.60 (m, 4H, may + min), 1.45–1.40 (m, 4H, may + min), 0.98–0.93 (m, 6H, may + min), 0.79–0.75 (m, 1H, may), 0.48–0.40 (m, 2H, may + min), 0.33–0.27 (m, 3H, may + min), 0.17–0.15 (m, 2H, may + min), 0.14–0.12 (m, 1H, min), -0.24–-0.29 (m, 1H, may) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 153.3 (C), 151.1 (C), 145.6 (C), 145.4 (C), 145.2 (C), 144.6 (C), 127.2 (CH), 126.9 (CH), 126.7 (CH), 126.6 (CH), 124.7 (CH), 123.7 (CH), 123.4 (CH), 123.2 (CH), 120.0 (CH), 119.8 (CH), 86.9 (CH), 85.8 (CH), 57.4 (CH_3), 57.3 (CH_3), 54.8 (CH), 54.5 (CH), 31.22 (CH_2), 31.18 (CH_2), 30.4 (CH_2), 30.1 (CH_2), 22.8 (CH_2), 22.7 (CH_2), 14.2 (CH_3), 14.1 (CH_3), 11.5 (CH), 10.9 (CH), 3.9 (CH_2), 2.8 (CH_2), 1.7 (CH_2), 1.4 (CH_2) ppm; LRMS (EI) *m/z* (%) 256 (M^+, <1), 128 (16), 85 (100); HRMS (ESI) calcd for $C_{18}H_{24}O^+$ [(M+Na)$^+$] 279.1719, found 279.1720.

Synthesis and characterization data of alkoxy-functionalized indenes 5:

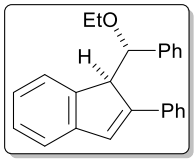


1 (R^2 = Ar)
3 (R^2 = Alk)

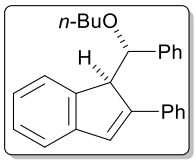
5

The corresponding nucleophile (0.6 mmol) was added to a solution of $IPrAuNTf_2$ (0.009 mmol, 7.8 mg) in CH_2Cl_2 (0.6 mL) and the solution mixture was stirred 5 minutes. A solution of the (*E*)-**1**,**3** (0.3 mmol) in CH_2Cl_2 (0.4 mL) was added subsequently. The resulting reaction mixture was stirred at RT until complete disappearance of the styrene derivate was observed by GC-MS (~1h). The mixture was filtered through a short pad of silica gel using a mixture 100/1 of hexane/EtOAc, the solvent was removed under reduced pressure, and the crude mixture was purified by flash column chromatography on silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding 1-α-alkoxybenzyl-1*H*-indenes **5** in the yields reported in Table 3.

The characterization data of novel compounds are reported below:

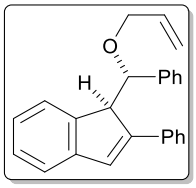


(*R)-1-((*S**)-1-(Ethoxy(phenyl)methyl)-2-phenyl-1*H*-indene (5a):** white oil; R_f = 0.37 (hexane/EtOAc, 50/1); 91% yield (89 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, J = 8.0 Hz, 2H), 7.43–7.05 (m, 13H), 4.88 (d, J = 4.3 Hz, 1H), 4.45 (d, J = 4.2 Hz, 1H), 3.39 (dq, J = 9.0, 7.0 Hz, 1H), 3.21 (dq, J = 9.0, 7.0 Hz, 1H), 1.01 (t, J = 7.0 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 149.3 (C), 144.8 (C), 144.3 (C), 140.5 (C), 136.7 (C), 129.2 (CH), 128.3 (2 x CH), 127.8 (2 x CH), 127.4 (2 x CH), 127.2 (CH), 127.14 (CH), 117.10 (CH), 127.0 (2 x CH), 124.8 (CH), 124.3 (CH), 121.0 (CH), 81.8 (CH), 65.0 (CH), 56.1 (CH_2), 15.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 326 (M^+, 24), 135 (100); HRMS (ESI) calcd for $C_{24}H_{22}O^+$ [$(M+Na)^+$] 327.1743, found 327.1744.

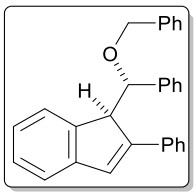


(*R)-1-((*S**)-Butoxy(phenyl)methyl)-2-phenyl-1*H*-indene (5b):** yellow oil; R_f = 0.25 (hexane/EtOAc, 100/1); 86% yield (94 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (d, J = 7.0 Hz, 2H), 7.44–7.14 (m, 12H), 7.03 (s, 1H), 4.90 (d, J = 4.2 Hz, 1H), 4.47 (d, J = 4.2 Hz, 1H), 3.33 (dt, J = 9.4, 6.3 Hz, 1H), 3.15 (dt, J = 9.4, 6.3 Hz, 1H), 1.41–1.27 (m, 4H), 0.86 (t, J = 7.2 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 149.4 (C), 144.9 (C), 144.4 (C), 140.3 (C), 136.8 (C), 129.3 (CH), 128.3 (2 x CH), 127.7 (2 x CH), 127.5 (2 x CH), 127.2 (CH), 127.1 (4 x CH), 124.8 (CH), 124.3 (CH), 121.0 (CH), 82.4 (CH), 69.4 (CH_2), 56.2 (CH), 31.9 (CH_2), 19.4 (CH_2), 14.0

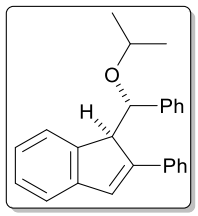
(CH_3) ppm; LRMS (EI) *m/z* (%) 354 (M^+, 38), 163 (85), 107 (100); HRMS (ESI) calcd for $C_{26}H_{26}NaO^+$ [$(M+Na)^+$] 377.1876, found 377.1873.



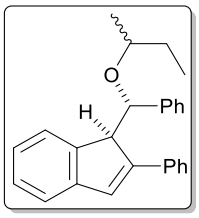
(*R)-1-((*S**)-2-Phenyl-1-(phenyl(vinyloxy)methyl)-1*H*-indene (5c):** yellow oil; R_f = 0.38 (hexane/EtOAc, 50/1); 82% yield (83 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.64 (d, J = 7.6 Hz, 2H), 7.47–7.18 (m, 12H), 7.09 (s, 1H), 5.69 (ddd, J = 22.1, 10.6, 5.4 Hz, 1H), 5.12–5.00 (m, 3H), 4.51 (d, J = 3.8 Hz, 1H), 3.94 (dd, J = 13.1, 4.8 Hz, 1H), 3.73 (dd, J = 13.1, 5.9 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$,) δ 149.2 (C), 144.8 (C), 144.0 (C), 139.9 (C), 136.6 (C), 134.7 (CH), 129.3 (CH), 128.4 (2 x CH), 127.8 (2 x CH), 127.4 (2 x CH), 127.3 (CH), 127.24 (CH), 127.21 (CH), 127.0 (2 x CH), 124.8 (CH), 124.4. (CH), 121.1 (CH), 116.4 (CH_2), 81.0 (CH), 70.2 (CH), 56.1 (CH_2) ppm; LRMS (EI) *m/z* (%) 338 (M^+, 7), 147 (100), 105 (69); HRMS (ESI) calcd for $C_{24}H_{20}O^+$ [$(M+H)^+$] 339.1743, found 339.1748.



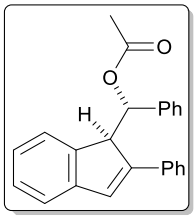
(*R)-1-((*S**)-1-(Benzyloxy)(phenyl)methyl)-2-phenyl-1*H*-indene (5d):** yellow oil; R_f = 0.30 (hexane/EtOAc, 100/1); 71% yield (83 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, J = 7.5 Hz, 2H), 7.44–7.21 (m, 17H), 7.09 (s, 1H), 5.10 (d, J = 4.1 Hz, 1H), 4.54 (dd, J = 19.8, 7.9 Hz, 2H), 4.29 (d, J = 11.9 Hz, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 149.2 (C), 144.8 (C), 144.1 (C), 139.5 (C), 138.4 (C), 136.7 (C), 129.5 (CH), 128.4 (2 x CH), 128.1 (2 x CH), 127.8 (2 x CH), 127.44 (3 x CH), 127.41 (3 x CH), 127.3 (CH), 127.2 (2 x CH), 127.1 (CH), 124.8 (CH), 124.4 (CH), 121.1 (CH), 81.9 (CH), 71.1 (CH), 56.1 (CH_2) ppm; LRMS (EI) *m/z* (%) 388 (M^+, 11), 282 (14), 191 (62), 91 (100); HRMS (ESI) calcd for $C_{29}H_{24}O^+$ [$(M+Na)^+$] 411.1719, found 411.1717.



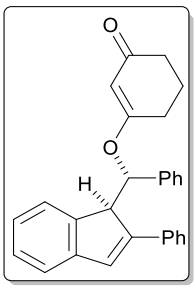
(*R)-1-((*S**)-1-(Isopropoxy(phenyl)methyl)-2-phenyl-1*H*-indene (5e):** white oil; R_f = 0.11 (hexane/EtOAc, 100/1); 80% yield (82 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (d, J = 7.1 Hz, 2H), 7.46–7.27 (m, 10H), 7.14–7.02 (m, 3H), 5.03 (d, J = 4.1 Hz, 1H), 4.42 (d, J = 3.9 Hz, 1H), 3.37 (hept, J = 6.1 Hz, 1H), 1.01 (d, J = 6.2 Hz, 3H), 0.90 (d, J = 6.0 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 149.3 (C), 144.9 (C), 144.4 (C), 141.4 (C), 136.7 (C), 129.2 (CH), 128.4 (2 x CH), 127.7 (2 x CH), 127.4 (2 x CH), 127.14 (CH), 127.10 (2 x CH), 127.07 (CH), 127.0 (CH), 124.9 (CH), 124.2 (CH), 120.9 (CH), 79.3 (CH), 70.1 (CH), 55.4 (CH), 23.1 (CH_3), 21.3 (CH_3) ppm; LRMS (EI) *m/z* (%) 340 (M^+, 9), 191 (26), 149 (46), 107 (100); HRMS (ESI) calcd for $C_{25}H_{24}O^+$ [$(M+H)^+$] 341.1900, found 341.1922.



(*R)-1-((*S**)-*sec*-Butoxy(phenyl)methyl)-2-phenyl-1*H*-indene (5f):** white solid; mp 102−104 ºC; 73% yield (82 mg); obtained with d.r. = 1.1/1 starting from (*E*)-**1a**; isolated with d.r. ~ 1/1 with traces of the other two minor diastereoisomers; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61–7.54 (m, 4H), 7.40–7.33 (m, 16H), 7.19–7.12 (m, 6H), 6.98–6.91 (m, 4H), 5.02−4.98 (m, 2H), 4.40−4.36 (m, 2H), 3.16−3.06 (m, 2H), 1.42-1.19 (m, 4H), 0.87−0.83 (m, 6H), 0.72−0.68 (m, 6H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 149.4 (C), 149.0 (C), 145.0 (C), 144.8 (C), 144.6 (C), 144.4 (C), 142.2 (C), 140.7 (C), 136.9 (C), 136.6 (C), 129.41 (CH), 129.38 (CH), 128.5 (2 x CH), 128.3 (2 x CH), 127.8 (2 x CH), 127.7 (2 x CH), 127.53 (2 x CH), 127.50 (2 x CH), 127.4 (2 x CH), 127.3 (CH), 127.2 (CH), 127.1 (CH), 127.04 (2 x CH), 127.02 (CH), 126.97 (CH), 124.9 (CH), 124.8 (CH), 124.2 (CH), 120.92 (CH), 120.88 (CH), 79.5 (CH), 76.7 (CH), 76.0 (CH), 74.0 (CH), 56.7 (CH), 56.5 (CH), 30.0 (CH_2), 28.6 (CH_2), 19.9 (CH_3), 18.2 (CH_3), 9.8 (CH_3), 9.6 (CH_3) ppm, two aromatic CH do not appear due to overlapping; LRMS (EI) *m/z* (%) 354 (M^+, 8), 191 (20), 163 (38), 107 (100); HRMS (ESI) calcd for $C_{26}H_{26}NaO^+$ [(M+Na)$^+$] 377.1876, found 377.1881.

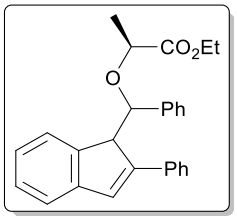


(*R)-1-((*S**)-Phenyl(2-phenyl-1*H*-inden-1-yl)methyl acetate (5g):** white solid; mp 165–167 ºC; 80% yield (88 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; isolated with d.r. = 20/1; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57–7.37 (m, 12H), 7.08–7.04 (m, 2H), 6.98 (s, 1H), 6.46 (d, J = 4.0 Hz, 1H), 4.62 (d, J = 3.8 Hz, 1H), 2.00 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC) δ 169.9 (C), 148.4 (C), 144.7 (C), 143.1 (C), 137.5 (C), 136.5 (C), 130.0 (CH), 128.5 (2 x CH), 127.7 (4 x CH), 127.5 (CH), 127.3 (2 x CH), 126.4 (2 x CH), 124.7 (CH), 124.5 (CH), 121. 2 (CH), 75.9 (CH), 54.3 (CH), 21.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 340 (M^+, 11), 280 (100), 192 (46), 107 (40); HRMS (ESI) calcd for $C_{24}H_{20}O^+$ [(M+Na)$^+$] 363.1356, found 363.1356.

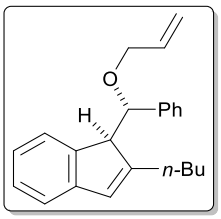


3-((*S)-Phenyl((*R**)-2-phenyl-1*H*-inden-1-yl)methoxy)cyclohex-2-en-1-one (5h):** yellow solid; mp 160–162 ºC; 86% yield (101 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.51 (d, J = 7.2 Hz, 2H), 7.41 (t, J = 7.3 Hz, 2H), 7.36–7.31 (m, 3H), 7.22–7.17 (m, 4H), 7.09 (d, J = 7.4 Hz, 1H), 6.96–6.94 (m, 3H), 5.66 (d, J = 4.0 Hz, 1H), 5.11 (s, 1H), 4.57 (d, J = 3.9 Hz, 1H), 2.35–2.22 (m, 4H), 1.96–1.89 (m, 2H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 199.4 (C), 176.3 (C), 148.1 (C), 144.7 (C), 142.5 (C), 136.3 (C), 136.0 (C), 129.9 (CH), 128.4 (2 x CH), 127.9 (CH), 127.8 (2 x CH), 127.53 (CH), 127.48 (CH), 127.2 (2 x CH), 126.1 (2 x CH), 124.6 (CH), 124.4 (CH), 121.2 (CH), 104.7 (CH), 80.7 (CH), 54.6 (CH), 36.5 (CH_2), 28.6

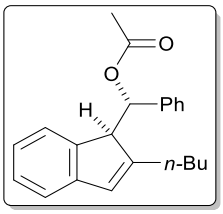
(CH_2), 20.9 (CH_2) ppm; LRMS (EI) *m/z* (%) 392 (M^+, 49), 301 (71), 281 (71), 207 (100); HRMS (ESI) calcd for $C_{28}H_{24}O_2^+$ [$(M+H)^+$] 393.1776, found 393.1774.



Ethyl(*S*)-2-(phenyl(2-phenyl-1H-inden-1-yl)methoxy) propanoate (5i): white oil; R_f = 0.15 (hexane/EtOAc, 100/1); 70% yield (83 mg); obtained with d.r. = 1.4/1 (the other two minor diastereoisomer are observed <10%) starting from (*E*)-**1a**; isolated one of the major diastereosiomers with d.r. = 20/1; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.54–7.50 (m, 2H), 7.39–7.22 (m, 10H), 7.10–7.04 (m, 3H), 4.97 (d, *J* = 4.1 Hz, 1H), 4.44 (d, *J* = 4.1 Hz, 1H), 3.89 (dtt, *J* = 10.7, 7.1, 3.6 Hz, 2H), 3.75 (q, *J* = 6.7 Hz, 1H), 1.16 (d, *J* = 6.7 Hz, 3H), 1.03 (t, *J* = 7.1 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$, 25 ºC) δ 172.7 (C), 148.8 (C), 144.7 (C), 144.1 (C), 140.2 (C), 136.3 (C), 129.6 (CH), 128.6 (2 x CH), 127.8 (2 x CH), 127.4 (CH), 127.3 (CH), 127.2 (4 x CH), 125.1 (CH), 124.5 (CH), 121. 1 (CH), 81.9 (CH), 74.6 (CH), 60.6 (CH_2), 56.1 (CH), 17.8 (CH_3), 13.9 (CH_3) ppm, one aromatic CH does not appear due to overlapping; LRMS (EI) *m/z* (%) 398 (M^+, 4), 207 (100); HRMS (ESI) calcd for $C_{24}H_{20}O^+$ [$(M+H)^+$] $C_{27}H_{26}NaO_3^+$ [$(M+Na)^+$] 421.1774, found 421.1773.

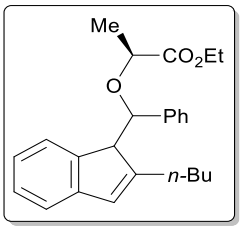


(*S)-1-((*S**)-(Allyloxy)(phenyl)methyl)-2-butyl-1*H*-indene (5j):** yellow oil; R_f = 0.20 (hexane/EtOAc, 40/1); 84% yield (89 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1h**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30–7.15 (m, 8H), 7.13–7.04 (m, 1H), 6.41 (s, 1H), 6.00–5.87 (m, 1H), 5.32–5.16 (m, 1H), 5.18 (d, *J* = 10.4 Hz, 1H), 4.75 (d, *J* = 5.5 Hz, 1H), 4.06–3.88 (m, 2H), 3.84 (d, *J* = 5.5 Hz, 1H), 2.35–2.25 (m, 2H), 1.55–1.49 (m, 2H), 1.34–1.29 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 151.8 (C), 145.1 (C), 144.4 (C), 139.6 (C), 135.0 (CH), 127.92 (CH), 127.88 (2 x CH), 127.6 (CH), 127.3 (2 x CH), 126.9 (CH), 124.5 (CH), 123.5 (CH), 119.9 (CH), 116.5 (CH_2), 82.4 (CH), 69.9 (CH), 56.9 (CH_2), 31.4 (CH_2), 30.6 (CH_2), 22.7 (CH_2), 14.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 318 (M^+, 2), 147 (100), 105 (63); HRMS (ESI) calcd for $C_{23}H_{26}NaO^+$ [$(M+Na)^+$] 341.1876, found 341.1876.

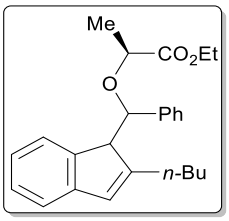


(*S)-((*S**)-2-Butyl-1H-inden-1-yl)(phenyl)methyl acetate (5k):** yellow solid; mp 101–103 ºC; 71% yield (93 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1h**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.30–7.28 (m, 3H), 7.22–7.18 (m, 4H), 7.04–7.02 (m, 2H), 6.47 (s, 1H), 6.39 (d, *J* = 4.6 Hz, 1H), 3.87 (d, *J* = 4.6 Hz, 1H), 2.48–2.40 (m, 2H), 2.10 (s, 3H), 1.62–1.55 (m, 2H), 1.47–1.33 (m, 2H), 0.95 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 170.0 (C), 150.7 (C), 145.2 (C), 142.9 (C), 138.2 (C), 128.4 (CH), 128.1 (2 x CH), 127.8 (CH), 127.2 (2 x CH), 126.4 (CH), 124.2 (CH), 123.7 (CH), 120.1 (CH), 75.3 (CH), 55.6 (CH), 31.3 (CH_2), 30.2 (CH_2), 22.7 (CH_2), 21.2

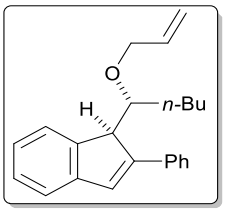
(CH_3), 14.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 320 (M^+, 2), 260 (100), 107 (78); HRMS (ESI) calcd for $C_{22}H_{24}NaO_2^+$ [$(M+Na)^+$] 343.1669, found 343.1667.



Ethyl(*S*)-2-(2-butyl-1*H*-inden-1-yl)(phenyl)methoxy)propanoate (5l): yellow oil; R_f = 0.15 (hexane/EtOAc, 40/1); 78% yield (90 mg); obtained with d.r. = 1.5/1 mixture of two major diastereoisomers (the other two minor diastereoisomer are observed <10%) starting from (*E*)-**1h**. Isolated one of the major diastereoisomers with d.r. >20/1; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, *J* = 7.0 Hz, 1H), 7.17–7.13 (m, 4H), 7.08–7.04 (m, 4H), 6.34 (s, 1H), 4.93 (d, *J* = 5.5 Hz, 1H), 4.26–4.14 (m, 2H), 3.98 (d, *J* = 5.5 Hz, 1H), 3.91 (q, *J* = 6.8 Hz, 1H), 2.39 (t, *J* = 8.6 Hz, 2H), 1.63–1.41 (m, 5H), 1.32–1.23 (m, 5H), 0.91 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 173.4 (C), 152.0 (C), 145.0 (C), 144.2 (C), 138.2 (C), 128.2 (CH), 127.8 (CH), 127.7 (2 x CH), 127.4 (2 x CH), 126.8 (CH), 124.4 (CH), 123.5 (CH), 119.8 (CH), 83.1 (CH_2), 72.4 (CH), 60.8 (CH), 56.7 (CH), 31.5 (CH_2), 31.1 (CH_2), 22.8 (CH_2), 19.0 (CH_3), 14.3 (CH_3) , 14.1 (CH_3) ppm; LRMS (EI) *m/z* (%) 378 (M^+, <1), 260 (52), 218 (90), 207 (100); HRMS (ESI) calcd for $C_{25}H_{30}NaO_3^+$ [$(M+Na)^+$] 401.2087, found 401.2095.

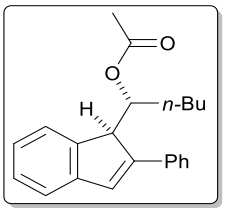


Ethyl(*S*)-2-(2-butyl-1*H*-inden-1-yl)(phenyl)methoxy)propanoate (diast-5l): yellow oil; R_f = 0.12 (hexane/EtOAc, 40/1); 84% yield (90 mg); obtained with d.r. = 1/1.5 mixture of two major diastereoisomers starting from (*E*)-**1h**. Isolated the other major diastereoisomer with d.r. 17/1; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.3 Hz, 1H), 7.20–7.07 (m, 8H), 6.40 (s, 1H), 4.67 (d, *J* = 6.2 Hz, 1H), 4.04–3.94 (m, 3H), 3.86 (d, *J* = 6.2 Hz, 1H), 2.27–2.19 (m, 1H), 2.15–2.06 (m, 1H), 1.41–1.27 (m, 5H), 1.25–1.22 (m, 2H), 1.14 (t, *J* = 7.1 Hz, 3H), 0.86 14 (t, *J* = 7.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 173.0 (C), 151.7 (C), 144.9 (C), 144.7 (C), 139.2 (C), 128.4 (CH), 127.9 (CH), 127.72 (2 x CH), 127.67 (2 x CH), 126.9 (CH), 124.7 (CH), 123.6 (CH), 119.9 (CH), 83.2 (CH_2), 73.9 (CH), 60.8 (CH), 56.7 (CH), 31.5 (CH_2), 30.7 (CH_2), 22.7 (CH_2), 18.1 (CH_3), 14.1 (CH_3) , 14.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 378 (M^+, <1), 260 (26), 218 (31), 207 (100). HRMS (ESI) calcd for $C_{25}H_{30}NaO_3^+$ [$(M+Na)^+$] 401.2087, found 401.2094.

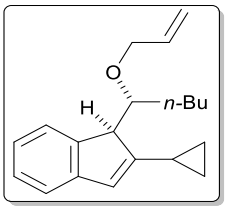


(*R)-1-((*R**)-1-(Allyloxy)pentyl)-2-phenyl-1*H*-indene (5m):** yellow oil; R_f = 0.19 (hexane/EtOAc, 40/1); 72% yield (88 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60–7.50 (m, 2H), 7.48 (d, *J* = 7.3 Hz, 1H), 7.42–7.37 (m, 3H), 7.32–7.29 (m, 2H), 7.23–7.18 (m, 1H), 7.09 (s, 1H), 5.81–5.75 (m, 1H), 5.13–5.07 (m, 2H), 4.28 (s, 1H), 4.12–3.89 (m, 3H), 1.54–1.36 (m, 2H), 1.28–1.21 (m, 4H), 0.82 (t, *J* = 7.0 Hz, 3H) ppm; ^{13}C{^{1}H} NMR

(75 MHz, $CDCl_3$) δ 150.4 (C), 145.0 (C), 144.9 (C), 136.8 (C), 125.2 (CH), 129.0 (2 x CH), 128.5 (2 x CH), 127.4 (CH), 127.1 (CH), 124.8 (CH), 123.7 (CH), 121.2 (CH), 116.9 (CH_2), 80.5 (CH_2), 71.1 (CH), 53.0 (CH), 31.9 (CH_2), 28.9 (CH_2), 22.7 (CH_2), 14.1 (CH_3) ppm, un CH aromático no aparece debido al solapamiento; LRMS (EI) *m/z* (%) 318 (M^+, 23), 191 (100), 127 (67), 85 (66); HRMS (ESI) calcd for $C_{23}H_{26}NaO^+$ [$(M+Na)^+$] 341.1876, found 341.1882.

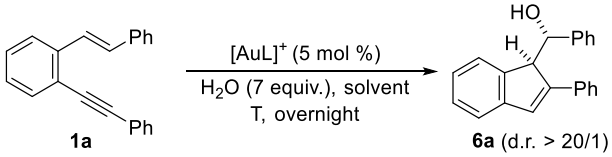


(*S)(R)-1-((R)-2-phenyl-1H-inden-1-yl)pentyl acetate (5n):** yellow solid; mp 101−103 ºC; 79% yield (72 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56 (d, J = 7.3 Hz, 1H), 7.48–7.41 (m, 2H), 7.38–7.36 (m, 3H), 7.33–7.24 (m, 2H), 7.22–7.19 (m, 1H), 7.01 (s, 1H), 5.42 (d, J = 9.5, 3.0 Hz, 1H), 4.40 (d, J = 3.0 Hz, 1H), 1.92 (s, 3H), 1.15–1.12 (m, 1H), 1.10–1.04 (m, 5H), 0.74 (t, J = 6.7 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 170.9 (C), 149.6 (C), 144.5 (C), 144.0 (C), 137.2 (C), 130.0 (CH), 128.4 (2 x CH), 127.52 (3 x CH), 127.48 (CH), 125.2 (CH), 123.7 (CH), 121.2 (CH), 75.4 (CH), 53.1 (CH), 28.8 (CH_2), 28.3 (CH_2), 22.3 (CH_2), 21.2 (CH_3), 13.9 (CH_3) ppm; LRMS (EI) *m/z* (%) 320 (M^+, 8), 260 (100), 204 (78), 43 (64); HRMS (ESI) calcd for $C_{22}H_{24}NaO_2^+$ [$(M+Na)^+$] 343.1669, found 343.1670.



(*S)-1-((*R**)-1-(Allyloxy)pentyl)-2-cyclopropyl-1*H*-indene (5o):** yellow oil; R_f = 0.30 (hexane/EtOAc, 40/1); 82% yield (77 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3f**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27–7.24 (m, 1H), 7.20–7.18 (m, 2H), 7.09–7.04 (m, 1H), 6.23 (s, 1H), 6.03 (ddt, J = 16.3, 11.2, 5.6 Hz, 1H), 5.36 (dd, J = 16.3, 1.3 Hz, 1H), 5.22 (dd, J = 11.2, 1.3 Hz, 1H), 4.37 (dd, J = 12.7, 5.6 Hz, 1H), 4.16 (dd, J = 12.7, 5.6 Hz, 1H), 3.99 (dt, J = 9.1, 3.0 Hz, 1H), 3.83 (d, J = 3.0 Hz, 1H), 1.96–1.90 (m, 1H), 1.44–1.38 (m, 2H), 1.18–1.12 (m, 3H), 0.91–0.75 (m, 7H), 0.58–0.53 (m, 1H) ppm; ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$) δ 156.3 (C), 145.3 (C), 144.4 (C), 135.5 (CH), 126.8 (CH), 123.6 (CH), 122.5 (2 x CH), 120.0 (CH), 116.8 (CH_2), 81.2 (CH_2), 70.6 (CH), 54.4 (CH), 29.9 (CH_2), 29.0 (CH_2), 22.6 (CH_2), 14.1 (CH_3), 11.2 (CH), 10.2 (CH_2), 9.0 (CH_2), ppm; LRMS (EI) *m/z* (%) 282 (M^+, 18), 127 (92), 85 (100), 41 (55); HRMS (ESI) calcd for $C_{20}H_{27}O^+$ [$(M+H)^+$] 283.2056, found 283.2055.

Effect of gold catalyst on hydroxycyclization of 1a

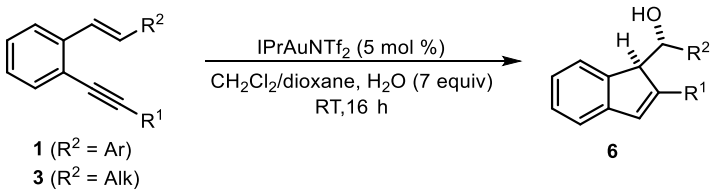


1a (*E*/*Z*)	[AuL]$^+$	Solvent	T (ºC)	Conversion (%)	Isolated yield (%)	**6a** (d.r.)
1/1	$IPrAuNTf_2$	CH_2Cl_2	RT	0	–	–
1/1	$IPrAuNTf_2$	DCE	80	–[b]	–	–
1/1	$IPrAuNTf_2$	CH_2Cl_2/dioxane (1/1)	RT	100	90	1/1
1/1	$IPrAuNTf_2$	DCE/dioxane (1/1)	80	–[b]	–	–
1/0	$IPrAuNTf_2$	CH_2Cl_2/dioxane (1/1)	RT	100	88	1/0
1/0	$Ph_3PAuNTf_2$	CH_2Cl_2/dioxane (1/1)	RT	0	–	–
1/0	$(PhO)_3PAuCl/AgSbF_6$	CH_2Cl_2/dioxane (1/1)	RT	0	–	–

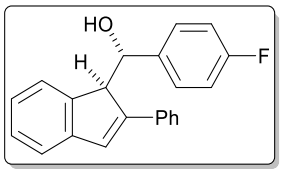
[a]Reactions conducted using **1a** (0.1 mmol) in the corresponding solvent or solvent mixture (0.8 mL). [b]Decomposition.

Synthesis and characterization data of hydroxy-functionalized indenes 6:

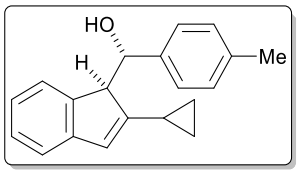
Water (2.2 mmol, 0.04 mL) was added to a solution of $IPrAuNTf_2$ (0.015 mmol, 13 mg) in a mixture of CH_2Cl_2 (0.4 mL) and dioxane (0.4 mL). After stirring at RT for 5 min, the corresponding starting *o*-(alkynyl)styrene **1**,**3** (0.3 mmol) was added in 0.8 mL of the same mixture of solvents and the resulting mixture was stirred overnight (complete consumption of starting material was confirmed by GC-MS). The mixture was diluted with water and extracted with CH_2Cl_2 (3 × 5 mL). The solvent was removed under reduced pressure, and the crude mixture was purified by flash column chromatography on deactivated silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding 1-α-hydroxybenzyl and 1-α-hydroxyalkyl-1*H*-indenes **6** in the yields reported in Table 3.



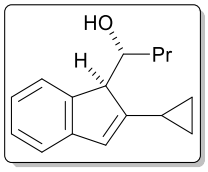
The characterization data of novel compounds are reported below:



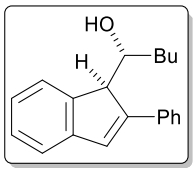
(*S)-(4-Fluorophenyl)((*R**)-2-phenyl-1*H*-inden-1-yl)methanol (6a):** yellow solid; mp 125−127 ºC; 62% yield (69 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, J = 7.1 Hz, 2H), 7.49–7.44 (m, 2H), 7.39−7.29 (m, 5H), 7.13 (s, 1H), 7.10−7.04 (m, 3H), 6.62 (d, J = 7.5 Hz, 1H), 5.33 (d, J = 2.5 Hz, 1H), 4.44 (d, J = 2.5 Hz, 1H), 1.58 (s, 1H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 162.1 (d, J = 245.1 Hz, C), 184.4 (C), 145.2 (C), 142.1 (C), 138.1 (d, J = 3.0 Hz, C), 135.3 (C), 129.6 (CH), 129.0 (2 x CH), 127.9 (CH), 127.8 (CH), 127.6 (CH), 127.5 (CH), 127.1 (2 x CH), 124.8 (d, J = 5.7 Hz, 2 x CH), 121.5 (CH), 115.0 (d, J = 21.3 Hz, 2 x CH) 72.4 (CH), 56.9 (CH) ppm; LRMS (EI) *m/z* (%) 316 (M^+, <1), 192 (100), 165 (18); HRMS (ESI) calcd for $C_{22}H_{16}F^+$ [$(M+H)^+(-H_2O)$] 299.1231, found 299.1237.



(*S)-((*S**)-2-Cyclopropyl-1H-inden-1-yl)(p-tolyl)methanol (6b):** yellow solid; mp 93−95 ºC; 74% yield (61 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1m**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (d, J = 8.1 Hz, 2H), 7.22–7.17 (m, 4H), 6.95−6.87 (m, 1H), 6.59 (d, J = 7.48 Hz, 1H), 6.32 (s, 1H), 5.48−5.45 (m, 1H), 3.92 (d, J = 3.5, 1H), 2.40 (s, 3H), 1.68–1.63 (m, 1H), 1.53 (d, J = 6.3 Hz, 1H), 0.95–0.89 (m, 2H), 0.72–0.70 (m, 2H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 153.8 (C), 145.7 (C), 142.0 (C), 139.8 (C), 136.9 (C), 129.0 (2 x CH), 127.4 (CH), 126.0 (2 x CH), 124.7 (CH), 124.2 (CH), 123.6 (CH), 120.3 (CH), 72.8 (CH), 59.9 (CH), 21.3 (CH_3), 10.6 (CH), 9.2 (CH_2), 8.0 (CH_2) ppm; LRMS (EI) *m/z* (%) 276 (M^+, <1), 156 (100), 141 (98), 115 (99); HRMS (ESI) calcd for $C_{20}H_{19}^+$ [$(M+H)^+(-H_2O)$] 259.1481, found 259.1484.



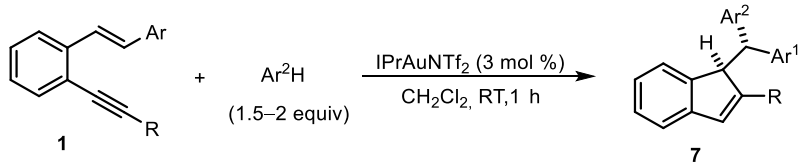
(*R)-1-((*S**)-2-Cyclopropyl-1*H*-inden-1-yl)butan-1-ol (6c):** yellow solid; mp 98-100 ºC; 63% yield (46 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3d**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.40 (d, J = 7.4 Hz, 1H), 7.28–7.23 (m, 2H), 7.15−7.09 (m, 3H), 6.32 (s, 1H), 4.38 (dd, J = 8.7, 3.2 Hz, 1H), 3.66 (d, J = 3.2 Hz, 1H), 1.75−1.47 (m, 5H), 1.37 (s, 1H), 1.00−0.95 (m, 5H), 0.75−0.71 (m, 2H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 154.5 (C), 145.7 (C), 142.9 (C), 127.2 (CH), 123.82 (CH), 123.77 (CH), 123.6 (CH), 120.7 (CH), 72.4 (CH), 58.6 (CH), 36.7 (CH_2), 20.0 (CH_2), 14.1 (CH_3), 10.8 (CH), 9.4 (CH_2), 8.1 (CH_2) ppm; LRMS (EI) *m/z* (%) 228 (M^+, 16), 156 (100), 141 (85); HRMS (ESI) calcd for $C_{16}H_{21}O^+$ [$(M+H)^+$] 229.1587, found 229.1591.



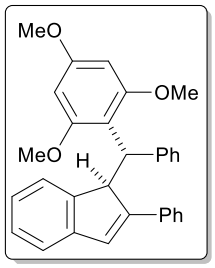
((*R)-1-((*R**)-2-Phenyl-1*H*-inden-1-yl)pentan-1-ol (6d):** uncolourless oil; R_f = 0.12 (hexane/EtOAc, 20/1); 68% yield (83 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**3e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59–7.52 (m, 3H), 7.46–7.40 (m, 3H), 7.35–7.30 (m, 2H), 7.22 (td, J = 7.40, 1.2 Hz, 1H), 7.12 (s, 1H), 4.24 (s, 1H), 4.19–4.14 (m, 1H), 1.67–1.62 (m, 2H),1.50–1.35 (m, 4H), 1.16 (s, 1H), 0.91 (t, J = 7.1 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 149.5 (C), 145.3 (C), 143.4 (C), 135.9 (C), 129.1 (CH), 128.9 (2 x CH), 127.8 (CH), 127.5 (CH), 127.3 (2 x CH), 124.9 (CH), 124.4 (CH), 121.5 (CH), 72.7 (CH), 55.5 (CH), 34.8 (CH_2), 28.9 (CH_2), 22.7 (CH_2), 14.2 (CH_3) ppm; LRMS (EI) *m/z* (%) 278 (M^+, <1), 192 (100), 165 (20); HRMS (ESI) calcd for $C_{20}H_{22}NaO^+$ [$(M+Na)^+$] 301.1563, found 301.1567.

Synthesis and characterization data of 1-diarylmethyl-1*H*-indenes 7:

The corresponding aromatic compound (0.45–0.6 mmol) was added to a solution of $IPrAuNTf_2$ (0.09 mmol, 7.8 mg) in CH_2Cl_2 (0.6 mL) and the solution mixture was stirred 5 minutes. A solution of the (*E*)-**1** (0.3 mmol, 0.084 g) in CH_2Cl_2 (0.4 mL) was added subsequently. The resulting reaction mixture was stirred at RT until complete disappearance of the styrene derivate was observed by GC-MS (~1h). The mixture was filtered through a short pad of silica gel using a mixture 100/1 of hexane/EtOAc, the solvent was removed under reduced pressure, and the crude mixture was purified by flash column chromatography on silica gel using mixtures of hexane and EtOAc as eluents to obtain the corresponding 1-diarylmethyl-1*H*-indenes **7** in the yields reported in Scheme 4.

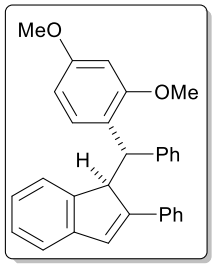


The characterization data of novel compounds are reported below:

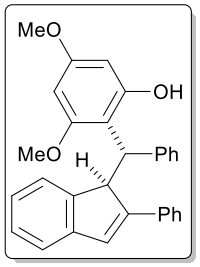


(*R)-1-[(*S**)-(2,4,6-Trimethoxyphenyl)(phenyl)methyl]-2-phenyl-1*H*-indene (7a):** yellow solid; mp 158–160 ºC; 84% yield (134 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1a**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42–7.40 (m, 3H), 7.37–7.11 (m, 9H), 6.98 (t, J = 7.5 Hz, 3H), 6.93 (s, 1H), 6.73 (d, J = 7.6 Hz, 1H), 6.04 (s, 1H), 5.26 (d, J = 9.0 Hz, 1H), 5.08 (d, J = 9.0 Hz, 1H), 3.84 (s, 3H), 3.40 (s, 6H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.7 (C), 159.5 (C), 152.8 (C), 148.7 (C), 144.0 (C), 142.9 (C), 137.6 (C), 129.3 (CH), 128.4 (CH), 127.7 (2 ×

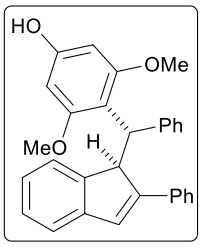
CH), 127.6 (2 × CH), 127.3 (2 × CH), 126.1 (CH), 1260 (CH), 125.6 (CH), 124.5 (CH), 124.0 (CH), 120.5 (CH), 111.2 (2 × C), 90.4 (2 × CH), 55.2 (CH_3), 55.2 (2 × CH_3), 52.6 (CH), 43.4 (CH) ppm, one aromatic CH signal does not appear due to overlapping ; LRMS (EI) *m/z* (%) 448 (M^+, 42), 281 (57), 257 (49), 207 (100); HRMS (ESI) calcd for $C_{31}H_{29}O_3^+$ [$(M+H)^+$] 449.2111, found: 449.2110.



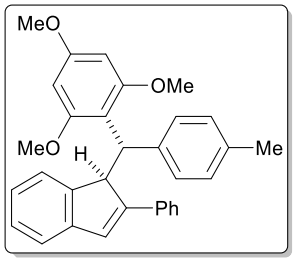
(*R)-1-[(*S**)-(2,4-Dimethoxyphenyl)(phenyl)methyl]-2-phenyl-1*H*-indene (7b):** orange oil; R_f = 0.26 (hexane/EtOAc, 100/1); 76% yield (94 mg); obtained with d.r. >8/1 starting from (*E*)-**1a**; isolated with d.r. ~ 11/1 along with trace amounts of starting 1,3-dimethoxybenzene. Data for the *(R*,S*)* diastereoisomer; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.42–7.25 (m, 12H), 6.81 (s, 1H), 6.61 (d, J = 7.6 Hz, 1H), 6.16–6.11 (m, 2H), 6.02 (d, J = 7.6, Hz, 1H), 5.50 (d, J = 5.3 Hz, 1H), 4.79 (d, J = 5.3 Hz, 1H), 3.69 (s, 3H), 3.12 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.2 (C), 158.1 (C), 151.4 (C), 146.0 (C), 145.3 (C), 143.3 (C), 136.5 (C), 129.5 (CH), 129.0 (2 × CH), 128.33 (2 × CH), 128.28 (2 × CH), 127.9 (CH), 127.3 (2 × CH), 127.0 (2 × CH), 126.2 (CH), 124.7 (CH), 124.3 (CH), 121.1 (CH), 119.6 (C), 103.1 (CH), 97.9 (CH), 55.2 (OCH_3), 55.0 (OCH_3), 54.5 (CH), 41.2 (CH) ppm; LRMS (EI) *m/z* (%) 418 (M^+, 58), 227 (100); HRMS (ESI) calcd for $C_{30}H_{26}O_2Na^+$ [$(M+Na)^+$] 441.1825, found: 441.1826.



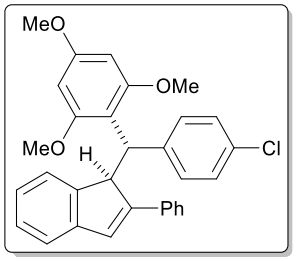
3,5-Dimethoxy-2-{(S*)-phenyl[(R*)-2-phenyl-1H-inden-1-yl]methyl}phenol (7c): white oil; R_f = 0.28 (hexane/EtOAc, 100/1); 45% yield (59 mg); obtained as a ~ 2/1 mixture of regioisomers with d.r. >20/1 starting from (*E*)-**1a**; isolated as a single regioisomer with d.r. >20/1; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35–7.08 (m, 12H), 6.94 (td, J = 7.5, 1.2 Hz, 1H), 6.89 (s, 1H), 6.68 (d, J = 7.5 Hz, 1H), 5.90 (s, 2H), 5.20 (d, J = 9.0 Hz, 1H), 5.03 (d, J = 9.0 Hz, 1H), 3.79 (s, 1H), 3.31 (s, 6H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.7 (C), 159.2 (C), 157.0 (C), 152.2 (C), 145.8 (C), 145.5 (C), 140.7 (C), 136.4 (C), 128.8 (2 × CH), 128.7 (2 × CH), 128.3 (2 × CH), 128.0 (CH), 127.4 (2 × CH), 127.1 (CH), 126.7 (CH), 125.1 (CH), 124.1 (CH), 121.9 (CH), 106.0 (C), 93.9 (CH), 90.9 (CH), 55.1 (CH_3), 55.0 (CH_3), 52.7 (CH), 40.6 (CH) ppm, one aromatic CH signal does not appear due to overlapping; LRMS (EI) *m/z* (%) 434 (M^+, 100), 243 (82); HRMS (ESI) calcd for $C_{30}H_{27}O_3^+$ [$(M+H)^+$] 435.1955, found 435.1955.



3,5-Dimethoxy-4-((S)-phenyl((R)-2-phenyl-1H-inden-1-yl)methyl)phenol (7'c): yellow oil; R_f = 0.28 (hexane/AcOEt, 100/1); 23% yield (26 mg); obtained as a ~ 2/1 mixture of regioisomers with d.r. >20/1 starting from (*E*)-**1a**; isolated as a single regioisomer with d.r. >20/1 slightly contaminated with trimethoxybenzene; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 2H), 7.43–7.28 (m, 10H), 7.02 (td, *J* = 7.5, 1.2 Hz, 1H), 6.92 (s, 1H), 6.80 (d, *J* = 7.5 Hz, 1H), 5.82–5.79 (m, 3H), 5.13 (d, *J* = 6.8 Hz, 1H), 4.19 (s, 1H), 3.71 (s, 3H), 3.11 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.6 (C), 155.7 (C), 152.7 (C), 148.6 (C), 144.0 (C), 142.9 (C), 137.6 (C), 129.3 (2 x CH), 128.4 (CH), 127.7 (2 × CH), 127.6 (2 × CH), 127.3 (2 x CH), 126.1 (CH), 126.0 (CH), 125.7 (CH), 1254.5 (CH), 124.0 (CH), 120.5 (CH), 110.9 (C), 94.3 (C), 91.8 (2 x CH), 55.1 (2 x CH_3), 52.6 (CH), 43.3 (CH) ppm; LRMS (EI) *m/z* (%) 434 (M^+, 100), 243 (82); HRMS (ESI) calcd for $C_{30}H_{27}O_3^+$ [$(M+H)^+$]

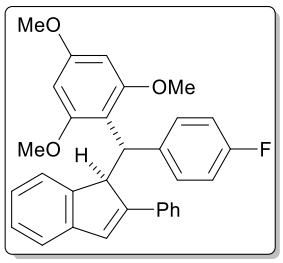


(*R)-2-Phenyl-1-((*S**)-*p*-tolyl(2,4,6-trimethoxyphenyl)methyl)-1*H*-indene (7d):** yellow solid; mp 167−169 ºC; 80% yield (120 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1b**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 (d, *J* = 7.4 Hz, 1H), 7.23–7.10 (m, 8H), 6.95–6.96 (m, 4H), 6.68 (d, *J* = 7.4 Hz, 1H), 5.96 (s, 2H), 5.17 (d, *J* = 8.9 Hz, 1H), 5.00 (d, *J* = 8.9 Hz, 1H), 3.78 (s, 3H), 3.32 (s, 6H), 2.23 (s, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.7 (C), 159.6 (C), 152.9 (C), 148.8 (C), 144.0 (C), 139.9 (C), 137.7 (C), 134.9 (C), 129.2 (2 x CH), 128.32 (2 x CH), 128.29 (CH), 127.7 (2 × CH), 127.3 (2 x CH), 125.94 (CH), 125.90 (CH), 124.5 (CH), 124.0 (CH), 120.5 (CH), 111.4 (2 × C), 90.4 (2 × CH), 55.3 (2 × CH_3), 55.1 (CH_3), 52.9 (CH), 43.0 (CH), 21.0 (CH_3) ppm; LRMS (EI) *m/z* (%) 462 (M^+, 100), 271 (92); HRMS (ESI) calcd for $C_{32}H_{31}O_3^+$ [$(M+H)^+$] 463.2268, found 463.2272.

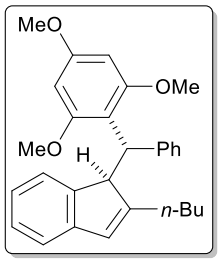


(*R)-1-((*S**)-(4-Chlorophenyl)(2,4,6-trimethoxyphenyl)methyl)-2-phenyl-1*H*-indene (7e):** yellow solid; mp 189–191 ºC; 83% yield (123 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1d**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.4 Hz, 1H), 7.20–7.10 (m, 8H), 6.96–6.89 (m, 4H), 6.69 (d, J = 7.4 HZ, 1H), 6.03 (s, 2H), 5.20 (d, *J* = 9.4 Hz, 1H), 4.80 (d, *J* = 9.4 Hz, 1H), 3.80 (s, 3H), 3.44 (s, 6H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 160.0 (C), 159.4 (C), 152.8 (C), 148.3 (C), 143.9 (C), 141.7 (C), 137.6 (C), 131.2 (C), 130.8 (2 x CH), 138.7 (CH), 127.8 (2 x CH), 127.5 (2 × CH), 127.3 (2 x CH), 126.3 (CH), 126.1 (CH), 124.4 (CH), 124.2 (CH), 120.7 (CH), 111.3 (2 × C), 90.7 (2 × CH), 55.3 (CH_3),

55.2 (2 × CH_3), 52.4 (CH), 43.6 (CH) ppm; LRMS (EI) *m/z* (%) 482 (M^+, 82), 291 (100), 125 (42); HRMS (ESI) calcd for $C_{31}H_{28}ClO_3^+$ [$(M+H)^+$] 483.1721, found 483.1723.



(*R)-1-((*S**)-(4-Fluorophenyl)(2,4,6-trimethoxyphenyl)methyl)-2-phenyl-1*H*-indene (7f):** yellow solid; mp 130−132 ºC; 74% yield (95 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1e**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (d, J = 7.4 Hz, 1H), 7.28–7.10 (m, 8H), 6.97–6.91 (m, 2H), 6.71–6.65 (m, 3H), 6.06 (s, 2H), 5.23 (d, J = 9.7 Hz, 1H), 4.79 (d, J = 9.7 Hz, 1H), 3.82 (s, 3H), 3.49 (s, 6H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 161.8 (d, J = 243.0 Hz, C), 159.9 (C), 159.4 (C), 153.0 (C), 148.4 (C), 143.9 (C), 138.8 (d, J = 3.0 Hz, C), 137.7 (C), 130.9 (CH), 130.8 (CH), 128.6 (CH), 127.7 (2 × CH), 127.3 (2 x CH), 126.2 (d, J = 8.1 Hz, 2 x CH), 124.3 (CH), 124.2 (CH), 120.7 (CH), 114.1 (d, J = 20.9 Hz, 2 x CH), 111.8 (2 × C), 90.7 (2 × CH), 55.3 (3 × CH_3), 52.5 (CH), 43.5 (CH) ppm; LRMS (EI) *m/z* (%) 466 (M^+, 75), 467 (25), 275 (100), 109 (51); HRMS (ESI) calcd for $C_{31}H_{28}FO_3^+$ [$(M+H)^+$] 467.2017, found 467.2023.



(*S)-2-Butyl-1-((*S**)-phenyl(2,4,6-trimethoxyphenyl)methyl)-1*H*-indene (7g):** white solid; mp 126−128 ºC; 83% yield (106 mg); obtained and isolated with d.r. >20/1 starting from (*E*)-**1h**; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, J = 7.8 Hz, 2H), 7.30–7.09 (m, 5H), 6.81 (t, J = 7.5 Hz, 3H), 6.50 (d, J = 7.5 Hz, 1H), 6.47 (s, 1H), 6.15 (s, 2H), 4.77 (d, J = 11.1 Hz, 1H), 4.45 (d, J = 11.1 Hz, 1H), 3.83 (s, 3H), 3.69 (s, 6H), 1.84–1.81 (m, 1H), 1.79–1.65 (m, 1H), 1.16–1.14 (m, 2H), 1.11–1.09 (m, 2H), 0.81 (t, J = 7.3 Hz, 3H) ppm; ^{13}C{^{1}H} NMR (75.4 MHz, $CDCl_3$) δ 159.7 (C), 159.1 (C), 156.3 (C), 147.6 (C), 144.7 (C), 144.6 (C), 129.0 (2 x CH), 127.9 (2 x CH), 126.2 (CH), 126.0 (2 × CH), 124.3 (CH), 123.2 (CH), 119.5 (CH), 93.0 (2 x C), 91.4 (2 x CH), 55.7 (2 x CH_3), 55.3 (CH_3), 52.1 (CH), 44.0 (CH), 31.4 (CH_2), 31.0 (CH_2), 22.7 (CH_2), 14.0 (CH_3) ppm, one aromatic CH signal does not appear due to overlapping ; LRMS (EI) *m/z* (%) 428 (M^+, 12), 261 (65), 257 (100), 217 (64); HRMS (ESI) calcd for $C_{29}H_{33}O_3^+$ [$(M+H)^+$] 429.2424, found 429.2430.

Computational Part

Computational methods:

Geometries of the molecules were optimized by using the M06 meta-hybrid functional[1] in combination with the Def2-SVP[2] basis set. Solvent effects were calculated with the PCM continuum solvation model[3] for dichloromethane. This method was applied previously in related reactions.[4] The nature of minimum and transition structure of all stationary points was confirmed by frequency analysis at the same level of theory. The wave function stability was confirmed in all stationary points.[5] All calculations were performed using the ultrafine grid implemented in Gaussian 09 E.01.[6] Note that racemic mixtures of **4** and **diast-4** are experimentally obtained.

Thermochemical analysis of the plausible final products:

We carried out an initial thermochemical stability study of all the plausible products which would form in the proposed and computed mechanistic routes. The calculation of the Gibbs reaction energy (Δ*G*rxn) was performed taking the most stable **3** (Alk = R= Me) stereoisomer as reactant, in this case that showing the (*E*) configuration at the C-C double bond. Note that racemic mixtures of **4** and **diast-4** are experimentally obtained.

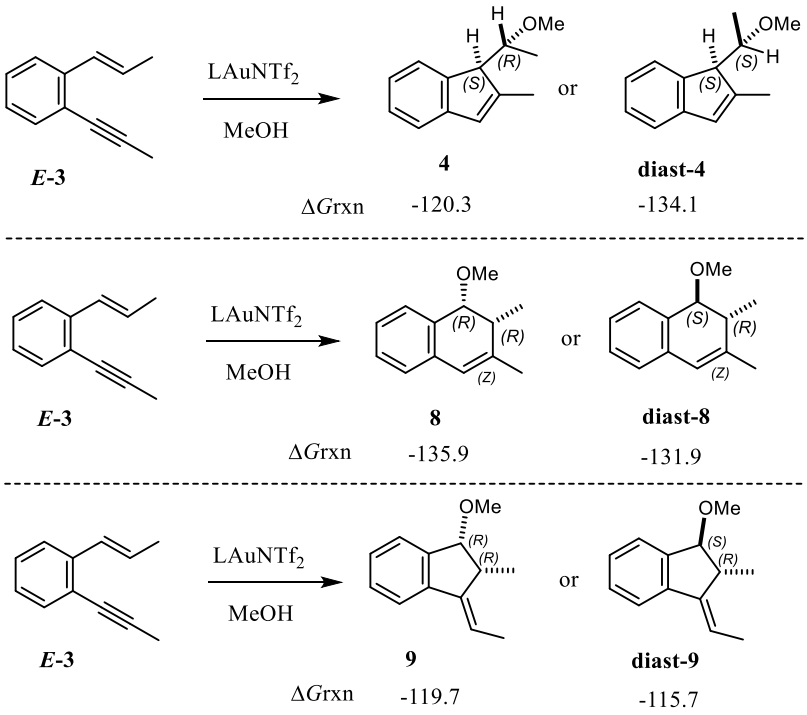
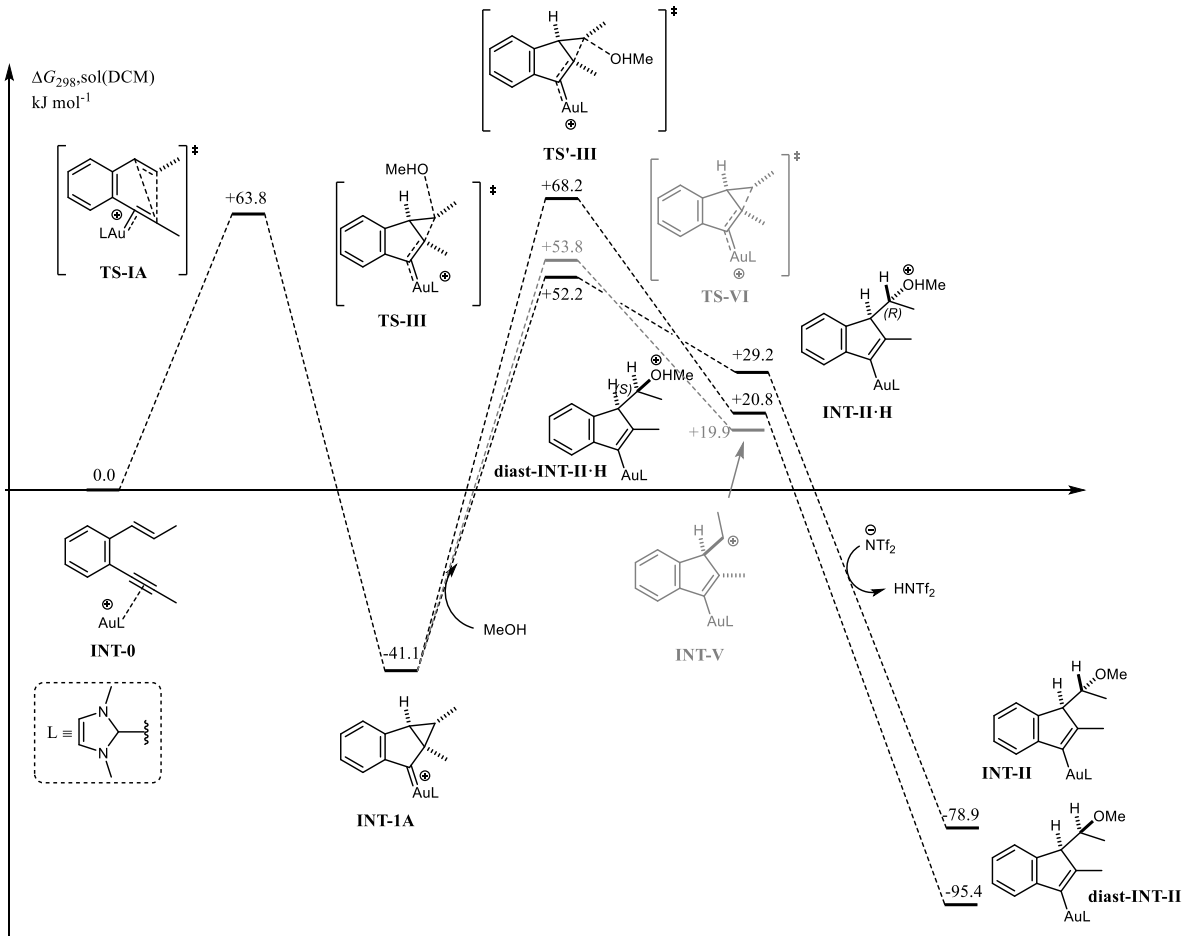


Figure 1. Computed Gibbs free energy of reactions (ΔG_{rxn}) for the transformation of ***E*-3** into different **4**, **8**, **9** products and their diastereoisomers (kJ/mol).

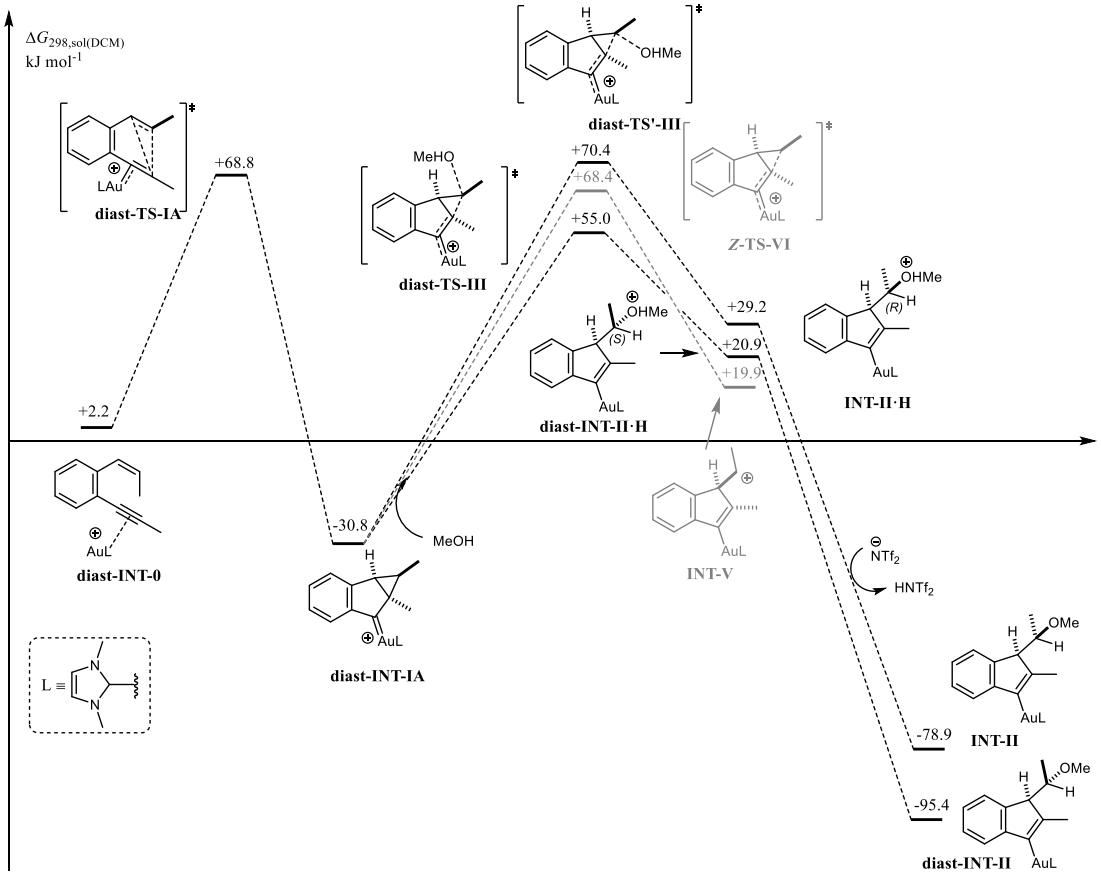
[1] (a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.(b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157.
[2] Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
[3] Tomasi, J.; Persico, M. *Chem. Rev.* **1994**, *94*, 2027.
[4] Marin-Luna, M.; Bolaño, I; Silva, C.; Nieto, O. *Comput. Theor. Chem.* **2019**, *1148*, 33.
[5] Bauernschmitdd, R.; Ahlrichs, R. *J. Chem. Phys.* **1996**, *104*, 9047.
[6] Gaussian 09, Revision E.01, Frisch M. J., Trucks G. W., Schlegel H. B., Scuseria G. E. et al, Gaussian, Inc., Wallingford CT, 2013.

Computed alternative mechanistic routes:

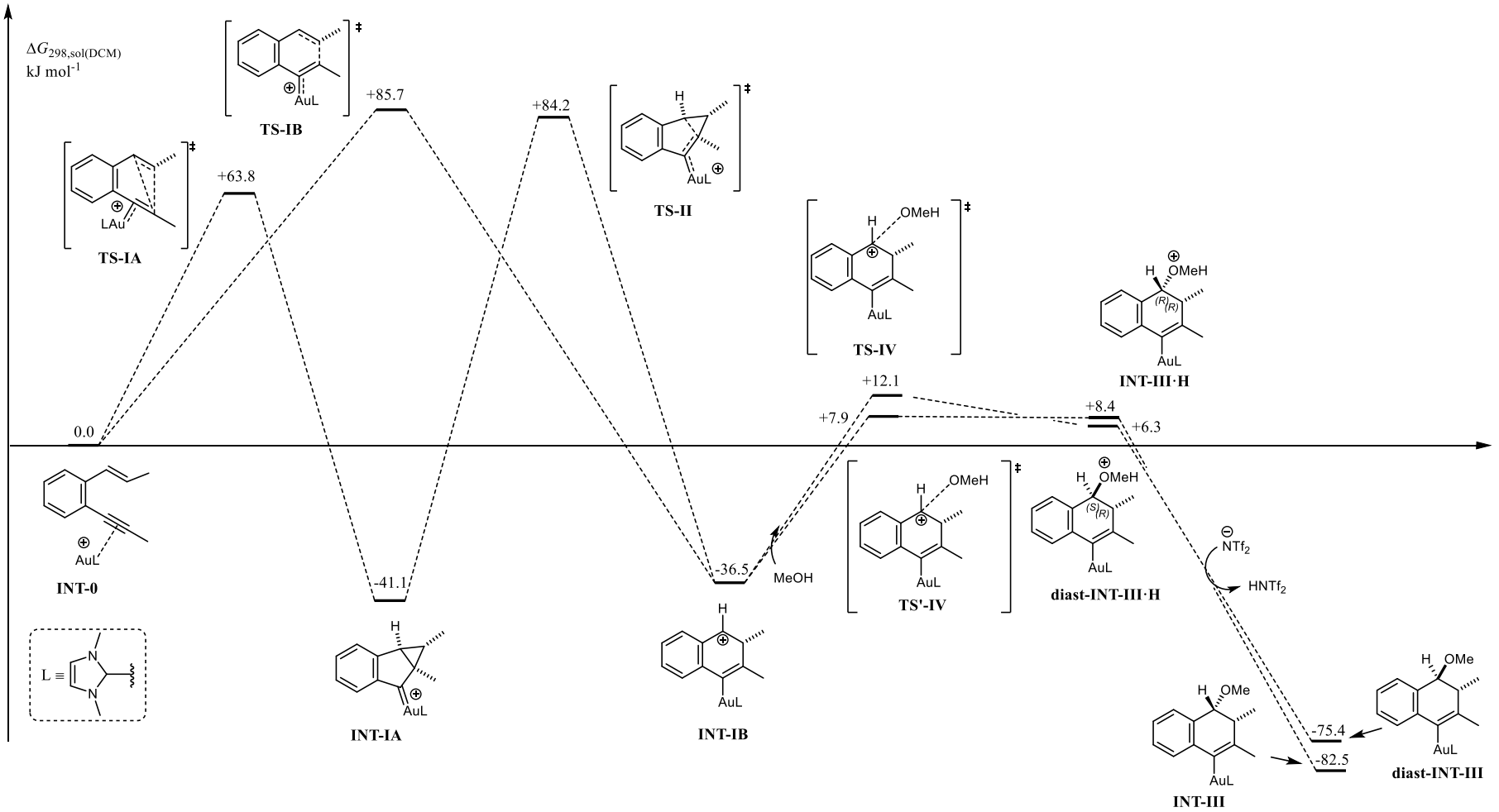
In the following we show all the computed mechanistic routes that were envisioned at the beginning of this project. For clarity, similar routes are split into two different Potential Energy Surface (PES) and they difference on the starting alkyne-gold complex **INT-0**. All the free Gibbs energies are referred to the most stable alkyne-complex ***(E)*-INT-0.**



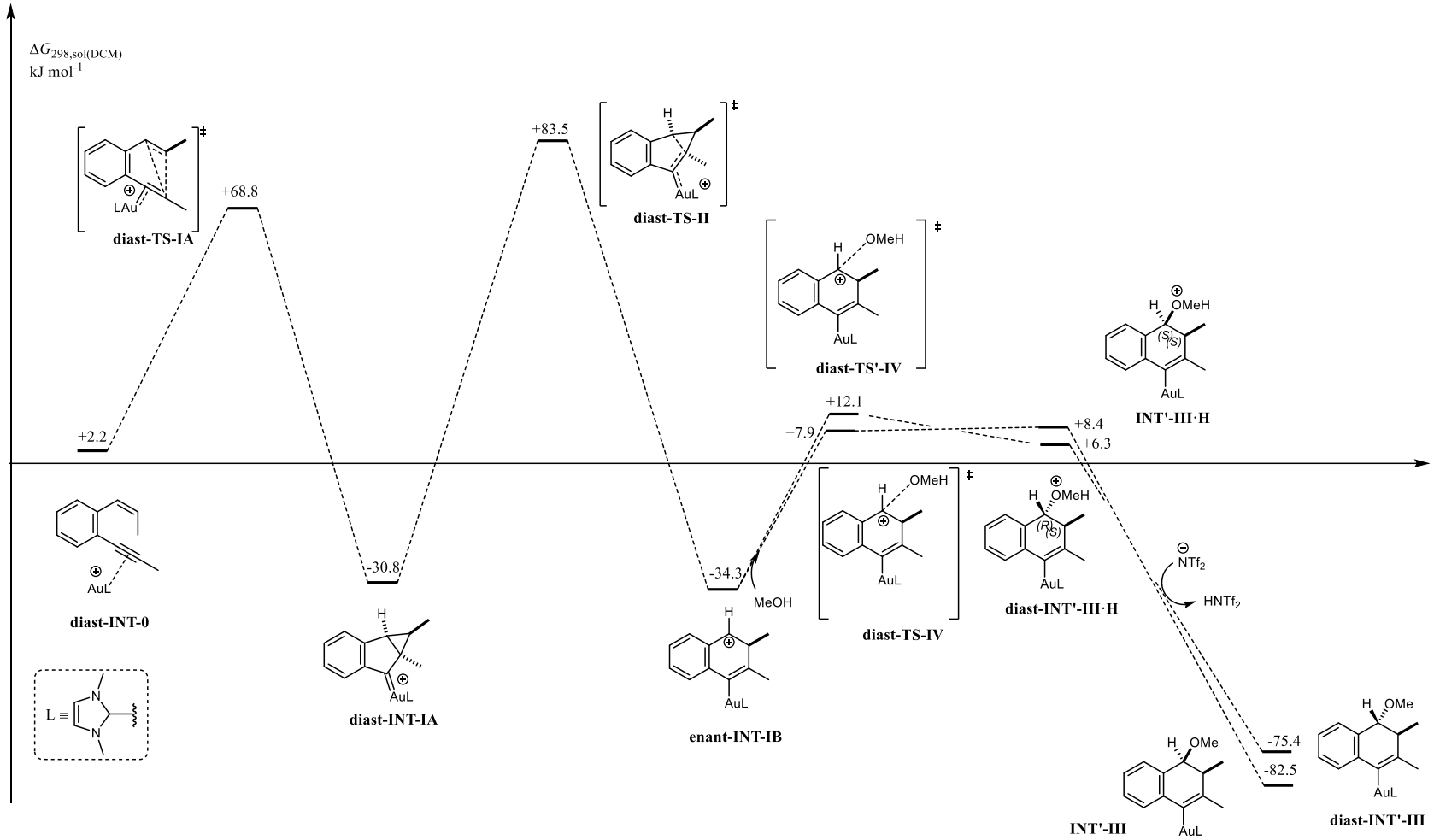
Scheme S1. Gold(I)-mediated transformation of alkynyl-gold complex **INT-0** into the methoxymethyl-1*H*-indenes **INT-II**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to **(*E*)-INT-0.**



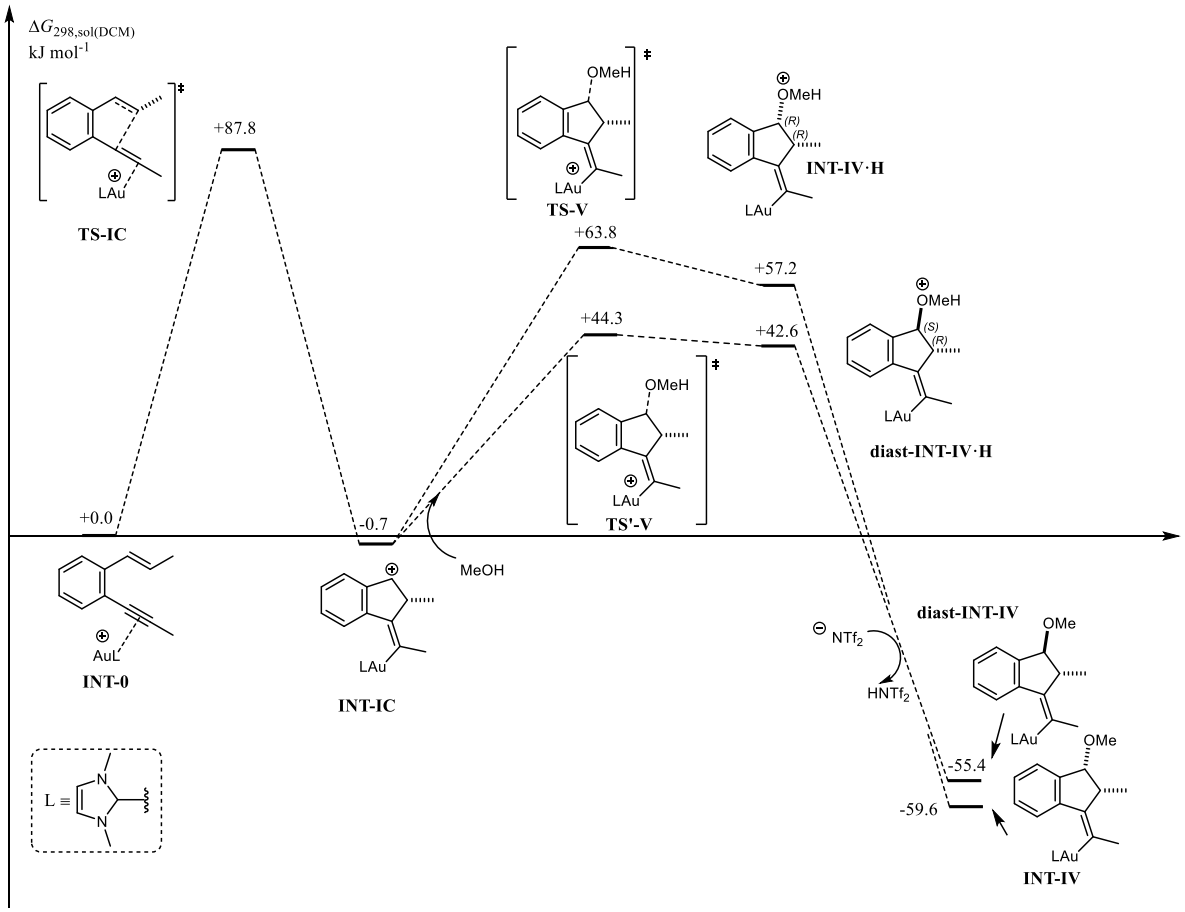
Scheme S2. Gold(I)-mediated transformation of alkynyl-gold complex **diast-INT-0** into the methoxymethyl-1*H*-indenes **INT-II**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to ***(E)*-INT-0.**



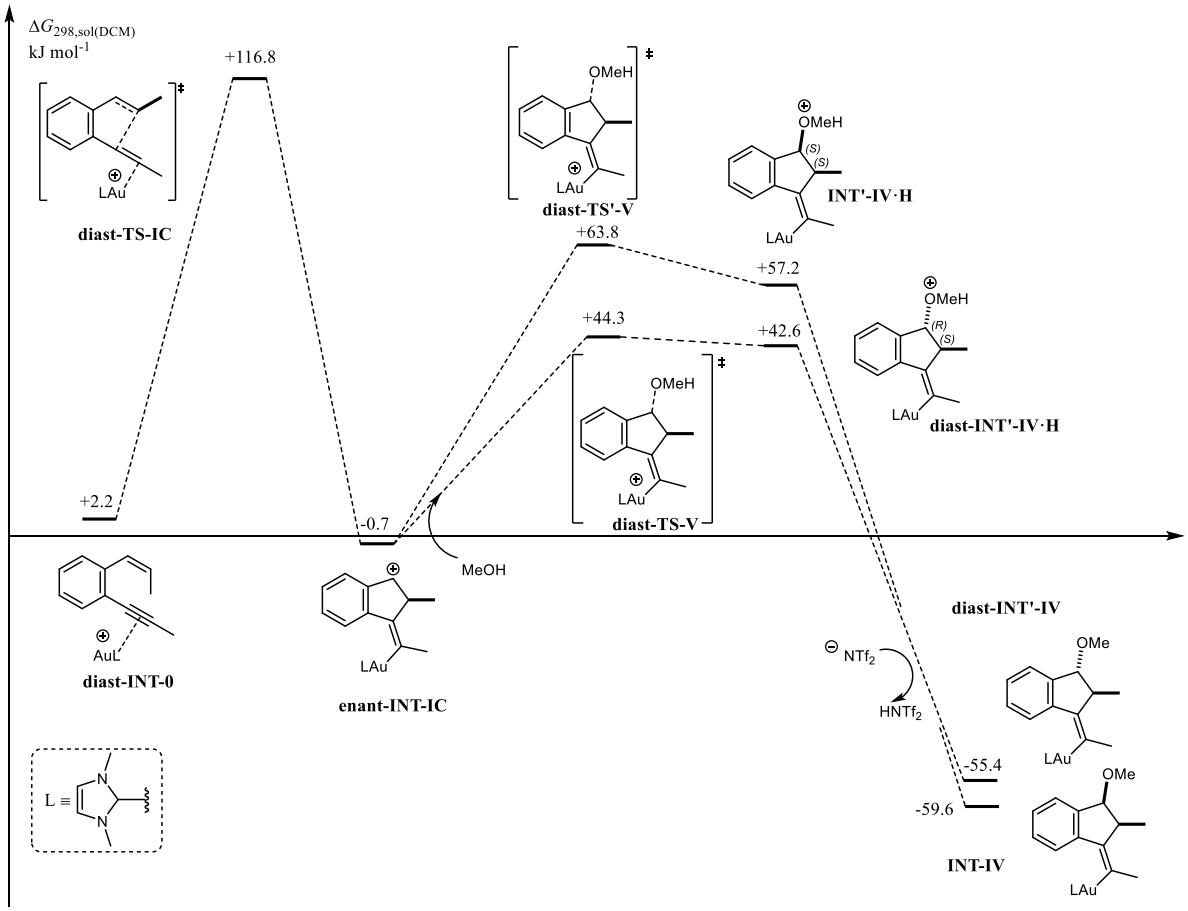
Scheme S3. Gold(I)-mediated transformation of alkynyl-gold complex **INT-0** into the 1-methoxy-dihydronaphthalene **(diast-)INT-III**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to **(E)-INT-0.**



Scheme S4. Gold(I)-mediated transformation of alkynyl-gold complex **diast-INT-0** into the 1-methoxy-dihydronaphthalene derivatives **INT'-III**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to **(*E*)-INT-0.**



Scheme S5. Gold(I)-mediated transformation of alkynyl-gold complex **INT-0** into the methoxymethyl derivatives **INT-IV**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to ***(E)*-INT-0.**



Scheme S6. Gold(I)-mediated transformation of alkynyl-gold complex **diast-INT-0** into the methoxymethyl derivatives **INT'-IV**. Calculations were performed at the PCM/M06/Def2-SVP (PCM, dichloromethane) theoretical level. Gibbs free energies are reported, in kJ mol^{-1} (1 atm and 298 K), relative to ***(E)*-INT-0.**

Computational data:

Table S1. Imaginary number and value of frequencies, electronic energies ($E_{SCF,298,sol}$), free ($G_{298,sol}$), and enthalpies ($H_{298,sol}$) energies for systems shown in Scheme S1-S6 (in Hartree) computed at PCM(DCM)/M06/def2-SVP level. Just the best conformer found is shown.

Filename	ImFreqs	Freq	$E_{SCF,298,sol}$ PCM(DCM)/M06/def2-SVP	$G_{,298,sol}$ PCM(DCM)/M06/def2-SVP	$H_{298,sol}$ PCM(DCM)/M06/def2-SVP
$LAuNTf_2$	0	-	-2265.940204	-2265.809715	-2265.729224
NTf_2 (-)	0	-	-1825.858659	-1825.842628	-1825.787915
MeOH	0	-	-115.5649533	-115.536774	-115.509757
$HNTf_2$	0	-	-1826.293849	-1826.269539	-1826.211132
***Z*-3**	0	-	-463.7218107	-463.563651	-463.511592
***E*-3**	0	-	-463.7268626	-463.569908	-463.516363
4	0	-	-579.3685373	-579.152512	-579.098763
diast-4	0	-	-579.3736938	-579.157759	-579.104065
diast-INT-0	0	-	-903.7742823	-903.503218	-903.424101
INT-0	0	-	-903.7751737	-903.504059	-903.425234
diast-TS-IA	1	-376.08	-903.750773	-903.477852	-903.402687
TS-IA	1	-389.22	-903.7499147	-903.479747	-903.402142
diast-INT-IA	0	-	-903.7943397	-903.515802	-903.4433
INT-IA	0	-	-903.7973497	-903.519699	-903.446266
diast-TS-III	1	-202.05	-1019.34335	-1019.019891	-1018.936599
diast-TS'-III	1	-161.46	-1019.334574	-1019.014018	-1018.928791
TS-III	1	-252.7	-1019.345873	-1019.020931	-1018.938638
TS'-III	1	-161.47	-1019.334574	-1019.014838	-1018.928791
diast-INT-II·H	0	-	-1019.361215	-1019.032889	-1018.951302
INT-II·H	0	-	-1019.358573	-1019.029706	-1018.948543
diast-INT-II	0	-	-1018.963639	-1018.650248	-1018.566955
INT-II	0	-	-1018.958381	-1018.643966	-1018.561481

diast-TS-VI	1	-254.09	-903.751828	-903.478021	-903.403804
TS-VI	1	-119.6	-903.7583753	-903.4835780	-903.4098900
INT-V	0	-	-903.773622	-903.496495	-903.423417
diast-8	0	-	-579.3751536	-579.15693	-579.104817
8	0	-	-579.3762701	-579.158461	-579.105941
TS1-IB	1	-544.61	-903.7443250	-903.4714120	-903.3961720
diast-TS-II	1	-455.71	-903.7488156	-903.472269	-903.399846
TS-II	1	-465.81	-903.7472821	-903.471984	-903.398749
INT-IB/enant-INT-IB	0	-	-903.7930285	-903.517963	-903.442536
diast-TS-IV/ TS'-IV	1	-253.36	-1019.363409	-1019.036208	-1018.955075
diast-TS'-IV/ TS-IV	1	-302.24	-1019.363166	-1019.037819	-1018.955023
diast-INT-III·H/diast-INT'-III·H	0	-	-1019.369056	-1019.038419	-1018.958617
INT-III·H/INT'-III·H	0	-	-1019.367003	-1019.037637	-1018.956959
diast-INT-III/diast-INT'-III	0	-	-1018.959306	-1018.642644	-1018.562235
INT-III/INT'-III	0	-	-1018.963166	-1018.645359	-1018.565746
9	0	-	-579.3680030	-579.1522660	-579.0981620
diast-9	0	-	-579.3669022	-579.1507510	-579.0970720
diast-TS-IC	1	-556.28	-903.7328443	-903.4595810	-903.3847710
TS-IC	1	-512.46	-903.7442003	-903.4706090	-903.3962360
INT-IC/enant-INT-IC	0	-	-903.7808633	-903.5043170	-903.4304740
diast-TS'-V/ TS-V	1	-303.03	-1019.3432276	-1019.0165480	-1018.9354450
diast-TS-V/ TS'-V	1	-271.29	-1019.3500243	-1019.0239490	-1018.9423690
diast-INT-IV·H/diast-INT'-IV·H	0	-	-1019.3538087	-1019.0245910	-1018.9438290
INT-IV·H/INT'-IV·H	0	-	-1019.3484862	-1019.0190430	-1018.9384690
diast-INT-IV/diast-INT'-IV	0	-	-1018.9504762	-1018.6350330	-1018.5537280
INT-IV/INT'-IV	0	-	-1018.9516146	-1018.6366150	-1018.5548180

Cartesian Coordinates:

In case of enantiomers just the structure of one of them is shown.

$LAuNTf_2$

SCF = -2265.94033016

Num. Imaginary Freq = 1

C	5.052209	-0.891824	0.458546
C	5.105062	0.464212	0.417911
H	5.829596	-1.634807	0.620893
H	5.939712	1.151504	0.535074
N	3.733973	-1.245017	0.248627
N	3.818000	0.906087	0.186649
C	2.972617	-0.142019	0.080860
C	3.257042	-2.614794	0.222950
H	2.177268	-2.614217	0.022744
H	3.769474	-3.178795	-0.568996
H	3.444766	-3.100674	1.190808
C	3.430058	2.296737	0.034980
H	4.251760	2.937045	0.378415
H	3.211625	2.525036	-1.018334
H	2.536028	2.505164	0.638328
Au	0.985349	-0.074121	-0.257603
N	-1.122704	-0.034378	-0.576128
S	-1.876680	-1.492434	-0.731119
S	-1.877071	1.410684	-0.829992
O	-0.834668	-2.506880	-0.765956
O	-2.952224	-1.492590	-1.702265
O	-3.313355	1.274417	-0.990455
O	-1.090627	2.225118	-1.740474
C	-2.684693	-1.724963	0.922235
C	-1.658216	2.231130	0.831262
F	-1.778027	-1.626849	1.875155
F	-3.222010	-2.927377	0.950630
F	-3.620624	-0.819058	1.106455
F	-0.394281	2.543619	1.041661
F	-2.078318	1.439127	1.796114

F	-2.380643	3.332215	0.818453

NTf_2 (-)

SCF = -1825.85865864

Num. Imaginary Freq = 0

N	0.034088	0.913035	0.763154
S	1.525242	0.874897	0.191785
S	-1.317486	0.950809	-0.098219
O	2.441979	1.200080	1.276751
O	1.735584	1.482397	-1.117873
O	-1.163966	1.099455	-1.541923
O	-2.290676	1.783536	0.597115
C	1.815721	-0.928059	-0.103009
C	-2.009758	-0.795873	0.114413
F	1.685615	-1.612527	1.018687
F	3.034570	-1.113757	-0.579539
F	0.936646	-1.381717	-0.986008
F	-1.389135	-1.455527	1.075757
F	-1.882956	-1.473556	-1.012298
F	-3.293834	-0.716549	0.414500

MeOH

SCF = -115.564953342

Num. Imaginary Freq = 0

C	0.649203	-0.019605	0.000000
H	1.095884	0.987232	-0.000002
H	1.036031	-0.547744	-0.893674
H	1.036031	-0.547741	0.893675
O	-0.741260	0.122942	0.000000
H	-1.133080	-0.757659	0.000000

$HNTf_2$

SCF = -1826.29384870

Num. Imaginary Freq = 0

N	0.000066	0.000220	-1.055326
S	-1.191054	-0.893502	-0.276747
S	1.191203	0.893683	-0.276351

O	-1.849400	-1.665156	-1.304318
O	-0.609207	-1.452134	0.922411
O	0.609320	1.452129	0.922912
O	1.849807	1.665431	-1.303678
C	-2.418428	0.427982	0.272574
C	2.418278	-0.428130	0.272745
F	-2.324636	1.473042	-0.514866
F	-3.615683	-0.100340	0.179273
F	-2.169704	0.767086	1.510297
F	2.169590	-0.767366	1.510433
F	3.615635	0.099937	0.179417
F	2.324109	-1.473036	-0.514857
H	0.000085	0.000398	-2.080957

***Z*-3**

SCF = -463.721810740

Num. Imaginary Freq = 0

C	-2.632570	-1.460217	0.376671
C	-1.262157	-1.675828	0.332801
C	-0.373426	-0.650619	-0.042086
C	-0.887484	0.629695	-0.363003
C	-2.278156	0.811347	-0.341814
C	-3.145173	-0.209503	0.029627
H	-3.304061	-2.271884	0.670202
H	-0.849469	-2.658816	0.578800
H	-2.678166	1.793526	-0.616136
H	-4.223994	-0.030572	0.048014
C	-0.040191	1.767750	-0.763400
H	-0.361943	2.280985	-1.680401
C	1.011222	2.281652	-0.107050
H	1.500867	3.148888	-0.570218
C	1.566019	1.849449	1.203583
H	0.920660	1.120182	1.716301
H	2.561235	1.385018	1.084887
H	1.705008	2.718613	1.868200
C	1.021558	-0.952163	-0.136820
C	2.198756	-1.244280	-0.219731
C	3.609397	-1.567128	-0.314678
H	3.882177	-2.388466	0.366739

H	3.884640	-1.880320	-1.334817
H	4.236272	-0.698082	-0.056177

***E*-3**

SCF = -463.726862641

Num. Imaginary Freq = 0

C	0.984346	-2.925365	-0.000008
C	-0.264161	-2.320089	0.000009
C	-0.393043	-0.919547	0.000009
C	0.769177	-0.105089	0.000018
C	2.018445	-0.745981	0.000022
C	2.131994	-2.129589	-0.000005
H	1.065294	-4.015797	-0.000013
H	-1.173787	-2.927900	0.000012
H	2.929545	-0.140355	0.000061
H	3.122974	-2.592457	-0.000007
C	0.639131	1.354097	0.000100
H	-0.392730	1.730671	0.000412
C	1.633306	2.255644	-0.000130
H	2.677202	1.912406	-0.000457
C	1.431602	3.728446	0.000028
H	0.363199	3.994441	0.000342
H	1.903149	4.198561	0.880448
H	1.902657	4.198690	-0.880587
C	-1.707885	-0.354216	-0.000005
C	-2.839609	0.091296	-0.000051
C	-4.188453	0.624413	-0.000032
H	-4.368442	1.264410	-0.878715
H	-4.938227	-0.182066	-0.018023
H	-4.379932	1.235269	0.896800

diast-*4*

SCF = -579.373693829

Num. Imaginary Freq = 0

C	0.670304	-0.215061	-0.281439
C	1.536924	0.879945	-0.082763
C	2.902944	0.673902	0.109929
C	3.390987	-0.634641	0.110061

C	2.530477	-1.718138	-0.078328
C	1.159787	-1.514102	-0.276446
C	-0.727488	0.304023	-0.471249
C	-0.559881	1.800245	-0.339932
C	0.740551	2.102016	-0.127317
H	3.579515	1.521187	0.260816
H	4.459944	-0.813651	0.261706
H	2.931412	-2.736180	-0.070483
H	0.483873	-2.363593	-0.413313
H	-1.066293	0.096307	-1.508755
C	-1.784990	-0.290849	0.475366
C	-1.700882	2.743624	-0.456131
H	-2.413683	2.630249	0.381050
H	-1.360285	3.789696	-0.462539
H	-2.280366	2.562531	-1.378400
C	-1.451761	-0.089269	1.934002
H	-2.247541	-0.511443	2.565734
H	-0.507451	-0.598134	2.186873
H	-1.343643	0.979443	2.175469
H	-2.749591	0.217828	0.243769
O	-1.952039	-1.675839	0.273694
C	-2.528016	-2.041727	-0.944012
H	-1.828994	-1.945203	-1.798966
H	-2.829278	-3.097584	-0.877687
H	-3.428872	-1.437123	-1.171023
H	1.143826	3.112579	-0.014249

4

SCF = -579.368537313

Num. Imaginary Freq = 0

C	-0.763442	-0.087800	0.342149
C	-1.552245	0.957237	-0.179947
C	-2.902618	0.758217	-0.465684
C	-3.461177	-0.498318	-0.224044
C	-2.682730	-1.533224	0.296940
C	-1.326720	-1.334617	0.583153
C	0.649356	0.411673	0.527180
C	0.550426	1.865786	0.103582

C	-0.711371	2.140500	-0.296547
H	-3.512880	1.572778	-0.868778
H	-4.519636	-0.672652	-0.440798
H	-3.137854	-2.509810	0.488233
H	-0.720924	-2.144015	0.997753
H	0.951018	0.361650	1.595970
C	1.660533	-0.453523	-0.237055
H	1.304333	-0.526196	-1.289621
C	1.653394	2.860598	0.211301
H	2.366609	2.800825	-0.628215
H	1.252394	3.885632	0.217666
H	2.242684	2.714894	1.132096
C	3.087693	0.053505	-0.217727
H	3.761929	-0.719628	-0.618900
H	3.225395	0.954116	-0.831650
H	3.404917	0.276573	0.814659
O	1.616382	-1.735707	0.361218
C	1.796167	-2.794332	-0.530212
H	1.811870	-3.731882	0.044956
H	0.971132	-2.851744	-1.269523
H	2.749822	-2.722334	-1.089972
H	-1.065466	3.123239	-0.622154

diast-INT-0

SCF = -903.774282263

Num. Imaginary Freq = 0

C	-2.454954	3.014223	0.083196
C	-1.671693	1.908922	-0.221711
C	-2.166213	0.609784	-0.032697
C	-3.478150	0.406120	0.467196
C	-4.238609	1.541558	0.779081
C	-3.740666	2.826643	0.588896
H	-2.060040	4.021893	-0.068097
H	-0.661090	2.042323	-0.621036
H	-5.234225	1.407253	1.210762
H	-4.359203	3.690300	0.847747
C	-3.992148	-0.952274	0.684382
H	-3.265999	-1.673810	1.081887
C	-5.232361	-1.402663	0.430507

H	-5.427880	-2.452054	0.687036
C	-6.369823	-0.670228	-0.189905
H	-7.137027	-0.410314	0.561115
H	-6.059628	0.261968	-0.685556
H	-6.877070	-1.305636	-0.933542
C	-1.375902	-0.541414	-0.377984
C	-0.957652	-1.665325	-0.691476
C	4.907180	0.359807	0.891165
C	4.698149	1.400704	0.043631
H	5.783937	0.068670	1.464889
H	5.352219	2.211336	-0.268936
N	3.732476	-0.361161	0.932864
N	3.403783	1.283765	-0.417131
C	2.806412	0.202759	0.128739
C	3.553852	-1.588926	1.686333
H	3.803887	-2.464172	1.069158
H	4.209874	-1.571149	2.565653
H	2.510923	-1.667215	2.019921
C	2.761393	2.236271	-1.304495
H	3.522679	2.714649	-1.933226
H	2.043648	1.712199	-1.949602
H	2.233396	3.010264	-0.727946
Au	0.882777	-0.427517	-0.192031
C	-0.724393	-3.033160	-1.132035
H	-0.167294	-3.613869	-0.381710
H	-1.694401	-3.526754	-1.300810
H	-0.156411	-3.057076	-2.074337

INT-0

SCF = -903.775173706

Num. Imaginary Freq = 0

C	-2.129481	3.345883	-0.250540
C	-1.613980	2.132609	-0.680346
C	-2.191617	0.915219	-0.273959
C	-3.337040	0.916880	0.563064
C	-3.812381	2.160539	1.007663
C	-3.228686	3.356122	0.609678
H	-1.669246	4.282193	-0.575593
H	-0.738445	2.106029	-1.337045

H	-4.680129	2.175063	1.674869
H	-3.635760	4.305006	0.969321
C	-4.048694	-0.290475	0.992741
H	-4.509090	-0.228855	1.989692
C	-4.255904	-1.399668	0.266866
H	-3.873408	-1.440071	-0.762404
C	-5.015066	-2.587657	0.734888
H	-5.374348	-2.464047	1.767921
H	-5.884748	-2.786768	0.085925
H	-4.391794	-3.497658	0.693326
C	-1.569500	-0.314220	-0.678031
C	-1.156752	-1.428779	-1.027570
C	4.665789	-0.000401	1.162100
C	4.586116	1.136189	0.421364
H	5.477525	-0.408624	1.759750
H	5.312059	1.925970	0.243176
N	3.450853	-0.640884	1.038576
N	3.326500	1.156758	-0.139831
C	2.626201	0.067269	0.239315
C	3.106796	-1.903892	1.668319
H	2.900950	-2.668001	0.905576
H	3.948625	-2.235155	2.287782
H	2.220142	-1.780634	2.305611
C	2.808919	2.226524	-0.974200
H	3.645119	2.841014	-1.329214
H	2.281580	1.804535	-1.840915
H	2.115523	2.860987	-0.402501
Au	0.708589	-0.408664	-0.290366
C	-1.028274	-2.781001	-1.560113
H	-0.541346	-3.456020	-0.840863
H	-2.029163	-3.181741	-1.788746
H	-0.432758	-2.786704	-2.485420

diast-TS-IA

SCF = 5

Num. Imaginary Freq = 4.0845

C	3.014374	3.046912	0.124313
C	1.986134	2.106723	0.112518
C	2.279382	0.767515	-0.150309

C	3.610115	0.377199	-0.412246
C	4.633206	1.319786	-0.391563
C	4.329690	2.656435	-0.125049
H	2.787716	4.096580	0.329285
H	0.952053	2.406435	0.308722
H	5.665139	1.015295	-0.588749
H	5.130249	3.401066	-0.115453
C	3.785263	-1.064119	-0.675784
H	3.833681	-1.402777	-1.720277
C	4.008268	-1.972676	0.315985
H	4.139524	-3.019557	0.012117
C	4.096051	-1.691538	1.763642
H	5.108555	-1.943930	2.122986
H	3.888818	-0.640359	2.009605
H	3.407472	-2.344293	2.325941
C	1.327440	-0.338683	-0.187869
C	1.723719	-1.569123	-0.339207
C	-4.838212	1.111417	0.227957
C	-5.026035	-0.230948	0.163712
H	-5.547561	1.931436	0.315164
H	-5.933999	-0.829617	0.183734
N	-3.475781	1.324955	0.160816
N	-3.773344	-0.802031	0.058145
C	-2.813368	0.150774	0.055174
C	-2.867215	2.640168	0.192920
H	-3.172960	3.225352	-0.686042
H	-3.169118	3.174755	1.104441
H	-1.775395	2.528055	0.187607
C	-3.548214	-2.230981	-0.032350
H	-2.469179	-2.417016	-0.109130
H	-3.937100	-2.735843	0.863244
H	-4.048571	-2.640280	-0.921434
Au	-0.768212	-0.126063	-0.078286
C	1.410639	-2.984552	-0.517402
H	0.322824	-3.067424	-0.675541
H	1.909050	-3.409846	-1.402831
H	1.674025	-3.595363	0.361791

TS-IA

SCF = -903.749914696

Num. Imaginary Freq = 1

C	2.769634	3.282498	0.369519
C	1.810315	2.272953	0.332248
C	2.198625	0.965854	0.034918
C	3.551815	0.674549	-0.234495
C	4.505951	1.686647	-0.188195
C	4.108870	2.991583	0.110583
H	2.470218	4.308176	0.601025
H	0.757114	2.491535	0.535304
H	5.556833	1.461105	-0.391323
H	4.855072	3.790273	0.138746
C	3.840228	-0.746269	-0.519829
H	3.953126	-1.071901	-1.565821
C	4.165603	-1.607430	0.485675
H	4.106133	-1.220866	1.513949
C	4.640031	-2.993014	0.309428
H	4.604868	-3.323419	-0.738749
H	5.688790	-3.048052	0.651044
H	4.087400	-3.701839	0.946538
C	1.327657	-0.200917	-0.044833
C	1.814871	-1.396508	-0.212181
C	-5.025269	-0.464149	0.140658
C	-4.925520	0.878174	-0.031915
H	-5.894105	-1.110006	0.246521
H	-5.689045	1.649047	-0.108109
N	-3.736102	-0.958003	0.164595
N	-3.578127	1.169365	-0.108804
C	-2.839536	0.043009	0.011414
C	-3.416947	-2.360855	0.343468
H	-3.916225	-2.964076	-0.427662
H	-2.330726	-2.494360	0.256504
H	-3.743249	-2.704528	1.335613
C	-3.054917	2.509319	-0.291084
H	-3.444935	2.946614	-1.220978
H	-3.341546	3.149751	0.555230
H	-1.959786	2.460036	-0.350271
Au	-0.778142	-0.111267	-0.024251
C	1.595390	-2.820703	-0.437092
H	2.132415	-3.191290	-1.324239

H	1.862225	-3.447998	0.427673
H	0.517455	-2.956135	-0.625429

diast-INT-IA

SCF = -903.794339690

Num. Imaginary Freq = 0

C	3.649730	0.068173	-0.316847
C	2.357337	0.660383	-0.258006
C	2.209099	2.055736	-0.148125
C	3.348577	2.843174	-0.109590
C	4.617814	2.245810	-0.160464
C	4.784705	0.860085	-0.245761
C	3.498801	-1.400278	-0.351936
C	2.005790	-1.643312	-0.351263
C	1.343335	-0.343623	-0.264490
H	1.207262	2.494718	-0.104840
H	3.267163	3.930290	-0.039215
H	5.504204	2.886167	-0.131564
H	5.785354	0.421603	-0.271375
H	4.174987	-2.030411	-0.938853
C	2.883902	-1.975387	0.894604
C	1.337993	-2.802892	-1.037745
H	2.003360	-3.679383	-1.061567
H	0.411365	-3.090200	-0.513802
H	1.076329	-2.549333	-2.076991
Au	-0.668893	-0.063267	-0.118075
C	-2.732513	0.213210	0.047915
N	-3.399103	1.382440	0.187284
N	-3.691678	-0.741327	0.038908
C	-4.758952	1.164180	0.264005
C	-2.792540	2.697907	0.244673
C	-4.943748	-0.177946	0.170561
C	-3.462204	-2.167190	-0.088652
H	-5.470552	1.979038	0.377588
H	-3.126664	3.310150	-0.604961
H	-3.067700	3.202232	1.181648
H	-1.701058	2.589541	0.202056
H	-5.850159	-0.779147	0.186250
H	-3.970667	-2.556685	-0.981973

H	-2.383539	-2.347870	-0.181398
H	-3.840155	-2.695012	0.798307
C	2.822692	-1.308393	2.234386
H	1.970852	-1.691169	2.817605
H	3.738057	-1.542702	2.800822
H	2.735690	-0.213223	2.182604
H	2.994959	-3.066106	0.964684

INT-IA

SCF = -903.797349742

Num. Imaginary Freq = 0

C	3.635152	-0.332262	0.258058
C	2.314220	-0.854797	0.171431
C	2.095742	-2.241277	0.063599
C	3.191891	-3.087510	0.059925
C	4.490188	-2.558468	0.143861
C	4.729256	-1.184537	0.225510
C	3.551707	1.140675	0.284803
C	2.079314	1.460073	0.304308
C	1.350529	0.198316	0.193050
H	1.073643	-2.627864	0.000280
H	3.054592	-4.169337	-0.005477
H	5.341241	-3.245748	0.146517
H	5.750432	-0.799465	0.280456
H	4.279295	1.763434	0.815190
C	2.940290	1.688701	-0.980248
H	2.779820	0.951460	-1.777090
C	1.455424	2.653376	0.973415
H	2.175819	3.473277	1.100721
H	0.601954	3.032887	0.386563
H	1.084052	2.381679	1.973509
C	3.198826	3.082401	-1.452788
H	3.987335	3.072944	-2.221392
H	2.298449	3.518285	-1.915137
H	3.528160	3.747891	-0.642180
Au	-0.677317	0.017920	0.071373
C	-2.754587	-0.156008	-0.048156
N	-3.674370	0.820032	0.131982
N	-3.471196	-1.270945	-0.320625

C	-4.951651	0.323106	-0.025144
C	-3.385788	2.204817	0.450401
C	-4.823225	-0.998024	-0.311664
C	-2.916741	-2.583726	-0.586977
H	-5.833885	0.950802	0.079285
H	-2.297768	2.341864	0.499183
H	-3.797577	2.866682	-0.324461
H	-3.825228	2.472673	1.421713
H	-5.570272	-1.763424	-0.509773
H	-3.256581	-3.303708	0.171028
H	-3.228317	-2.934369	-1.581012
H	-1.821452	-2.518354	-0.556174

diast-TS-III

SCF = -1019.34334972

Num. Imaginary Freq = 1

C	0.802779	-0.143251	-0.333555
C	1.562884	-1.263533	-0.563085
C	3.045182	-0.842726	-0.772816
C	3.004563	0.642350	-0.657603
C	1.682346	1.027585	-0.362895
C	1.111464	-2.680593	-0.695342
H	0.058865	-2.711118	-1.017008
H	1.710456	-3.233905	-1.438524
H	1.169155	-3.246394	0.252917
C	3.484768	-1.528707	0.420355
O	5.654433	-1.196395	0.073112
C	6.513666	-0.679860	1.068316
H	7.519227	-0.486761	0.660895
H	6.093411	0.278578	1.406766
H	6.609230	-1.354488	1.937321
H	3.475525	-1.264203	-1.695845
H	6.041734	-1.999055	-0.304600
C	4.038333	1.565247	-0.721509
C	1.389166	2.377968	-0.151604
C	2.420682	3.312078	-0.232912
C	3.731250	2.913455	-0.516385
Au	-1.247478	-0.079446	-0.106483
C	-3.321911	-0.007006	0.136895
N	-4.074050	1.067947	0.471386

N	-4.206769	-1.022497	-0.001693
C	-5.411325	0.731136	0.541875
C	-3.566188	2.400121	0.730525
C	-5.495259	-0.589749	0.242234
C	-3.873724	-2.385217	-0.364839
H	-6.179175	1.458169	0.797065
H	-4.031752	3.125533	0.048288
H	-3.777196	2.696709	1.768046
H	-2.480108	2.402326	0.570234
H	-6.351611	-1.257618	0.180378
H	-4.354152	-2.657276	-1.315624
H	-2.784746	-2.467195	-0.477443
H	-4.208236	-3.081537	0.417424
H	5.061643	1.242723	-0.937554
H	4.522240	3.665895	-0.582511
H	2.204791	4.372723	-0.074858
H	0.363685	2.689483	0.074113
C	3.370118	-1.043034	1.801531
H	3.175112	0.035181	1.877571
H	2.563604	-1.606424	2.302967
H	4.281119	-1.302671	2.362949
H	3.665463	-2.607036	0.311287

diast-TS'-III

SCF = -1019.33457429

Num. Imaginary Freq = 1

C	1.071601	-0.003527	-0.492332
C	1.837464	-1.083314	-0.806216
C	3.347319	-0.642012	-0.889997
C	3.277737	0.829130	-0.626322
C	1.939976	1.171683	-0.352064
C	1.434794	-2.483893	-1.102804
H	0.337105	-2.546917	-1.156446
H	1.841296	-2.829754	-2.069524
H	1.766123	-3.212019	-0.340069
C	4.014038	-1.392382	0.153377
O	2.353367	-1.732301	1.933073
C	2.468618	-0.714455	2.902903
H	1.714688	-0.823468	3.701070

H	3.462053	-0.794672	3.369073
H	2.367710	0.296089	2.462576
H	3.731232	-0.946042	-1.885424
H	1.538943	-1.572027	1.428506
C	4.299496	1.764638	-0.547057
C	1.621411	2.486561	-0.009457
C	2.644004	3.433308	0.059254
C	3.969289	3.080152	-0.207377
Au	-0.983622	0.003875	-0.249266
C	-3.050812	0.019296	0.044067
N	-3.829613	1.080883	0.359158
N	-3.902742	-1.030612	-0.027027
C	-5.151489	0.701427	0.484799
C	-3.364078	2.440455	0.545893
C	-5.197682	-0.632505	0.240535
C	-3.533438	-2.395852	-0.342585
H	-5.936292	1.411981	0.734550
H	-3.562601	2.776285	1.573799
H	-2.282772	2.474356	0.359482
H	-3.870868	3.117206	-0.156740
H	-6.031470	-1.331055	0.232300
H	-4.059605	-2.735230	-1.246200
H	-2.451165	-2.439441	-0.520878
H	-3.787785	-3.064298	0.492432
H	5.338951	1.488524	-0.751835
H	4.754334	3.839396	-0.152771
H	2.406673	4.467875	0.323569
H	0.583417	2.764358	0.201986
C	4.499172	-2.750055	-0.003322
H	4.149406	-3.256355	-0.911892
H	5.604197	-2.654787	-0.059386
H	4.314663	-3.344959	0.904619
H	4.312929	-0.856588	1.061935

TS-III

SCF = -1019.34587295

Num. Imaginary Freq = 1

C	0.826277	-0.083626	-0.370244
C	1.582476	-1.185360	-0.688361

C	3.064846	-0.785124	-0.831815
C	3.029391	0.705505	-0.677739
C	1.712504	1.080410	-0.343437
C	1.085160	-2.565078	-0.967180
H	1.775425	-3.136867	-1.608584
H	0.908882	-3.164133	-0.054308
H	0.116578	-2.509857	-1.489172
C	3.505648	-1.429128	0.404192
O	5.436104	-0.753603	0.547971
C	5.764992	-0.201564	1.814681
H	6.814723	0.126681	1.829362
H	5.121084	0.676336	1.965539
H	5.597769	-0.923022	2.632935
H	3.555772	-1.188460	-1.734333
H	6.055717	-1.466366	0.325694
C	4.050917	1.642815	-0.753273
C	1.417577	2.422288	-0.084721
C	2.438219	3.366642	-0.172709
C	3.740606	2.983557	-0.509384
Au	-1.217802	-0.038090	-0.099984
C	-3.288881	-0.002930	0.179442
N	-4.141310	-1.054109	0.136295
N	-4.071394	1.070394	0.441141
C	-5.439879	-0.645179	0.367395
C	-3.766104	-2.429835	-0.121650
C	-5.395794	0.697361	0.560288
C	-3.605161	2.435374	0.579737
H	-6.274229	-1.343094	0.373882
H	-4.253510	-2.795343	-1.036973
H	-2.676678	-2.482331	-0.249579
H	-4.060732	-3.071041	0.721476
H	-6.183446	1.417380	0.771036
H	-4.078001	3.079835	-0.175102
H	-3.843404	2.821936	1.581000
H	-2.516701	2.454691	0.436778
C	3.803824	-2.865310	0.533705
H	4.429453	-3.064096	1.415412
H	2.856511	-3.404001	0.710953
H	4.263836	-3.283701	-0.373819
H	3.227550	-0.889741	1.321211

H	5.071119	1.341112	-1.006442
H	4.524054	3.742822	-0.587689
H	2.220062	4.421697	0.016944
H	0.394945	2.718582	0.173167

TS'-III

SCF = -1019.33457429

Num. Imaginary Freq = 1

C	3.277800	0.829031	-0.626298
C	1.940040	1.171643	-0.352114
C	1.621501	2.486538	-0.009548
C	2.644125	3.433247	0.059199
C	3.969411	3.080035	-0.207358
C	4.299589	1.764503	-0.546998
C	3.347334	-0.642123	-0.889922
C	1.837458	-1.083366	-0.806187
C	1.071624	-0.003530	-0.492400
H	0.583503	2.764360	0.201842
H	2.406822	4.467828	0.323486
H	4.754482	3.839250	-0.152723
H	5.339043	1.488346	-0.751717
H	3.731289	-0.946211	-1.885315
C	4.013941	-1.392492	0.153518
C	1.434724	-2.483935	-1.102731
H	1.765926	-3.212043	-0.339923
H	0.337034	-2.546875	-1.156462
H	1.841280	-2.829881	-2.069397
C	4.498965	-2.750214	-0.003090
H	4.314300	-3.345073	0.904849
H	4.149246	-3.256513	-0.911679
H	5.604005	-2.655058	-0.059035
H	4.312828	-0.856677	1.062064
O	2.353149	-1.732174	1.933178
C	2.468443	-0.714283	2.902953
H	2.367603	0.296248	2.462576
H	1.714490	-0.823204	3.701112
H	3.461861	-0.794537	3.369152
Au	-0.983604	0.003930	-0.249382
C	-3.050790	0.019329	0.044012
N	-3.902710	-1.030593	-0.027055

N	-3.829580	1.080882	0.359253
C	-5.197622	-0.632533	0.240706
C	-3.533435	-2.395843	-0.342609
C	-5.151429	0.701383	0.485050
C	-3.364081	2.440460	0.546044
H	-6.031403	-1.331093	0.232498
H	-2.451309	-2.439313	-0.521816
H	-3.786967	-3.064160	0.492762
H	-4.060316	-2.735493	-1.245703
H	-5.936226	1.411910	0.734896
H	-3.561575	2.775876	1.574288
H	-2.282983	2.474631	0.358492
H	-3.871741	3.117379	-0.155800
H	1.538760	-1.571869	1.428564

diast-INT-II·H

SCF = -1019.36121508

Num. Imaginary Freq = 0

C	3.042875	0.707698	-0.417432
C	1.695663	1.073306	-0.216741
C	1.370206	2.419150	-0.049360
C	2.382487	3.382561	-0.087446
C	3.708509	3.018254	-0.312910
C	4.045425	1.668723	-0.490002
C	3.107209	-0.791333	-0.516590
C	1.640496	-1.196227	-0.443707
C	0.829686	-0.118439	-0.255039
H	0.326031	2.713401	0.103766
H	2.129825	4.438722	0.044673
H	4.486107	3.784427	-0.371603
H	5.082970	1.416881	-0.751861
H	3.548351	-1.127101	-1.476943
C	3.890889	-1.424938	0.627313
C	1.256666	-2.628912	-0.570788
H	1.628020	-3.247665	0.268699
H	0.161370	-2.738433	-0.595578
H	1.668813	-3.081878	-1.490615
C	3.370176	-1.194347	2.015061
H	4.068552	-1.597066	2.761446

H	3.201826	-0.123611	2.213051
H	2.407174	-1.711194	2.130089
H	4.084587	-2.493689	0.440026
O	5.297108	-0.850405	0.632294
C	6.230789	-1.271391	-0.403429
H	5.857781	-0.973684	-1.392319
H	7.189534	-0.794450	-0.175306
H	6.313697	-2.360005	-0.320048
Au	-1.228419	-0.083778	-0.091566
C	-3.315786	-0.037610	0.065129
N	-4.179775	-1.073308	-0.060365
N	-4.100041	1.040015	0.307017
C	-5.485158	-0.650620	0.099804
C	-3.809335	-2.448084	-0.328396
C	-5.434828	0.685177	0.332043
C	-3.625367	2.393911	0.507279
H	-6.327856	-1.335380	0.034441
H	-2.715911	-2.512583	-0.403945
H	-4.152913	-3.103367	0.484978
H	-4.255380	-2.788024	-1.274216
H	-6.224040	1.412011	0.512139
H	-2.527939	2.391988	0.476262
H	-4.006212	3.056240	-0.283634
H	-3.956830	2.775027	1.483854
H	5.235775	0.132939	0.702663

INT-II·H

SCF = -1019.35857289

Num. Imaginary Freq = 0

C	3.001560	0.832414	-0.362526
C	1.649843	1.157396	-0.125778
C	1.292486	2.484629	0.110413
C	2.277376	3.475744	0.100345
C	3.607461	3.156535	-0.164487
C	3.977663	1.825279	-0.405105
C	3.103761	-0.664267	-0.510652
C	1.637138	-1.097452	-0.480098
C	0.809626	-0.044147	-0.229816
H	0.242879	2.741724	0.291297

H	1.999743	4.517825	0.283540
H	4.363624	3.944866	-0.205695
H	5.016345	1.613312	-0.694265
H	3.594765	-0.974960	-1.455860
C	3.842844	-1.274535	0.675204
C	1.226101	-2.509857	-0.732414
H	1.262684	-3.142393	0.174028
H	0.185129	-2.543997	-1.090909
H	1.865142	-3.000118	-1.487229
O	5.165564	-0.535209	0.876051
C	6.294001	-0.822103	-0.000098
H	5.973932	-0.802301	-1.050848
H	7.045889	-0.051572	0.199878
H	6.682141	-1.805650	0.280944
Au	-1.249312	-0.059860	-0.073771
C	-3.336018	-0.073904	0.083335
N	-4.155656	-1.152239	0.084623
N	-4.163534	0.990814	0.210242
C	-5.476586	-0.768961	0.211937
C	-3.726764	-2.531529	-0.027557
C	-5.481655	0.585473	0.291347
C	-3.745393	2.377216	0.255307
H	-6.289869	-1.491064	0.232991
H	-2.637113	-2.553680	-0.161945
H	-3.988869	-3.091484	0.881859
H	-4.205694	-3.010995	-0.893297
H	-6.300309	1.294005	0.396978
H	-2.654158	2.421767	0.141891
H	-4.214699	2.944910	-0.560911
H	-4.026281	2.832796	1.215861
H	4.963065	0.433947	0.896887
H	3.320975	-1.004064	1.608380
C	4.166509	-2.736239	0.624874
H	4.843572	-3.017664	1.444808
H	3.239894	-3.308034	0.761946
H	4.602998	-3.036708	-0.340261

diast-INT-II

SCF = -1018.96363889

Num. Imaginary Freq = 0

C	3.057904	0.746260	-0.382471
C	1.698330	1.115381	-0.296520
C	1.349148	2.467734	-0.307922
C	2.354412	3.434102	-0.395918
C	3.697758	3.060390	-0.471732
C	4.057283	1.706730	-0.465689
C	3.139065	-0.751414	-0.362865
C	1.685590	-1.162671	-0.237346
C	0.848805	-0.085875	-0.209084
H	0.294482	2.761433	-0.246516
H	2.087577	4.496045	-0.403725
H	4.473933	3.829497	-0.535819
H	5.109998	1.410382	-0.514053
H	3.512473	-1.119709	-1.343118
C	4.058129	-1.346461	0.715620
C	1.315524	-2.604290	-0.179335
H	1.656307	-3.087058	0.756694
H	0.223633	-2.737141	-0.239315
H	1.779860	-3.179149	-1.002040
C	3.681549	-0.924259	2.115232
H	4.356862	-1.391772	2.847748
H	3.762919	0.169731	2.222588
H	2.647390	-1.217218	2.352706
H	3.979949	-2.455836	0.633949
O	5.410903	-0.985845	0.524552
C	6.020884	-1.522625	-0.608724
H	5.704423	-1.025267	-1.547608
H	7.108691	-1.388470	-0.510788
H	5.813937	-2.607008	-0.713769
Au	-1.211876	-0.075263	-0.076516
C	-3.308978	-0.066028	0.062364
N	-4.202927	-0.433003	-0.887553
N	-4.066769	0.302181	1.123672
C	-5.498945	-0.296996	-0.428729
C	-3.865848	-0.910062	-2.213104
C	-5.412806	0.168038	0.842876
C	-3.554576	0.775721	2.393285
H	-6.360989	-0.541957	-1.045489
H	-2.773753	-0.897963	-2.324207
H	-4.231395	-1.937238	-2.356912

H	-4.313104	-0.260597	-2.979405
H	-6.183908	0.414723	1.569503
H	-2.457598	0.779776	2.351037
H	-3.911093	1.796261	2.595112
H	-3.881071	0.114818	3.209277

INT-II

SCF = -1018.95838101

Num. Imaginary Freq = 0

C	3.008289	0.893523	-0.319043
C	1.658586	1.178215	-0.025385
C	1.294889	2.454212	0.410542
C	2.278204	3.436356	0.548644
C	3.612084	3.150594	0.252162
C	3.985127	1.872544	-0.183160
C	3.109595	-0.552669	-0.729491
C	1.657089	-1.005233	-0.691691
C	0.823902	-0.005508	-0.281632
H	0.245029	2.676448	0.635688
H	2.001384	4.440004	0.887821
H	4.371993	3.931618	0.356454
H	5.028980	1.646715	-0.418569
H	3.508247	-0.649910	-1.763597
C	4.090200	-1.316256	0.169366
H	3.792686	-1.117550	1.224151
C	1.224288	-2.357141	-1.158009
H	1.334174	-3.141183	-0.387457
H	0.160041	-2.341963	-1.443550
H	1.809230	-2.698510	-2.030287
C	4.159499	-2.811464	-0.063120
H	5.012952	-3.235931	0.489624
H	3.256171	-3.334217	0.279739
H	4.307890	-3.029265	-1.134095
O	5.372687	-0.757293	-0.065815
C	6.192159	-0.702422	1.060571
H	7.177476	-0.319314	0.755141
H	5.779909	-0.024129	1.835943
H	6.344427	-1.696544	1.527038
Au	-1.231263	-0.057462	-0.077813

C	-3.322571	-0.098315	0.132829
N	-4.252184	0.296954	-0.770241
N	-4.039669	-0.520432	1.202211
C	-5.530274	0.125836	-0.274409
C	-3.965897	0.833072	-2.085189
C	-5.395899	-0.391138	0.972796
C	-3.479299	-1.043216	2.431472
H	-6.415458	0.386410	-0.850722
H	-2.877862	0.847175	-2.230437
H	-4.425366	0.206211	-2.863043
H	-4.354463	1.857830	-2.175606
H	-6.139099	-0.677057	1.714035
H	-2.384320	-1.023153	2.355679
H	-3.792405	-0.428272	3.287584
H	-3.810184	-2.079161	2.594938

diast-TS-VI

SCF = -903.751828

Num. Imaginary Freq = 1

C	3.572427	0.267625	-0.393675
C	2.262901	0.755855	-0.163069
C	2.084943	2.123345	0.076096
C	3.197708	2.957933	0.084078
C	4.487619	2.455867	-0.143205
C	4.690228	1.097363	-0.371321
C	1.970438	-1.484589	-0.500033
C	1.287444	-0.319787	-0.256153
H	1.080993	2.519629	0.258949
H	3.067616	4.028343	0.266965
H	5.340751	3.139356	-0.147804
H	5.694532	0.701632	-0.548513
C	1.441681	-2.872074	-0.591657
H	1.946724	-3.453282	-1.381331
H	1.565963	-3.435276	0.351682
H	0.362278	-2.850496	-0.806463
Au	-0.760091	-0.089888	-0.113037
C	-2.827109	0.149231	0.057858
N	-3.769973	-0.822424	0.067011
N	-3.516085	1.306132	0.197857

C	-5.032453	-0.281889	0.211185
C	-3.514425	-2.243567	-0.055112
C	-4.871943	1.063050	0.293955
C	-2.933624	2.632158	0.245508
H	-5.927105	-0.900033	0.239915
H	-2.435139	-2.400613	-0.180811
H	-3.852331	-2.772810	0.847437
H	-4.041733	-2.652756	-0.928703
H	-5.597253	1.865330	0.410452
H	-3.346700	3.258724	-0.557782
H	-3.141646	3.108219	1.214514
H	-1.847281	2.547453	0.112193
C	3.479577	-1.220174	-0.619581
C	4.106435	-1.798127	0.553023
H	4.959486	-2.480327	0.408636
C	3.682588	-1.620012	1.928443
H	3.931059	-1.577328	-1.557714
H	4.557765	-1.395755	2.564583
H	2.872879	-0.893172	2.074134
H	3.352087	-2.614908	2.297488

TS-VI

SCF = -903.7583753

Num. Imaginary Freq = 1

C	3.522690	0.410465	-0.346173
C	2.186793	0.853428	-0.138966
C	1.958867	2.220226	0.084276
C	3.038958	3.090539	0.083721
C	4.355128	2.633265	-0.121924
C	4.613945	1.285242	-0.319088
C	1.989480	-1.392421	-0.478918
C	1.251721	-0.249528	-0.235176
H	0.940412	2.584657	0.251868
H	2.869783	4.158878	0.245465
H	5.179083	3.351478	-0.127488
H	5.633434	0.917693	-0.470171
C	1.507554	-2.786701	-0.665728
H	1.610410	-3.097239	-1.720731
H	2.081937	-3.517862	-0.072101

H	0.447011	-2.877241	-0.387687
Au	-0.801261	-0.093662	-0.083558
C	-2.876313	0.075045	0.078852
N	-3.788532	-0.925369	0.088258
N	-3.602510	1.210976	0.202034
C	-5.068605	-0.423386	0.215800
C	-3.486834	-2.338214	-0.023336
C	-4.950882	0.926663	0.287864
C	-3.060480	2.554121	0.247742
H	-5.943930	-1.068683	0.241905
H	-2.399174	-2.462065	-0.105601
H	-3.844398	-2.877185	0.865670
H	-3.966195	-2.763042	-0.916953
H	-5.702046	1.706606	0.391235
H	-3.499181	3.169210	-0.550718
H	-3.273994	3.022222	1.219490
H	-1.973300	2.501795	0.104582
C	3.473008	-1.076038	-0.511751
C	3.876932	-1.388931	0.847079
H	3.242360	-0.962494	1.634346
C	4.977752	-2.261726	1.219017
H	4.089441	-1.536749	-1.297487
H	5.356110	-2.079577	2.233195
H	4.548402	-3.289065	1.221788
H	5.782503	-2.273548	0.468648

INT-V

SCF = -903.773621957

Num. Imaginary Freq = 0

C	3.562366	0.134584	-0.182836
C	2.204022	0.647749	-0.126074
C	2.014610	2.035764	-0.073297
C	3.108908	2.870895	-0.212935
C	4.425619	2.376589	-0.405727
C	4.660049	1.028019	-0.414591
C	1.907356	-1.566275	-0.449624
C	1.214759	-0.396066	-0.238477
H	1.002886	2.442149	0.015676
H	2.955440	3.954016	-0.203001

H	5.249421	3.079553	-0.545700
H	5.673638	0.637114	-0.535184
C	1.372310	-2.941391	-0.560243
H	1.792699	-3.591280	0.227687
H	0.275789	-2.952559	-0.478813
H	1.663187	-3.402646	-1.519953
Au	-0.830960	-0.128148	-0.075463
C	-2.893206	0.143394	0.091171
N	-3.853832	-0.810625	0.070019
N	-3.564004	1.309994	0.241660
C	-5.108830	-0.249903	0.204626
C	-3.622129	-2.233853	-0.072177
C	-4.925777	1.090148	0.312673
C	-2.959152	2.624435	0.315145
H	-6.014376	-0.852646	0.211890
H	-2.541623	-2.411268	-0.151345
H	-4.011763	-2.774054	0.802497
H	-4.116771	-2.614227	-0.977473
H	-5.637864	1.903591	0.433564
H	-3.290120	3.247376	-0.528283
H	-3.235913	3.119652	1.256825
H	-1.867604	2.515194	0.273910
C	3.400733	-1.352700	-0.410116
C	3.905391	-1.032510	0.933271
H	3.154447	-0.969886	1.732048
C	5.306825	-1.293629	1.358160
H	4.081830	-1.852935	-1.108552
H	5.320050	-2.252405	1.901615
H	5.997627	-1.385022	0.508049
H	5.676623	-0.523142	2.050703

diast-8

SCF = -579.375153566

Num. Imaginary Freq = 0

C	3.415269	-0.804041	-0.049763
C	2.311250	-1.627787	0.159671
C	1.016436	-1.096169	0.176094
C	0.841969	0.291074	0.005726
C	1.946764	1.106268	-0.218232

C	3.233133	0.562873	-0.250327
C	-0.163964	-1.940725	0.315412
C	-0.556627	0.835558	0.150534
C	-1.607422	-0.083864	-0.466772
C	-1.403982	-1.509451	0.008431
C	-3.000471	0.464555	-0.202180
H	-3.783482	-0.114935	-0.713319
H	-3.225532	0.458702	0.879539
H	-3.071099	1.503365	-0.556927
C	-2.576878	-2.430570	0.024410
H	-3.355845	-2.098665	0.732385
H	-3.062961	-2.470029	-0.967322
H	-2.280195	-3.453490	0.299366
H	-1.433594	-0.079017	-1.567466
H	1.795124	2.178514	-0.373597
H	4.095122	1.212232	-0.429477
H	4.421670	-1.232777	-0.065012
H	2.444564	-2.706258	0.299001
H	-0.781272	0.866100	1.245042
O	-0.669598	2.130556	-0.387300
C	-0.781481	3.154043	0.559260
H	-0.811791	4.114619	0.024473
H	-1.708340	3.061753	1.159983
H	0.077984	3.173787	1.258321
H	-0.007545	-2.988936	0.599823

8

SCF = -579.376270086

Num. Imaginary Freq = 0

C	-3.288382	-1.021108	-0.016844
C	-2.099097	-1.648760	-0.380239
C	-0.865654	-1.012345	-0.190778
C	-0.845242	0.285815	0.358525
C	-2.038798	0.902528	0.724204
C	-3.262376	0.254574	0.544619
C	0.395671	-1.671308	-0.506191
C	0.483535	0.995630	0.430423
C	1.613809	0.042641	0.794323
C	1.581179	-1.206319	-0.065238

C	2.952344	0.764935	0.812978
H	3.754116	0.138712	1.232100
H	3.250083	1.075581	-0.200218
H	2.885976	1.674282	1.431915
C	2.854310	-1.940226	-0.315397
H	3.580473	-1.323633	-0.872936
H	3.351748	-2.213891	0.632613
H	2.680241	-2.863503	-0.887620
H	1.392204	-0.296164	1.831013
H	-2.008679	1.909782	1.156896
H	-4.193438	0.747301	0.838913
H	-4.243030	-1.533952	-0.167578
H	-2.116782	-2.656895	-0.808811
H	0.426596	1.796510	1.202854
O	0.812294	1.587125	-0.813244
C	0.016222	2.672139	-1.179628
H	0.445056	3.118488	-2.088787
H	-1.029957	2.382442	-1.399574
H	-0.008991	3.449455	-0.387982
H	0.350907	-2.610678	-1.071388

TS-IB

SCF = -903.7443250

Num. Imaginary Freq = 1

C	2.639094	3.273201	0.158753
C	1.795059	2.174058	0.272143
C	2.275195	0.867564	0.114287
C	3.657020	0.687012	-0.180291
C	4.480786	1.812894	-0.348290
C	3.987112	3.095031	-0.156267
C	1.386125	-0.288483	0.135164
C	4.200143	-0.627824	-0.401707
C	3.787303	-1.758283	0.249363
C	1.716153	-1.544445	0.099637
H	4.972260	-0.720397	-1.179882
C	1.256675	-2.927092	0.248608
H	0.154996	-2.920870	0.259891
H	1.583281	-3.574959	-0.579412
H	1.592501	-3.375295	1.198166
Au	-0.733873	-0.100638	0.037823

C	-2.786010	0.093953	-0.047076
N	-3.532427	1.218600	0.004757
N	-3.672298	-0.919924	-0.167281
C	-4.876738	0.914708	-0.083956
C	-3.018576	2.570124	0.108014
C	-4.964586	-0.435906	-0.190491
C	-3.309998	-2.323800	-0.232643
H	-5.645811	1.683488	-0.064279
H	-3.545299	3.110431	0.906436
H	-1.948880	2.528426	0.349007
H	-3.153952	3.108967	-0.840920
H	-5.827571	-1.091887	-0.279030
H	-2.565391	-2.485185	-1.024842
H	-2.892491	-2.660801	0.727734
H	-4.205339	-2.915372	-0.459818
C	4.388238	-3.096037	-0.035130
H	5.227682	-3.287425	0.653720
H	3.678846	-3.923077	0.109455
H	4.773967	-3.150914	-1.064004
H	3.381886	-1.609313	1.266602
H	5.534009	1.661065	-0.602863
H	4.647917	3.958631	-0.264694
H	2.236134	4.280294	0.293957
H	0.732306	2.323790	0.483737

diast-TS-II

SCF = -903.748815600

Num. Imaginary Freq = 1

C	3.641994	0.446080	-0.389571
C	2.289114	0.667201	-0.005059
C	1.911369	1.965766	0.293281
C	2.845813	3.017320	0.251379
C	4.154639	2.791410	-0.146446
C	4.551120	1.497090	-0.502180
C	3.974405	-0.918937	-0.680758
C	1.910304	-1.712906	-0.229493
C	1.360889	-0.489653	-0.097749
H	0.863783	2.175436	0.533877
H	2.520849	4.030747	0.501303

H	4.866956	3.617073	-0.208297
H	5.575918	1.299370	-0.827925
H	4.546022	-1.159425	-1.589510
C	3.467822	-1.959726	0.147047
C	1.246800	-3.017851	-0.517784
H	1.646696	-3.475215	-1.438711
H	1.410779	-3.744624	0.297451
H	0.163577	-2.873110	-0.647940
Au	-0.697554	-0.176673	-0.041988
C	-2.743954	0.193959	0.005971
N	-3.328835	1.413093	0.063133
N	-3.768889	-0.688223	0.001283
C	-4.703694	1.296762	0.098541
C	-2.602479	2.667980	0.114837
C	-4.982447	-0.031405	0.057773
C	-3.638033	-2.130010	-0.061095
H	-5.358653	2.163809	0.146782
H	-3.301531	3.496628	-0.054044
H	-2.121789	2.799812	1.095791
H	-1.830500	2.687840	-0.667051
H	-5.930128	-0.565119	0.059746
H	-2.571686	-2.388418	-0.088465
H	-4.098385	-2.593707	0.822984
H	-4.126618	-2.519609	-0.965641
C	3.618244	-1.871855	1.660783
H	2.941132	-2.596235	2.136423
H	4.650014	-2.120290	1.953175
H	3.373649	-0.867835	2.035892
H	3.759295	-2.951377	-0.226566

TS-II

SCF = -903.7472821

Num. Imaginary Freq = 1

C	3.607994	0.645612	-0.330613
C	2.249783	0.866165	0.027690
C	1.822599	2.178527	0.146840
C	2.714951	3.248123	-0.049425
C	4.029362	3.018013	-0.426558
C	4.475734	1.702644	-0.599685

C	4.008040	-0.731673	-0.395502
C	1.963837	-1.535443	0.133322
C	1.370484	-0.327820	0.080127
H	0.768845	2.380576	0.362272
H	2.352048	4.273570	0.058987
H	4.708204	3.853321	-0.612318
H	5.506768	1.501348	-0.903446
H	4.624016	-1.092425	-1.235002
C	3.550918	-1.642676	0.588755
H	3.519127	-1.191041	1.596601
C	1.332401	-2.881525	0.004131
H	1.825048	-3.500846	-0.762278
H	1.359944	-3.450541	0.948623
H	0.280150	-2.756673	-0.290807
C	4.158894	-3.022529	0.584238
H	5.194642	-2.964819	0.951321
H	3.617082	-3.711104	1.245221
H	4.183374	-3.455557	-0.427412
Au	-0.704988	-0.114832	0.040016
C	-2.777402	0.097646	-0.018380
N	-3.689201	-0.840622	-0.366708
N	-3.504838	1.201284	0.274056
C	-4.970787	-0.331889	-0.293120
C	-3.390326	-2.203793	-0.757123
C	-4.854304	0.958038	0.111200
C	-2.966148	2.480783	0.689289
H	-5.846209	-0.931550	-0.532470
H	-3.829284	-2.913087	-0.040842
H	-3.792940	-2.410163	-1.758924
H	-2.301189	-2.338022	-0.774148
H	-5.606649	1.721235	0.297326
H	-3.421963	2.794420	1.639030
H	-1.882088	2.381511	0.828287
H	-3.162754	3.247724	-0.073810

INT-IB/*enant*-INT-IB

SCF = -903.793028477

Num. Imaginary Freq = 0

C	-2.620233	3.152283	0.416047

C	-1.776301	2.076012	0.256033
C	-2.274419	0.768687	0.038997
C	-3.719186	0.632856	0.004131
C	-4.570680	1.775477	0.170084
C	-4.032968	3.012631	0.371336
C	-1.386843	-0.351984	-0.133276
C	-4.258403	-0.618633	-0.154965
C	-3.432903	-1.801733	-0.370204
C	-1.955087	-1.596147	-0.325595
H	-5.347599	-0.747331	-0.150744
C	-3.959612	-3.033696	0.378717
H	-3.490089	-3.955679	0.012616
H	-3.748102	-2.939497	1.454728
H	-5.046791	-3.131460	0.246234
C	-1.136096	-2.825743	-0.533360
H	-1.088297	-3.421924	0.397139
H	-1.568991	-3.484952	-1.304008
H	-0.104097	-2.576223	-0.819777
Au	0.692100	-0.102640	-0.054215
C	2.765254	0.119512	0.028974
N	3.492977	1.225951	-0.252868
N	3.677082	-0.817680	0.380871
C	4.841881	0.985909	-0.078859
C	2.953120	2.504899	-0.668039
C	4.958209	-0.305316	0.321199
C	3.376387	-2.181769	0.766686
H	5.593933	1.751613	-0.255795
H	3.129799	3.267773	0.104159
H	3.424704	2.829343	-1.606463
H	1.872461	2.398959	-0.829071
H	5.833238	-0.903612	0.565396
H	3.740912	-2.380346	1.784740
H	2.288398	-2.326782	0.740854
H	3.851002	-2.889641	0.072014
H	-3.630741	-1.997395	-1.459750
H	-5.653648	1.625520	0.132126
H	-4.671586	3.889244	0.499137
H	-2.191462	4.144625	0.582508
H	-0.692044	2.218953	0.293463

diast-TS-IV/*E*-TS'-IV

SCF = -1019.36340933

Num. Imaginary Freq = 1

C	2.231643	3.122067	-0.787365
C	1.403670	2.014029	-0.663354
C	1.920985	0.732827	-0.403563
C	3.338296	0.636643	-0.278538
C	4.168545	1.770330	-0.382587
C	3.621987	3.012690	-0.644742
C	1.047404	-0.439690	-0.248659
C	3.894218	-0.648187	-0.005614
C	3.127553	-1.845183	-0.408449
C	1.635713	-1.671000	-0.241817
C	3.491620	-2.133090	-1.880754
H	2.970172	-3.041946	-2.214162
H	3.182120	-1.299922	-2.530931
H	4.572941	-2.297604	-2.004122
C	0.889751	-2.960952	-0.139375
H	1.114568	-3.624837	-0.994089
H	1.187644	-3.522418	0.764635
H	-0.198490	-2.803678	-0.107611
Au	-1.016987	-0.164264	-0.064763
C	-3.072998	0.149412	0.118714
N	-3.692726	1.349604	0.216755
N	-4.073073	-0.761715	0.145341
C	-5.062151	1.192713	0.300045
C	-3.008391	2.628036	0.190223
C	-5.302999	-0.142313	0.257060
C	-3.902167	-2.198484	0.073250
H	-5.739871	2.039327	0.384746
H	-2.138466	2.601399	0.861032
H	-2.665895	2.866994	-0.827996
H	-3.695627	3.413674	0.528773
H	-6.233457	-0.704067	0.299075
H	-4.444707	-2.604521	-0.792459
H	-2.833389	-2.422605	-0.035947
H	-4.279316	-2.676948	0.988560
H	3.479257	-2.707610	0.187371
H	5.251003	1.648393	-0.267778

H	4.260201	3.894022	-0.740560
H	1.787797	4.099889	-0.995943
H	0.319515	2.127590	-0.770939
H	4.988438	-0.739540	0.005987
O	3.746866	-0.849580	1.893410
C	4.232624	0.248855	2.658197
H	3.713123	1.186510	2.400864
H	4.101309	0.034349	3.727952
H	5.304235	0.349167	2.439592
H	2.792749	-0.969581	2.052260

diast-TS'-IV/*E*-TS-IV

SCF = -1019.36316562

Num. Imaginary Freq = 1

C	2.120764	3.255055	-0.807901
C	1.323978	2.123431	-0.695309
C	1.879834	0.846372	-0.498734
C	3.298580	0.779813	-0.423994
C	4.099133	1.932419	-0.516295
C	3.516201	3.171282	-0.717018
C	1.041889	-0.354967	-0.373821
C	3.889653	-0.507495	-0.195693
C	3.153087	-1.703549	-0.655449
C	1.652404	-1.574761	-0.455566
C	0.899374	-2.866348	-0.466807
H	-0.184583	-2.691650	-0.406822
H	1.100716	-3.437346	-1.391428
H	1.187168	-3.526987	0.369692
Au	-1.023022	-0.136265	-0.110339
C	-3.082954	0.100965	0.162487
N	-3.746166	1.247021	0.448954
N	-4.048866	-0.843870	0.068758
C	-5.106974	1.023726	0.530027
C	-3.135760	2.548603	0.628414
C	-5.298152	-0.297774	0.290188
C	-3.829975	-2.244620	-0.229018
H	-5.812582	1.821146	0.752707
H	-3.399699	3.219152	-0.202620
H	-3.475084	2.998445	1.572119

H	-2.045059	2.428476	0.660906
H	-6.205537	-0.896989	0.261133
H	-4.309180	-2.515299	-1.180934
H	-2.750629	-2.426557	-0.307351
H	-4.243784	-2.874040	0.571688
C	3.792230	-3.013399	-0.215008
H	3.402513	-3.864414	-0.789499
H	4.881723	-2.980345	-0.369632
H	3.610905	-3.210941	0.852466
H	3.313108	-1.612873	-1.760088
H	5.187382	1.832617	-0.442435
H	4.132676	4.068921	-0.804704
H	1.648475	4.228750	-0.967284
H	0.234822	2.213146	-0.767557
H	4.986345	-0.571520	-0.224012
O	3.782568	-0.752233	1.640814
C	4.363541	0.279787	2.437598
H	3.900131	1.257831	2.232337
H	4.241327	0.022059	3.498187
H	5.433498	0.315109	2.194000
H	2.827608	-0.827207	1.826788

diast-INT-III·H/diast-INT'-III·H

SCF = -1019.36905593

Num. Imaginary Freq = 0

C	2.322160	3.087416	-0.946690
C	1.471195	1.994323	-0.796727
C	1.954035	0.742117	-0.391286
C	3.340783	0.645463	-0.130288
C	4.191894	1.740651	-0.266788
C	3.686151	2.970078	-0.682720
C	1.067472	-0.438446	-0.249714
C	3.834011	-0.675836	0.325305
C	3.164230	-1.827379	-0.375337
C	1.654147	-1.669763	-0.258496
C	0.913249	-2.967003	-0.217597
H	-0.177071	-2.819581	-0.219369
H	1.175429	-3.596157	-1.088196
H	1.184941	-3.559334	0.675078

Au	-0.993480	-0.151543	-0.080092
C	-3.054718	0.157934	0.102190
N	-3.694204	1.337222	0.291039
N	-4.042543	-0.767190	0.049358
C	-5.061741	1.153172	0.355152
C	-3.054828	2.632548	0.401918
C	-5.281852	-0.176815	0.202618
C	-3.852245	-2.190195	-0.144187
H	-5.751180	1.981602	0.502803
H	-3.362767	3.285574	-0.427607
H	-3.326117	3.111769	1.353515
H	-1.966119	2.495596	0.365957
H	-6.203878	-0.753892	0.189976
H	-4.362324	-2.524234	-1.059102
H	-2.778092	-2.394345	-0.238359
H	-4.251474	-2.750735	0.713265
C	3.630882	-1.917805	-1.826482
H	4.723430	-2.045822	-1.891196
H	3.161174	-2.782234	-2.318542
H	3.351646	-1.014520	-2.391827
H	3.469873	-2.755481	0.144130
H	5.259536	1.623393	-0.048846
H	4.350376	3.830329	-0.797562
H	1.912364	4.047568	-1.273304
H	0.401390	2.099965	-1.009214
H	4.931268	-0.757089	0.368173
O	3.427040	-0.864712	1.798489
C	3.903313	0.103748	2.769032
H	3.483449	1.094674	2.551361
H	3.594314	-0.258851	3.754771
H	4.996450	0.110998	2.687631
H	2.440407	-0.955110	1.793587

INT-III·H/INT'-III·H

SCF = -1019.36700268

Num. Imaginary Freq = 0

C	2.142874	3.286360	-0.844030
C	1.345513	2.148179	-0.753024
C	1.896262	0.890887	-0.463283

C	3.293893	0.837048	-0.260482
C	4.091930	1.978248	-0.330569
C	3.519320	3.211239	-0.631221
C	1.068562	-0.333867	-0.374021
C	3.855937	-0.492339	0.068162
C	3.214723	-1.611999	-0.707145
C	1.698876	-1.538689	-0.507014
C	0.967720	-2.842796	-0.562424
H	-0.115548	-2.691371	-0.445890
H	1.135255	-3.350805	-1.529751
H	1.301139	-3.550931	0.216047
Au	-0.995280	-0.136291	-0.112225
C	-3.058608	0.087931	0.149009
N	-3.733425	1.236718	0.394142
N	-4.014996	-0.869114	0.086599
C	-5.092044	1.003012	0.481429
C	-3.135538	2.548805	0.534997
C	-5.269893	-0.327903	0.287582
C	-3.781467	-2.277547	-0.159583
H	-5.805840	1.801053	0.673719
H	-3.457473	3.209599	-0.283023
H	-3.427754	2.999050	1.494357
H	-2.042924	2.445889	0.504949
H	-6.171438	-0.936480	0.276153
H	-4.288812	-2.595262	-1.081838
H	-2.702350	-2.444759	-0.269110
H	-4.155552	-2.880092	0.680536
C	3.864818	-2.955859	-0.414188
H	3.482116	-3.742897	-1.078397
H	4.953569	-2.895725	-0.568471
H	3.690787	-3.278971	0.624544
H	3.423202	-1.350717	-1.767477
H	5.170383	1.893966	-0.155943
H	4.141313	4.107383	-0.697940
H	1.681502	4.249367	-1.081200
H	0.265019	2.221322	-0.920095
H	4.956523	-0.528094	0.072852
O	3.513543	-0.814297	1.541272
C	4.008663	0.079357	2.569888
H	3.584000	1.083181	2.435850

H	3.720943	-0.354280	3.533215
H	5.099982	0.093629	2.467319
H	2.530442	-0.936335	1.565490

diast-INT-III/diast-INT'-III

SCF = -1018.95930627

Num. Imaginary Freq = 0

C	1.982713	3.344618	-0.672452
C	1.208445	2.188973	-0.595261
C	1.771588	0.940819	-0.283344
C	3.160850	0.898343	-0.032385
C	3.935585	2.052324	-0.115508
C	3.353958	3.279764	-0.435938
C	0.963083	-0.297118	-0.250653
C	3.750295	-0.430629	0.351175
C	3.137038	-1.555267	-0.470290
C	1.616563	-1.487002	-0.364121
C	0.895750	-2.794575	-0.485047
H	-0.195506	-2.649092	-0.481265
H	1.163630	-3.313792	-1.424788
H	1.147262	-3.497001	0.329681
Au	-1.109350	-0.139333	-0.063656
C	-3.188810	0.043851	0.157832
N	-3.890745	1.174510	0.414723
N	-4.126999	-0.930179	0.069966
C	-5.245595	0.912779	0.485258
C	-3.318409	2.493553	0.590347
C	-5.395049	-0.417838	0.267388
C	-3.859687	-2.328601	-0.195306
H	-5.977346	1.692805	0.684078
H	-3.676983	3.176999	-0.193202
H	-3.592561	2.901717	1.573835
H	-2.225028	2.415603	0.527070
H	-6.284249	-1.043839	0.236381
H	-4.348411	-2.643865	-1.128629
H	-2.775425	-2.468121	-0.293720
H	-4.229062	-2.953284	0.630837
C	3.740654	-2.887263	-0.051932
H	3.394601	-3.724030	-0.676349

H	4.837546	-2.846430	-0.128213
H	3.484522	-3.120946	0.997569
H	3.417134	-1.365507	-1.532604
H	5.012786	1.981486	0.063174
H	3.972013	4.180318	-0.502287
H	1.511568	4.299867	-0.924723
H	0.131309	2.238762	-0.796556
H	3.467997	-0.635645	1.413073
O	5.155044	-0.434462	0.231722
C	5.845964	-0.402121	1.444952
H	5.656135	-1.308650	2.054727
H	6.923480	-0.353865	1.227774
H	5.577473	0.481524	2.058046

INT-III/INT'-III

SCF = -1018.96316618

Num. Imaginary Freq = 0

C	2.014142	3.328508	0.613549
C	1.239480	2.172410	0.538018
C	1.787410	0.938125	0.155675
C	3.163500	0.909207	-0.168657
C	3.936689	2.064287	-0.095233
C	3.369463	3.277768	0.298042
C	0.972869	-0.298127	0.107796
C	3.736770	-0.402735	-0.624497
C	3.151029	-1.549729	0.192378
C	1.634665	-1.485639	0.127616
C	0.968947	-2.824739	0.148341
H	-0.127063	-2.745591	0.224009
H	1.210634	-3.407341	-0.760550
H	1.329379	-3.433978	0.998947
Au	-1.104423	-0.152215	0.015588
C	-3.193365	0.017845	-0.106730
N	-3.914112	1.148748	-0.303305
N	-4.119306	-0.966770	-0.008215
C	-5.268526	0.876575	-0.327182
C	-3.360003	2.477184	-0.466998
C	-5.398395	-0.460864	-0.140660
C	-3.829604	-2.368860	0.210102

H	-6.014018	1.654982	-0.474872
H	-3.657697	2.899994	-1.437412
H	-3.711056	3.142012	0.335670
H	-2.264752	2.411093	-0.426268
H	-6.280647	-1.095456	-0.091009
H	-4.230654	-2.976325	-0.614098
H	-2.740897	-2.500849	0.256654
H	-4.273642	-2.711195	1.156151
C	3.659220	-1.555776	1.630797
H	3.215589	-2.386993	2.202292
H	4.755299	-1.663355	1.670959
H	3.394713	-0.616848	2.145902
H	3.464671	-2.498241	-0.286527
H	4.997840	2.002426	-0.351028
H	3.986639	4.179683	0.355228
H	1.554674	4.272649	0.922816
H	0.173543	2.211060	0.793970
H	3.405574	-0.564666	-1.681387
O	5.140784	-0.342428	-0.592065
C	5.786386	-1.390239	-1.249360
H	5.383012	-1.543434	-2.270688
H	6.853532	-1.137135	-1.333511
H	5.708326	-2.353116	-0.707510

9

SCF = -579.368003000

Num. Imaginary Freq = 0

C	-3.301901	0.163928	0.073297
C	-2.224319	1.028093	-0.129492
C	-0.946540	0.489753	-0.210672
C	-0.726260	-0.887338	-0.080207
C	-1.807498	-1.750085	0.113760
C	-3.092414	-1.214545	0.186885
C	0.351581	1.192212	-0.483530
C	0.716541	-1.160573	-0.154545
C	1.419661	0.177834	0.001124
C	1.288352	-2.366117	-0.303386
C	2.748141	-2.649453	-0.361253
H	3.015067	-3.204939	-1.276731

H	3.358538	-1.734145	-0.330880
H	3.064637	-3.288820	0.481974
H	2.329110	0.230935	-0.623304
C	1.792020	0.410830	1.461267
H	2.487054	-0.369467	1.809841
H	2.270513	1.390300	1.615050
H	0.895854	0.374185	2.103621
H	0.620781	-3.234624	-0.393874
H	-2.374375	2.108207	-0.220900
H	-4.317135	0.565057	0.146451
H	-3.947009	-1.878626	0.347782
H	-1.651861	-2.827783	0.228871
O	0.388985	2.455419	0.116039
C	1.393699	3.286633	-0.388758
H	1.322671	4.260395	0.116365
H	2.408603	2.879246	-0.212317
H	1.280518	3.446443	-1.479383
H	0.458774	1.313237	-1.587817

diast-9

SCF = -579.366902245

Num. Imaginary Freq = 0

C	2.929300	-1.255237	0.291380
C	2.348756	-0.002995	0.504183
C	0.981370	0.148877	0.299737
C	0.186031	-0.940084	-0.090341
C	0.769454	-2.190584	-0.305363
C	2.143006	-2.336458	-0.117653
C	0.132191	1.396128	0.372510
C	-1.220828	-0.521626	-0.159641
C	-1.294564	0.847162	0.496027
H	0.412460	2.047965	1.230126
C	-2.238463	-1.234809	-0.666036
C	-3.663086	-0.809294	-0.726972
H	-4.059669	-0.881760	-1.754071
H	-4.304393	-1.462749	-0.108945
H	-3.809162	0.225301	-0.381148
C	-1.726034	0.729237	1.952533
H	-2.726197	0.275949	2.036663

H -1.024822 0.089106 2.515930

H -1.753406 1.715064 2.444719

H -1.974693 1.527822 -0.044828

O 0.197039 2.148675 -0.823049

C 1.425995 2.764653 -1.061486

H 2.227276 2.040369 -1.307157

H 1.307648 3.443877 -1.918425

H 1.764459 3.360058 -0.188416

H -2.007296 -2.225167 -1.083121

H 2.961243 0.843390 0.834141

H 4.002663 -1.393953 0.450156

H 2.609792 -3.313227 -0.276524

H 0.159020 -3.051257 -0.597969

diast-TS-IC

SCF = -903.7328443

Num. Imaginary Freq = 1

C -2.358059 0.957794 2.838619

C -1.843206 0.974827 1.552454

C -2.478498 0.203192 0.564349

C -3.684023 -0.482035 0.864678

C -4.173765 -0.511321 2.180492

C -3.511744 0.214851 3.154740

C -4.202808 -1.102055 -0.313823

H -4.643408 -2.105905 -0.275601

C -3.891079 -0.492980 -1.520587

H -3.940187 -1.148247 -2.402090

C -4.175946 0.957731 -1.852680

H -4.213594 1.599563 -0.961004

H -5.162602 0.995640 -2.344455

H -3.450360 1.383657 -2.560112

C -2.014008 -0.012638 -0.772353

C -1.054385 -0.009148 -1.642197

C 4.822665 0.011297 0.814235

C 4.175398 -0.205186 1.987515

H 5.881988 0.106575 0.586850

H 4.551812 -0.334195 2.999791

N 3.852606 0.091904 -0.165149

N 2.827384 -0.254100 1.693523

C 2.622229 -0.069711 0.369531

C 4.143027 0.317127 -1.567507

H 3.203210 0.294293 -2.133801

H 4.812369 -0.467535 -1.947371

H 4.622746 1.296473 -1.705687

C 1.781582 -0.423695 2.684102

H 2.147334 -1.066541 3.495235

H 0.908864 -0.899097 2.216105

H 1.478516 0.547413 3.104513

Au 0.795823 -0.033222 -0.595291

C -1.013283 -0.064586 -3.126093

H -0.501759 0.828290 -3.521300

H -2.011993 -0.127915 -3.586856

H -0.420135 -0.928162 -3.465473

H -5.083349 -1.070593 2.414626

H -3.890689 0.222531 4.179913

H -1.849107 1.517687 3.628118

H -0.934148 1.535222 1.315088

INT-IC/*enant*-INT-IC

SCF = -903.780863255

Num. Imaginary Freq = 0

C	-3.627969	3.221913	0.422688
C	-4.503387	2.193643	0.222549
C	-3.972198	0.880327	0.039432
C	-2.547254	0.625760	0.056291
C	-1.681709	1.718210	0.272652
C	-2.222781	2.971608	0.452012
C	-4.625973	-0.310448	-0.162515
C	-2.307975	-0.767910	-0.178279
C	-3.672504	-1.429698	-0.270649
H	-5.712518	-0.437543	-0.189490
C	-1.086542	-1.389067	-0.343536
C	-1.051301	-2.834596	-0.710673
H	-0.318105	-3.010820	-1.515444
H	-0.662894	-3.415137	0.148286
H	-2.012191	-3.277271	-1.019875
Au	0.786949	-0.523945	-0.141369
C	2.703394	0.292394	0.031613

N	3.816968	-0.294958	0.526450
N	3.091782	1.540448	-0.321041
C	4.889821	0.573566	0.486833
C	3.901430	-1.652794	1.026616
C	4.430924	1.733960	-0.047108
C	2.217916	2.561404	-0.865225
H	5.880037	0.287455	0.834440
H	2.908767	-2.116722	0.963340
H	4.612167	-2.238260	0.426091
H	4.232551	-1.652900	2.074859
H	4.936664	2.673144	-0.260368
H	2.787024	3.205482	-1.548332
H	1.402625	2.083731	-1.424757
H	1.790468	3.182633	-0.062972
C	-3.965087	-2.469346	0.825032
H	-3.279312	-3.324291	0.751624
H	-3.841000	-2.014831	1.820701
H	-4.994757	-2.847993	0.740768
H	-3.809802	-1.916080	-1.260238
H	-5.584445	2.351793	0.199542
H	-3.989798	4.242322	0.567837
H	-1.549737	3.816002	0.629199
H	-0.598829	1.568982	0.308695

diast-TS'-V/*E*-TS-V

SCF = -1019.34322758

Num. Imaginary Freq = 1

C	2.926107	3.436259	-0.881241
C	3.861574	2.436868	-0.678039
C	3.409339	1.115072	-0.569097
C	2.042098	0.763700	-0.638540
C	1.114638	1.793550	-0.864714
C	1.562169	3.102932	-0.973600
C	4.178354	-0.075126	-0.311913
C	1.876057	-0.690030	-0.535743
C	3.304750	-1.260785	-0.587824
C	0.702921	-1.376946	-0.472165
C	0.689893	-2.877788	-0.575468
H	-0.265472	-3.244787	-0.981975

H	1.492893	-3.286909	-1.212193
H	0.787672	-3.345996	0.422422
H	3.541454	-1.459651	-1.659024
C	3.666438	-2.500229	0.214792
H	3.260880	-3.415339	-0.231427
H	4.760154	-2.626273	0.261585
H	3.276373	-2.440595	1.244046
H	5.253488	-0.128722	-0.523791
O	4.423572	0.023758	1.460717
C	5.506413	-0.593944	2.164021
H	6.361589	-0.616881	1.476155
H	5.763810	0.025682	3.033516
H	5.256305	-1.616271	2.479051
Au	-1.167004	-0.535618	-0.122326
C	-3.066237	0.245513	0.283106
N	-3.352910	1.455396	0.820348
N	-4.270807	-0.328011	0.054612
C	-4.717978	1.639008	0.922308
C	-2.368624	2.452614	1.191472
C	-5.298129	0.510743	0.440435
C	-4.479086	-1.646783	-0.508419
H	-5.152826	2.548848	1.330418
H	-2.205765	3.169430	0.371668
H	-2.712575	2.998759	2.080032
H	-1.418130	1.953715	1.423516
H	-6.344136	0.228165	0.344076
H	-5.011141	-2.289915	0.207280
H	-5.067607	-1.578527	-1.434556
H	-3.501788	-2.092290	-0.735116
H	3.580096	-0.004505	1.945699
H	4.929439	2.663598	-0.605641
H	3.239992	4.478351	-0.979612
H	0.832714	3.899698	-1.149376
H	0.049155	1.564698	-0.969652

diast-TS-V/*E*-TS'-V

SCF = -1019.35002427

Num. Imaginary Freq = 1

C	-3.205024	3.297545	0.070989

C	-4.075331	2.224051	0.016065
C	-3.536619	0.935656	-0.138914
C	-2.140085	0.699374	-0.247743
C	-1.280520	1.805705	-0.185694
C	-1.818013	3.075627	-0.026478
C	-4.217706	-0.321698	-0.190917
C	-1.887070	-0.728497	-0.439939
C	-3.262077	-1.355978	-0.684718
C	-0.696345	-1.387228	-0.435825
C	-0.672153	-2.869772	-0.664729
H	-0.081022	-3.379207	0.115771
H	-1.660002	-3.360829	-0.709796
H	-0.144136	-3.093738	-1.610140
H	-3.418358	-2.309950	-0.151706
C	-3.529720	-1.587414	-2.178184
H	-2.816532	-2.324455	-2.574584
H	-4.549059	-1.965023	-2.354148
H	-3.398724	-0.653247	-2.748200
Au	1.179690	-0.543039	-0.140077
C	3.098063	0.248551	0.147652
N	3.624407	1.351006	-0.436833
N	4.074589	-0.212718	0.963454
C	4.911225	1.579469	0.009753
C	2.923463	2.212450	-1.368487
C	5.196559	0.589975	0.893490
C	3.981038	-1.391446	1.801129
H	5.507678	2.417998	-0.342997
H	2.442172	3.051686	-0.843184
H	3.632268	2.613197	-2.105333
H	2.155072	1.629672	-1.893596
H	6.095017	0.381804	1.470186
H	4.107304	-1.120569	2.859260
H	2.991388	-1.845545	1.661849
H	4.755182	-2.121106	1.523559
O	-4.430370	-0.868979	1.597201
C	-5.165062	0.028248	2.427212
H	-6.170167	0.120273	1.995004
H	-5.244345	-0.394952	3.437780
H	-4.686485	1.019664	2.474124
H	-5.293054	-0.403396	-0.388725

H	-5.158499	2.367106	0.082214
H	-3.586347	4.315374	0.182209
H	-1.142194	3.935299	0.013459
H	-0.197603	1.670993	-0.272943
H	-3.532807	-0.994871	1.954145

diast-INT-IV·H/diast-INT'-IV·H

SCF = -1019.35380874

Num. Imaginary Freq = 0

C	-3.161909	3.313087	0.152198
C	-4.038275	2.232249	0.131740
C	-3.512164	0.952219	-0.039402
C	-2.131653	0.715998	-0.207268
C	-1.266403	1.816372	-0.182037
C	-1.787007	3.094235	0.000152
C	-4.221375	-0.346926	-0.047885
C	-1.883863	-0.719948	-0.426067
C	-3.266767	-1.327640	-0.697963
C	-0.703021	-1.388153	-0.435061
C	-0.684828	-2.865399	-0.708594
H	-0.124405	-3.407059	0.073335
H	-1.676880	-3.342361	-0.800357
H	-0.134317	-3.069543	-1.645378
H	-3.400993	-2.326428	-0.246347
C	-3.557425	-1.421286	-2.193223
H	-2.833826	-2.095426	-2.674802
H	-4.571395	-1.805322	-2.389462
H	-3.461650	-0.433128	-2.673297
Au	1.176785	-0.553723	-0.129617
C	3.098380	0.239069	0.147186
N	3.630685	1.318330	-0.474718
N	4.072221	-0.196803	0.980206
C	4.917914	1.557222	-0.034489
C	2.934010	2.150501	-1.435631
C	5.197933	0.598187	0.883734
C	3.972909	-1.346525	1.856250
H	5.518454	2.380394	-0.415408
H	2.460461	3.012052	-0.940200
H	3.643447	2.518451	-2.188885

H	2.159184	1.554929	-1.936371
H	6.094729	0.406729	1.468788
H	4.119078	-1.043820	2.903156
H	2.974073	-1.788251	1.745543
H	4.731047	-2.097689	1.591677
O	-4.392875	-0.846950	1.415196
C	-5.257364	-0.086197	2.300577
H	-6.230663	-0.025257	1.800500
H	-5.341497	-0.656146	3.231591
H	-4.834674	0.912115	2.475197
H	-5.263528	-0.368471	-0.399943
H	-5.117403	2.384337	0.240540
H	-3.543928	4.329455	0.277259
H	-1.106032	3.950733	0.009405
H	-0.189420	1.673417	-0.320904
H	-3.507741	-0.997093	1.808835

INT-IV·H/INT'-IV·H

SCF = -1019.34848616

Num. Imaginary Freq = 0

C	-2.865022	3.440130	0.398818
C	-3.767481	2.464979	-0.018949
C	-3.320374	1.150920	-0.122261
C	-1.994767	0.775532	0.151658
C	-1.102728	1.768386	0.574446
C	-1.543486	3.083986	0.691483
C	-4.070931	-0.047589	-0.580475
C	-1.818198	-0.669988	-0.064703
C	-3.239516	-1.254822	-0.139205
C	-0.666292	-1.375731	-0.167713
C	-0.706652	-2.864354	-0.369882
H	-0.081851	-3.166430	-1.228347
H	-0.261846	-3.378743	0.502163
H	-1.712316	-3.294924	-0.523920
C	-3.645932	-1.795473	1.230542
H	-2.938582	-2.580463	1.534534
H	-3.592722	-1.009975	2.005635
H	-4.650381	-2.251203	1.250192

H	-3.317207	-2.060601	-0.887209
Au	1.247062	-0.565096	-0.096783
C	3.190952	0.217818	-0.050178
N	3.565339	1.488375	-0.334423
N	4.339766	-0.415498	0.284654
C	4.928114	1.649266	-0.176179
C	2.660637	2.557507	-0.706832
C	5.418068	0.445267	0.213281
C	4.447713	-1.810131	0.661850
H	5.425306	2.599508	-0.358727
H	2.408556	3.181193	0.164928
H	3.128052	3.189420	-1.474125
H	1.737962	2.122874	-1.114090
H	6.432642	0.123397	0.438085
H	4.872157	-1.901510	1.672042
H	3.444831	-2.256414	0.651286
H	5.091125	-2.351328	-0.046891
H	-4.305912	-0.041002	-1.658552
O	-5.458979	-0.009454	0.009374
C	-6.469873	-0.905703	-0.538814
H	-6.167559	-1.949068	-0.382565
H	-7.409957	-0.673906	-0.029024
H	-6.539395	-0.666872	-1.605038
H	-5.446026	0.030411	0.988465
H	-0.069088	1.506458	0.825172
H	-0.842574	3.854321	1.027725
H	-3.187812	4.479510	0.500819
H	-4.804634	2.723396	-0.254657

diast-INT-IV/diast-INT'-IV

SCF = -1018.95047624

Num. Imaginary Freq = 0

C	-3.138696	3.312127	0.111628
C	-4.016950	2.227019	0.153003
C	-3.511401	0.938578	0.016418
C	-2.138681	0.703238	-0.185843
C	-1.268438	1.798362	-0.226903
C	-1.771461	3.089170	-0.071319
C	-4.243605	-0.376619	0.100260

C	-1.898435	-0.740219	-0.381715
C	-3.287733	-1.352230	-0.587227
C	-0.717242	-1.404526	-0.416044
C	-0.701498	-2.890597	-0.659328
H	-0.127273	-3.419263	0.122631
H	-1.699019	-3.362241	-0.712772
H	-0.177993	-3.123855	-1.605580
H	-3.387399	-2.331515	-0.088083
C	-3.611092	-1.495688	-2.068940
H	-2.885745	-2.155436	-2.570928
H	-4.620782	-1.910755	-2.228796
H	-3.566372	-0.514233	-2.573469
Au	1.162817	-0.563647	-0.141282
C	3.083958	0.243911	0.140986
N	3.595216	1.359380	-0.434179
N	4.071823	-0.210825	0.948261
C	4.881098	1.601513	0.009249
C	2.878231	2.220333	-1.353065
C	5.183388	0.607344	0.881755
C	3.995995	-1.398321	1.774449
H	5.464280	2.452244	-0.336652
H	2.423097	3.071200	-0.822846
H	3.567686	2.603917	-2.117388
H	2.085476	1.640654	-1.844426
H	6.086657	0.406279	1.453620
H	4.149163	-1.139486	2.832098
H	3.000947	-1.846350	1.655052
H	4.759982	-2.128541	1.470343
O	-4.411504	-0.807166	1.439824
C	-5.301865	-0.042919	2.191516
H	-6.282367	0.068627	1.682765
H	-5.467977	-0.554140	3.151481
H	-4.918954	0.974038	2.407986
H	-5.241727	-0.335450	-0.392428
H	-5.093365	2.388925	0.282529
H	-3.519031	4.332870	0.213842
H	-1.085677	3.941820	-0.111358
H	-0.196805	1.643338	-0.396751

INT-IV/INT'-IV

SCF = -1018.95161460

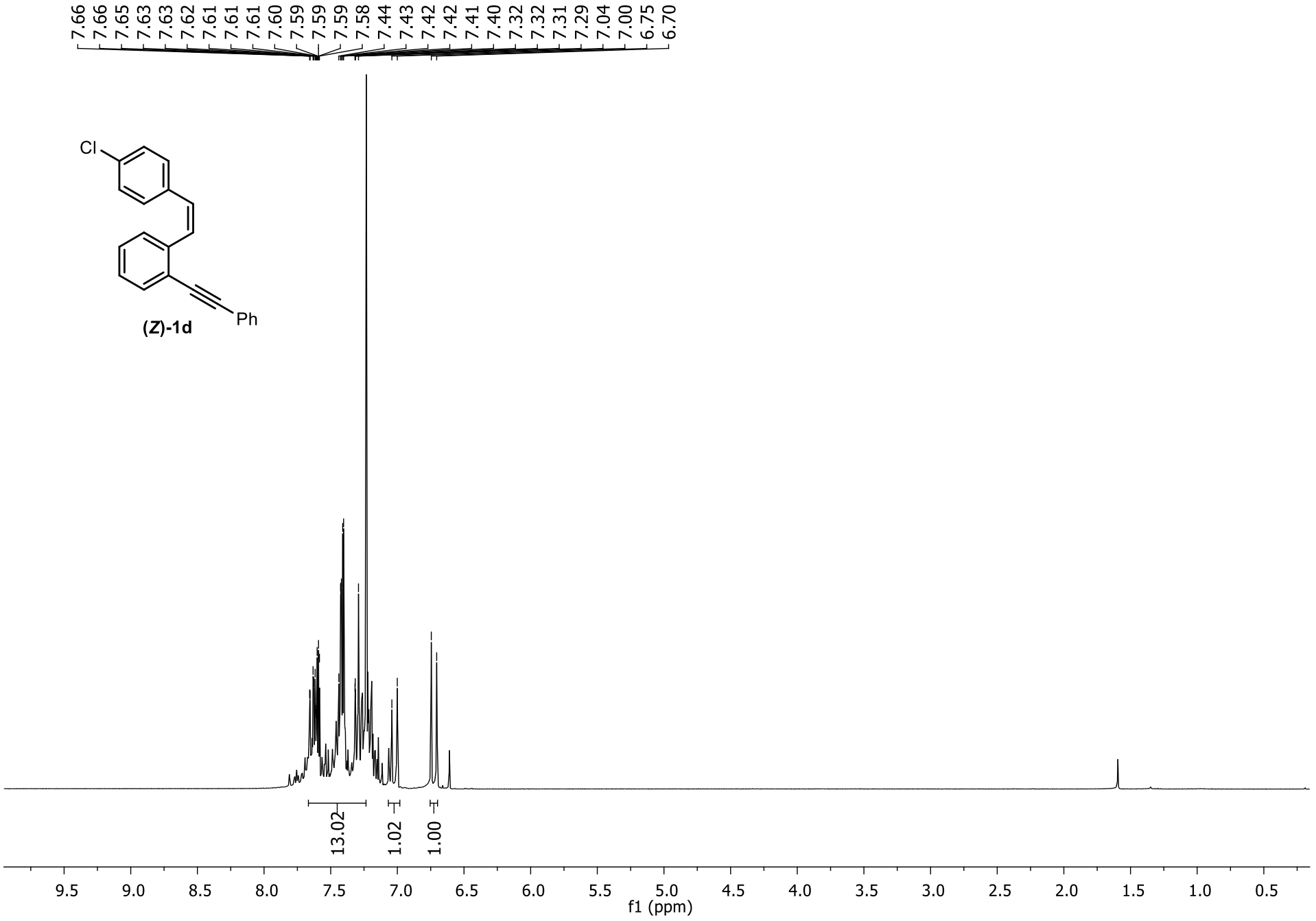
Num. Imaginary Freq = 0

C	2.860352	3.461688	-0.500317
C	3.766744	2.411719	-0.662188
C	3.330037	1.111572	-0.447779
C	2.010396	0.821273	-0.065656
C	1.111563	1.881645	0.093630
C	1.540634	3.190172	-0.128765
C	4.104196	-0.161675	-0.607803
C	1.861206	-0.634888	0.141339
C	3.293387	-1.175701	0.227659
C	0.718480	-1.356315	0.253292
C	0.779953	-2.840159	0.500805
H	0.190697	-3.398376	-0.248916
H	1.797741	-3.269845	0.508981
H	0.314193	-3.089351	1.472683
H	3.372566	-2.187117	-0.207657
C	3.766267	-1.213263	1.676410
H	3.121852	-1.878561	2.273149
H	4.805343	-1.567560	1.770959
H	3.716812	-0.207729	2.128529
H	4.053587	-0.472578	-1.679423
O	5.449558	0.004592	-0.250500
C	6.276548	-1.031151	-0.691214
H	6.241358	-1.141139	-1.793756
H	7.310386	-0.798728	-0.397330
H	6.004046	-2.009733	-0.248977
Au	-1.206438	-0.588140	0.099630
C	-3.167456	0.156063	-0.055343
N	-3.693938	1.210224	0.613951
N	-4.171002	-0.281333	-0.852731
C	-5.004802	1.432099	0.238245
C	-2.970593	2.034351	1.561130
C	-5.307284	0.487514	-0.687680
C	-4.088012	-1.409466	-1.757366
H	-5.603018	2.234885	0.663895
H	-2.575238	2.939536	1.074877
H	-3.638654	2.332268	2.380658
H	-2.133209	1.455975	1.973791

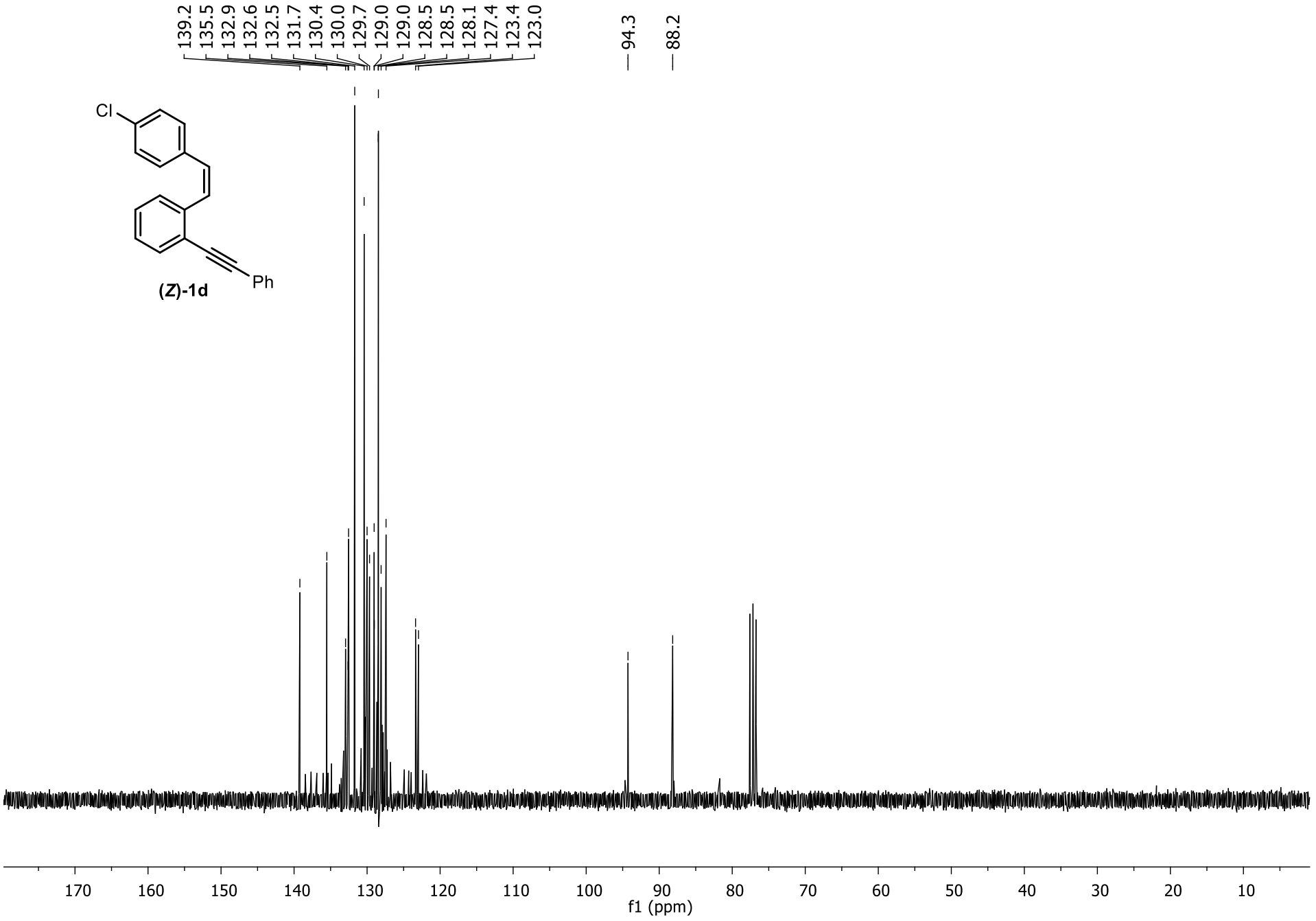
H	-6.225291	0.290676	-1.237163
H	-4.299777	-1.090179	-2.788031
H	-3.072127	-1.822946	-1.710815
H	-4.808544	-2.188587	-1.468805
H	4.806409	2.599958	-0.948438
H	3.182084	4.495705	-0.657605
H	0.835841	4.017346	0.004897
H	0.079969	1.687283	0.408762

^{1}H and ^{13}C NMR Spectra of Characterized Compounds

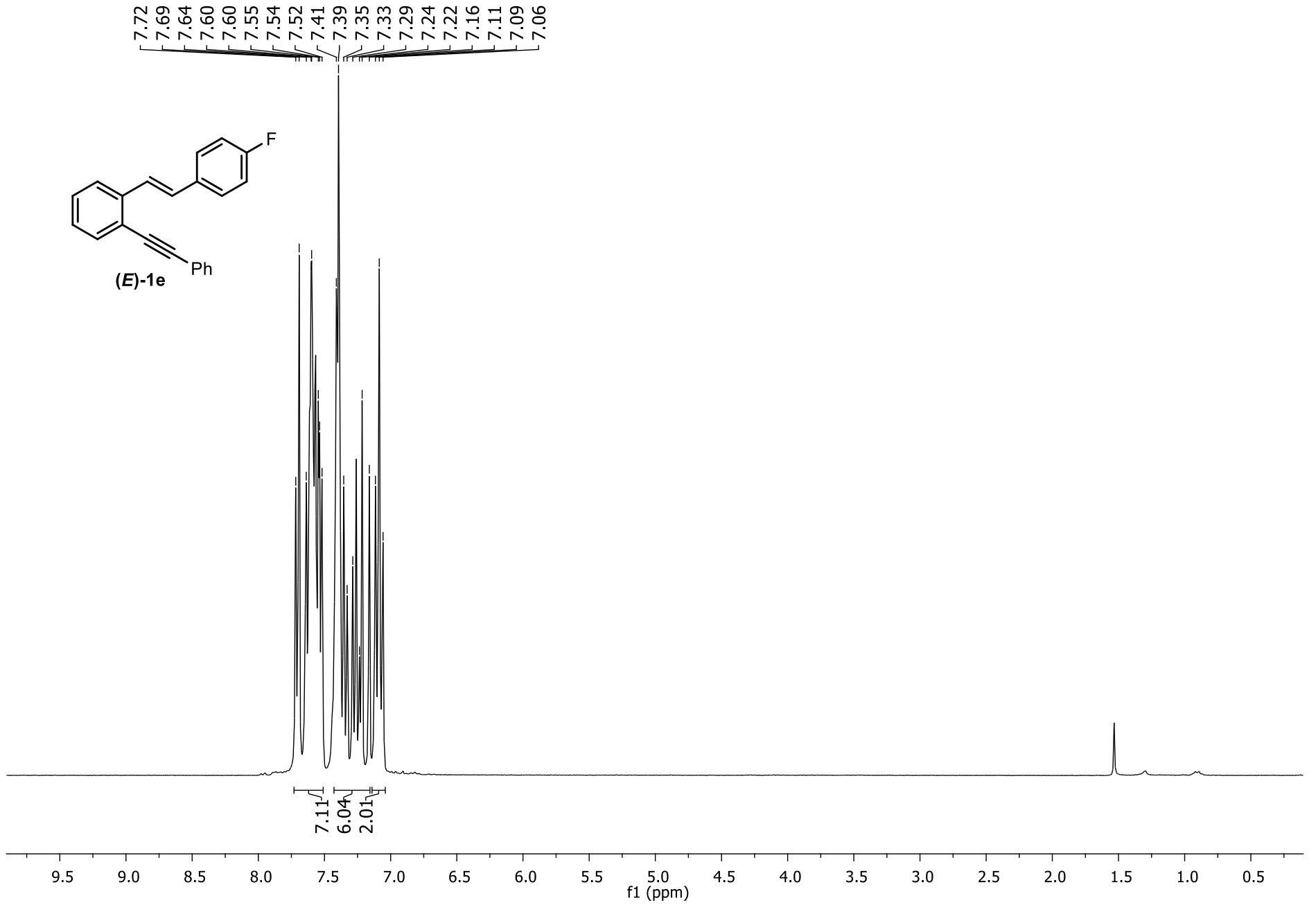
^{1}H NMR (300 MHz, $CDCl_3$)



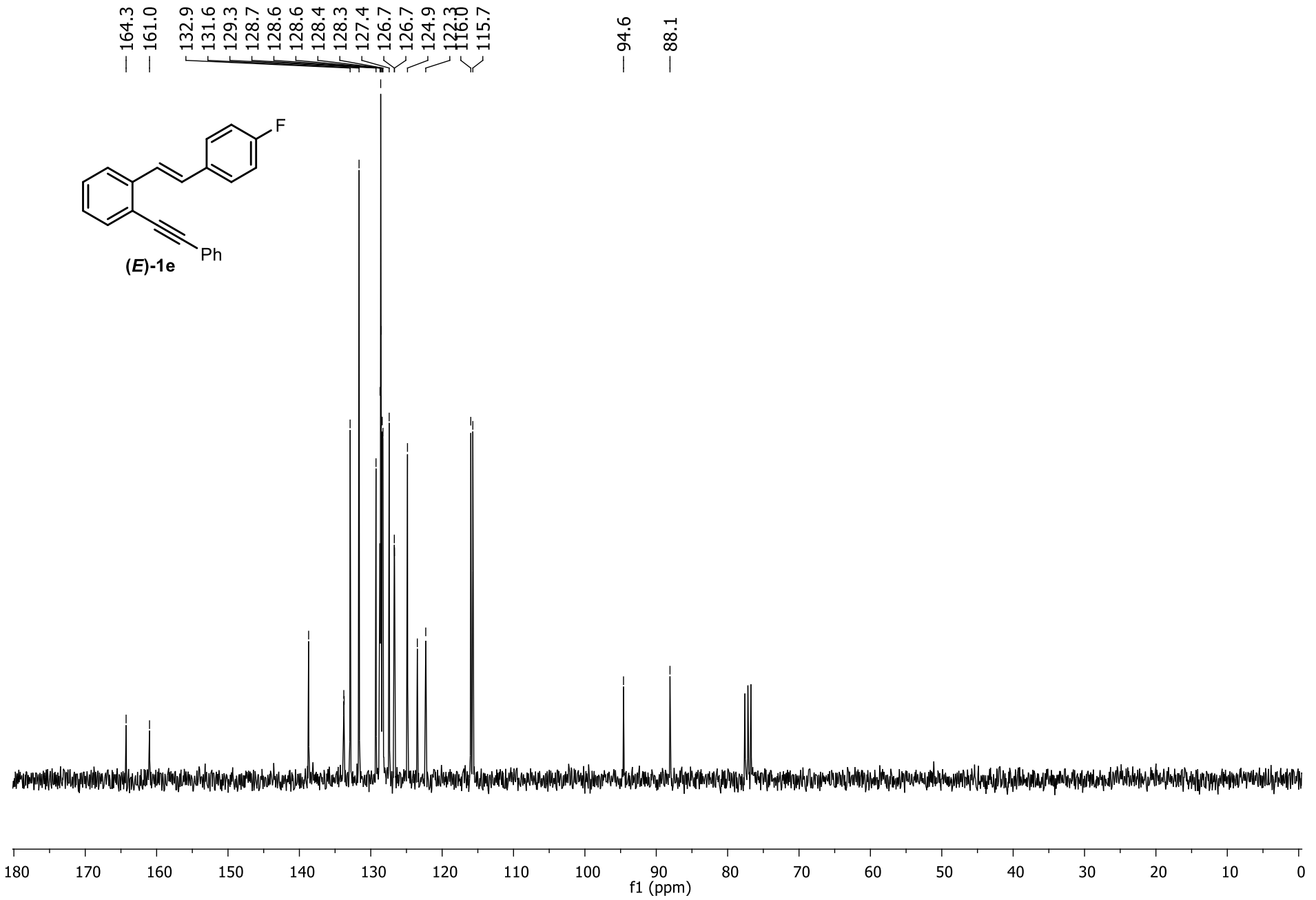
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



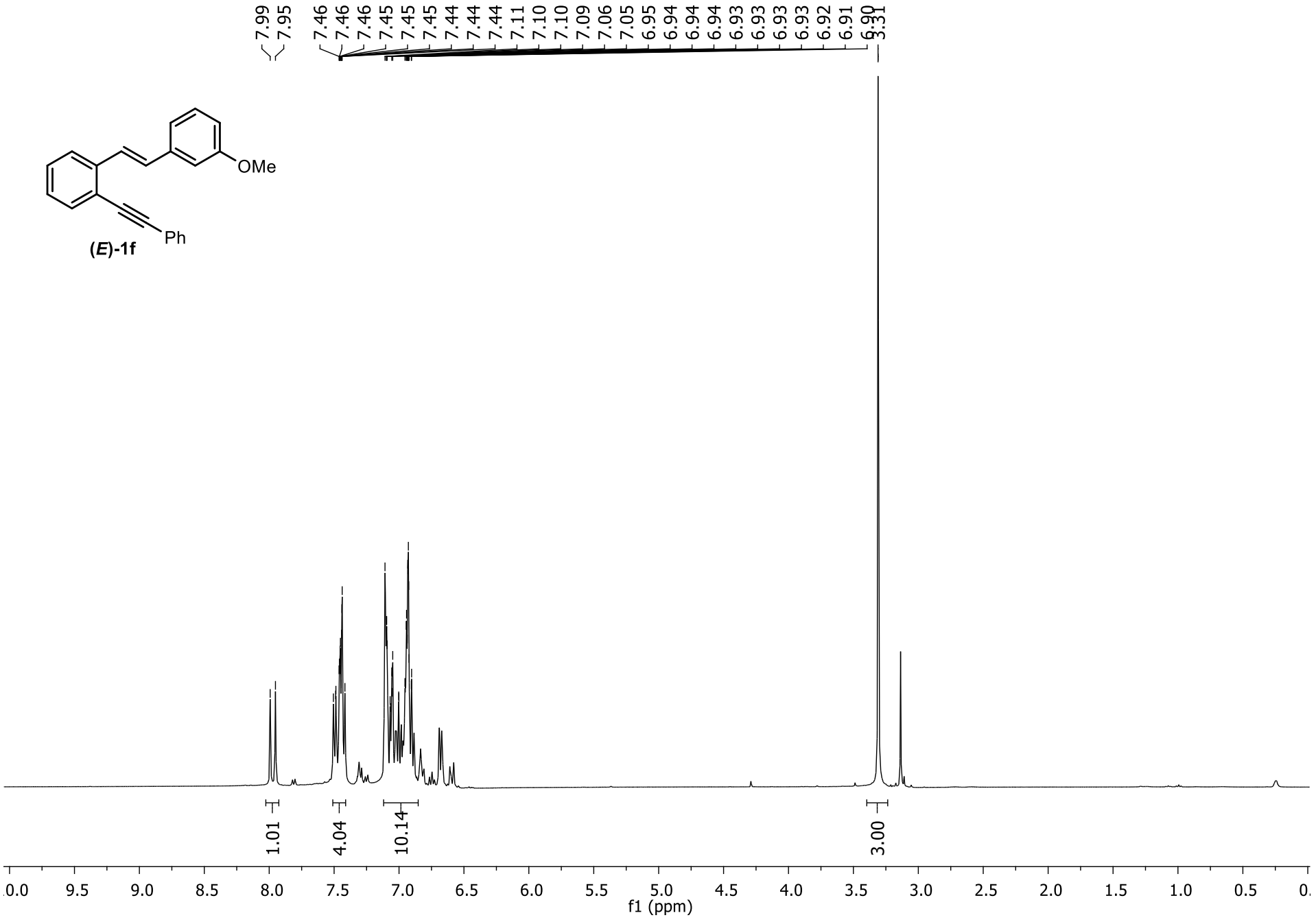
^{1}H NMR (300 MHz, $CDCl_3$)



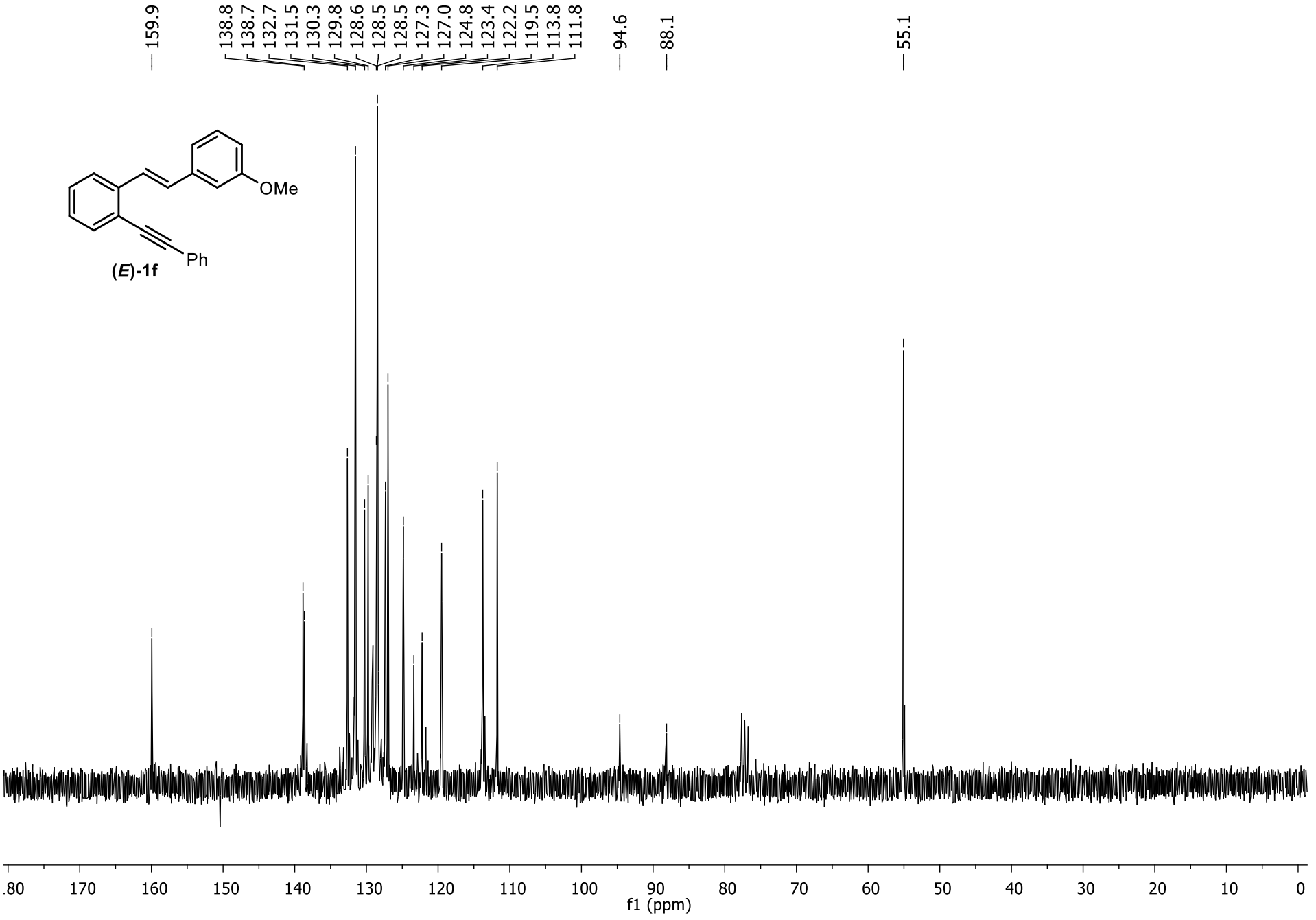
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



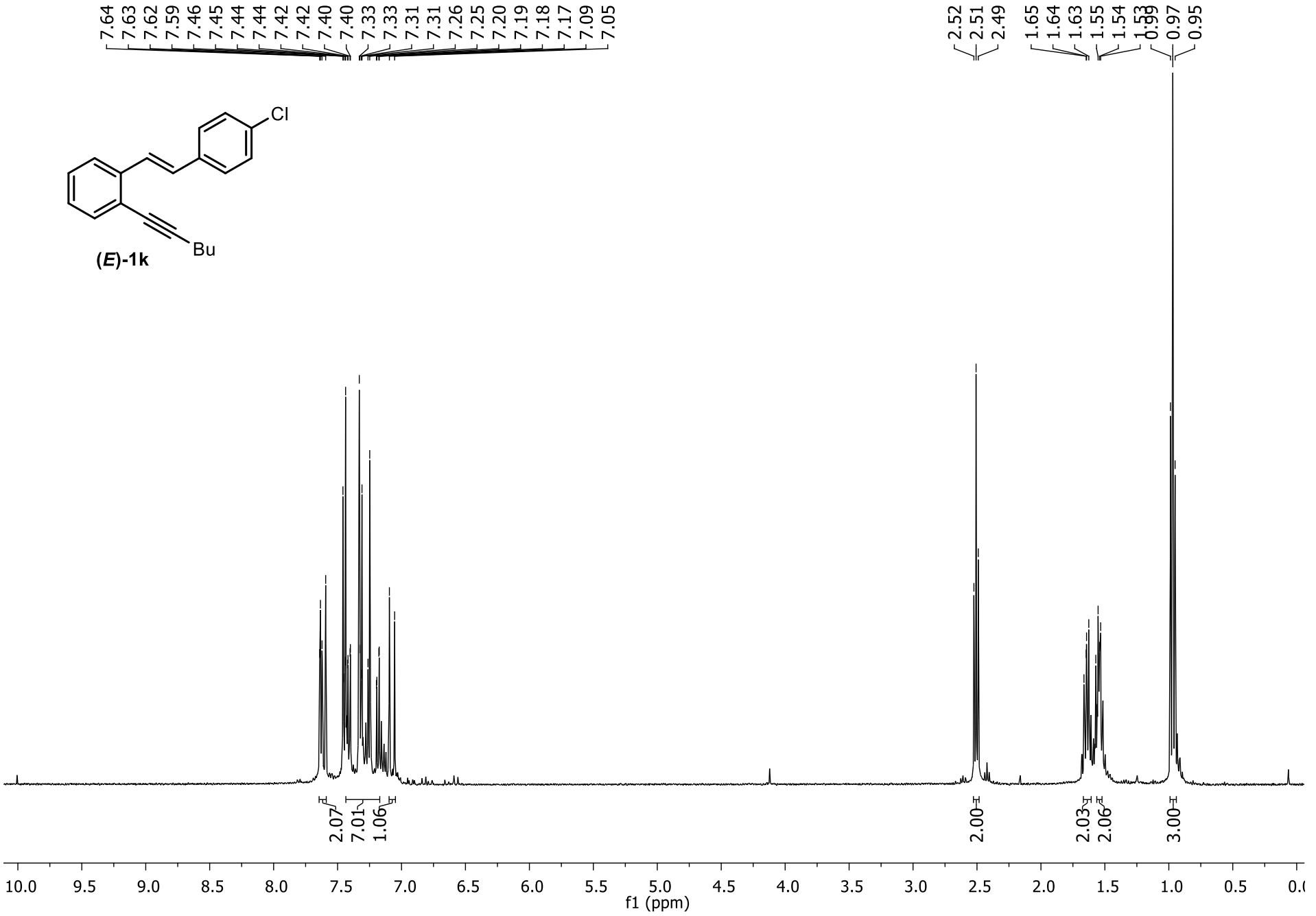
^{1}H NMR (300 MHz, $CDCl_3$)



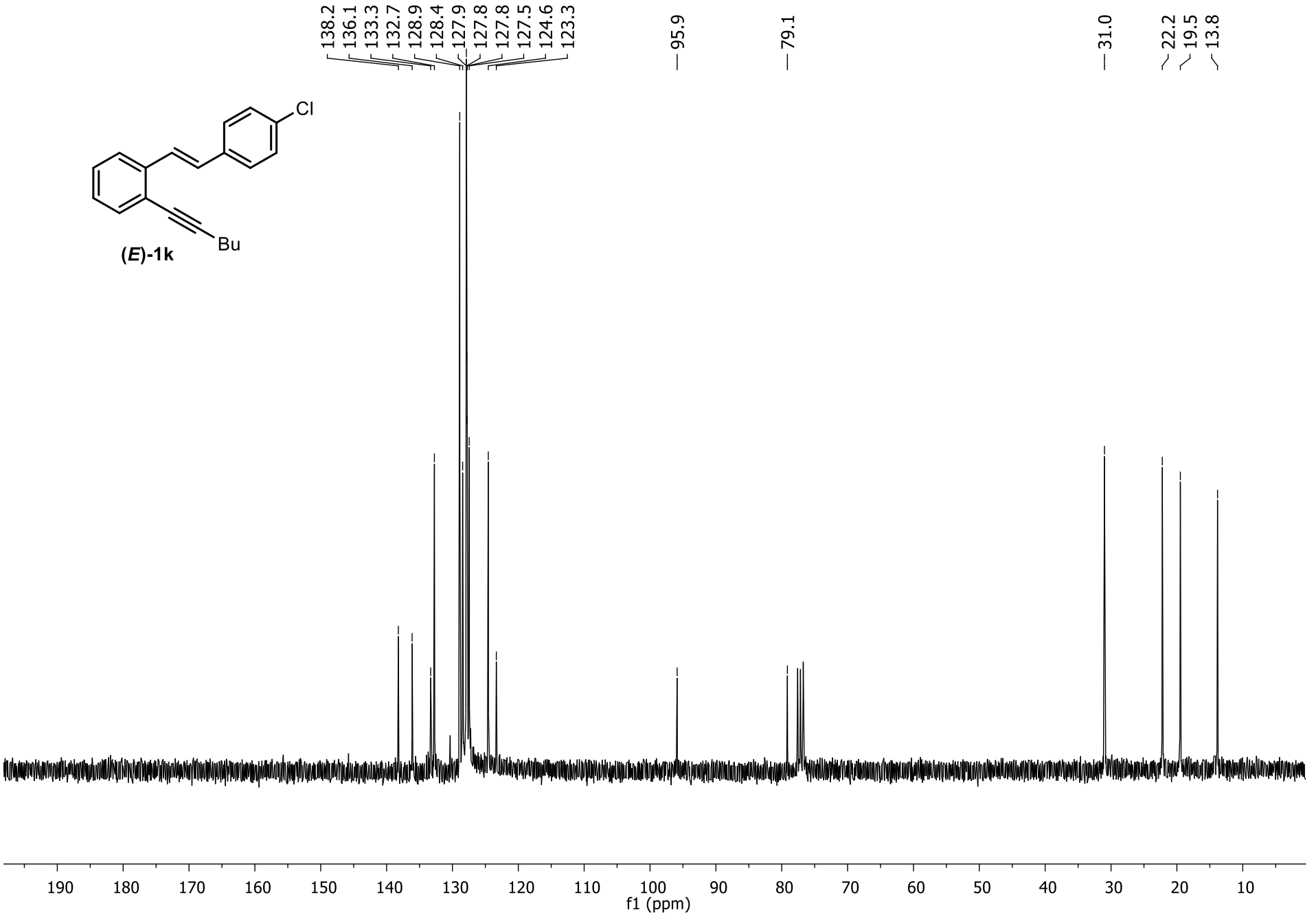
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



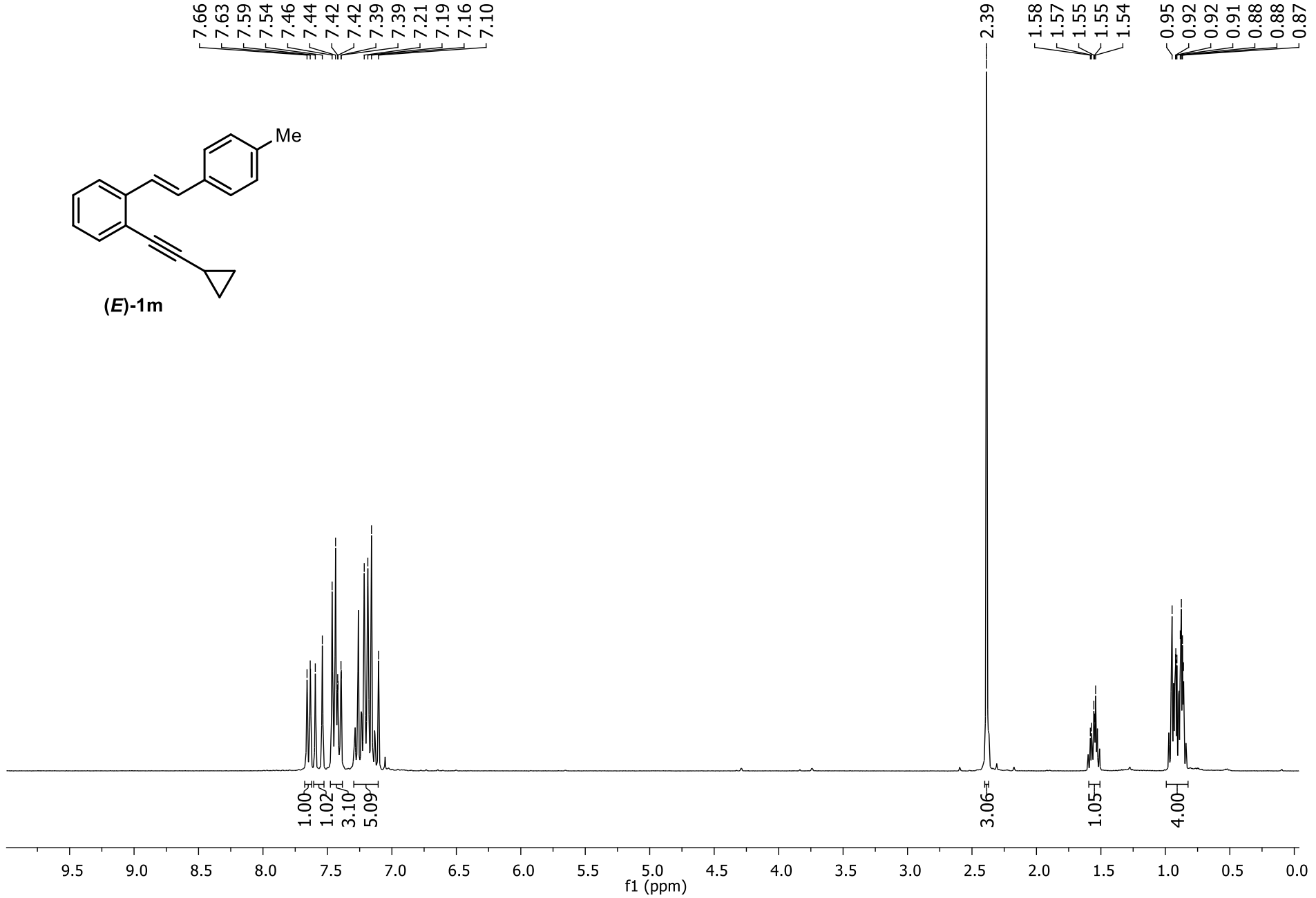
^{1}H NMR (300 MHz, $CDCl_3$)



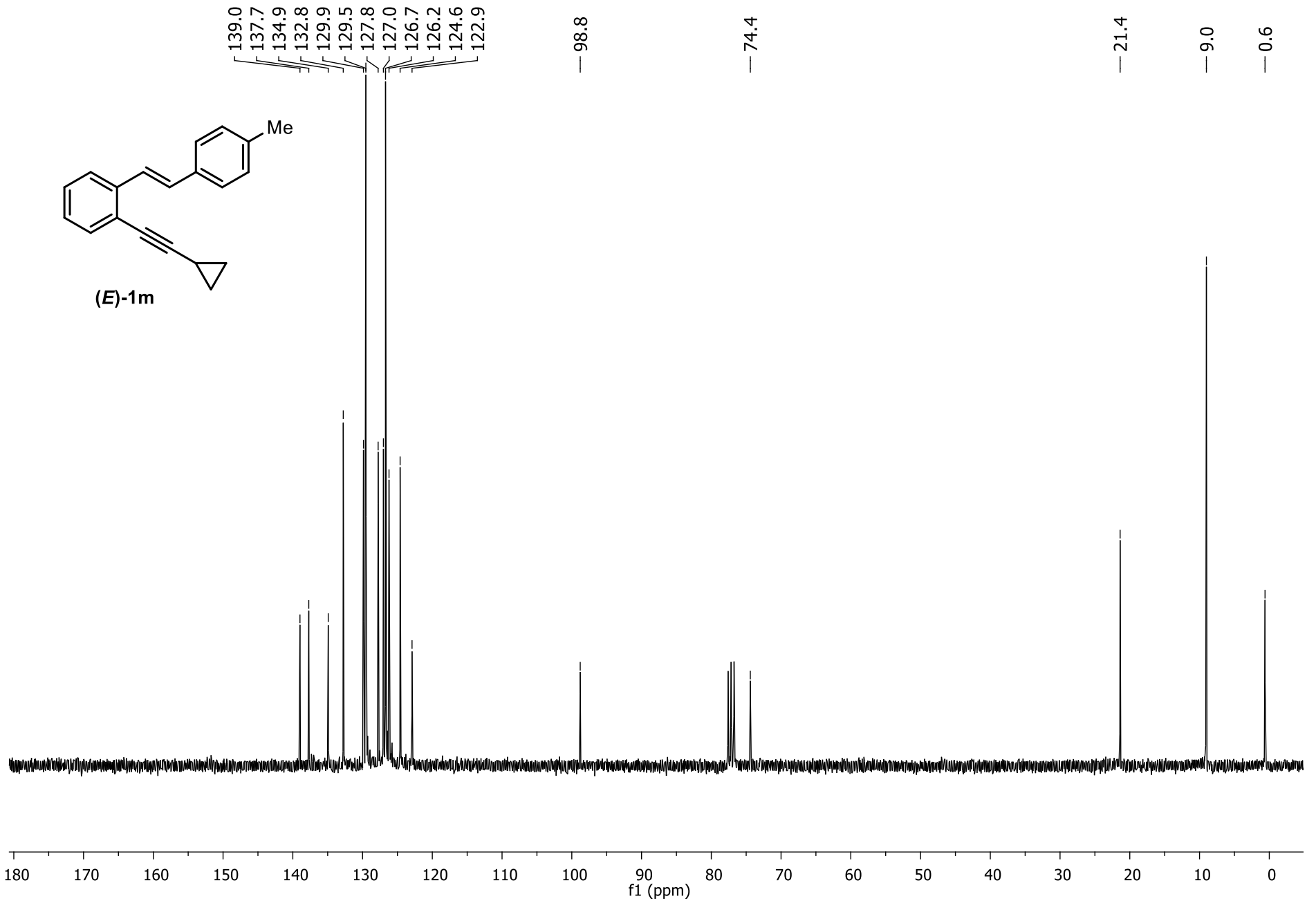
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



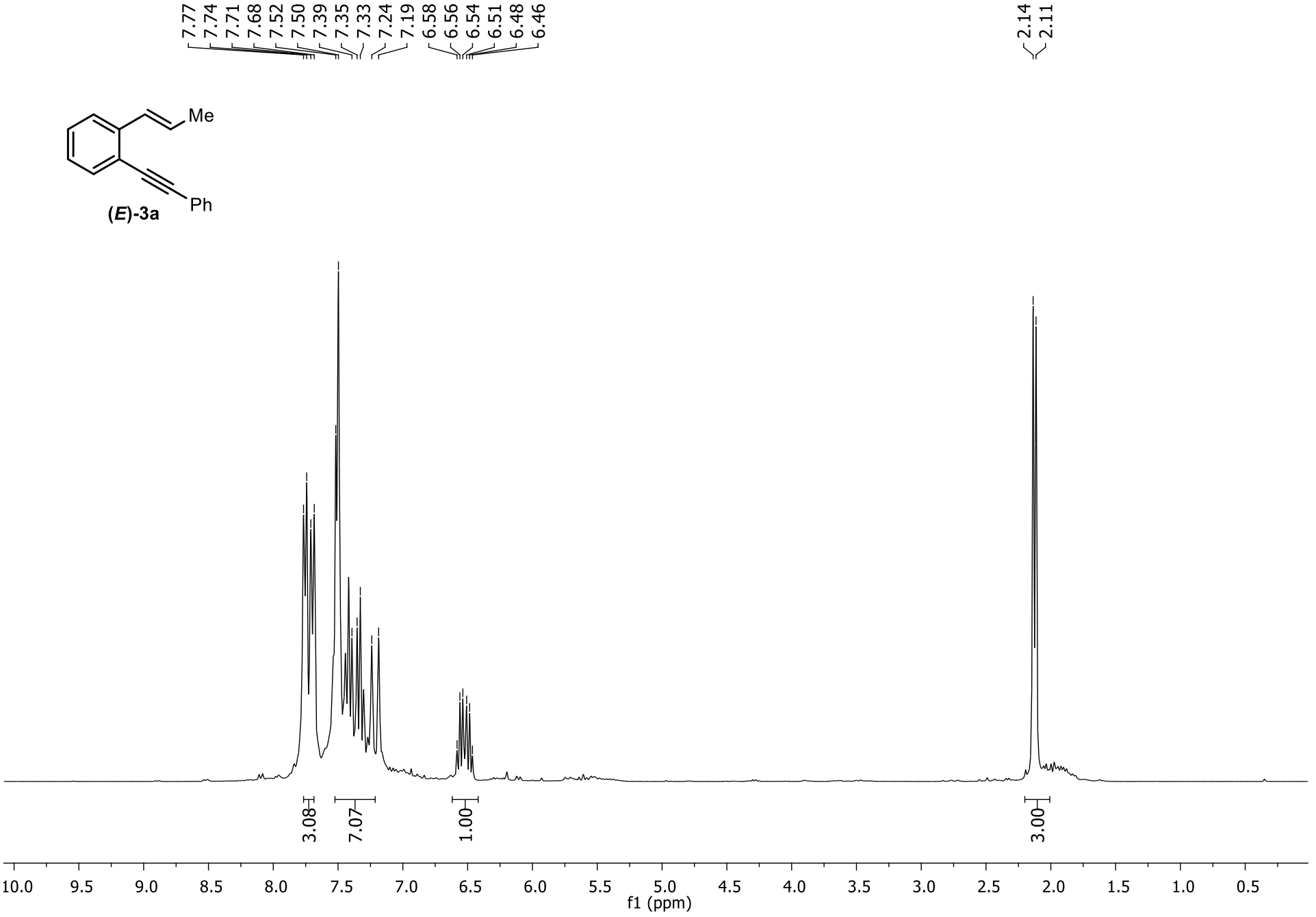
^{1}H NMR (300 MHz, $CDCl_3$)



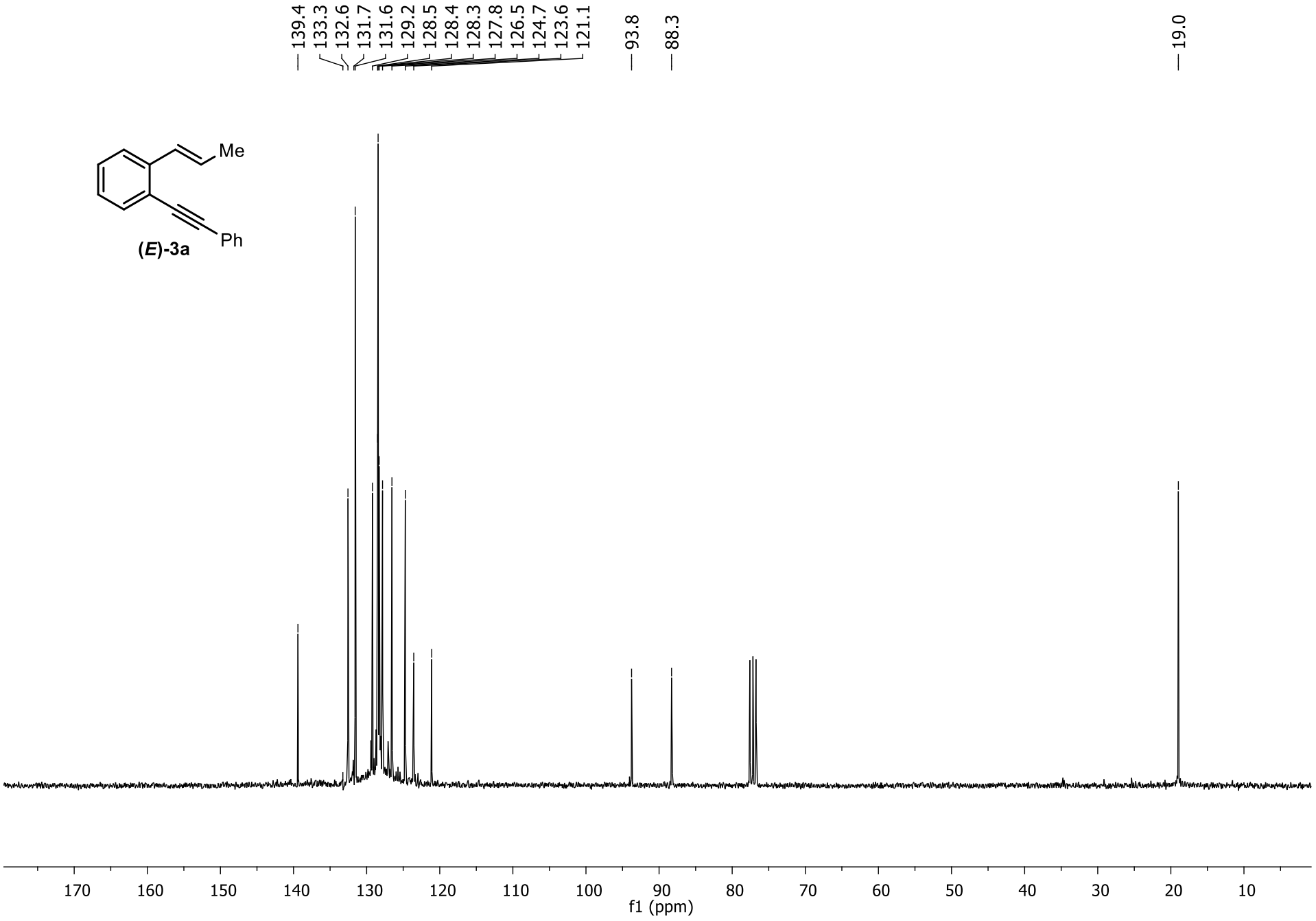
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



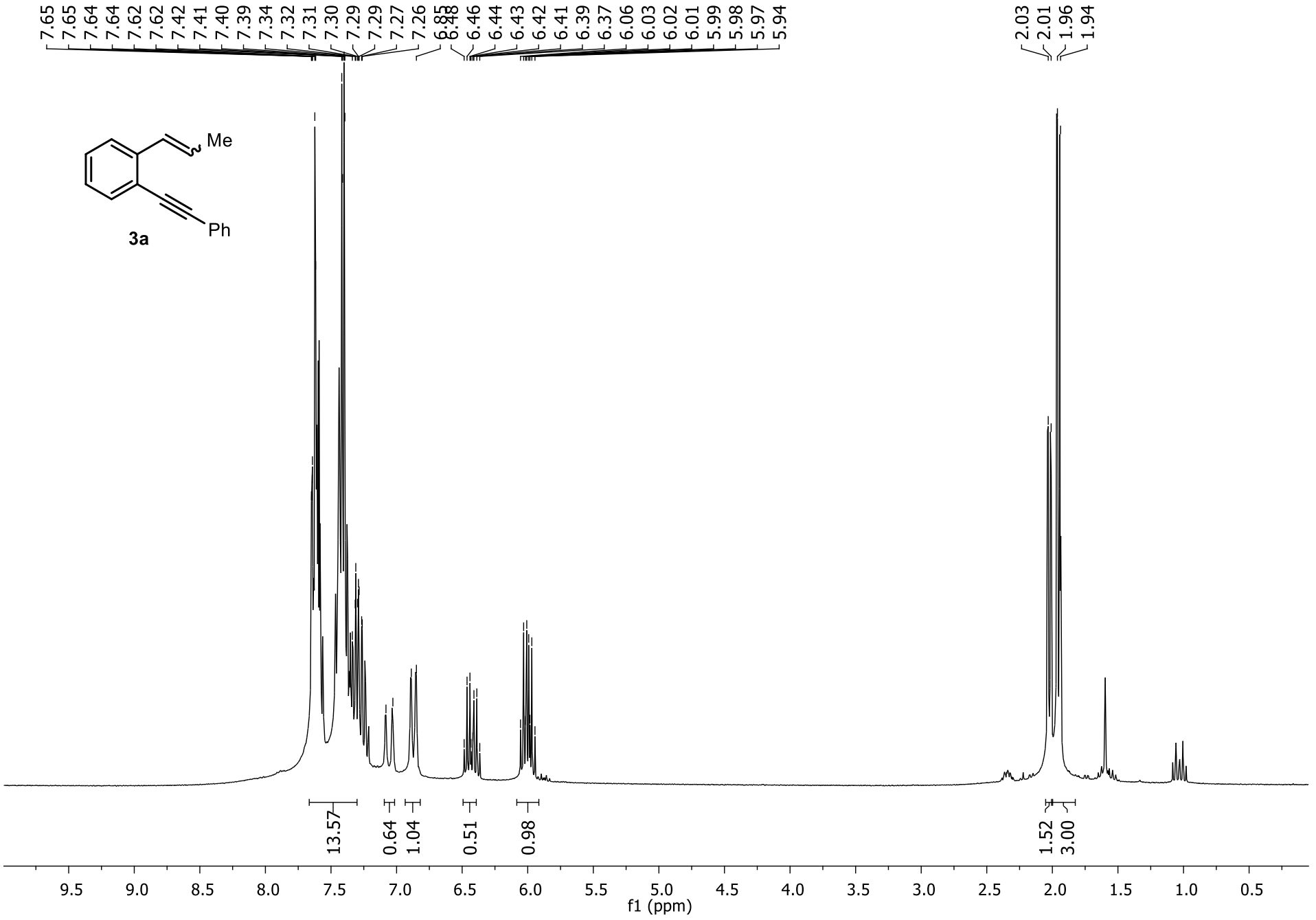
^{1}H NMR (300 MHz, $CDCl_3$)



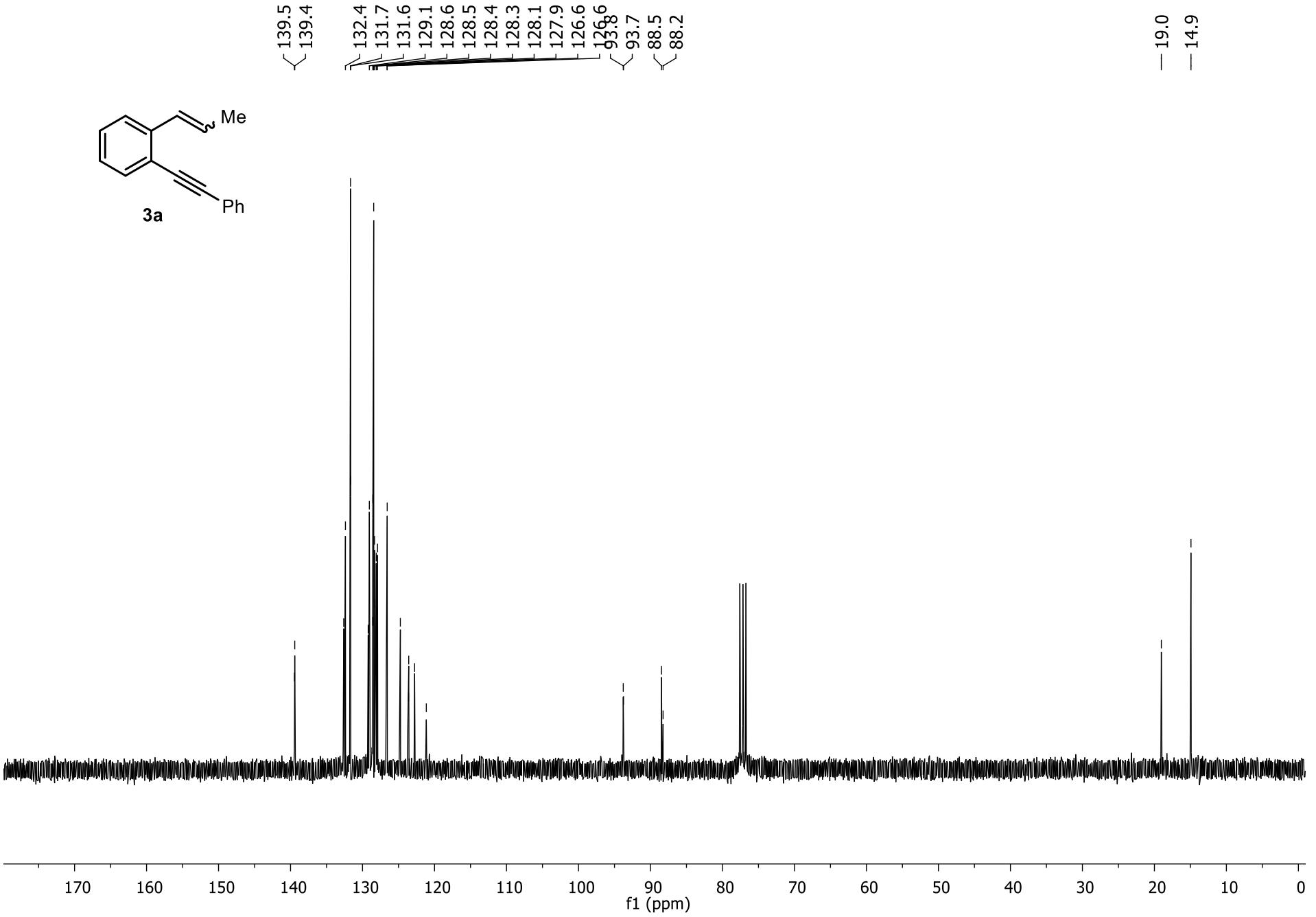
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



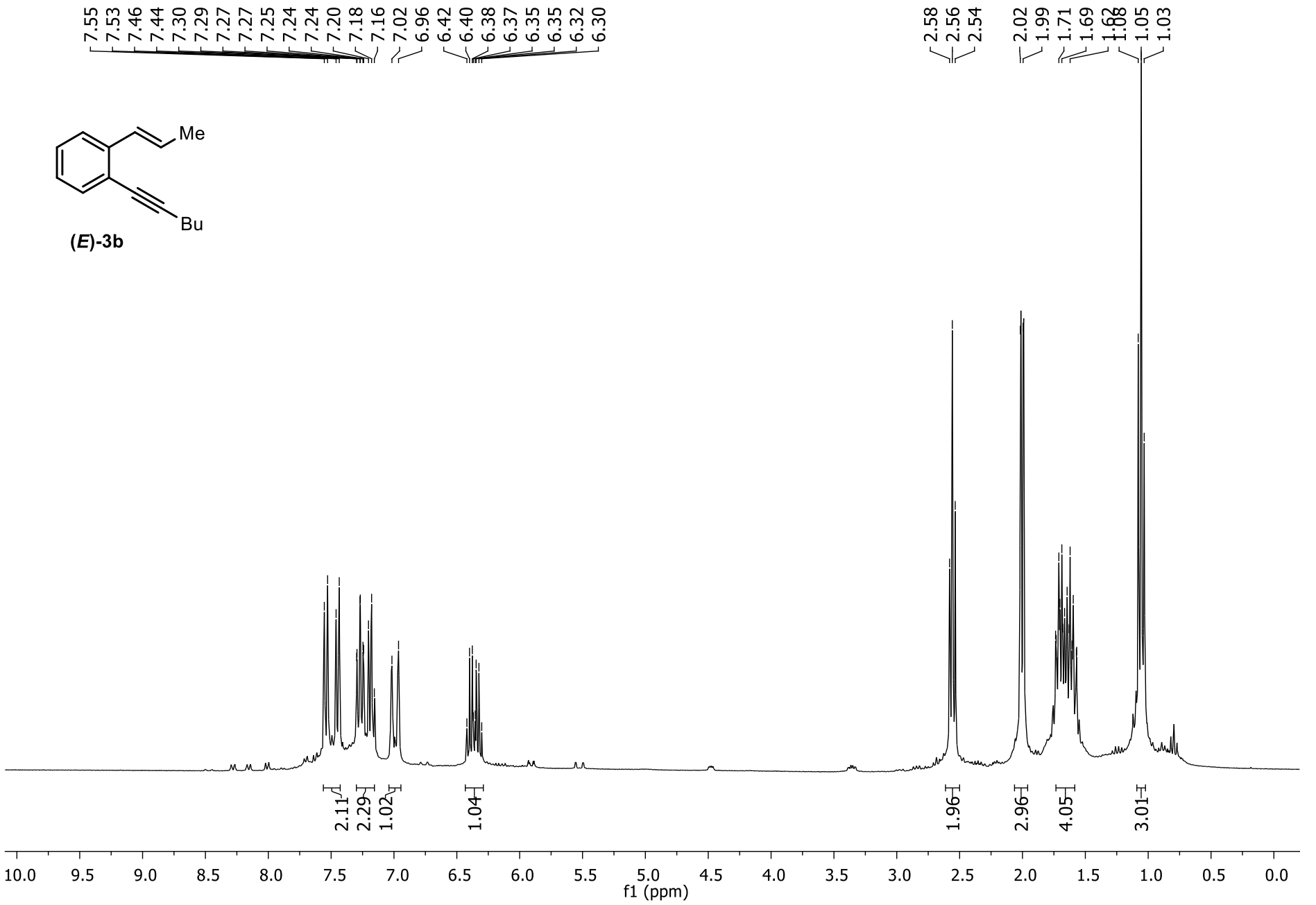
^{1}H NMR (300 MHz, $CDCl_3$)



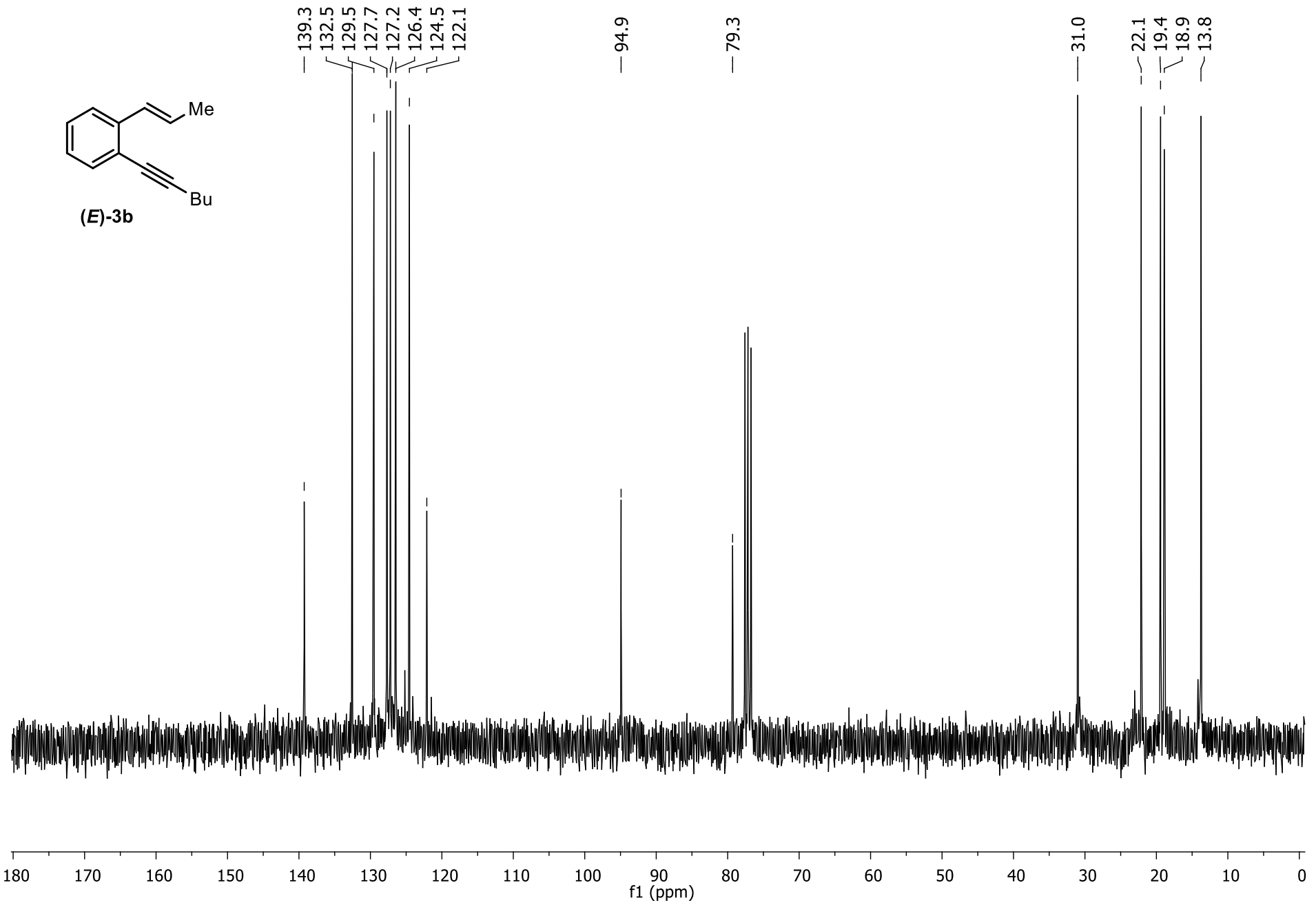
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



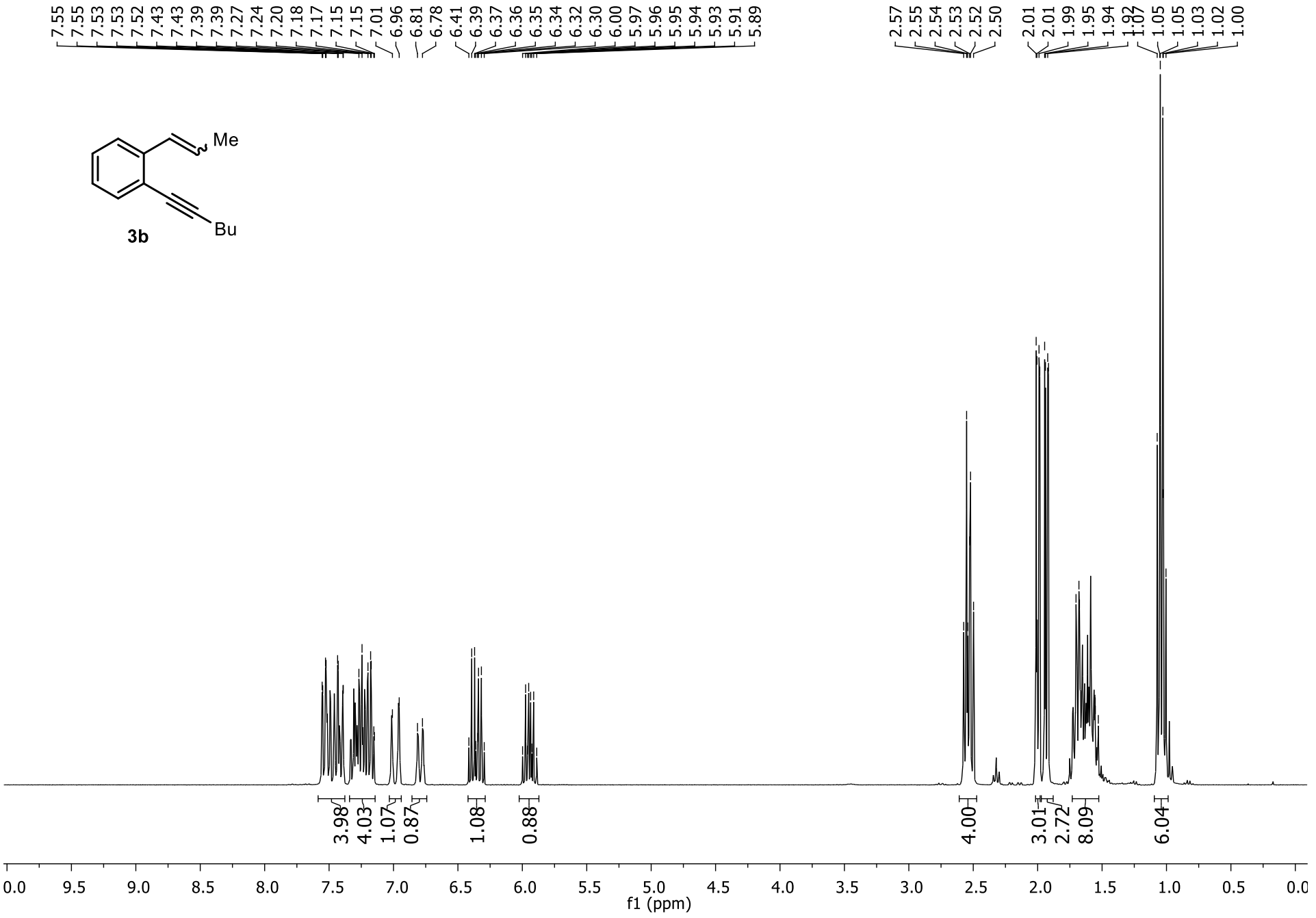
^{1}H NMR (300 MHz, $CDCl_3$)



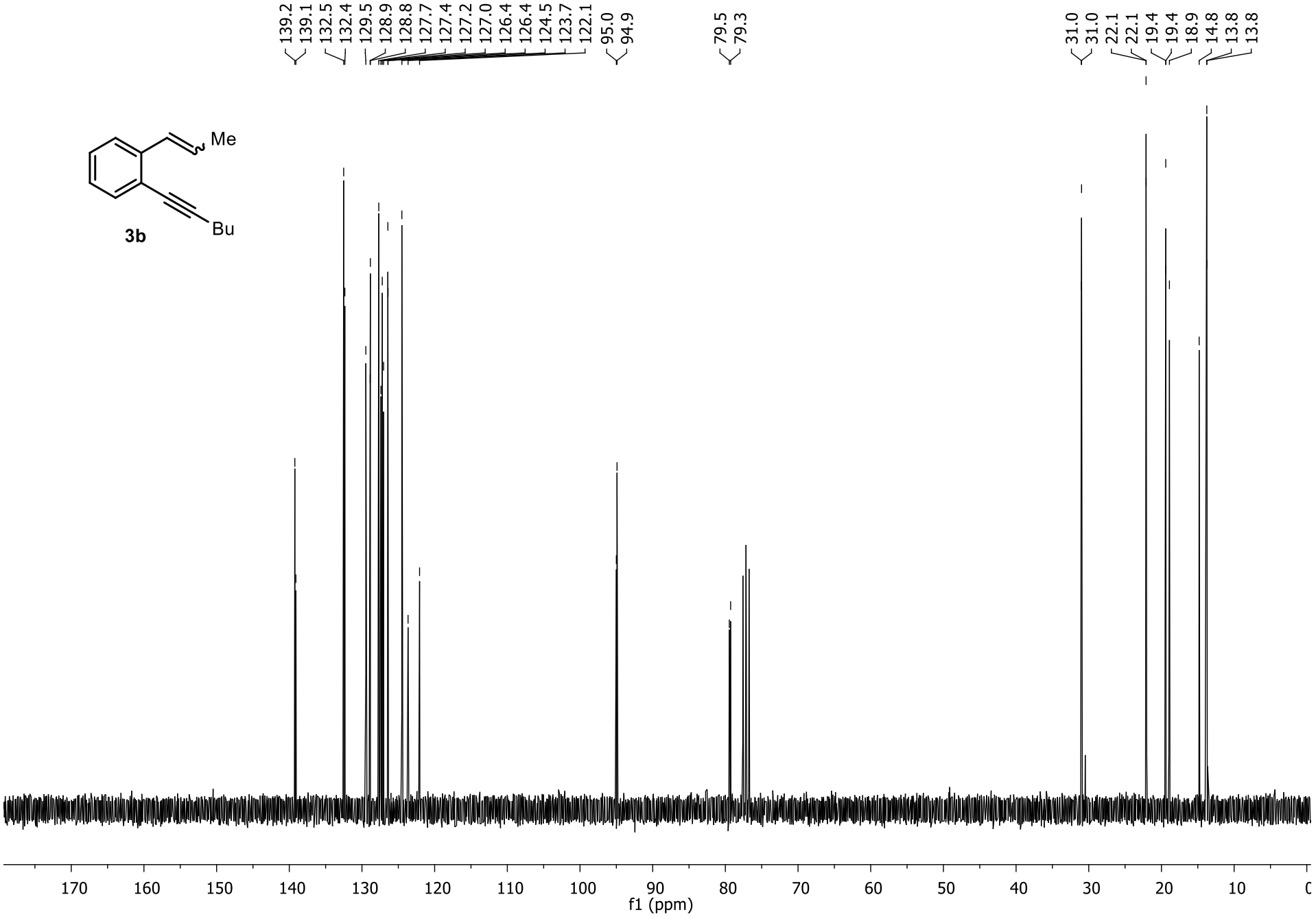
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



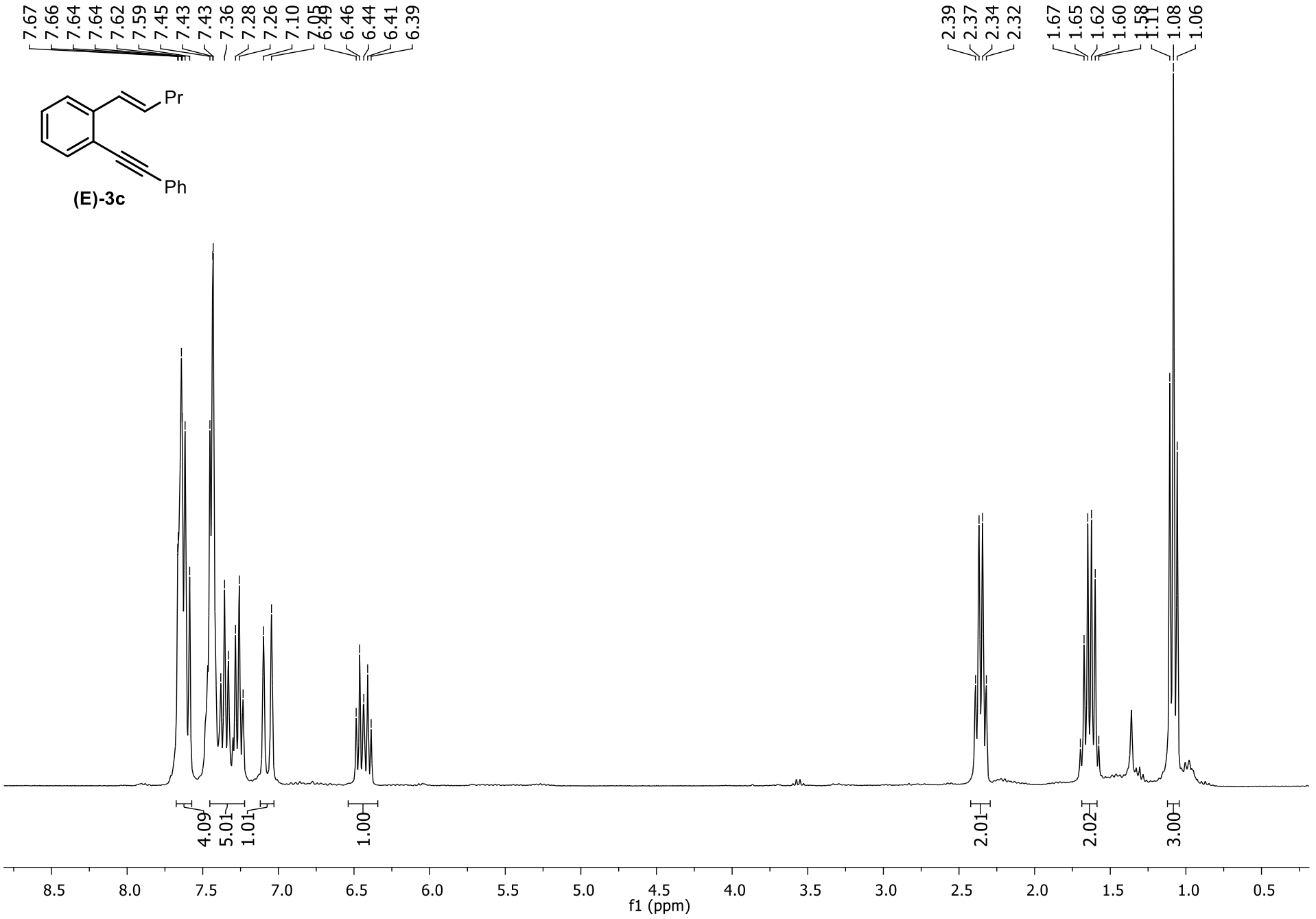
^{1}H NMR (300 MHz, $CDCl_3$)



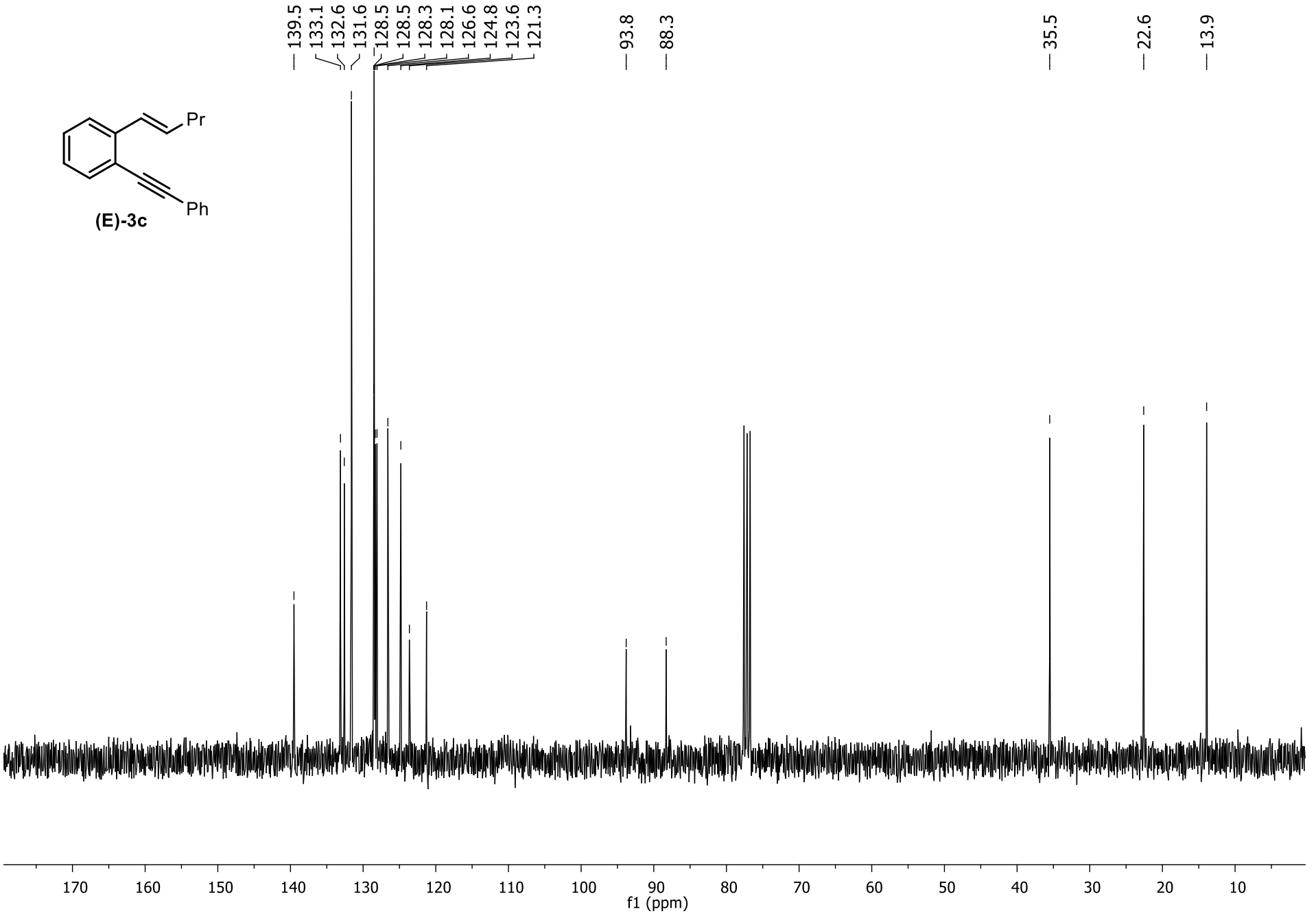
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



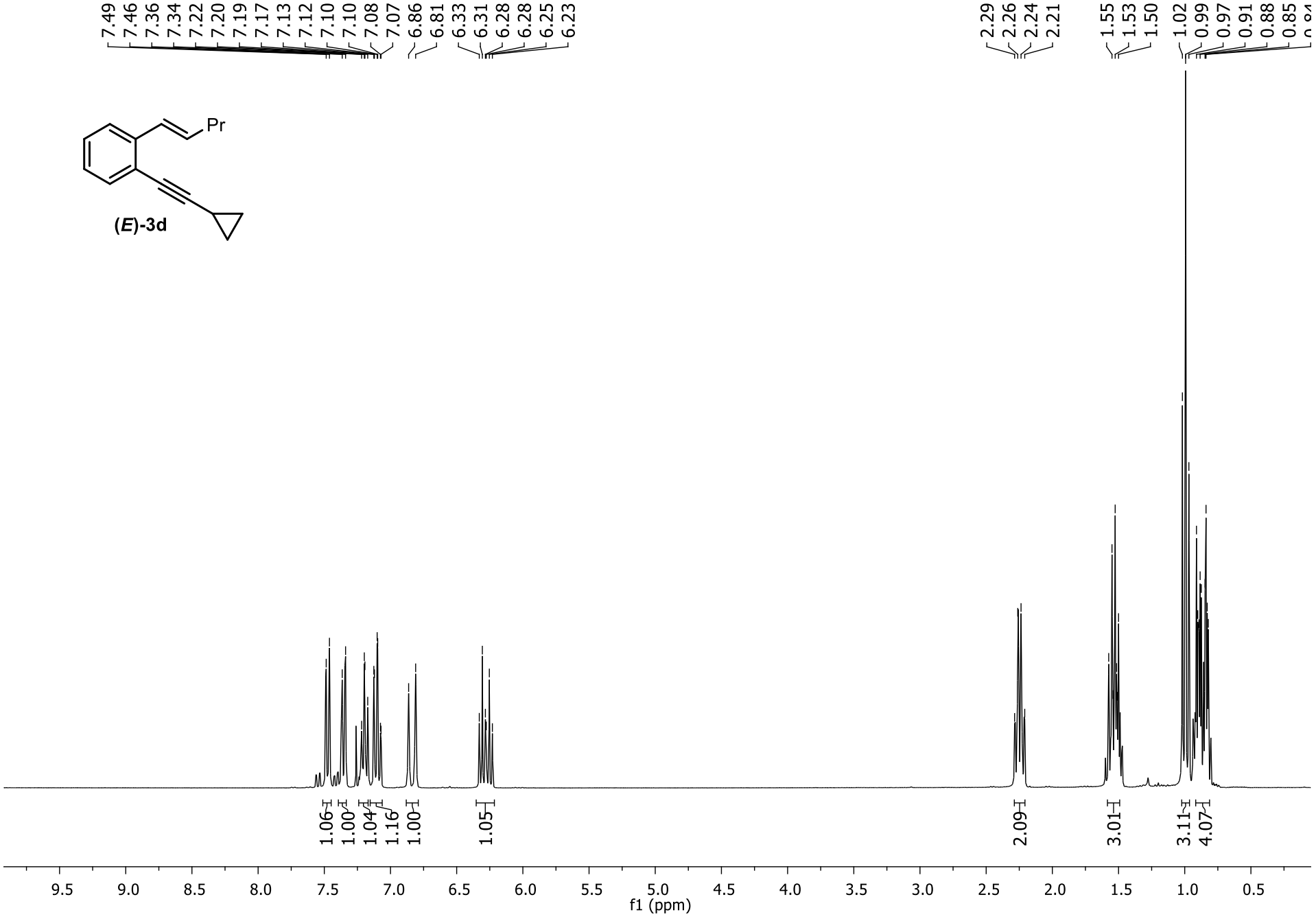
^{1}H NMR (300 MHz, $CDCl_3$)



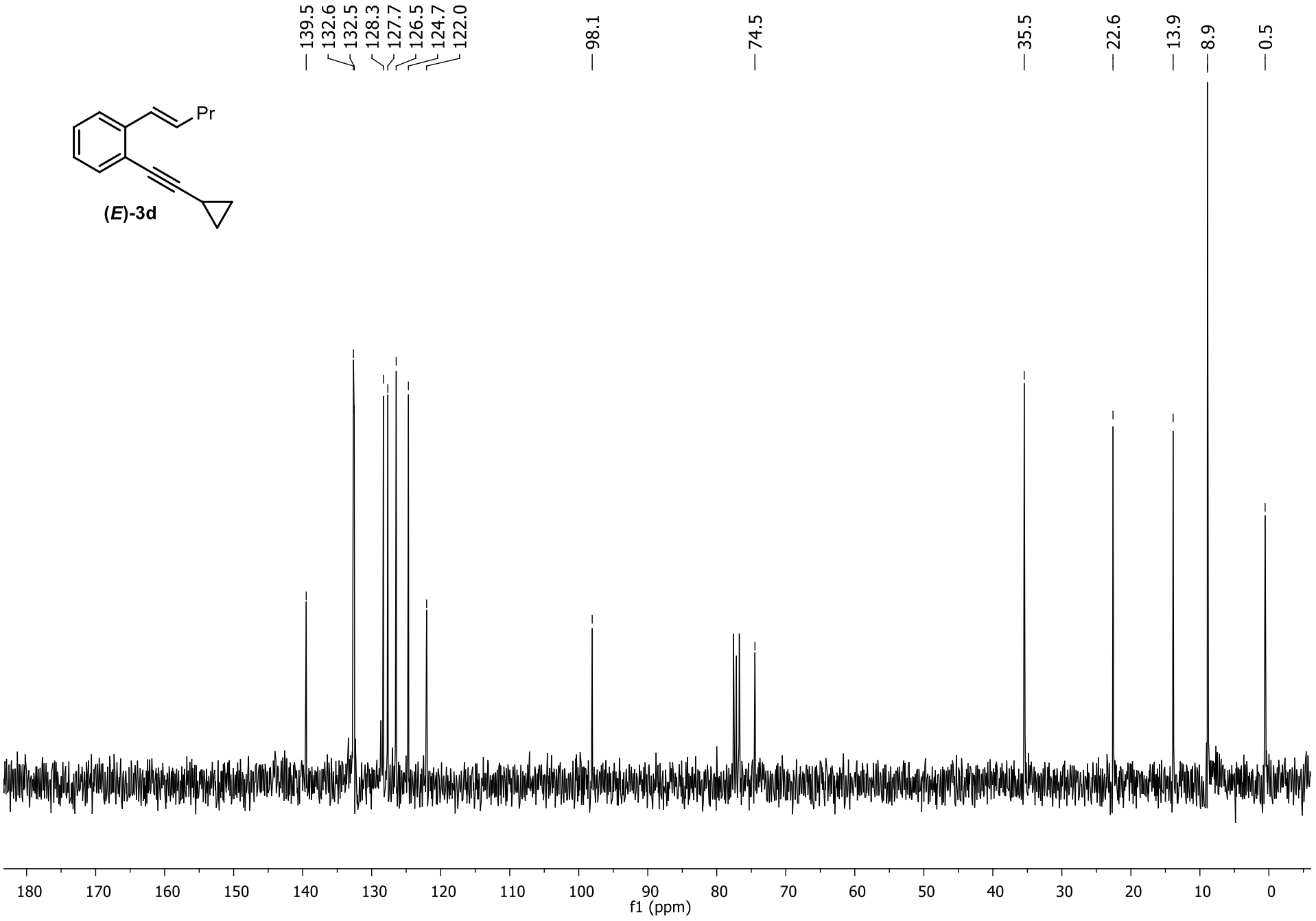
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



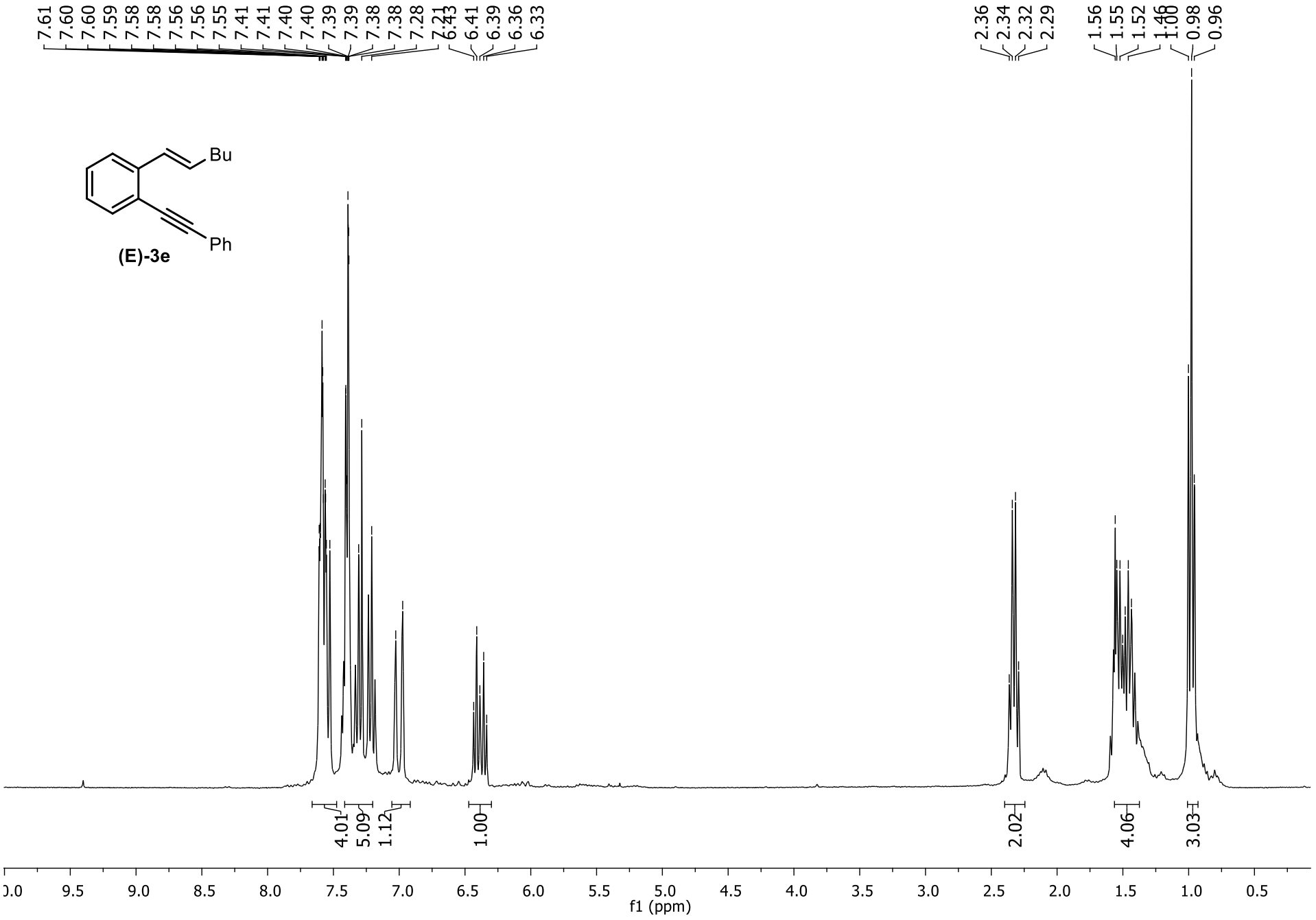
^{1}H NMR (300 MHz, $CDCl_3$)



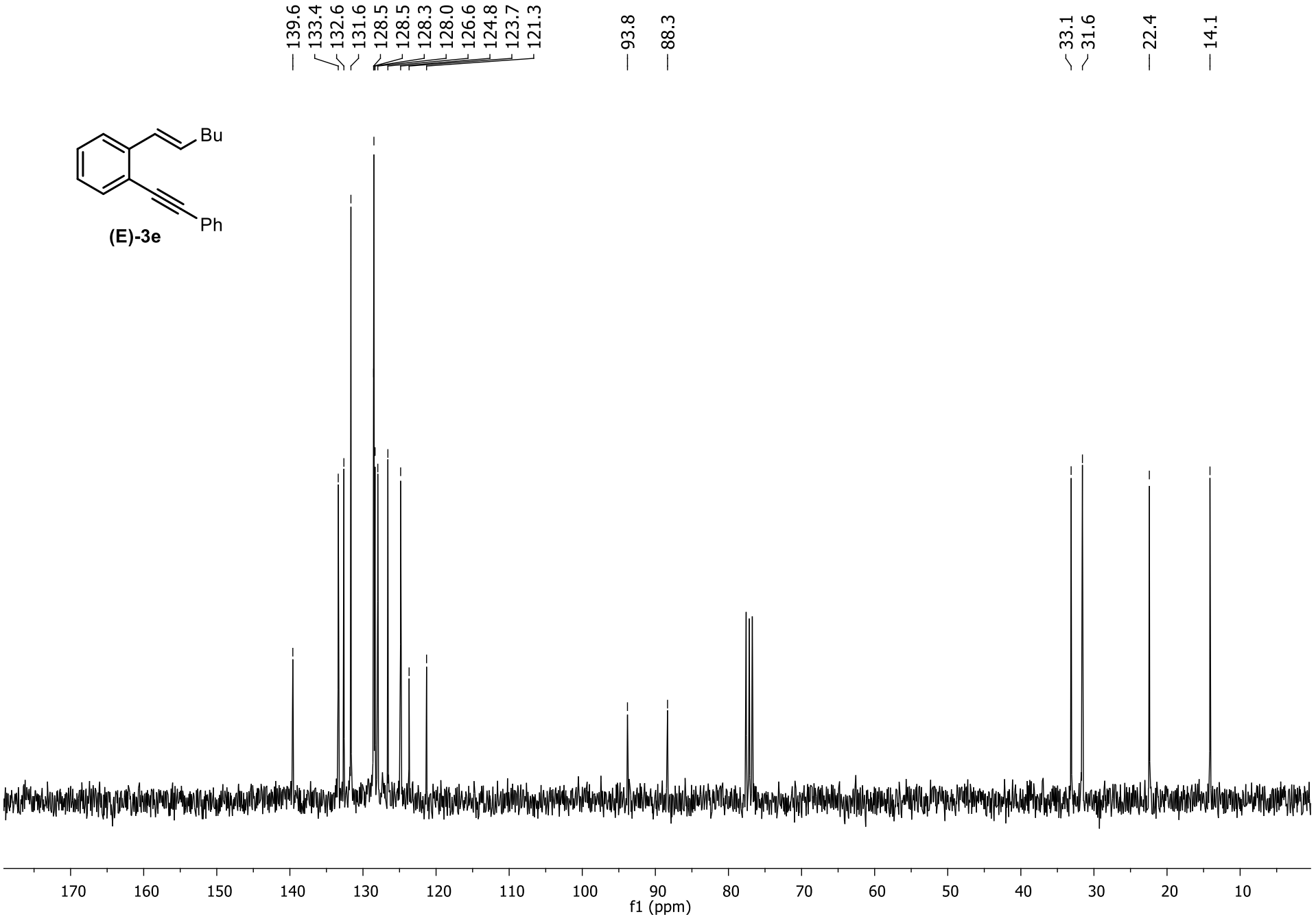
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



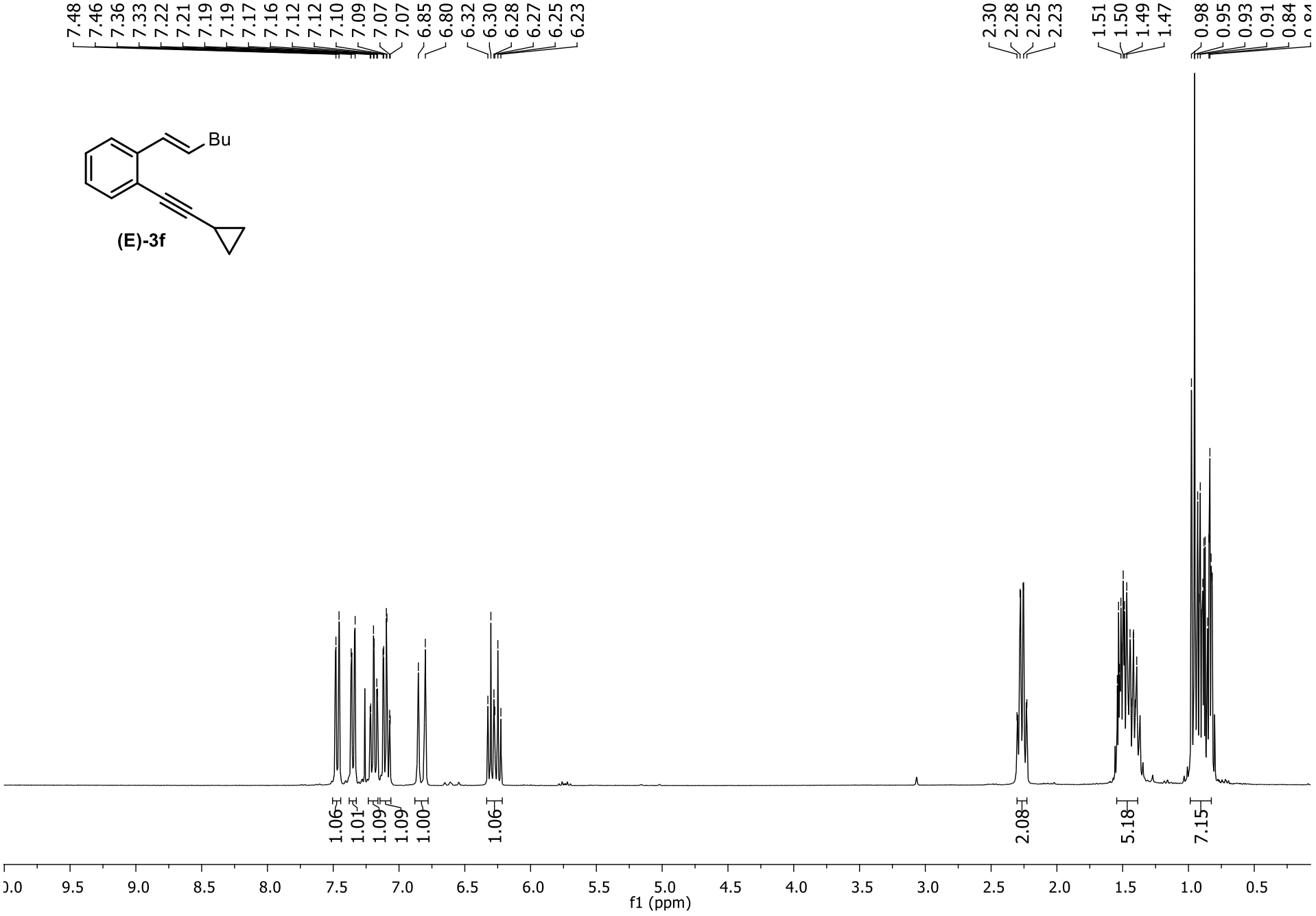
^{1}H NMR (300 MHz, $CDCl_3$)



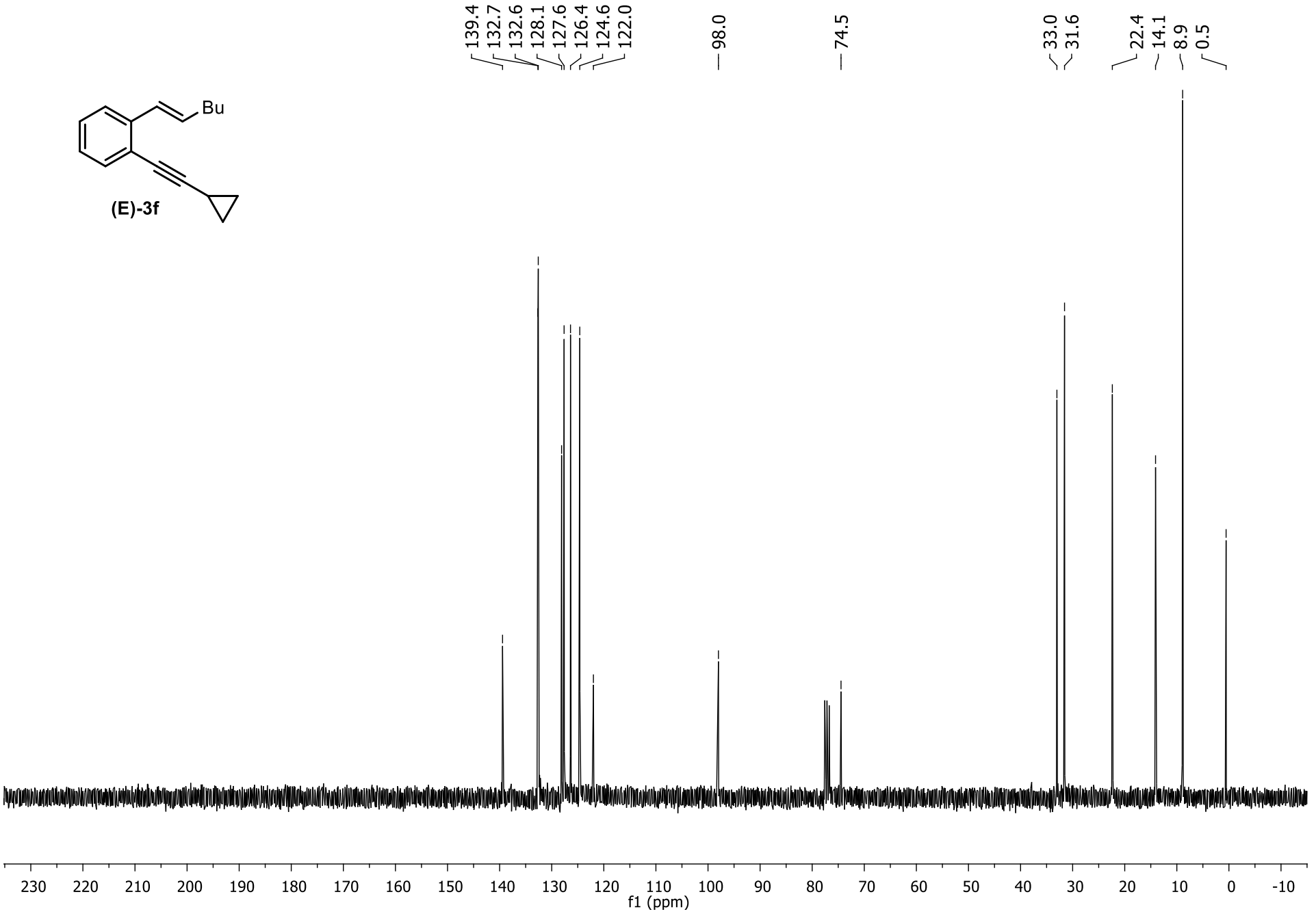
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



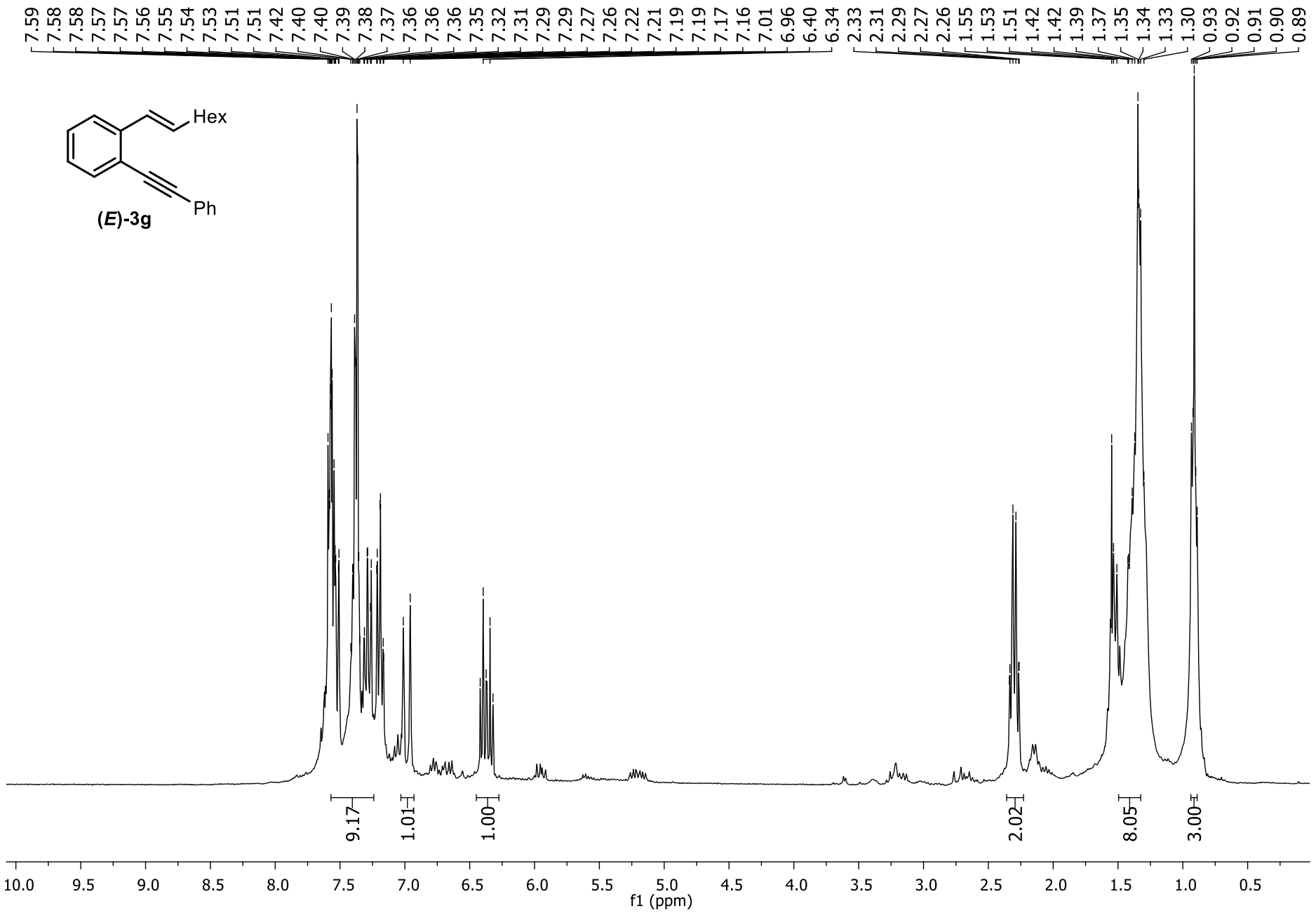
^{1}H NMR (300 MHz, $CDCl_3$)



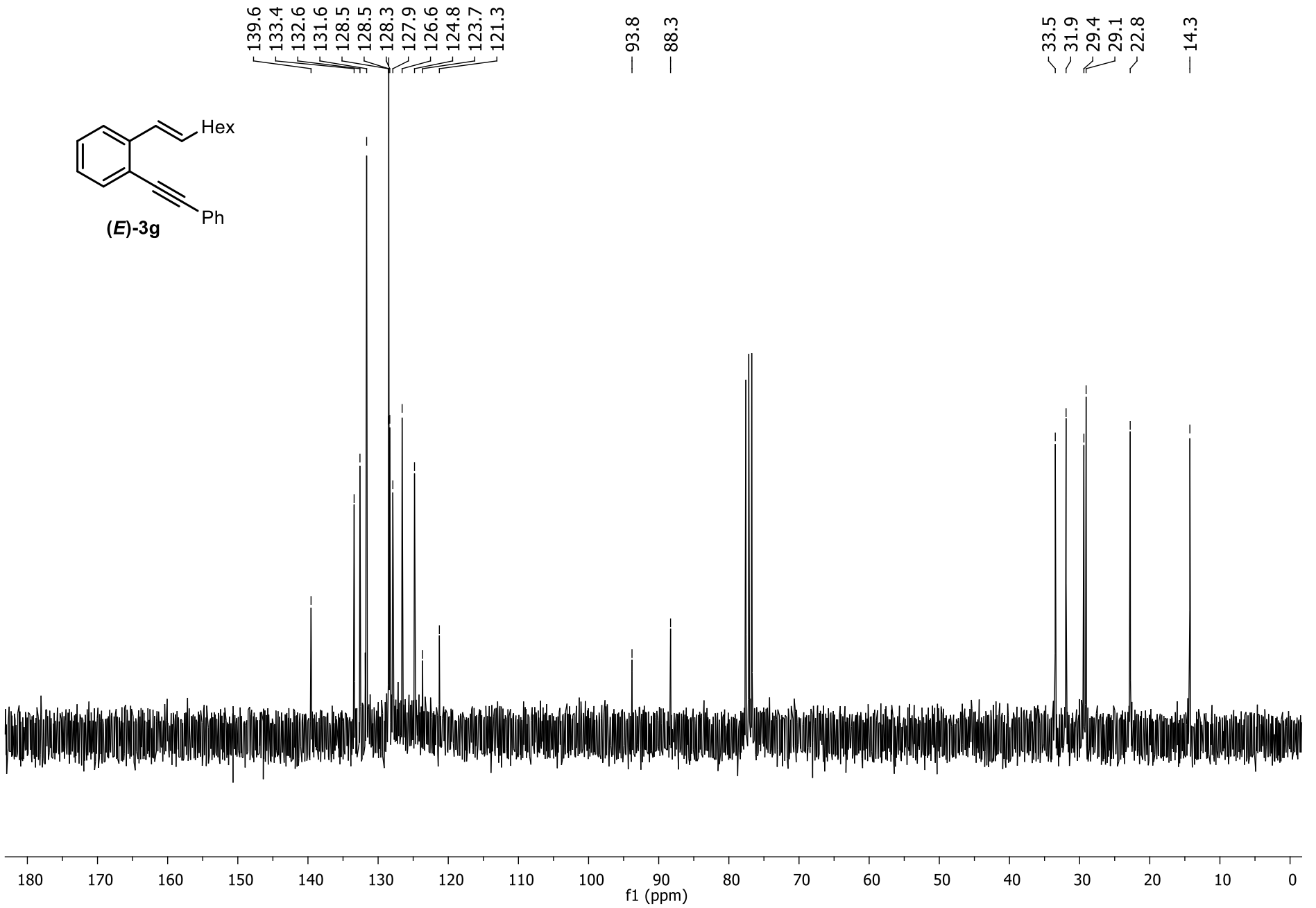
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



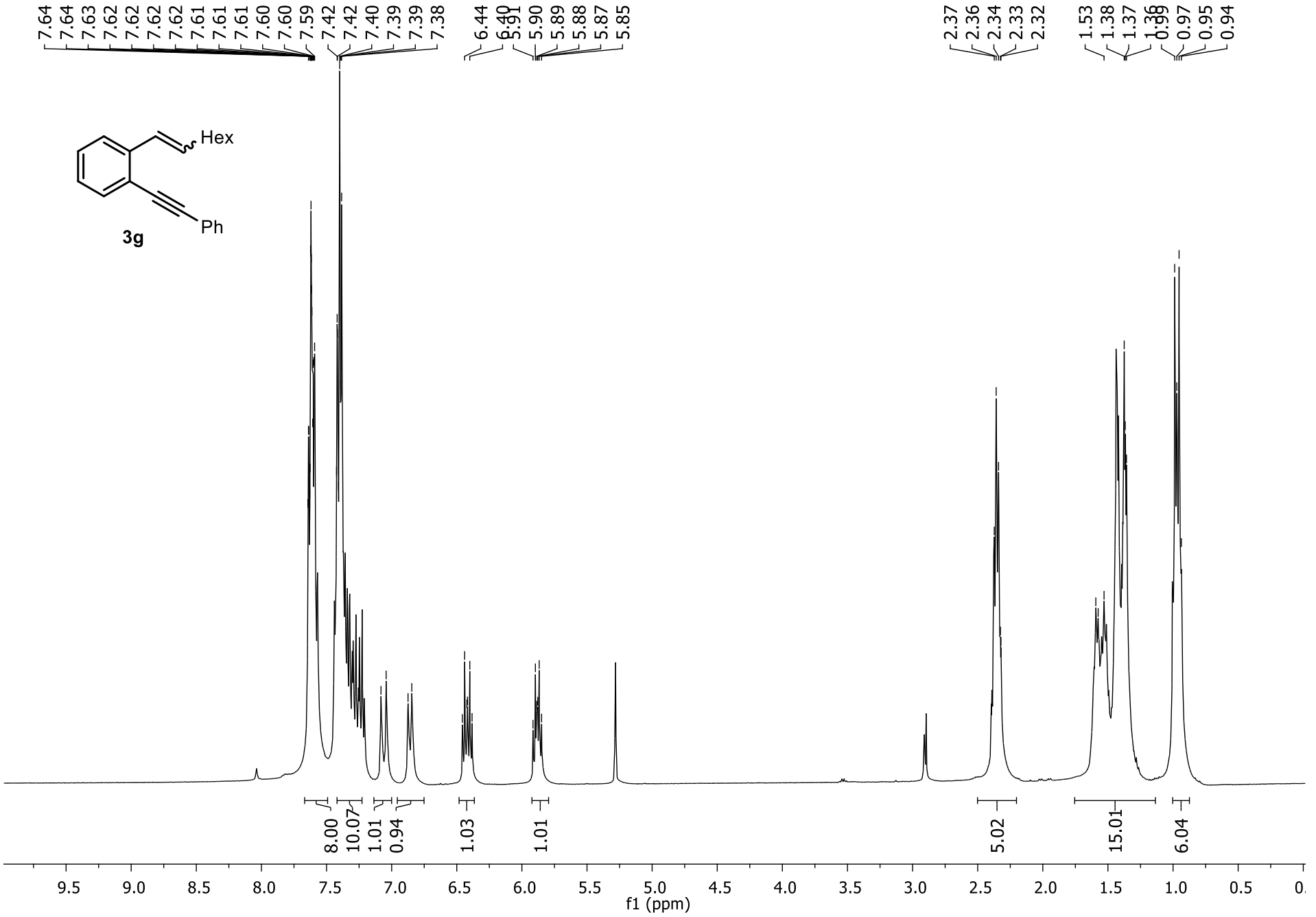
^{1}H NMR (300 MHz, $CDCl_3$)



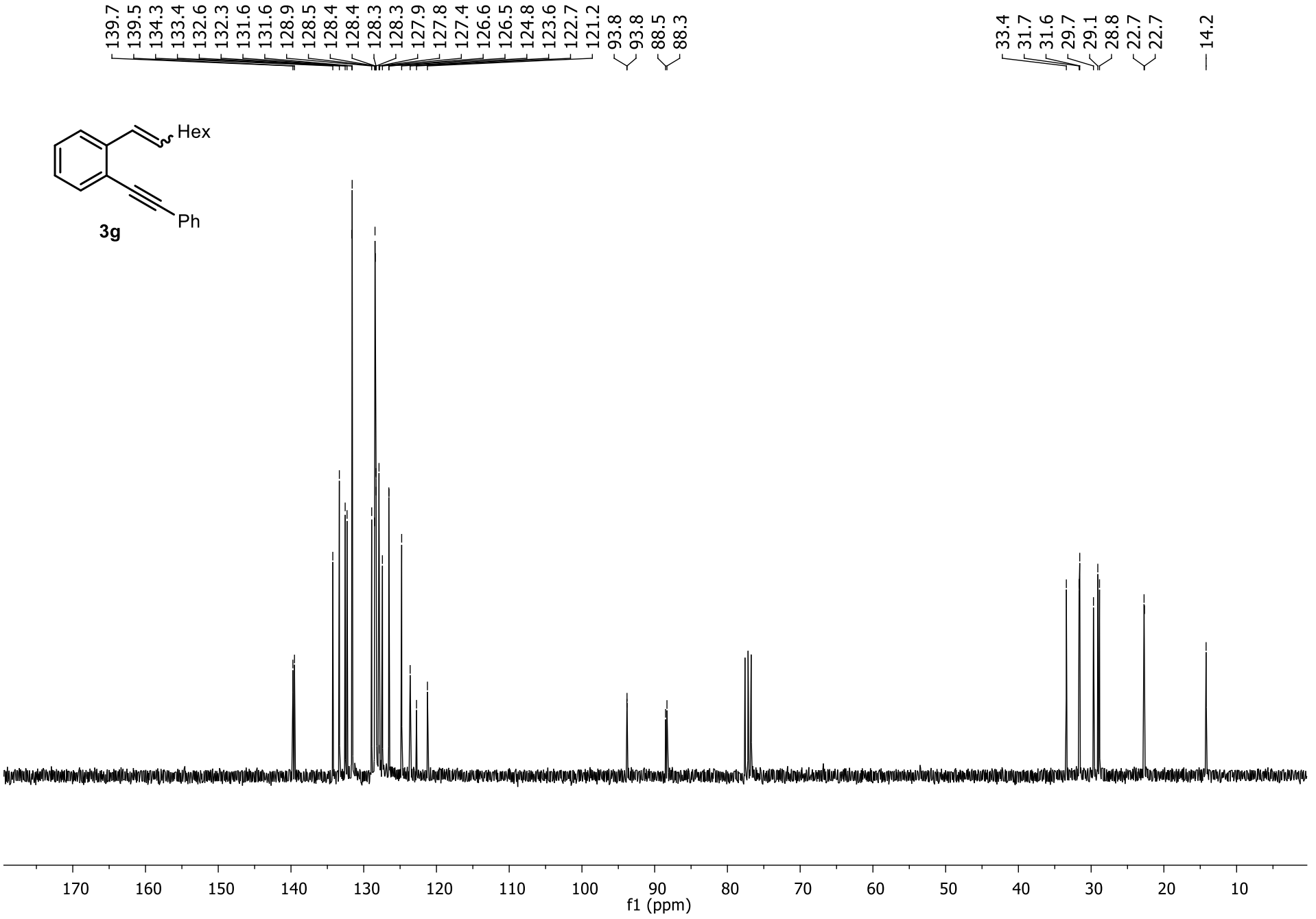
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



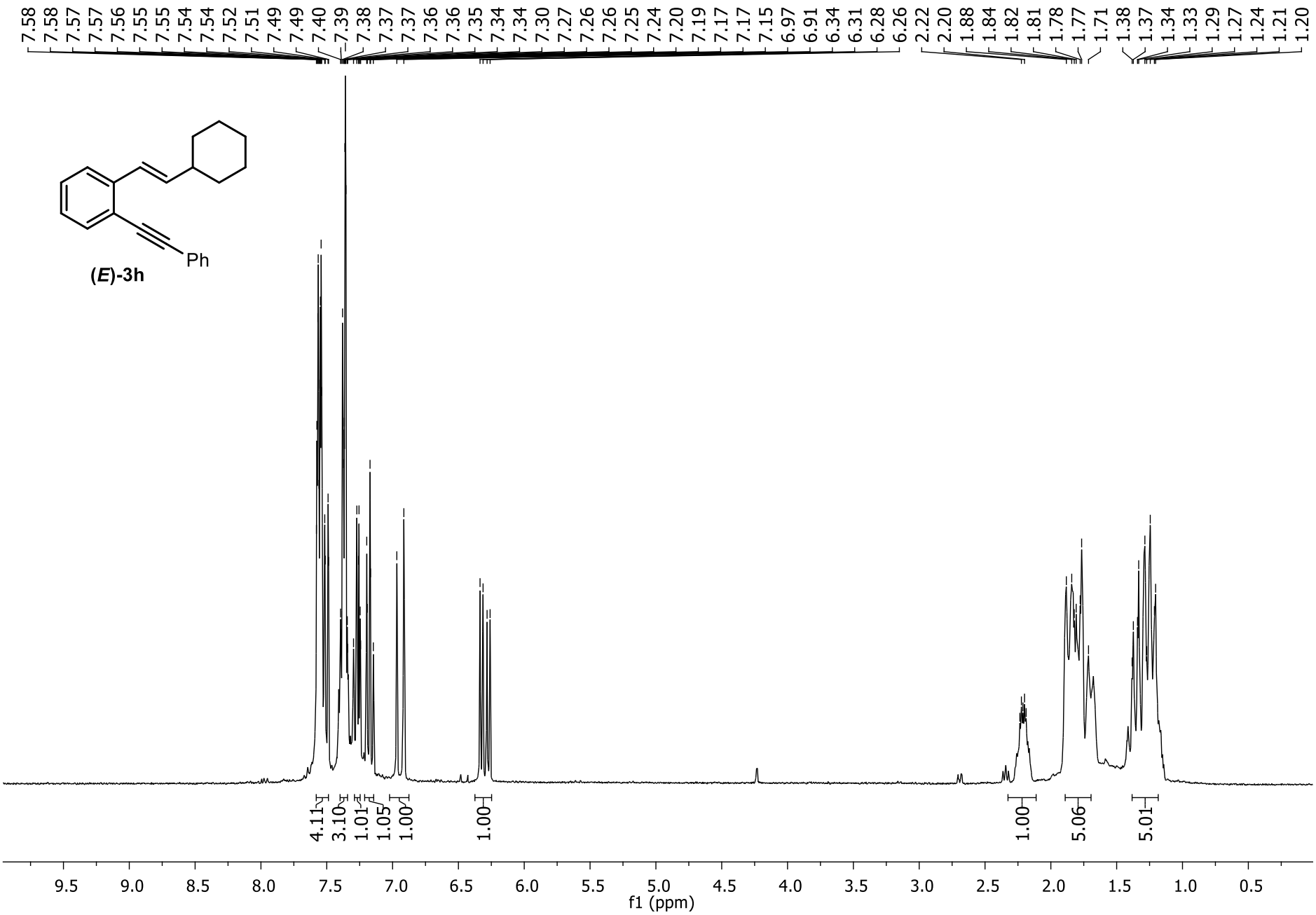
^{1}H NMR (300 MHz, $CDCl_3$)



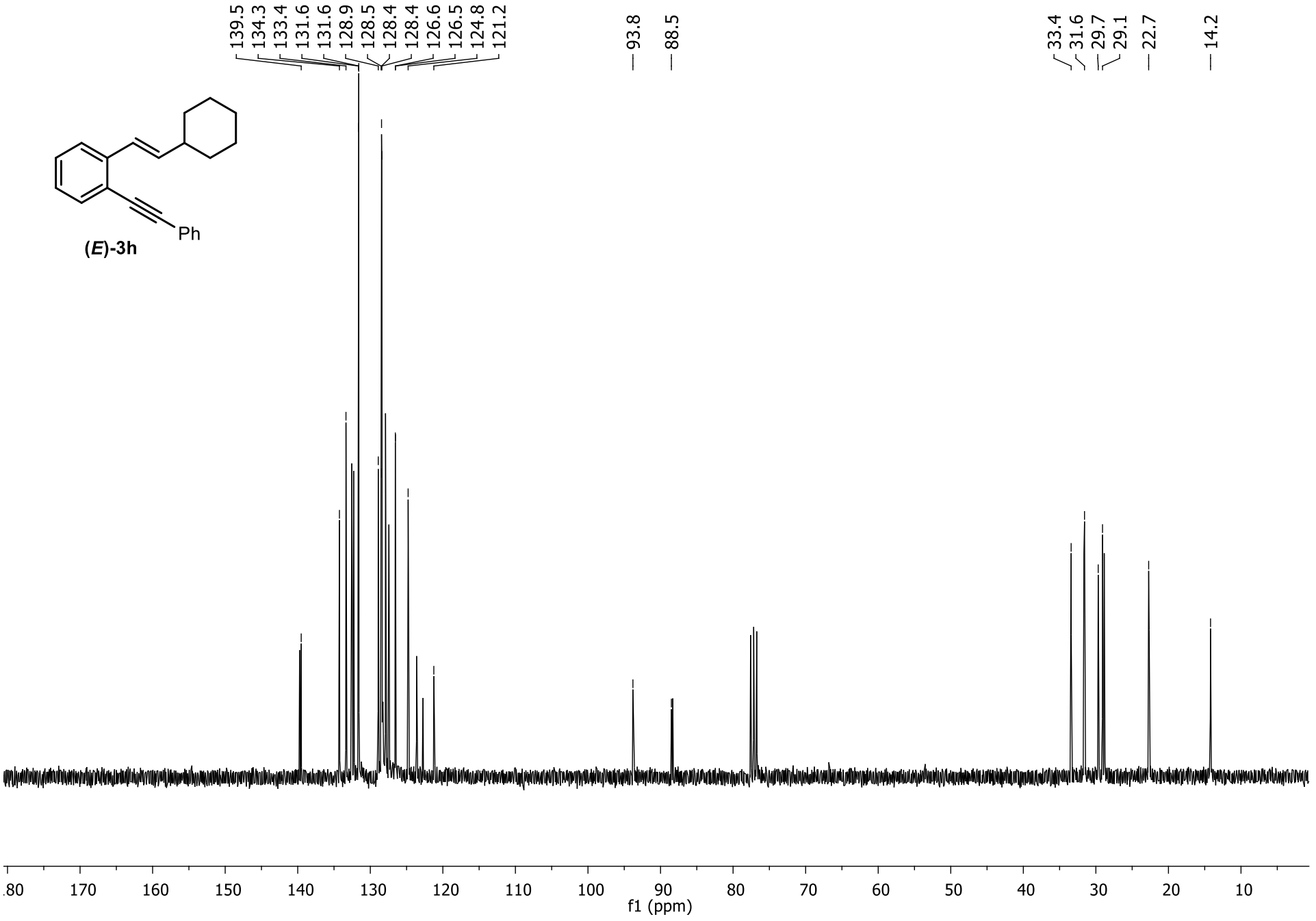
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



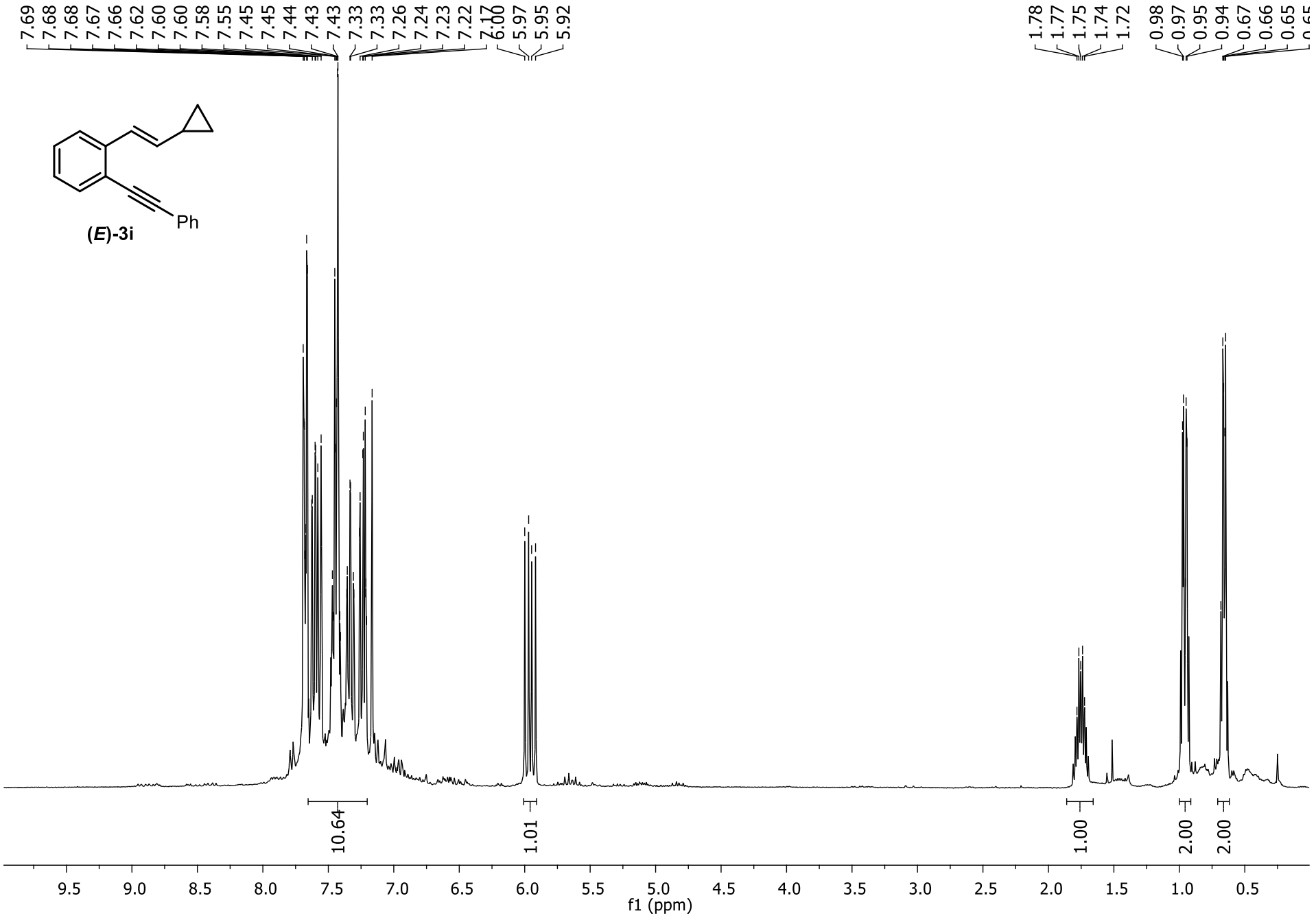
^{1}H NMR (300 MHz, $CDCl_3$)



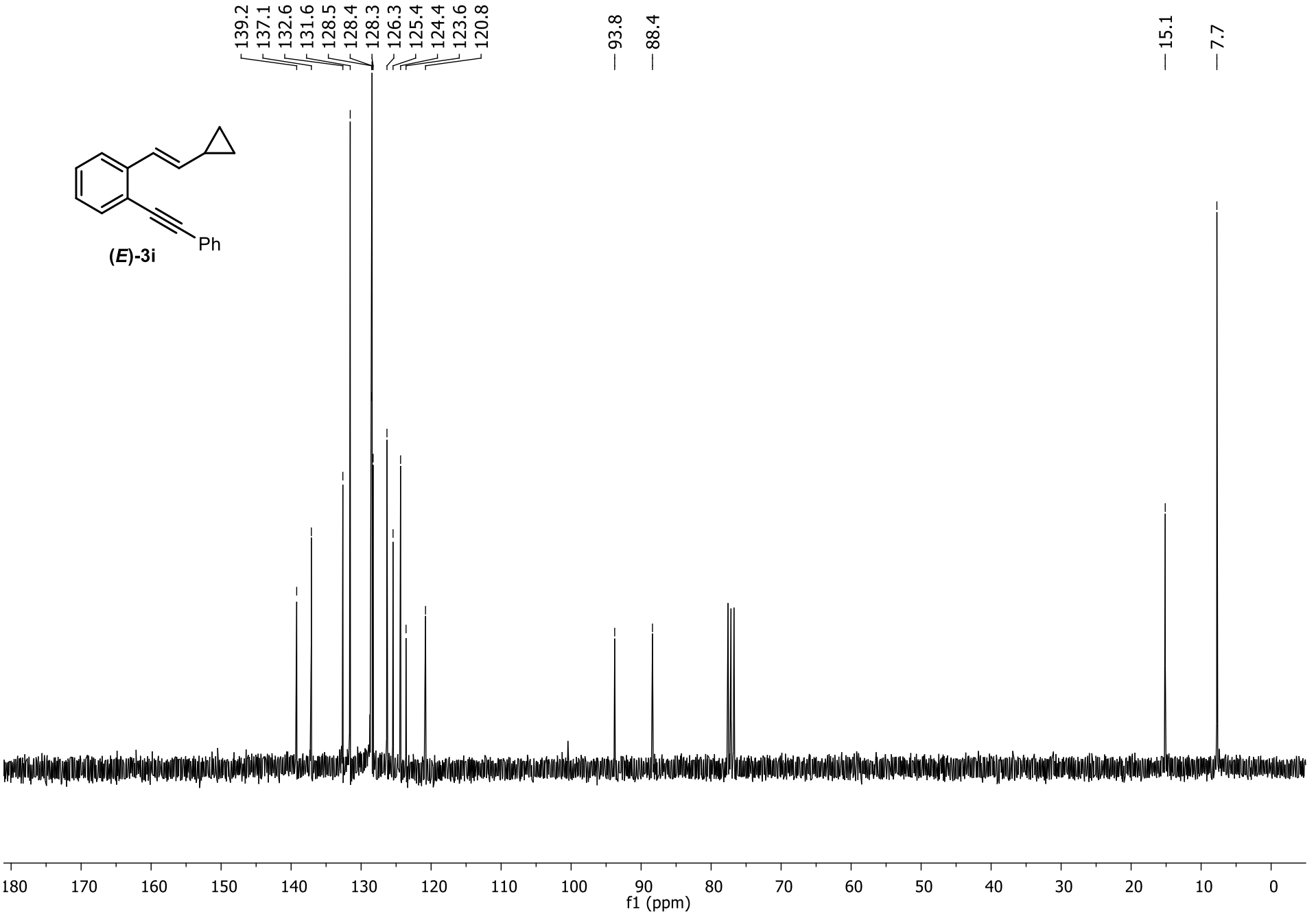
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



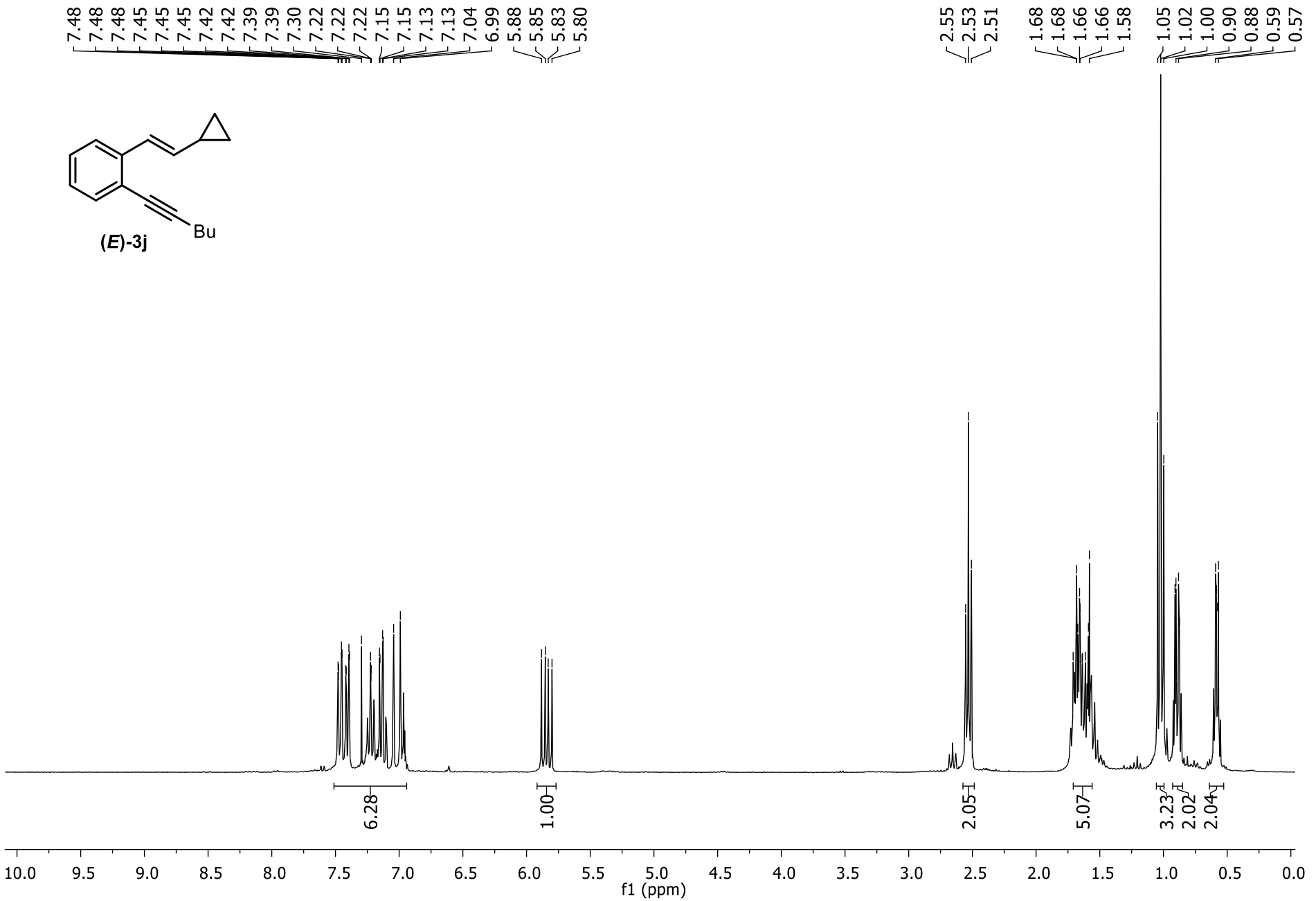
^{1}H NMR (300 MHz, $CDCl_3$)



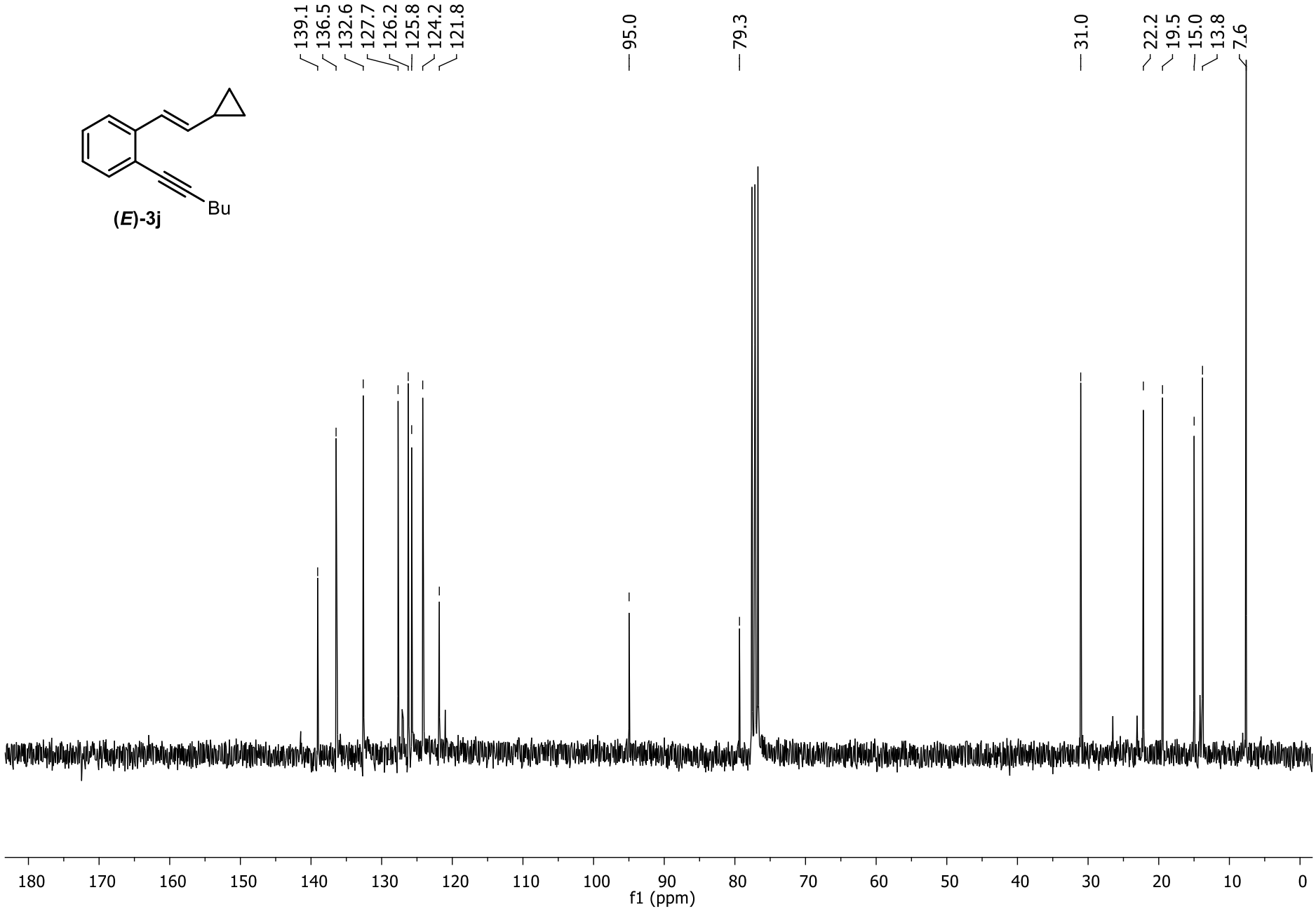
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



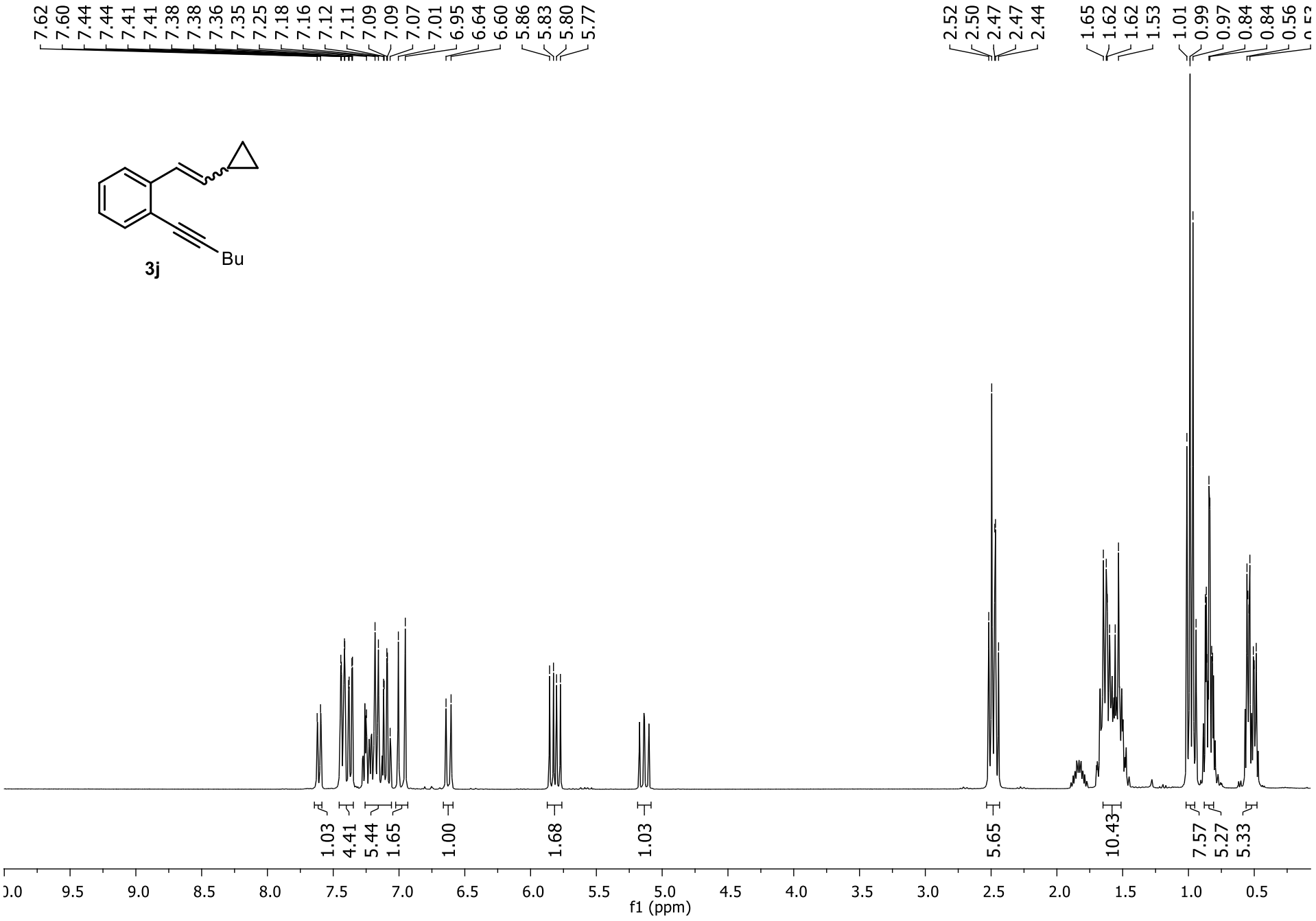
^{1}H NMR (300 MHz, $CDCl_3$)



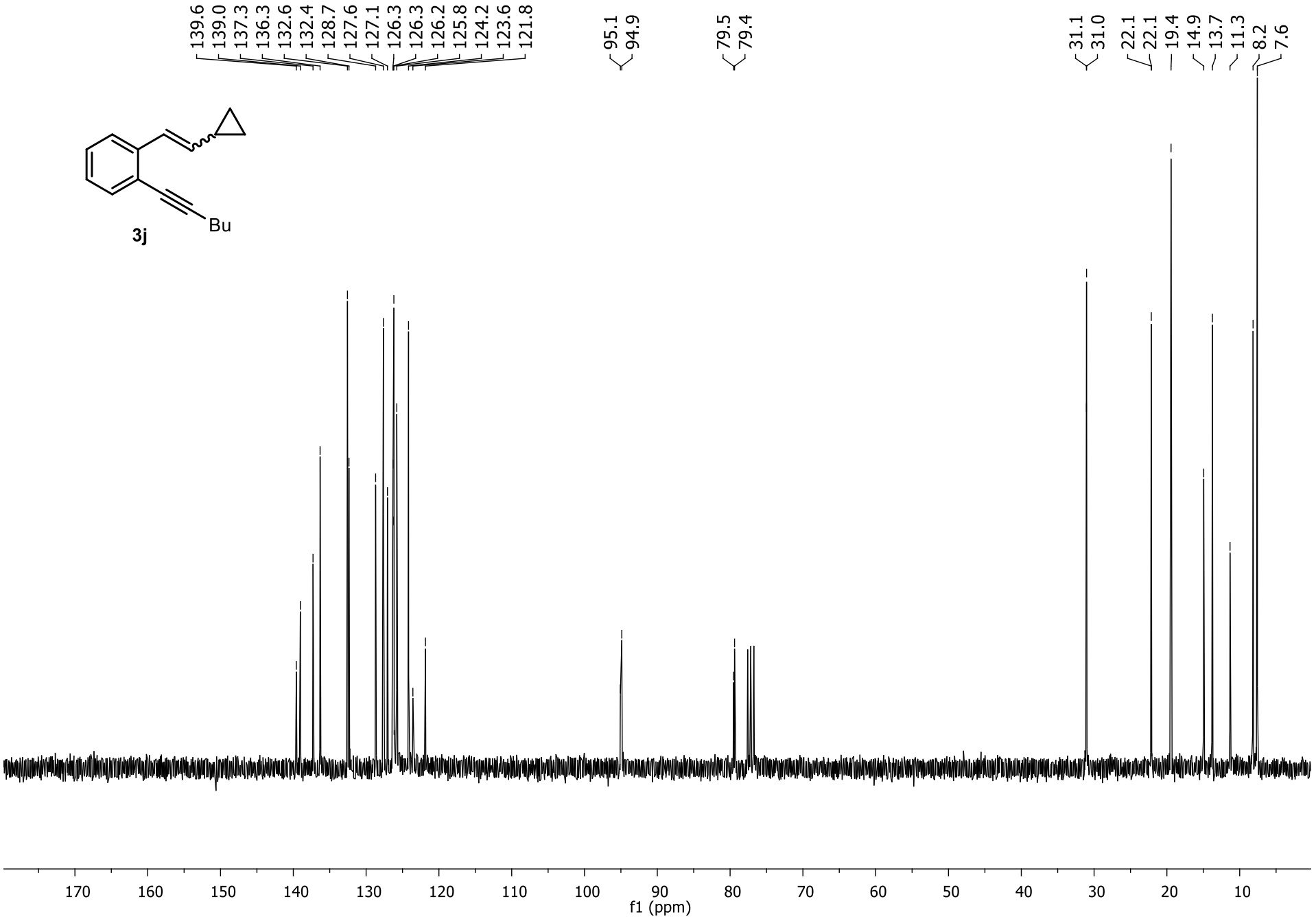
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



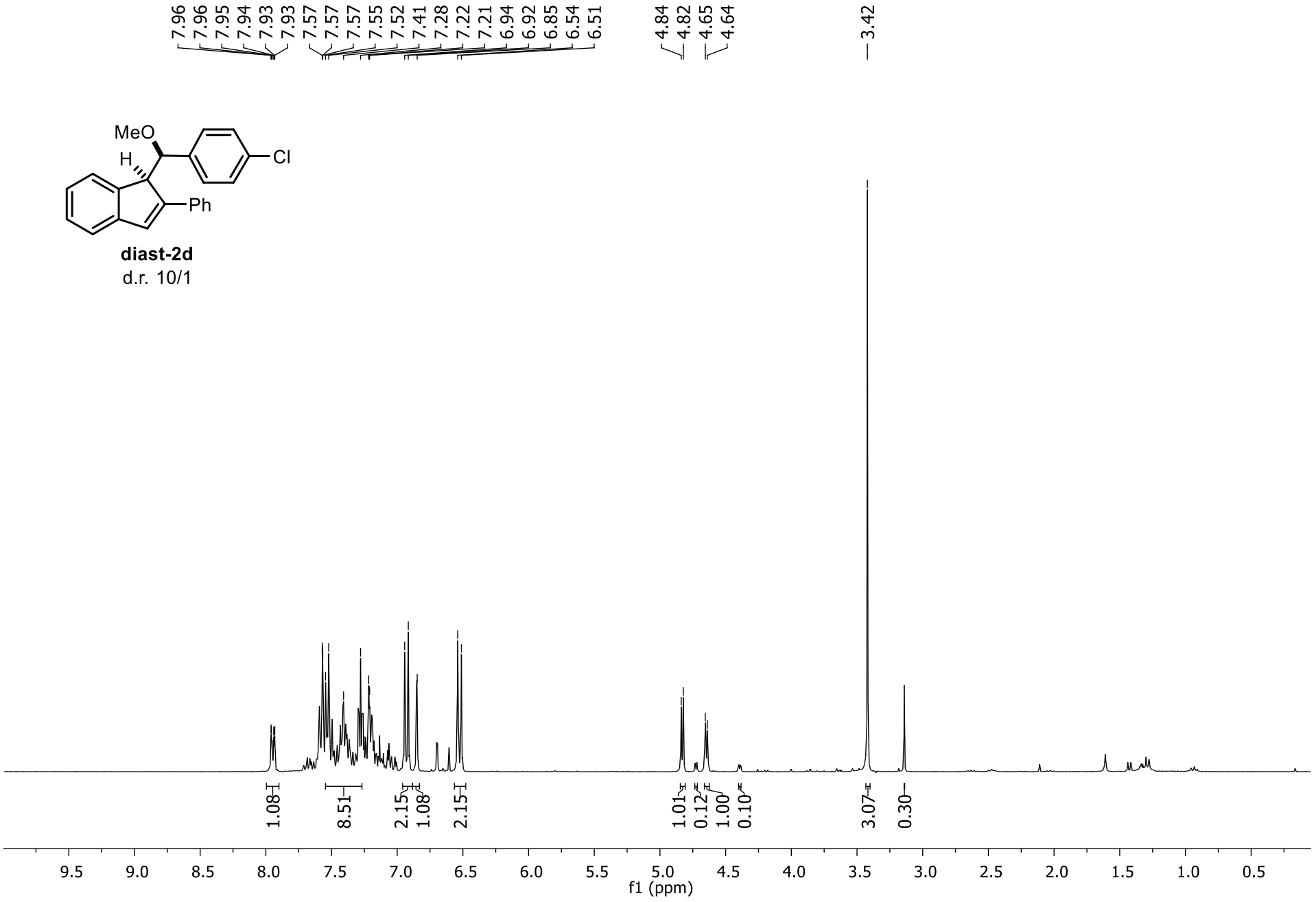
^{1}H NMR (300 MHz, $CDCl_3$)



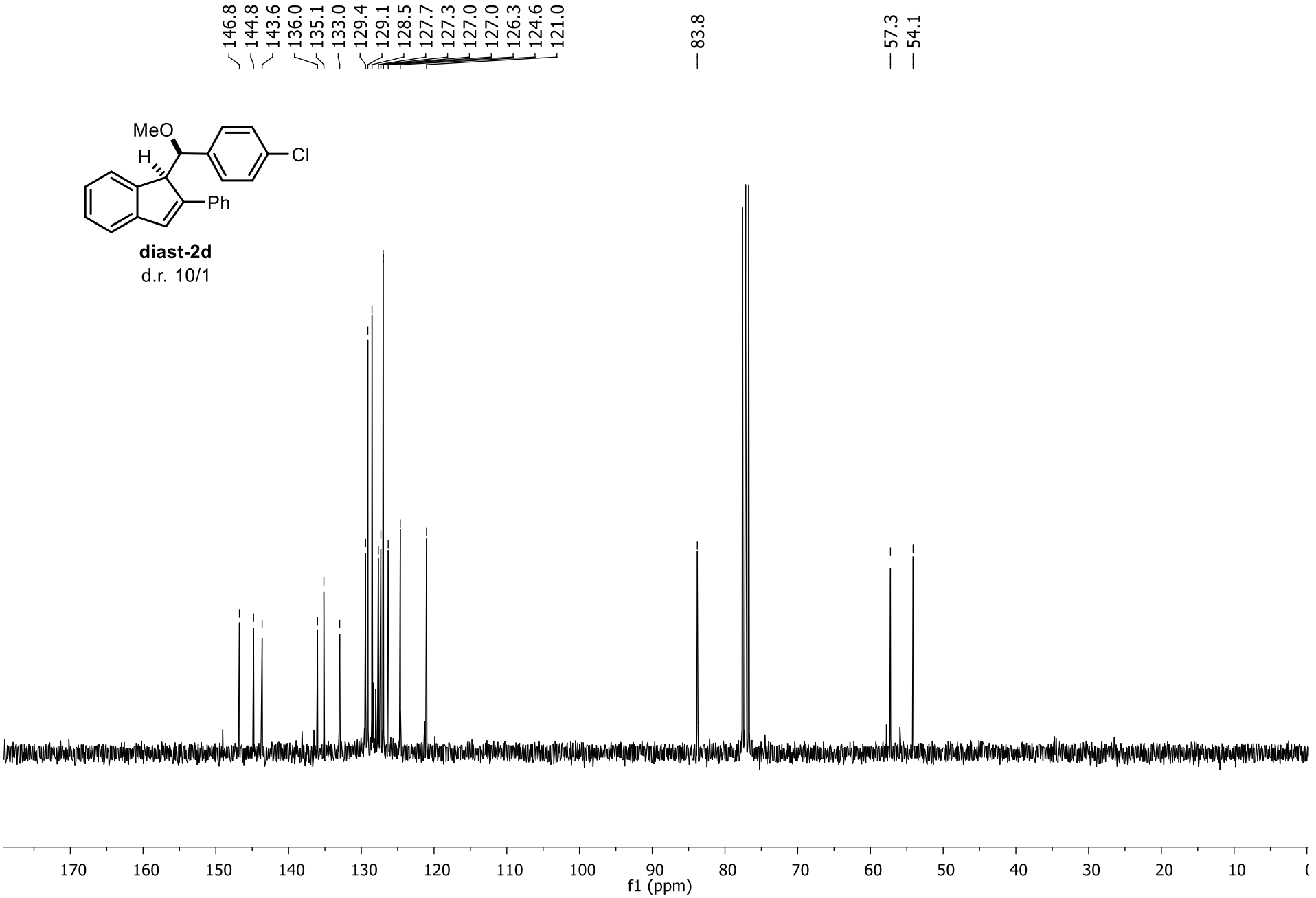
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



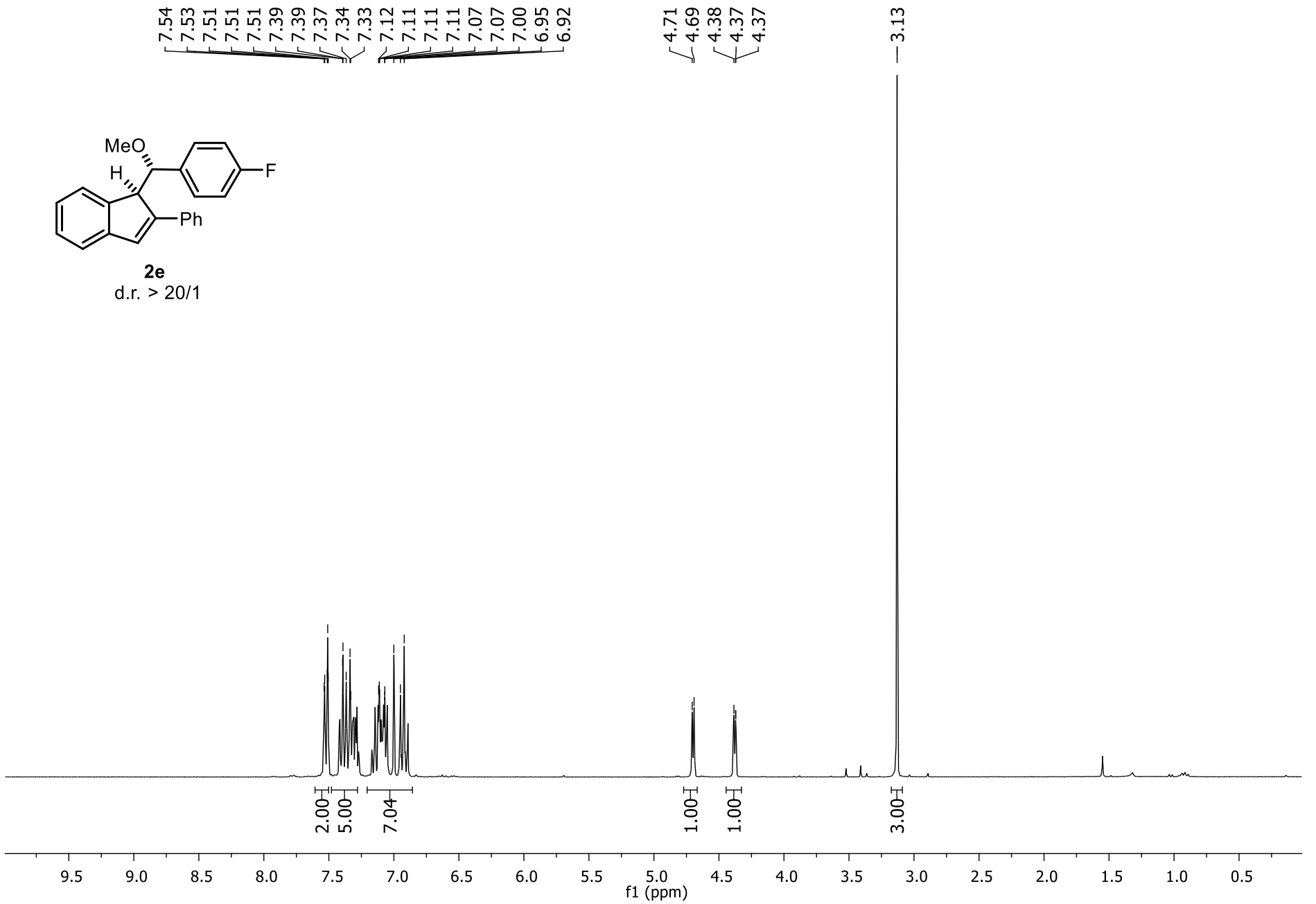
^{1}H NMR (300 MHz, $CDCl_3$)



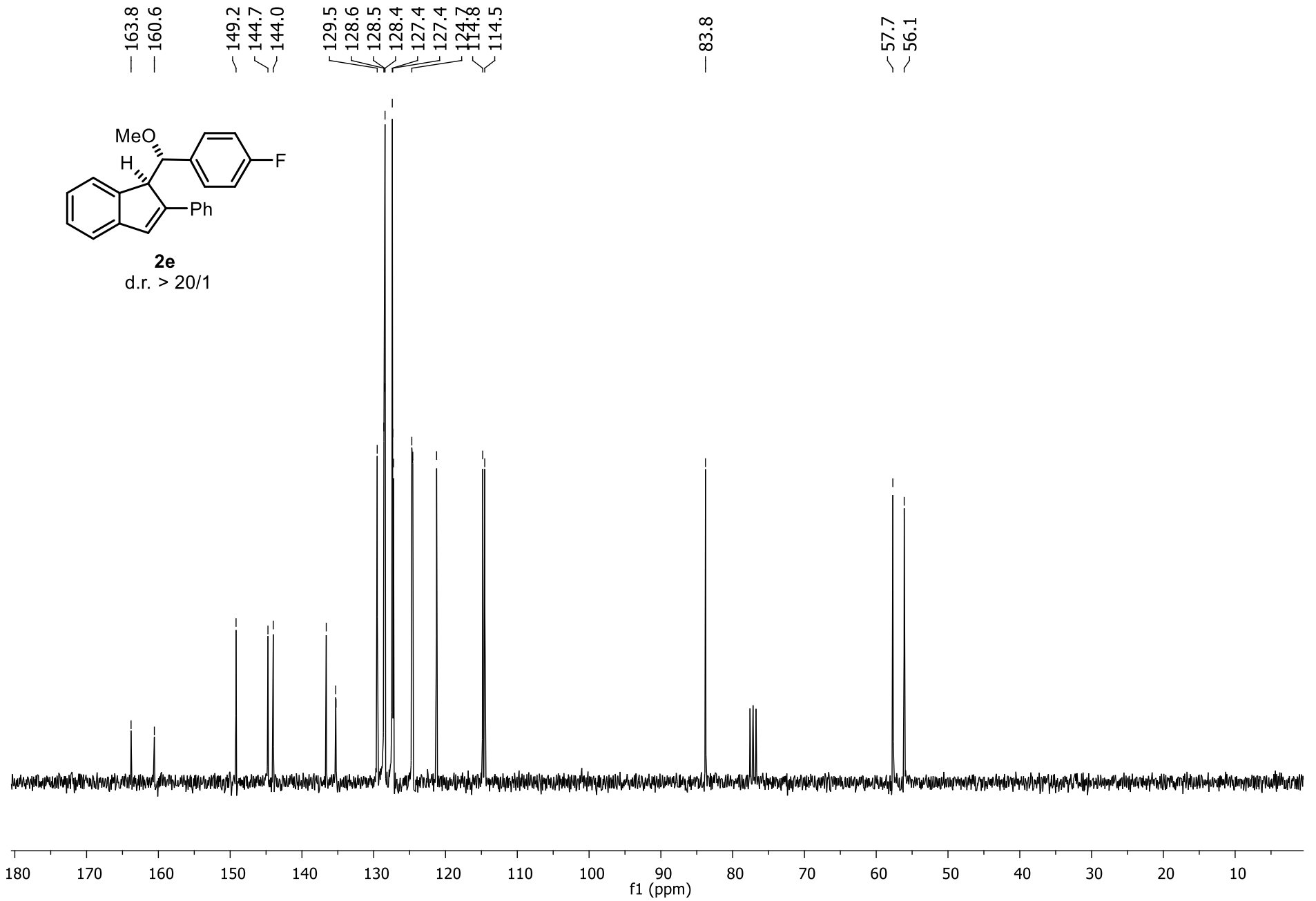
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



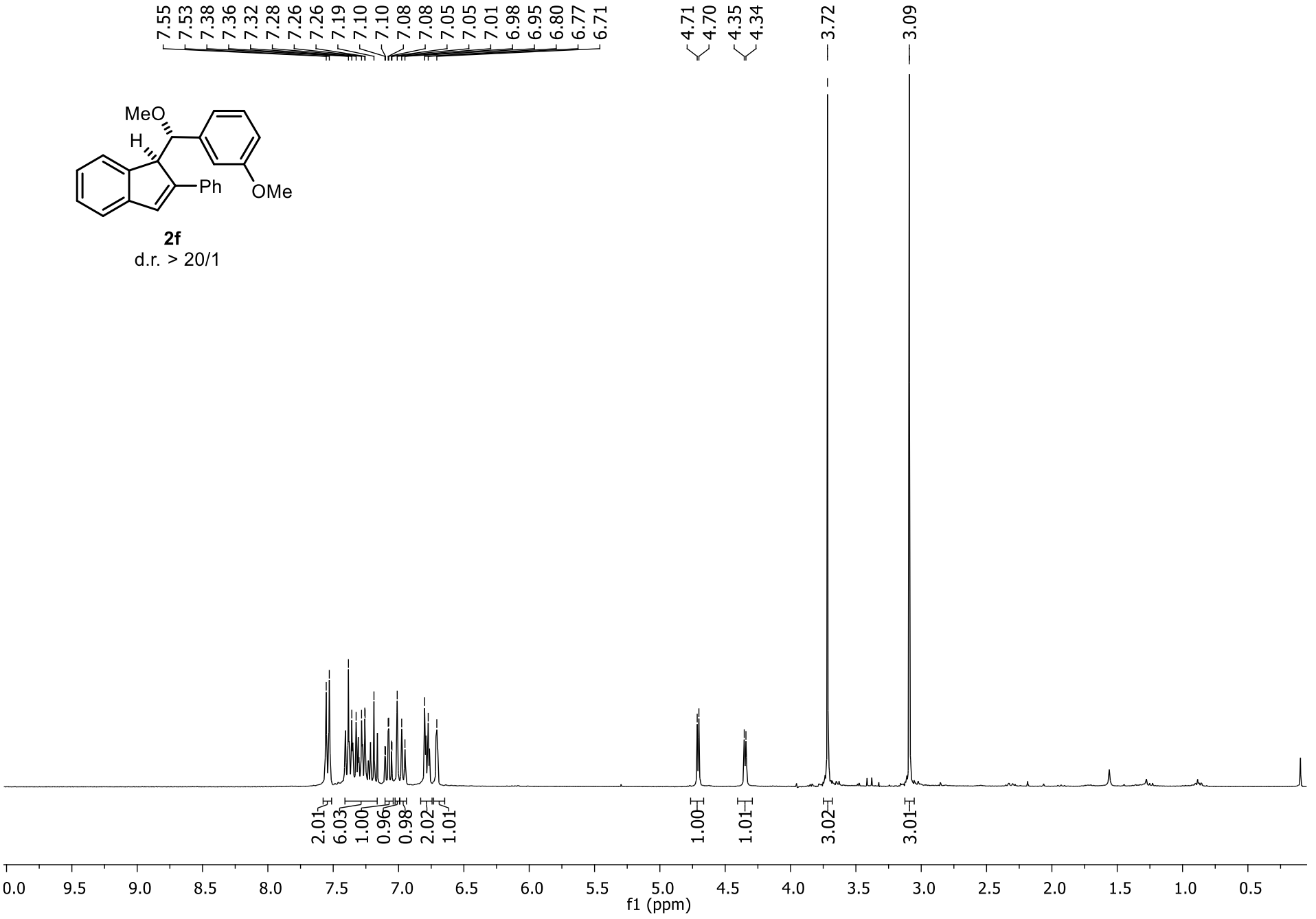
^{1}H NMR (300 MHz, $CDCl_3$)



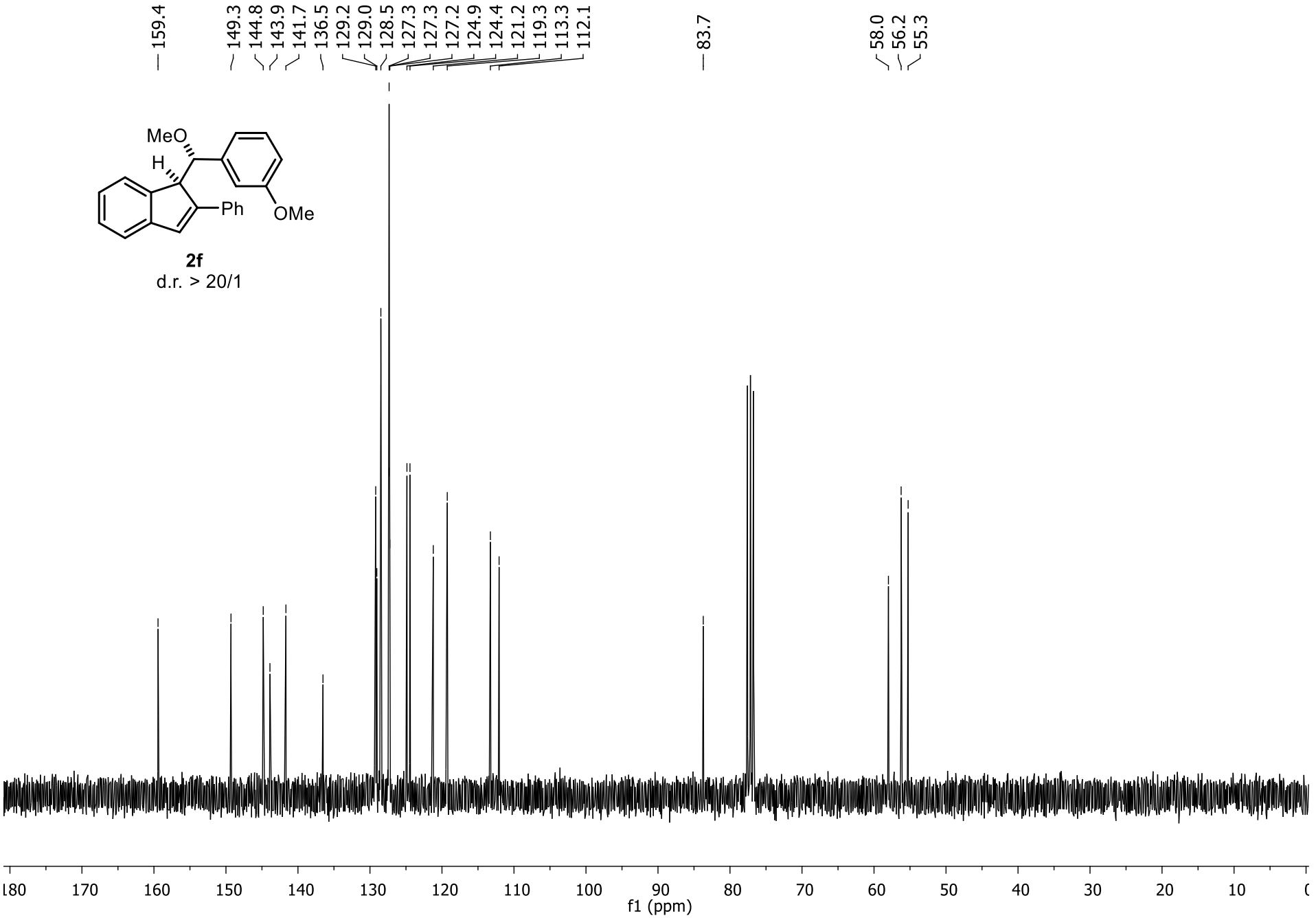
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



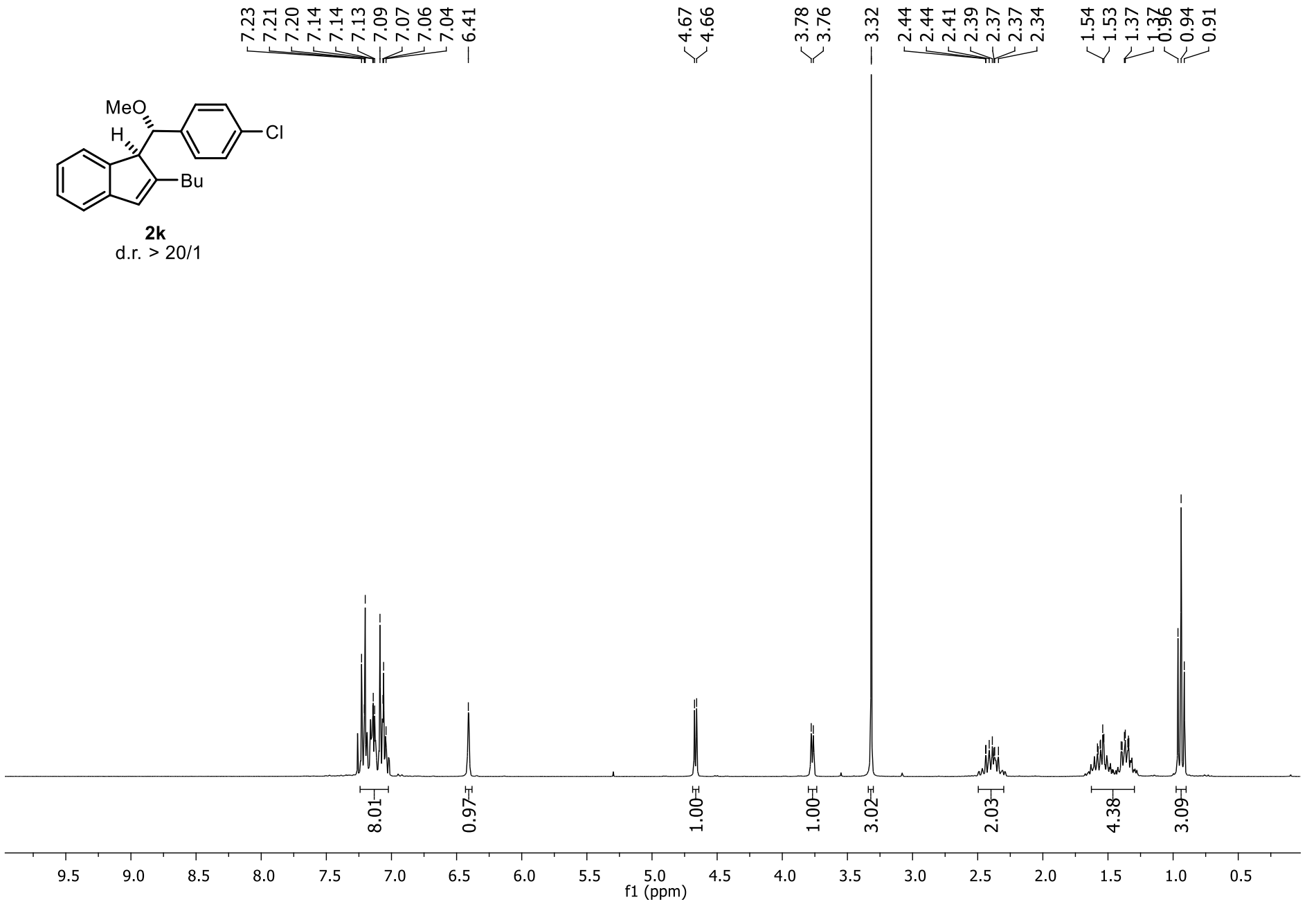
^{1}H NMR (300 MHz, $CDCl_3$)



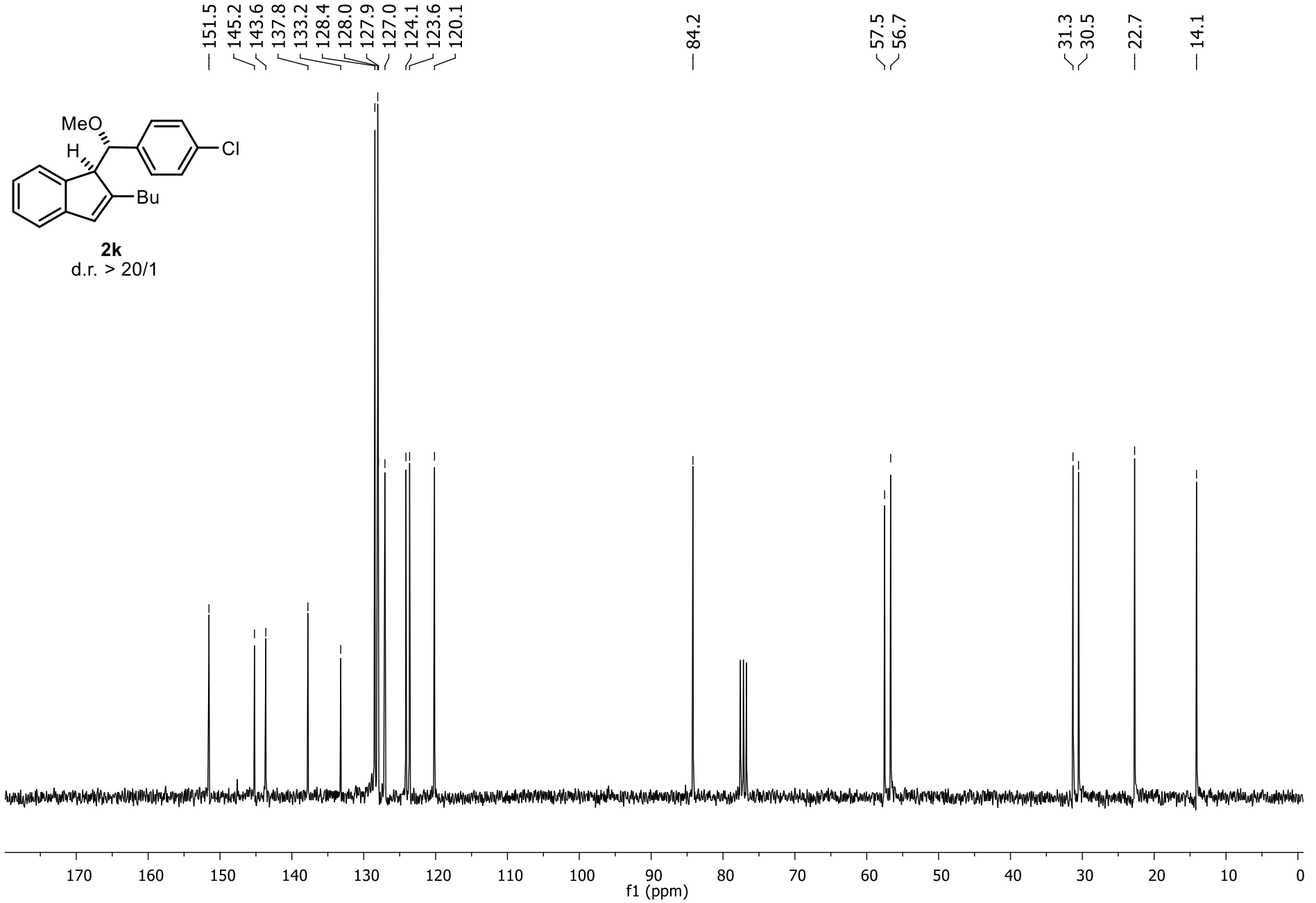
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



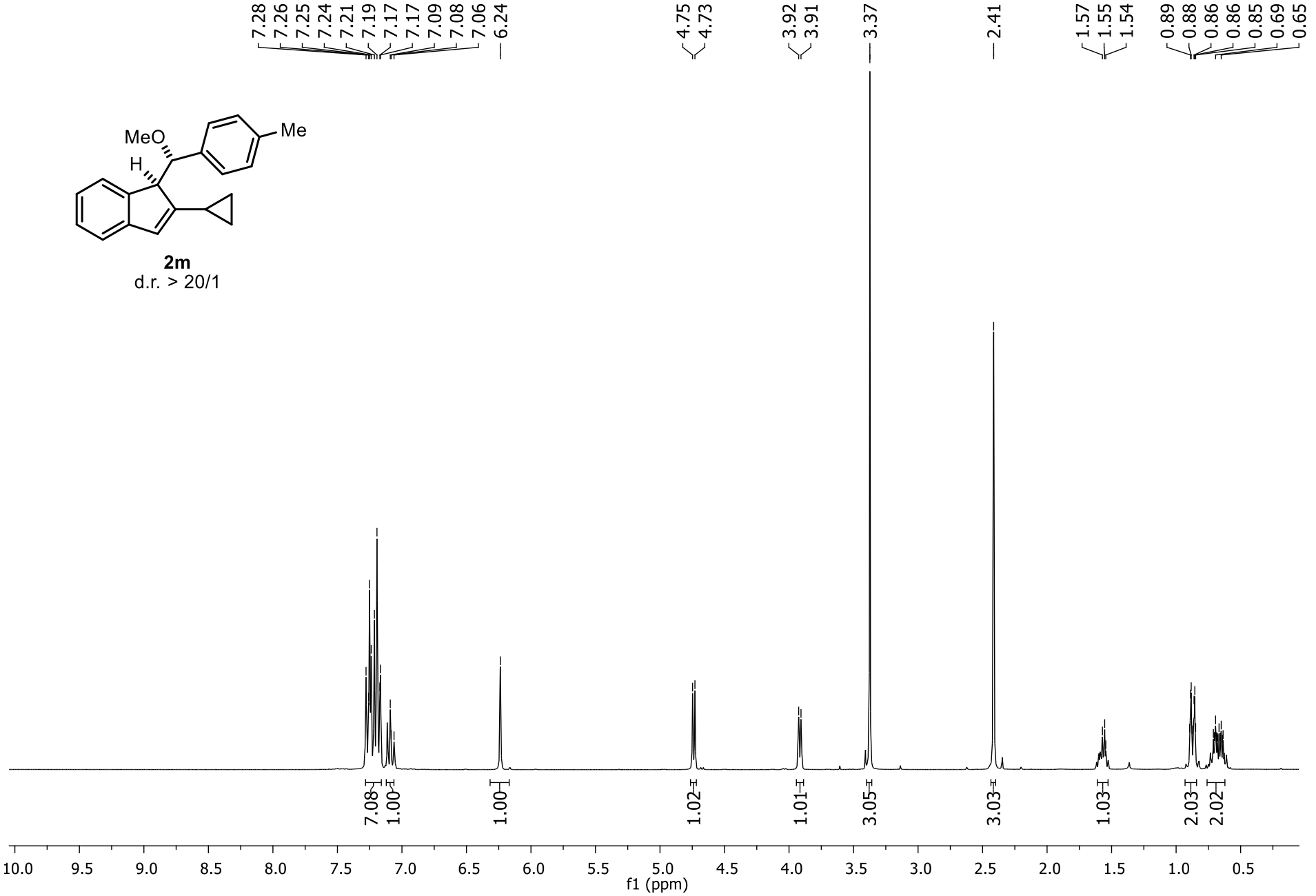
^{1}H NMR (300 MHz, $CDCl_3$)



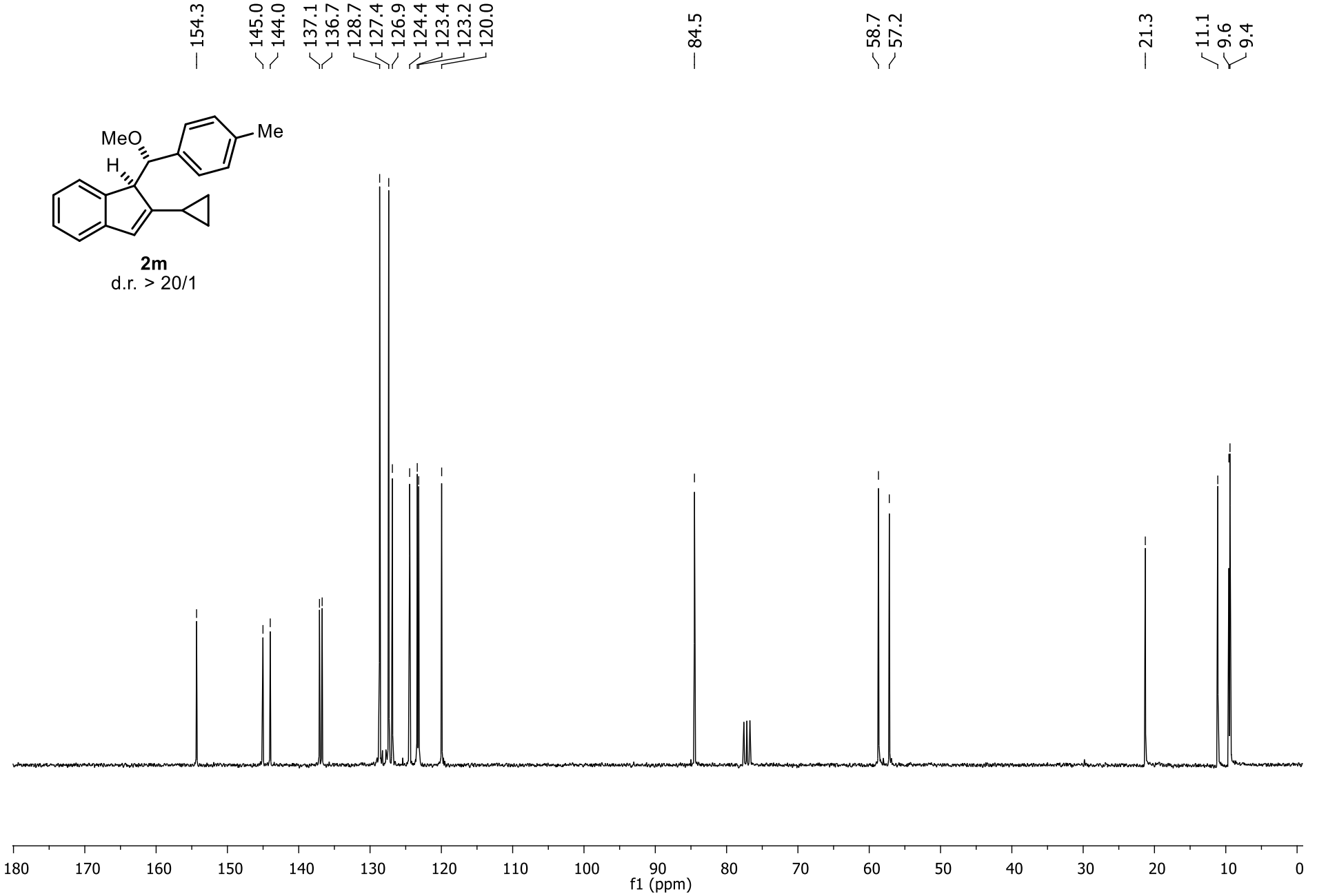
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



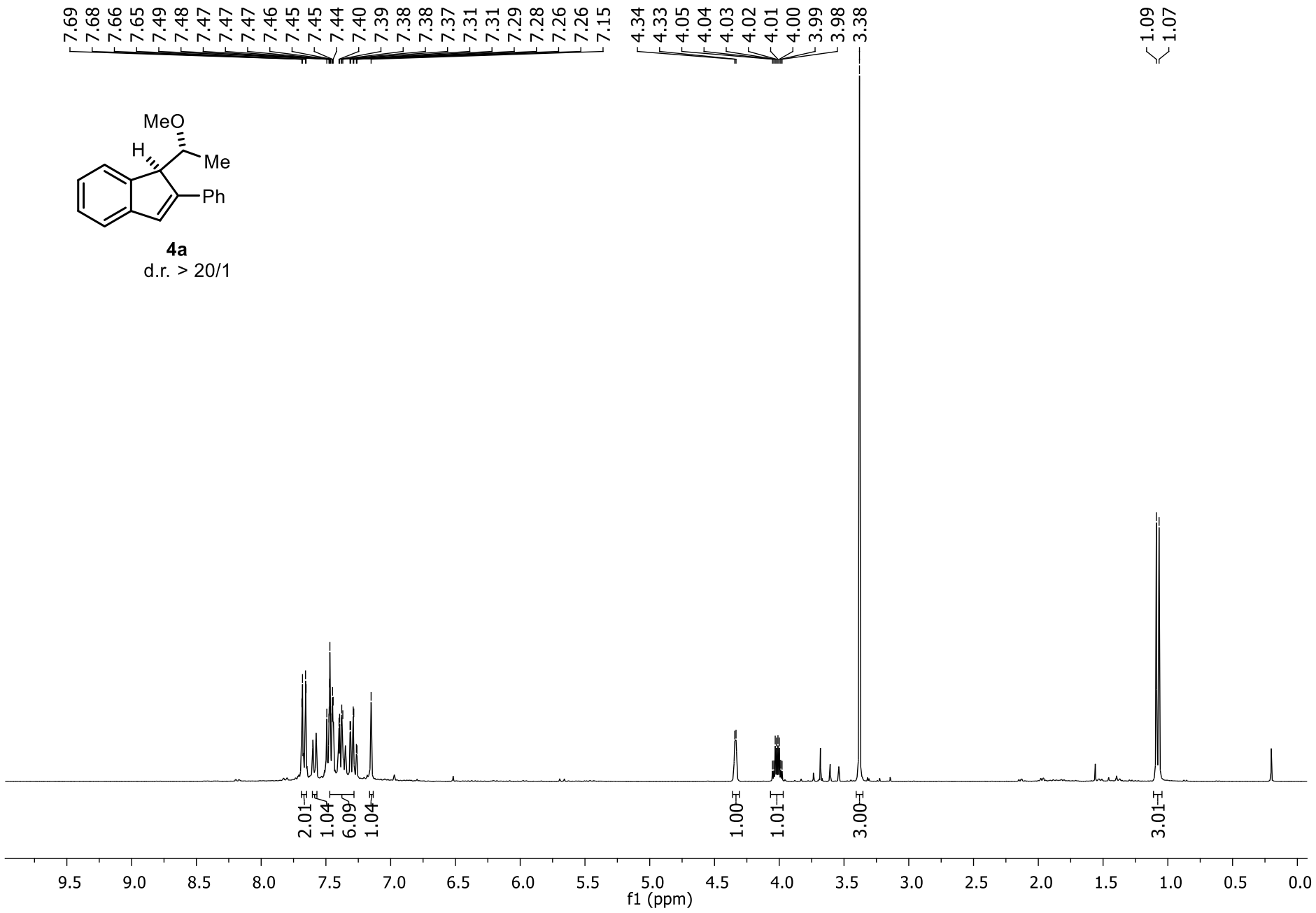
^{1}H NMR (300 MHz, $CDCl_3$)



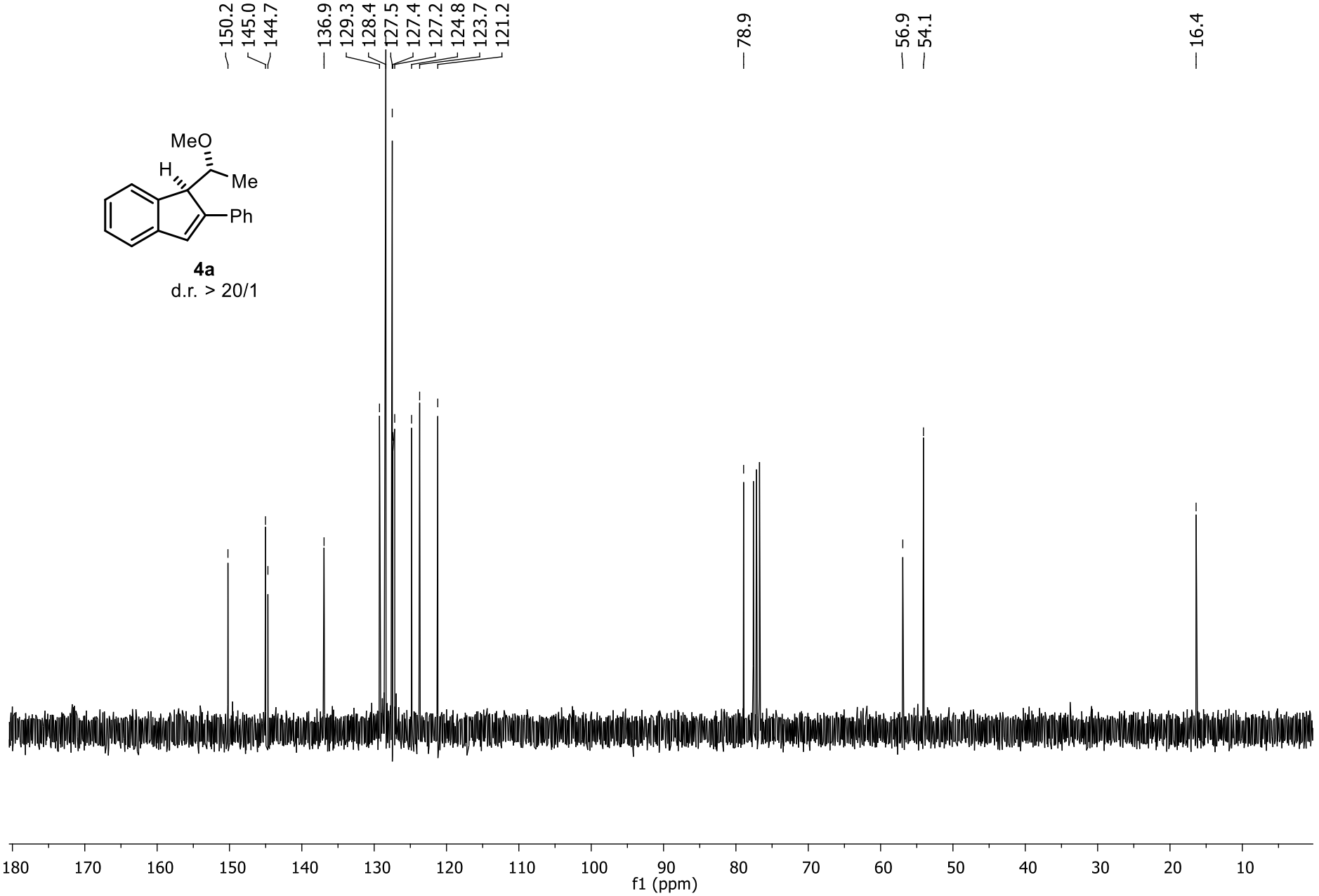
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



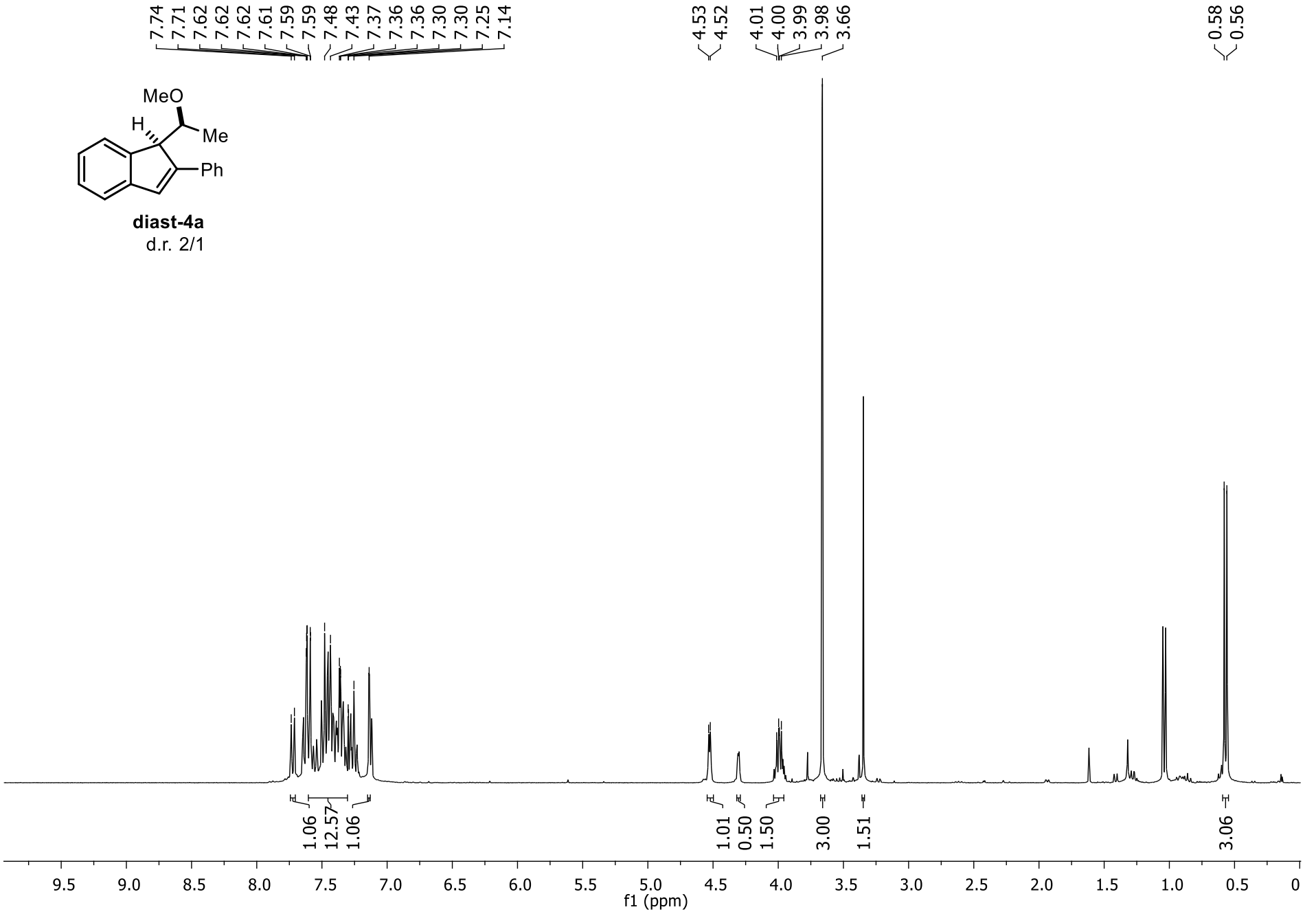
^{1}H NMR (300 MHz, $CDCl_3$)



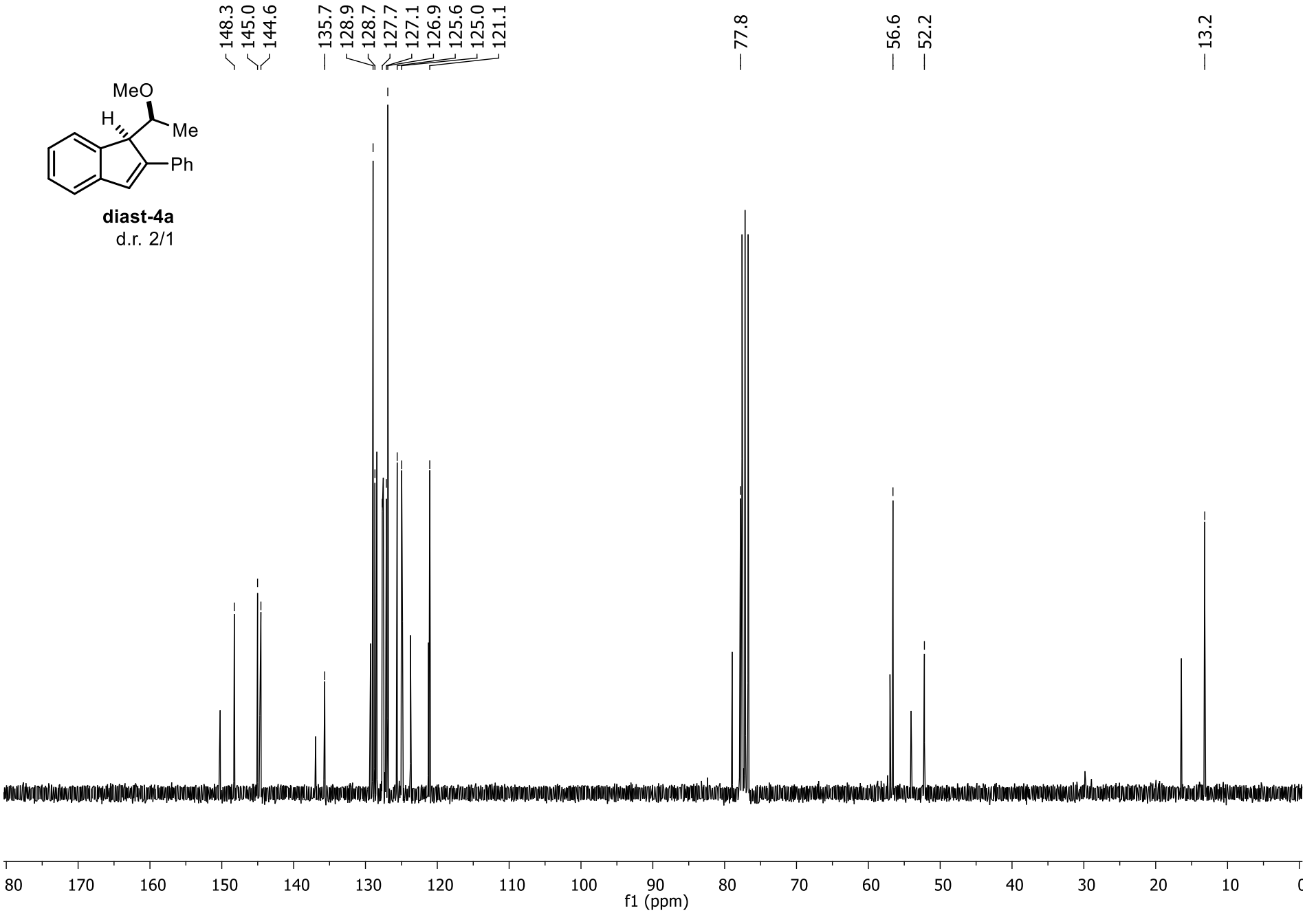
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



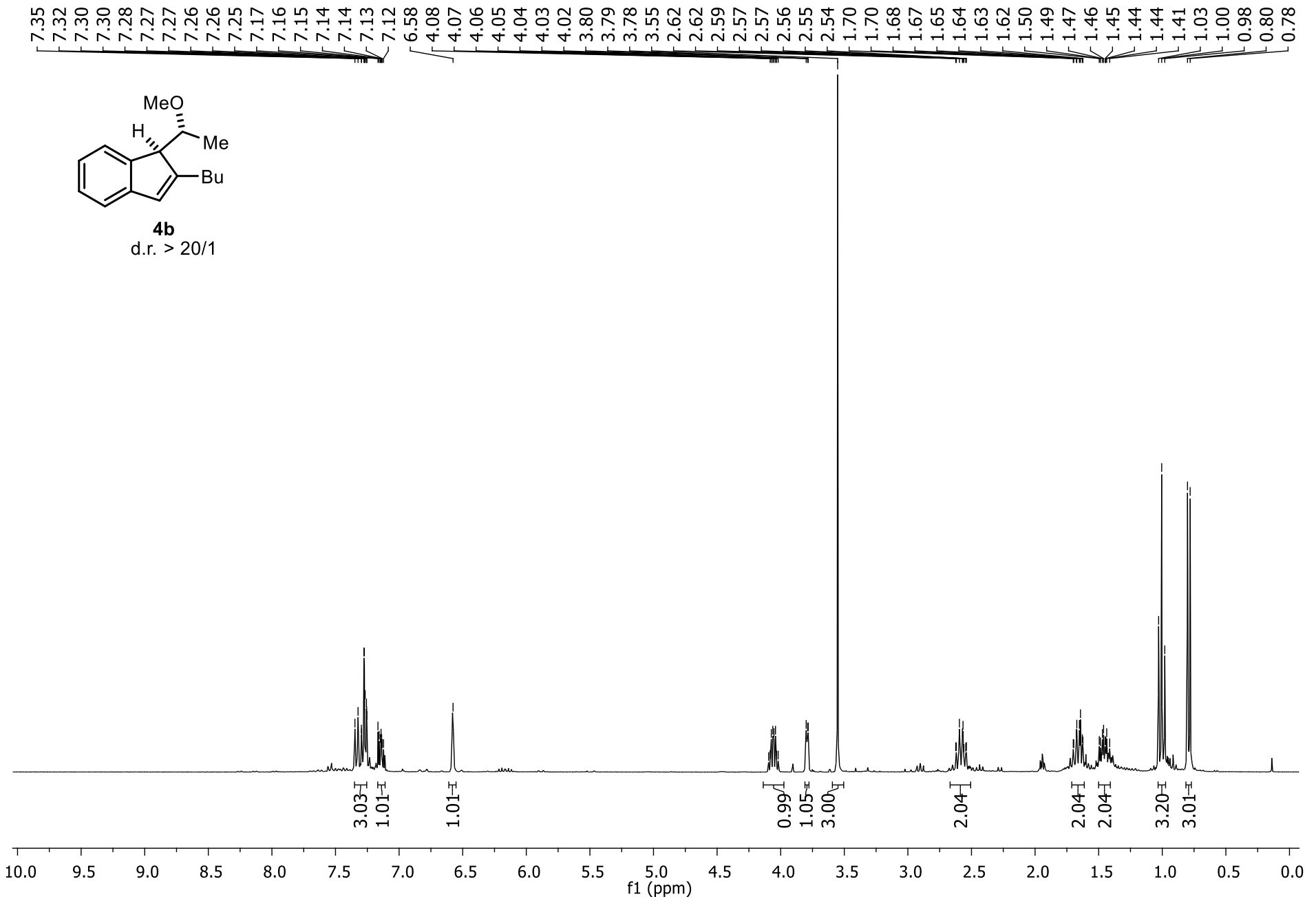
^{1}H NMR (300 MHz, $CDCl_3$)



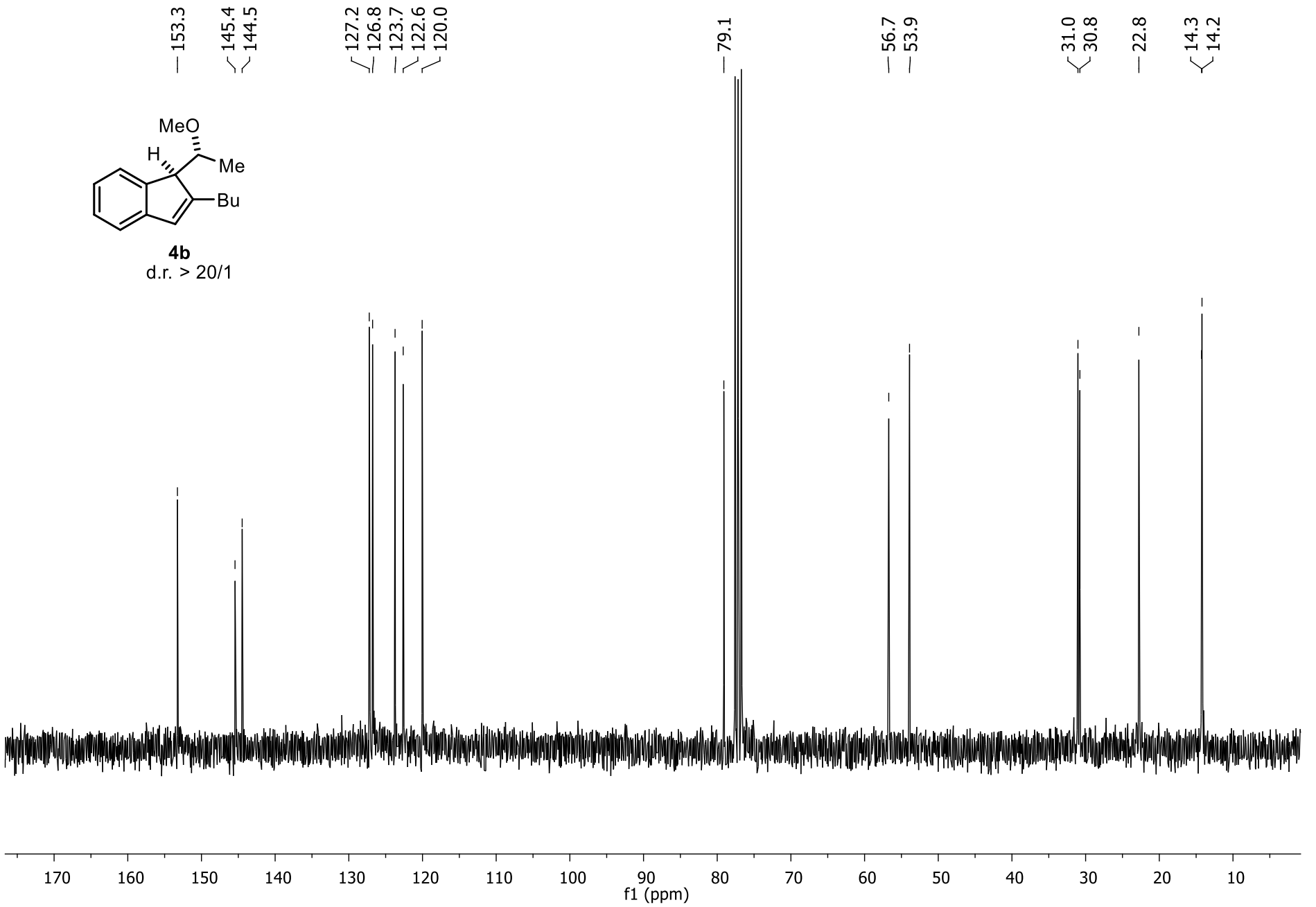
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



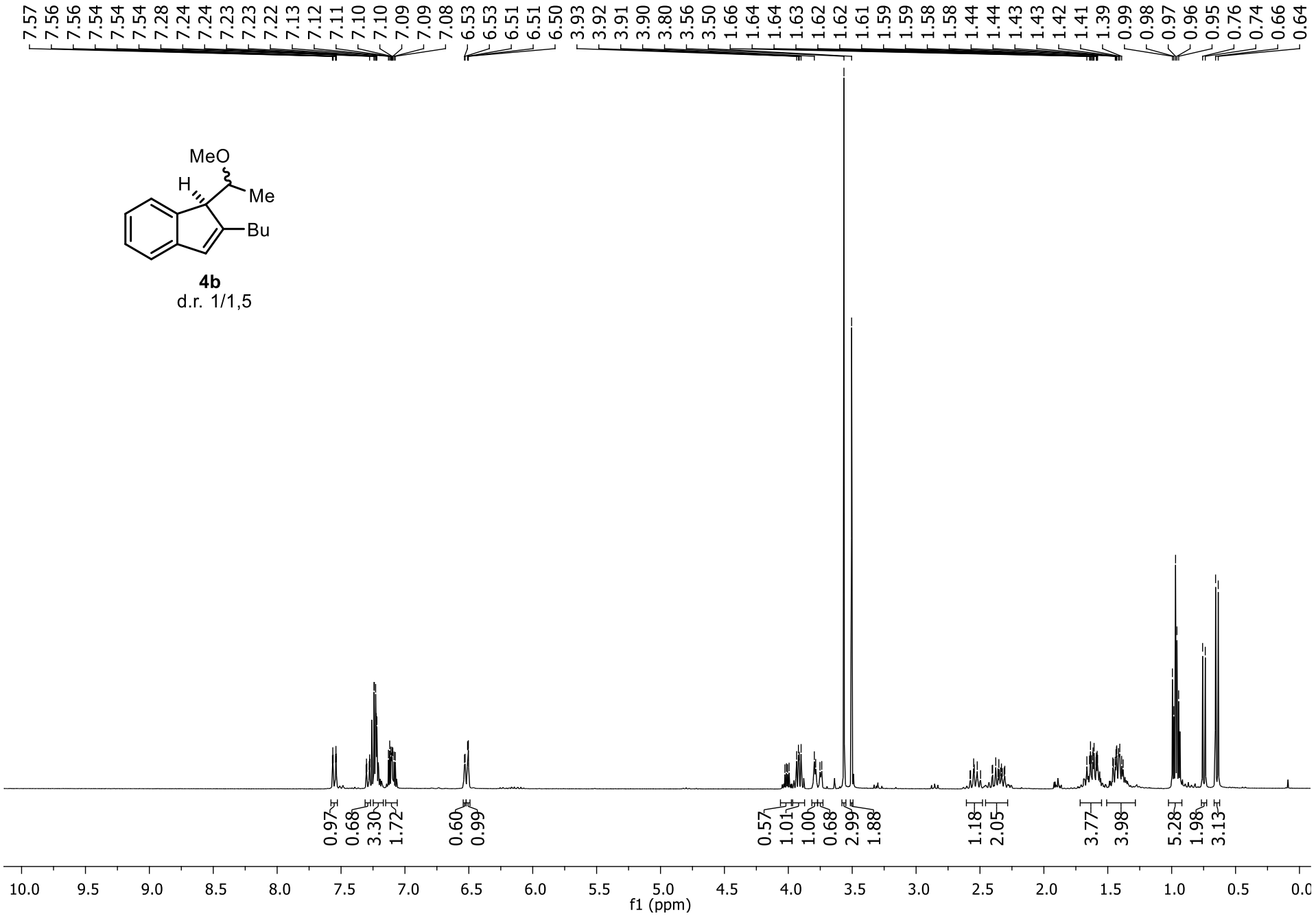
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

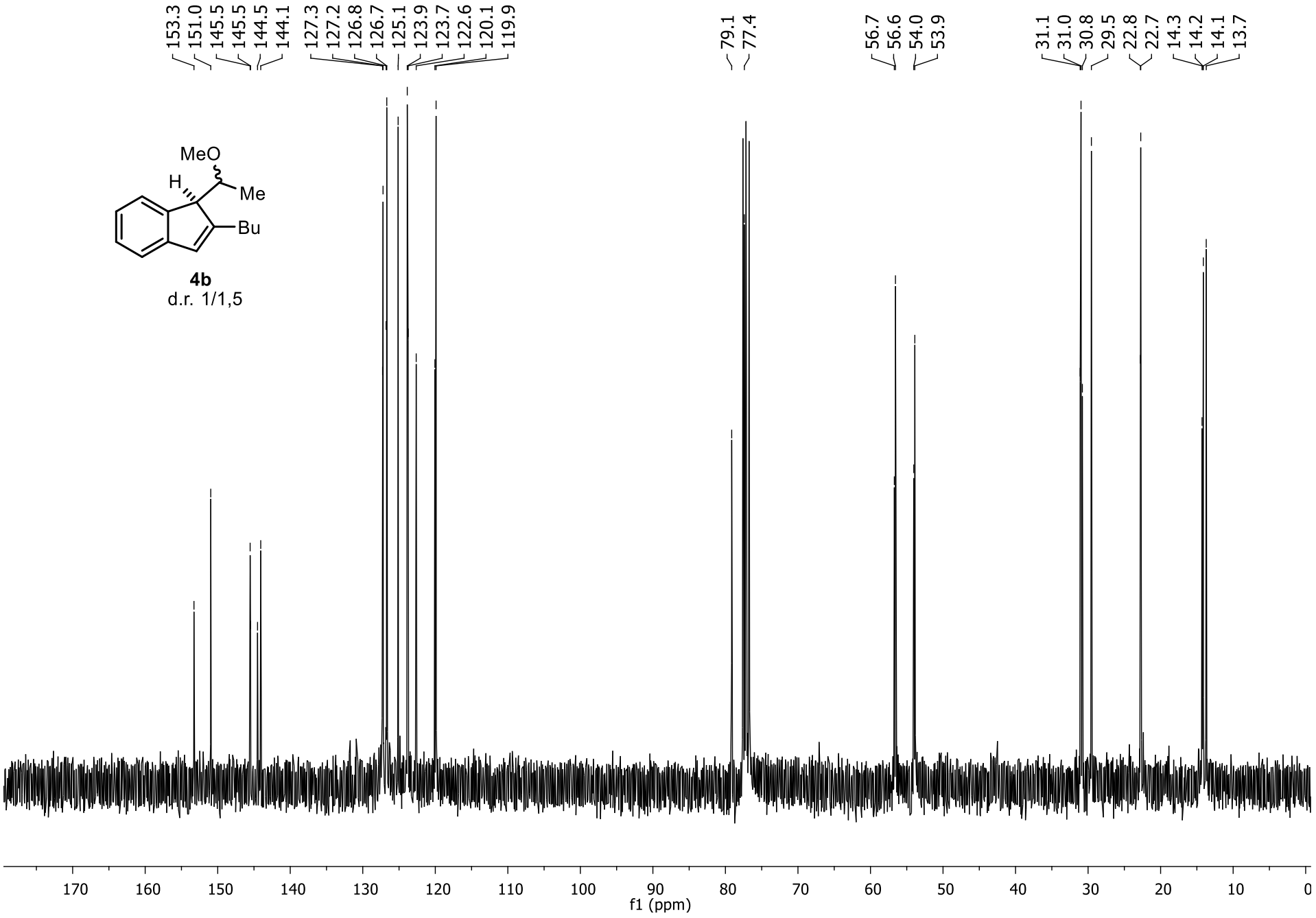


^{1}H NMR (300 MHz, $CDCl_3$)

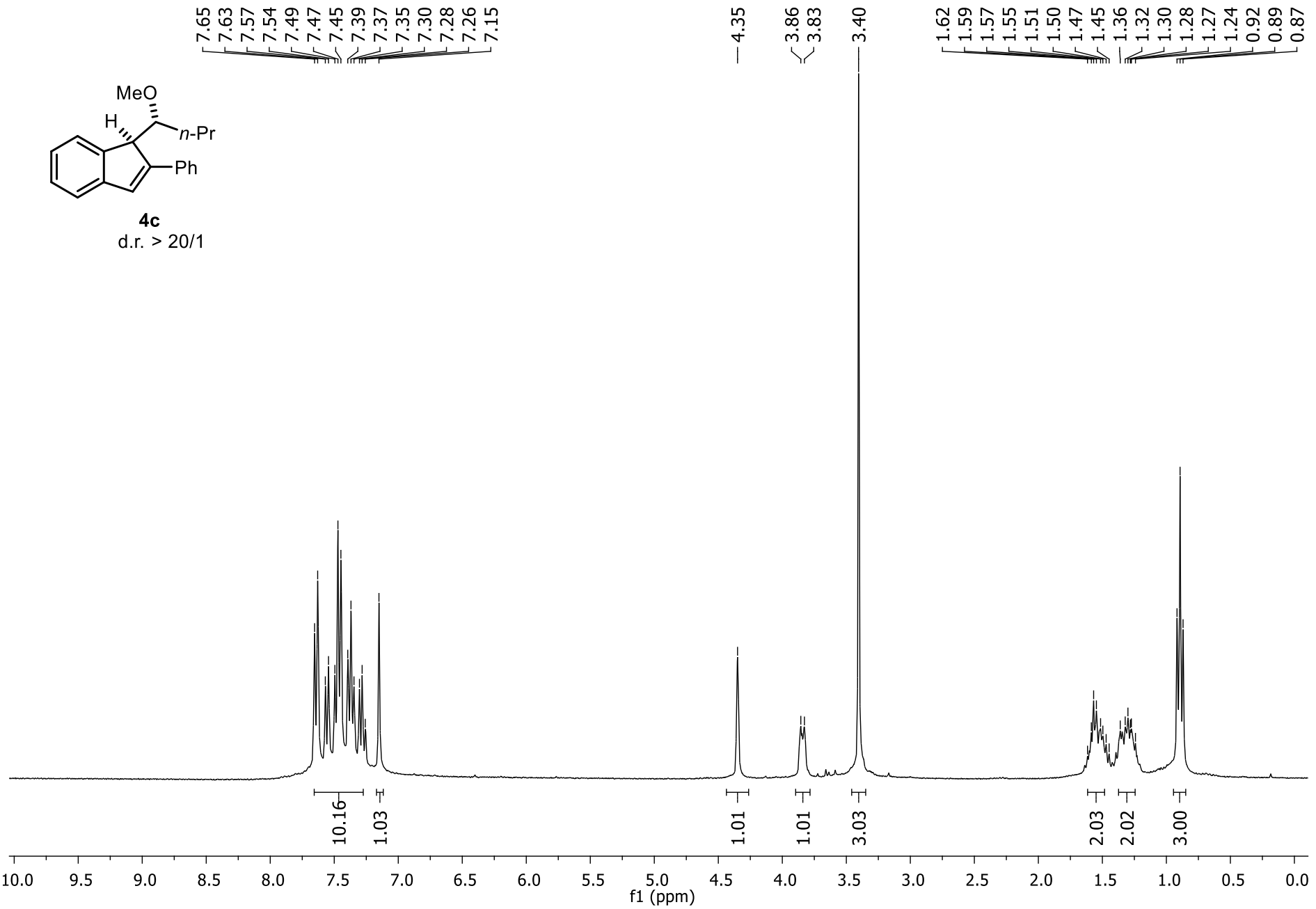


4b
d.r. 1/1,5

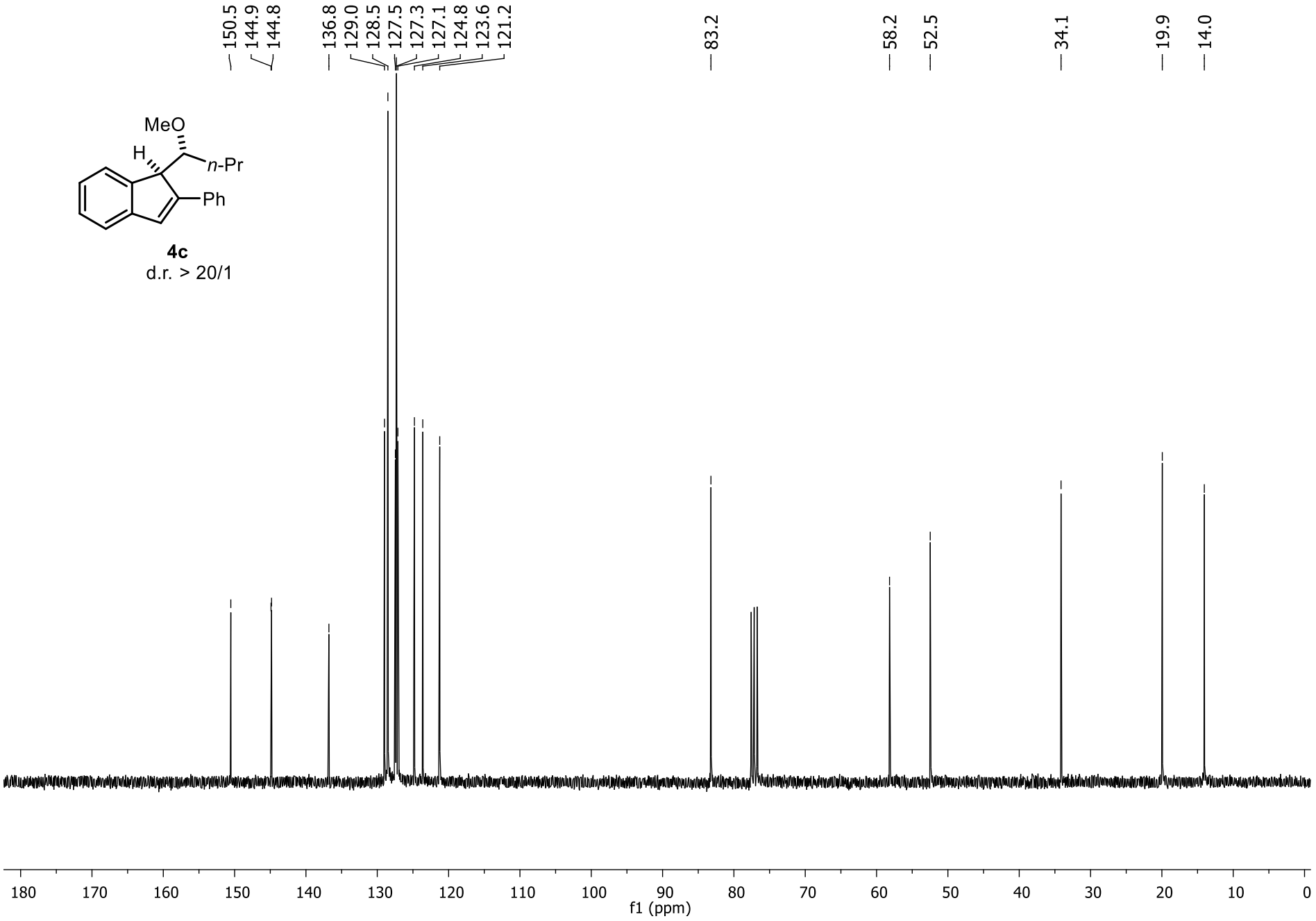
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



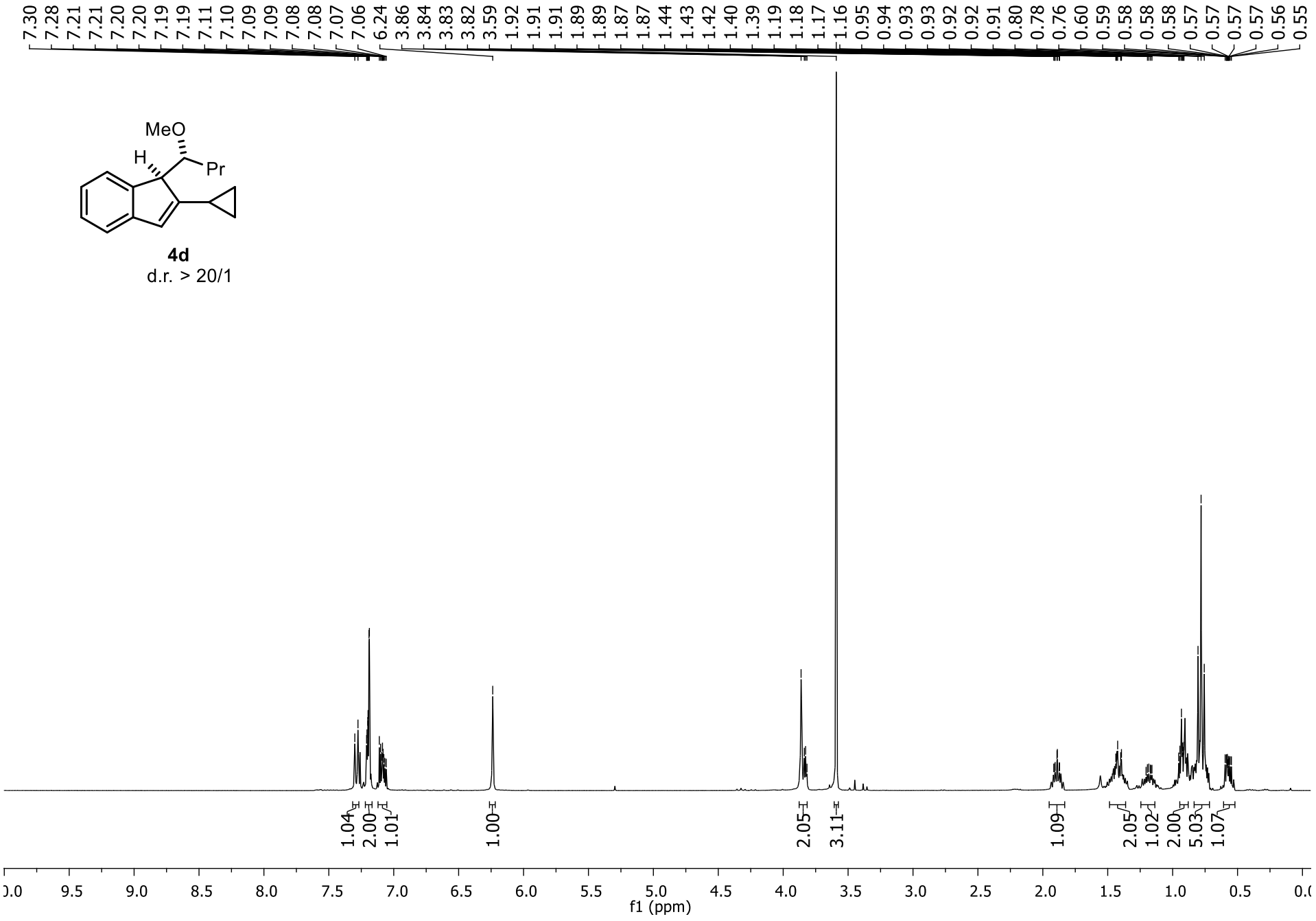
^{1}H NMR (300 MHz, $CDCl_3$)



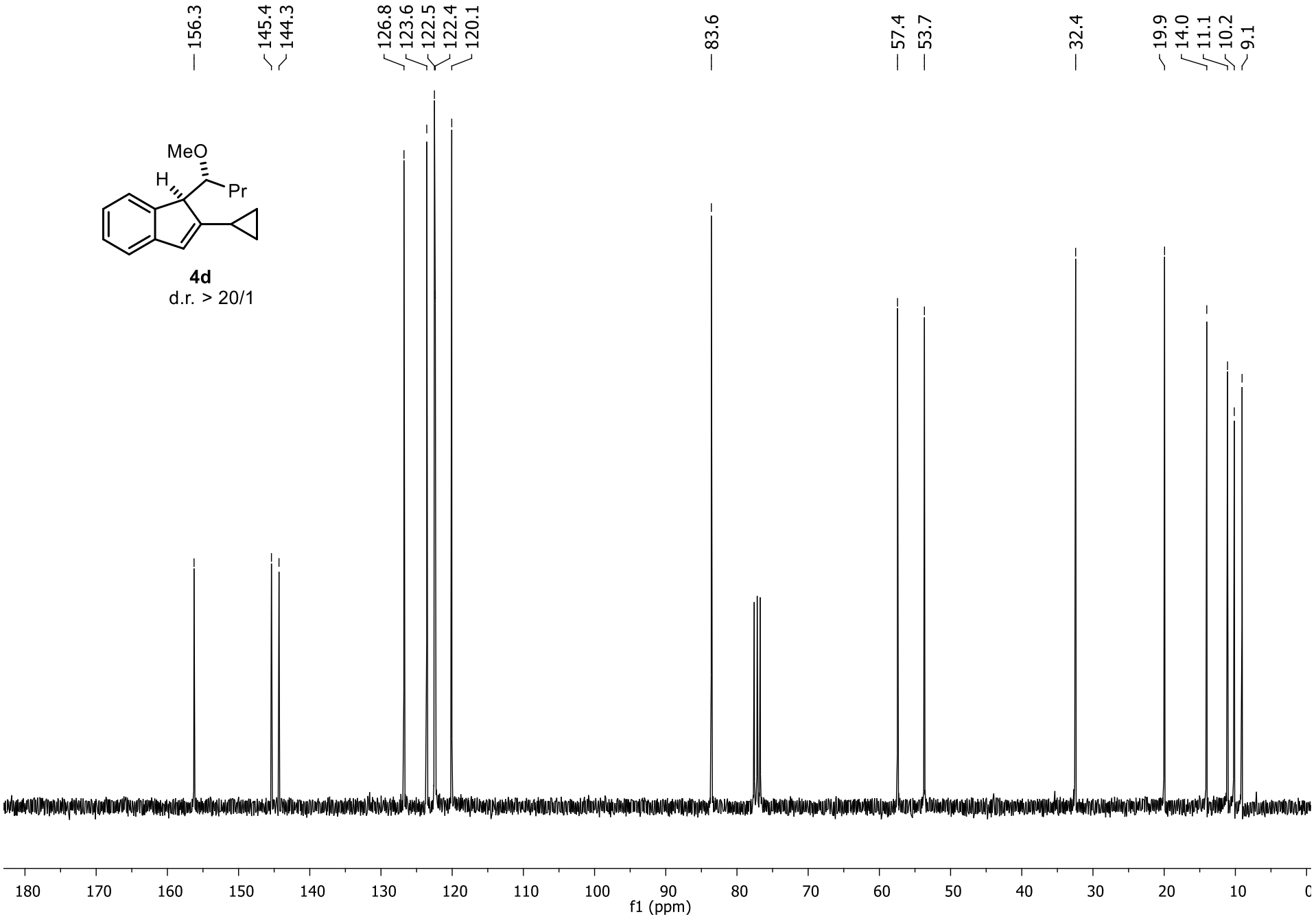
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



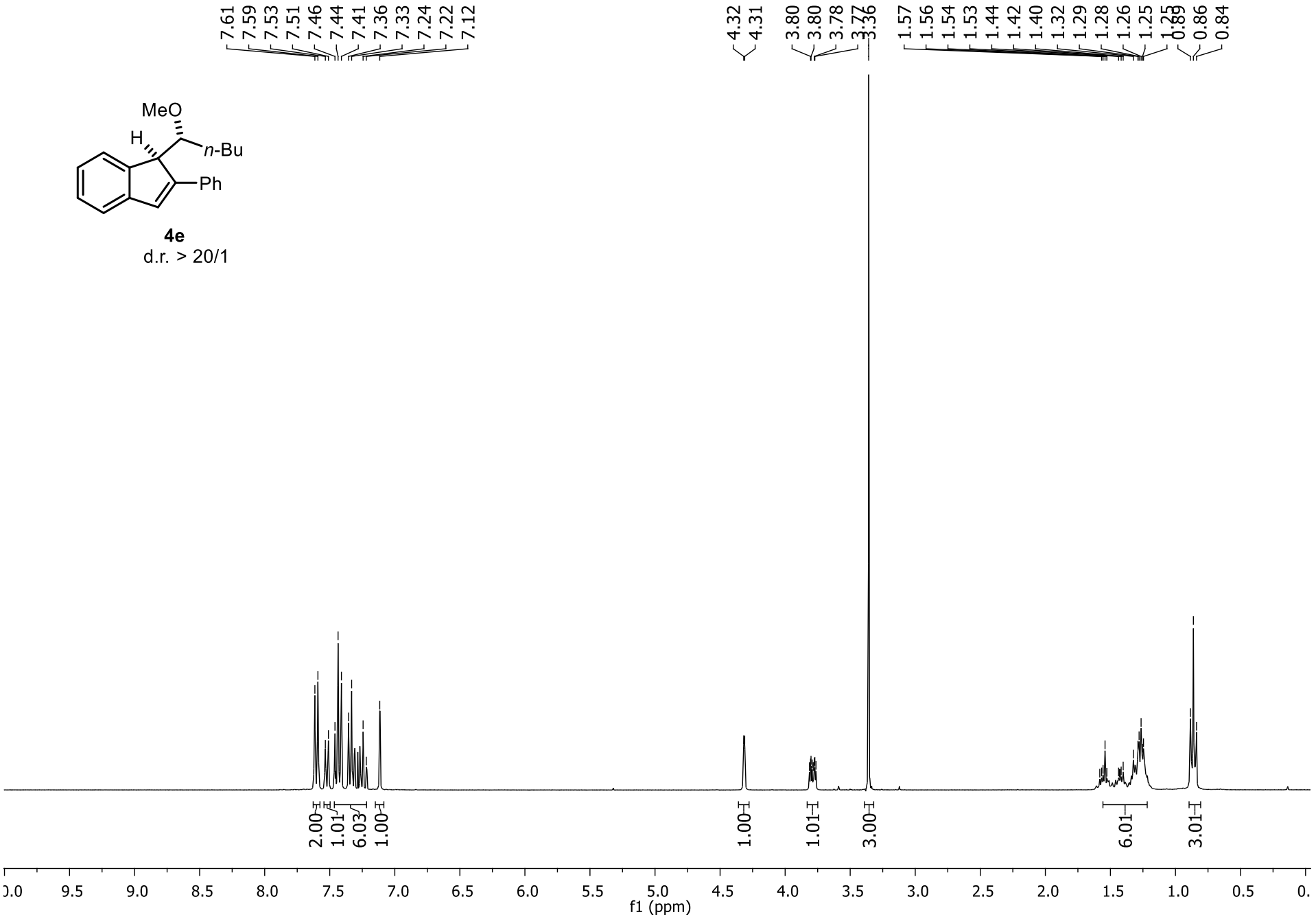
^{1}H NMR (300 MHz, $CDCl_3$)



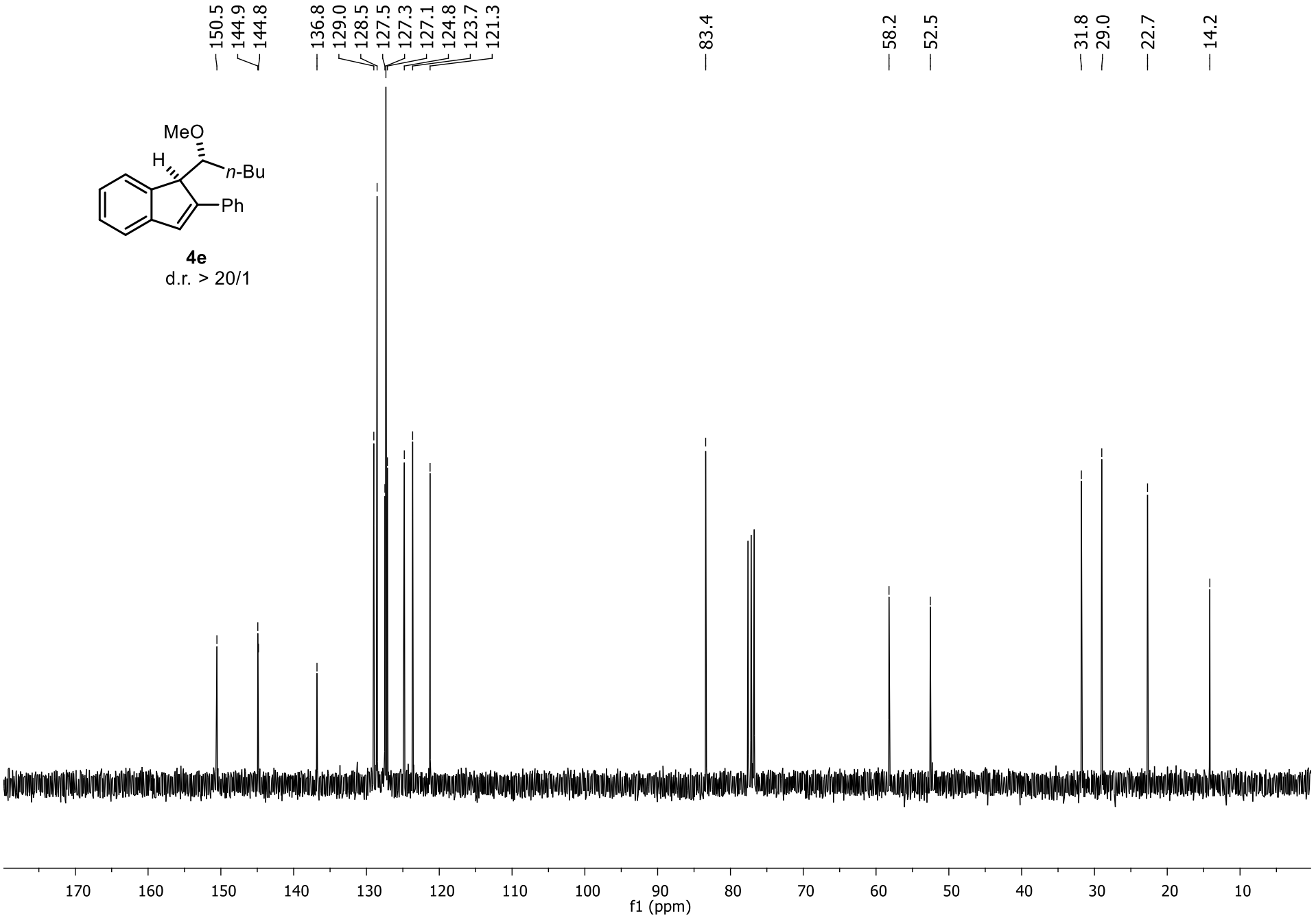
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



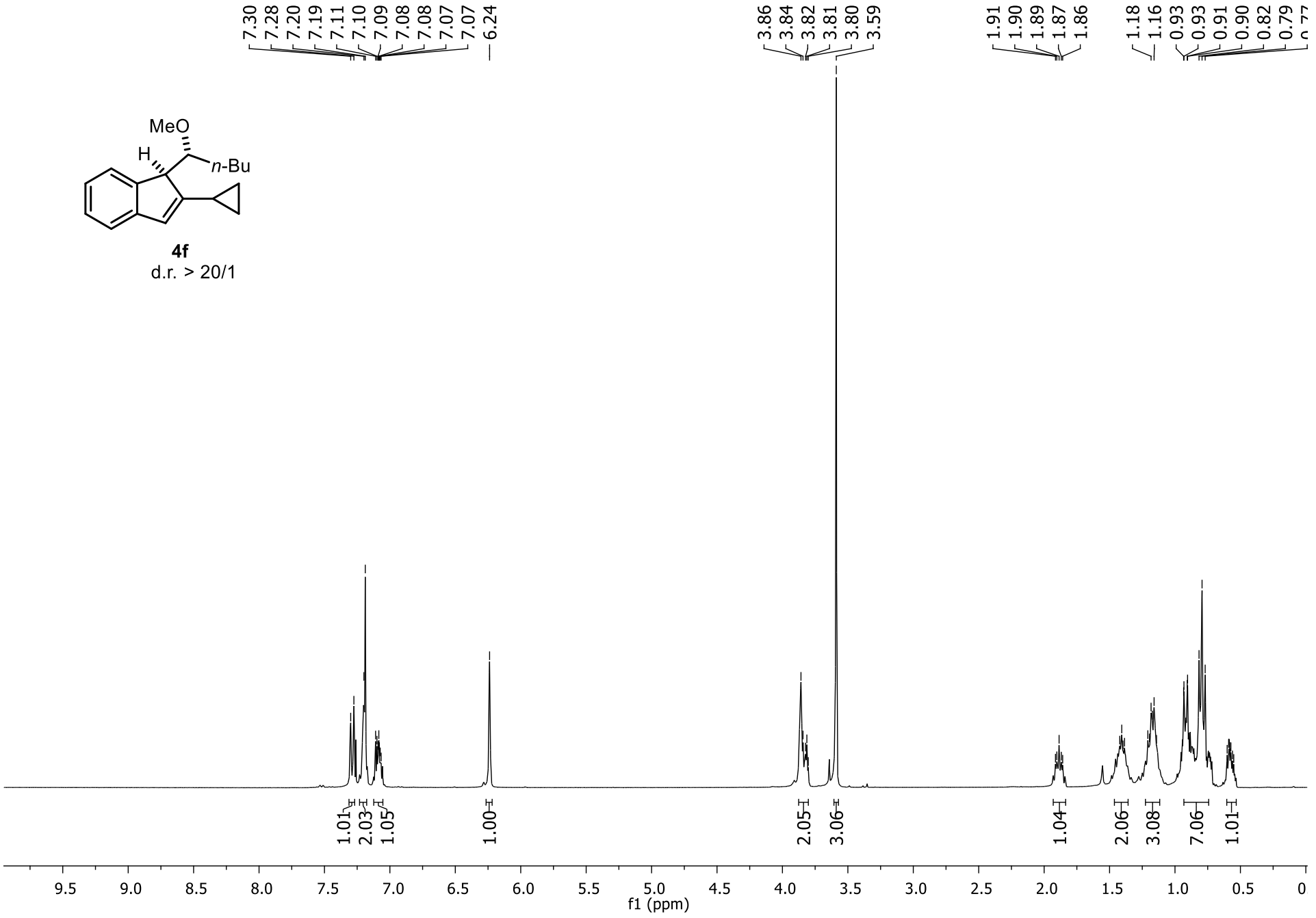
^{1}H NMR (300 MHz, $CDCl_3$)



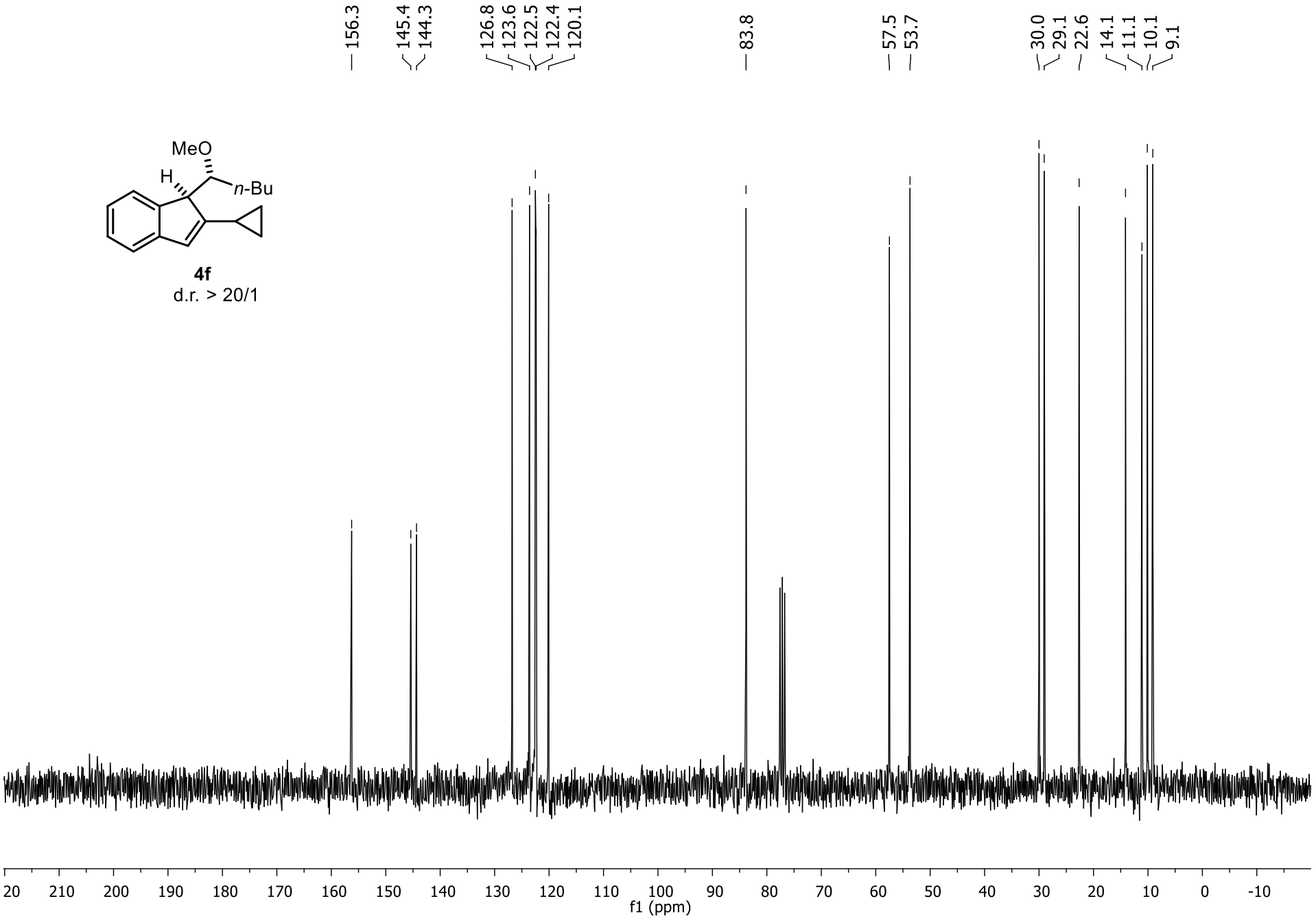
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



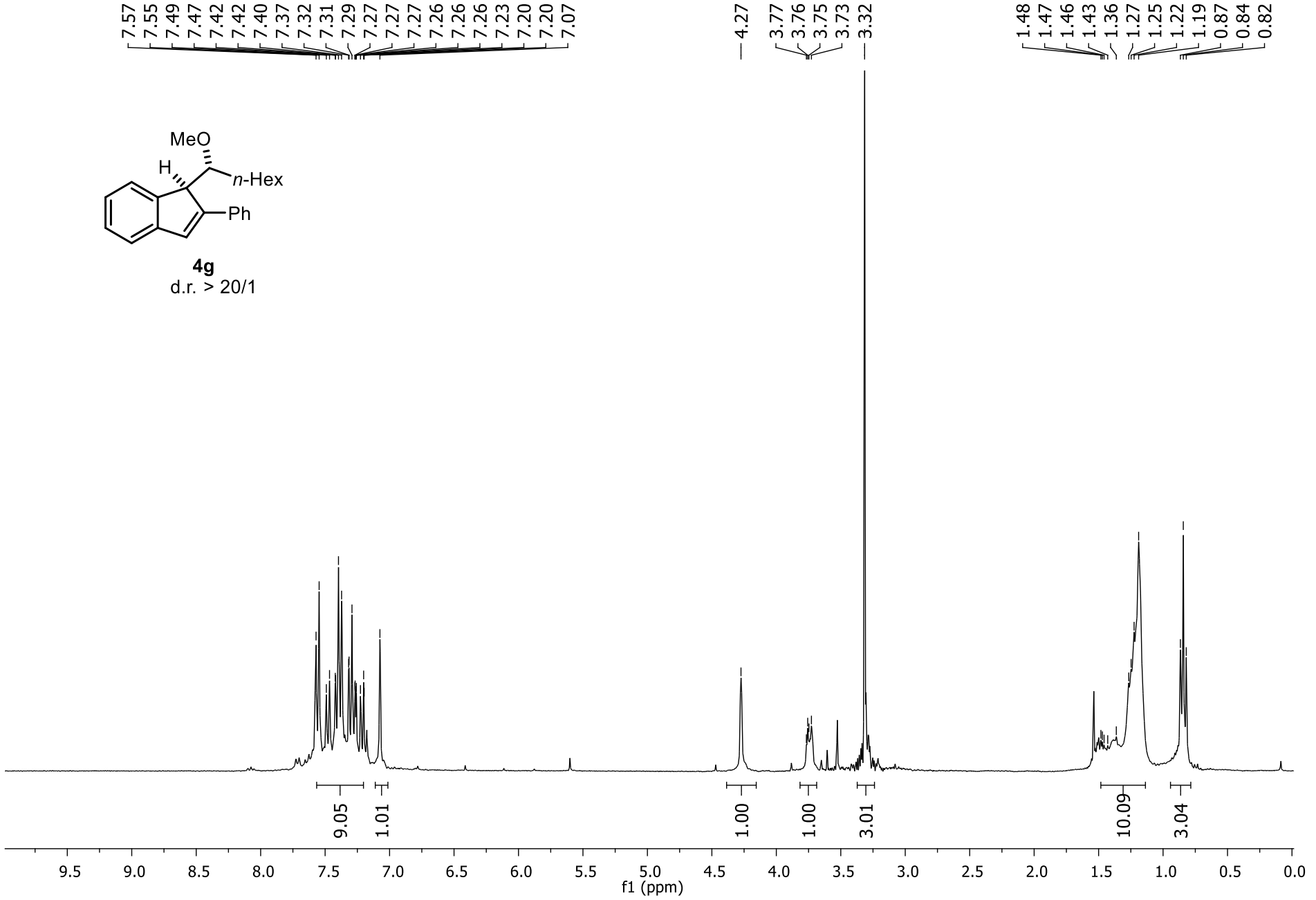
^{1}H NMR (300 MHz, $CDCl_3$)



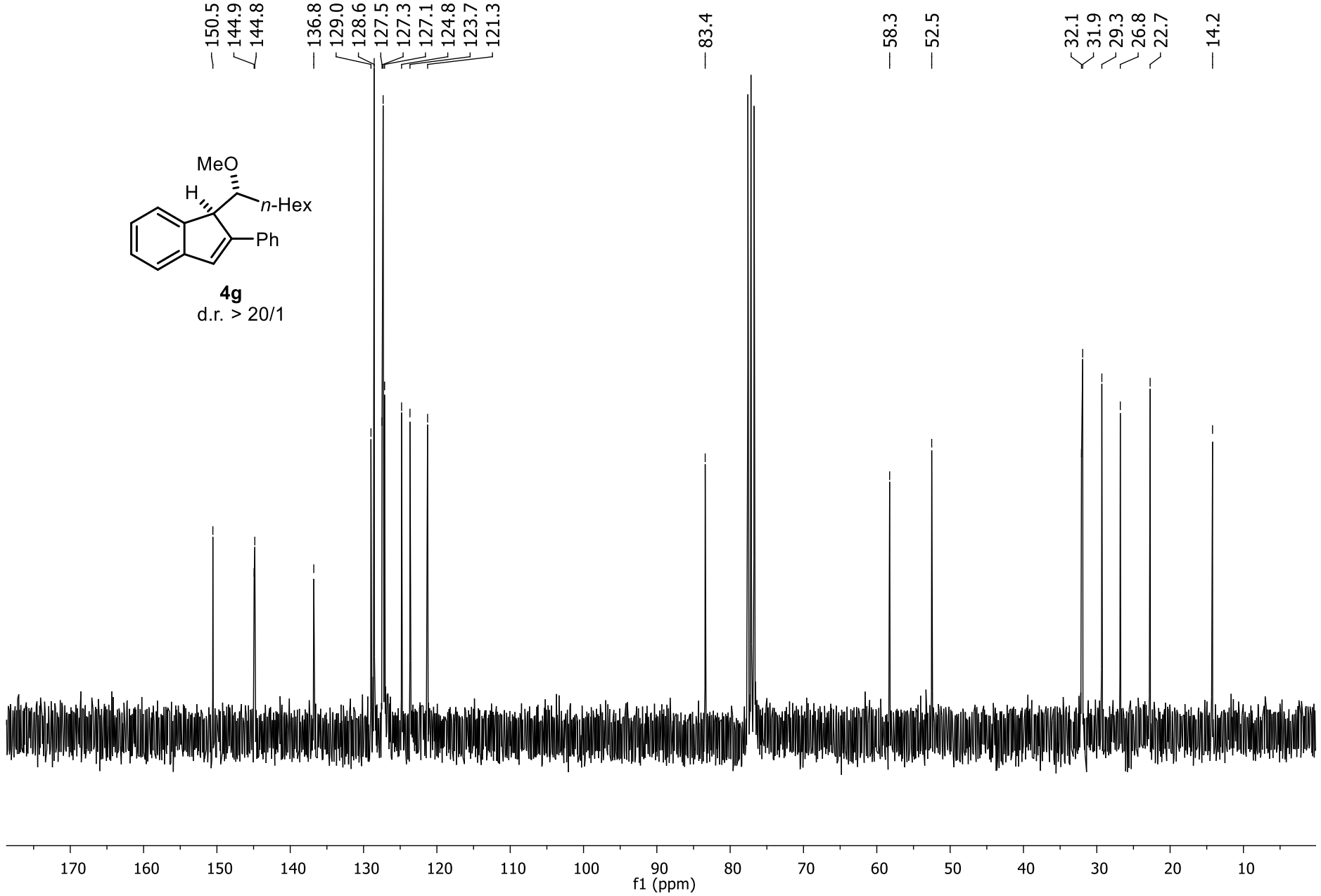
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



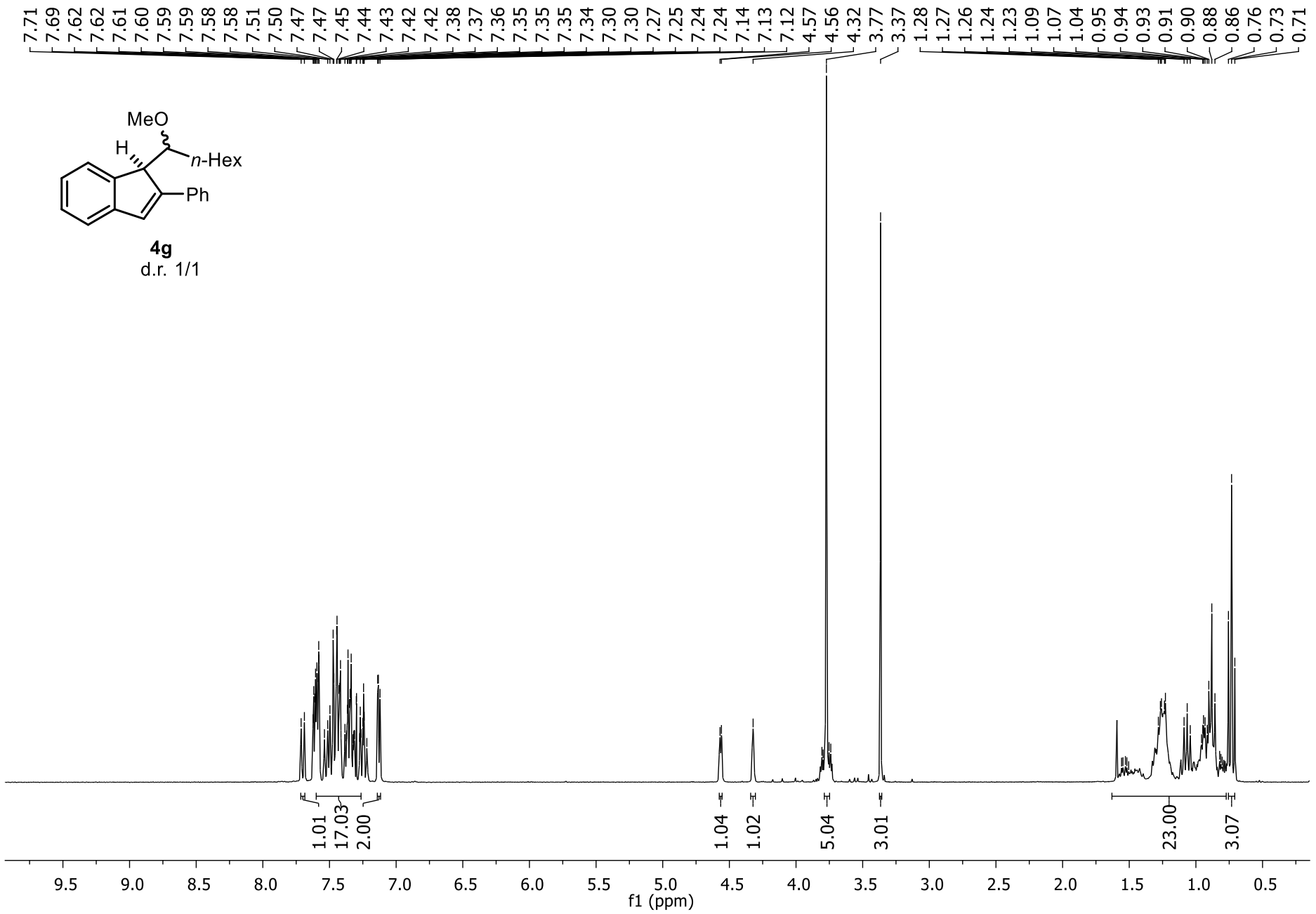
^{1}H NMR (300 MHz, $CDCl_3$)



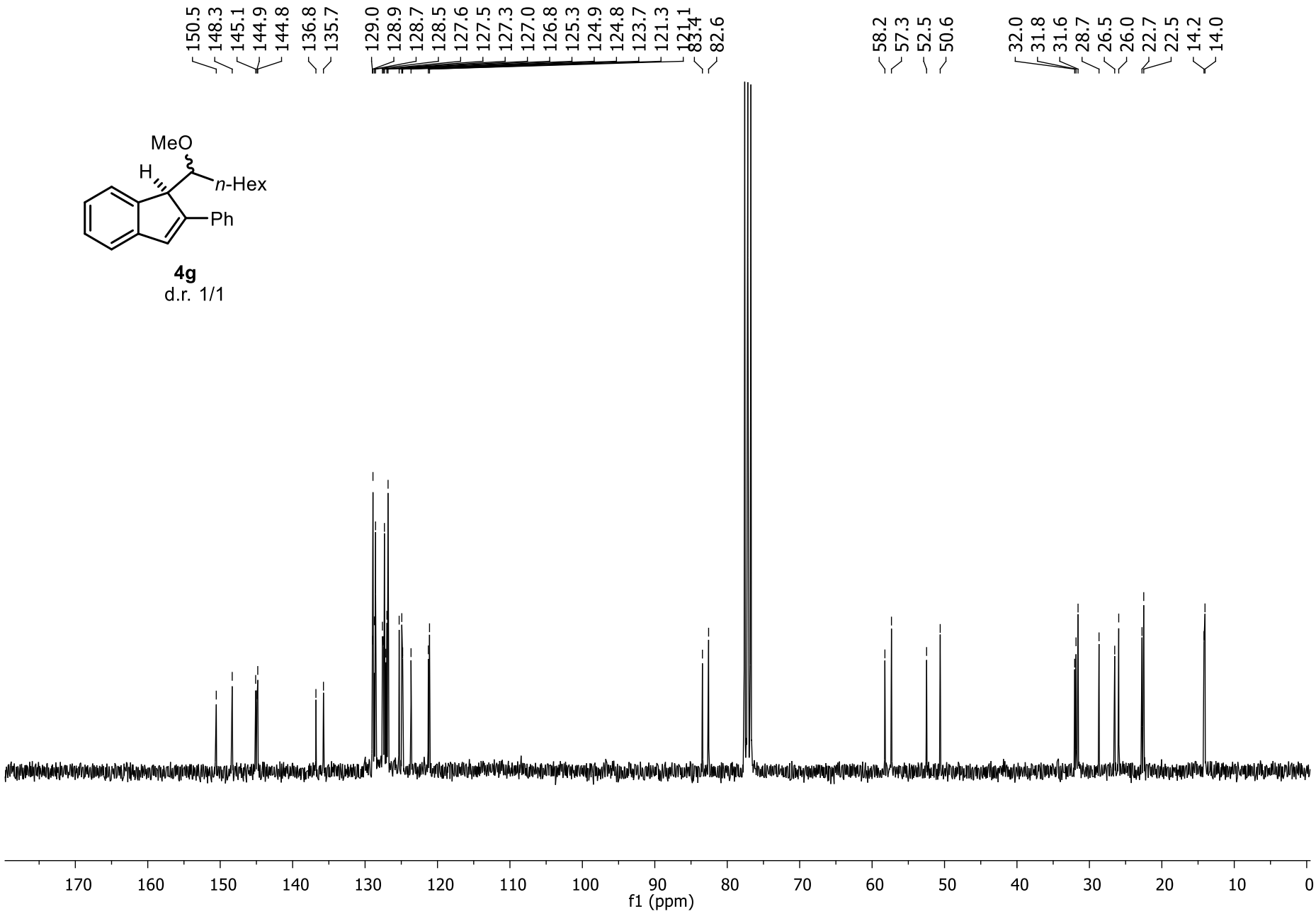
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



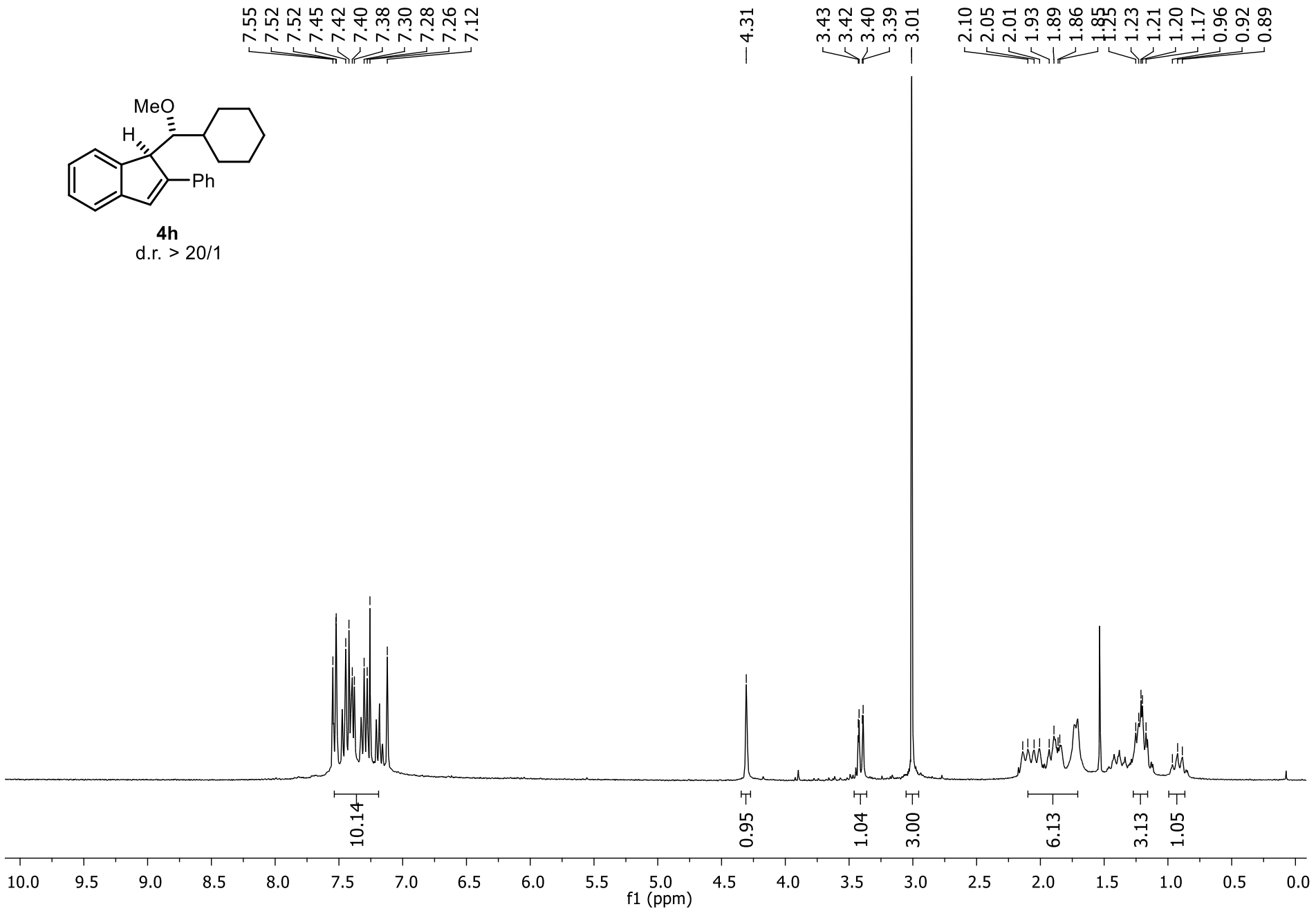
^{1}H NMR (300 MHz, $CDCl_3$)



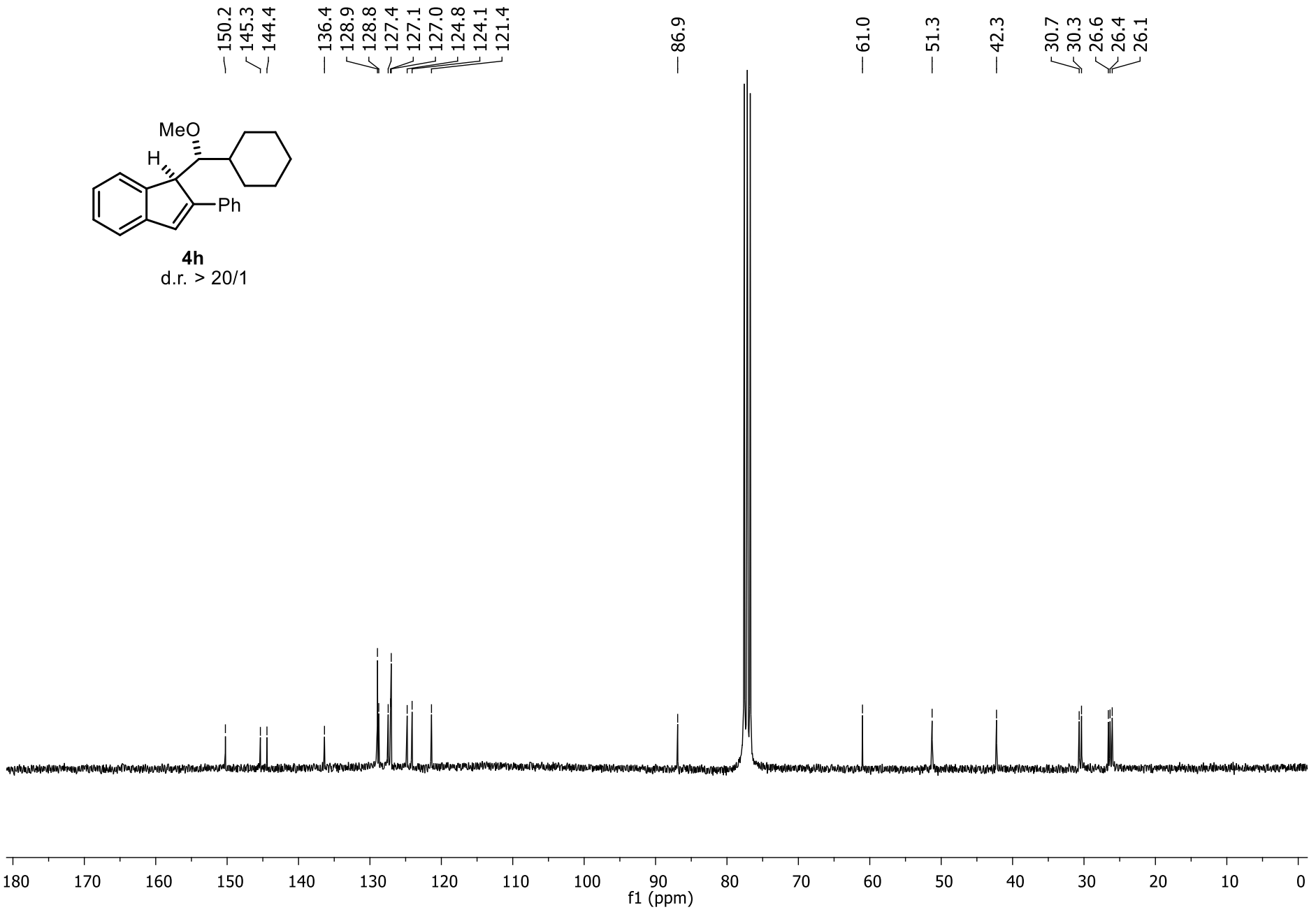
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



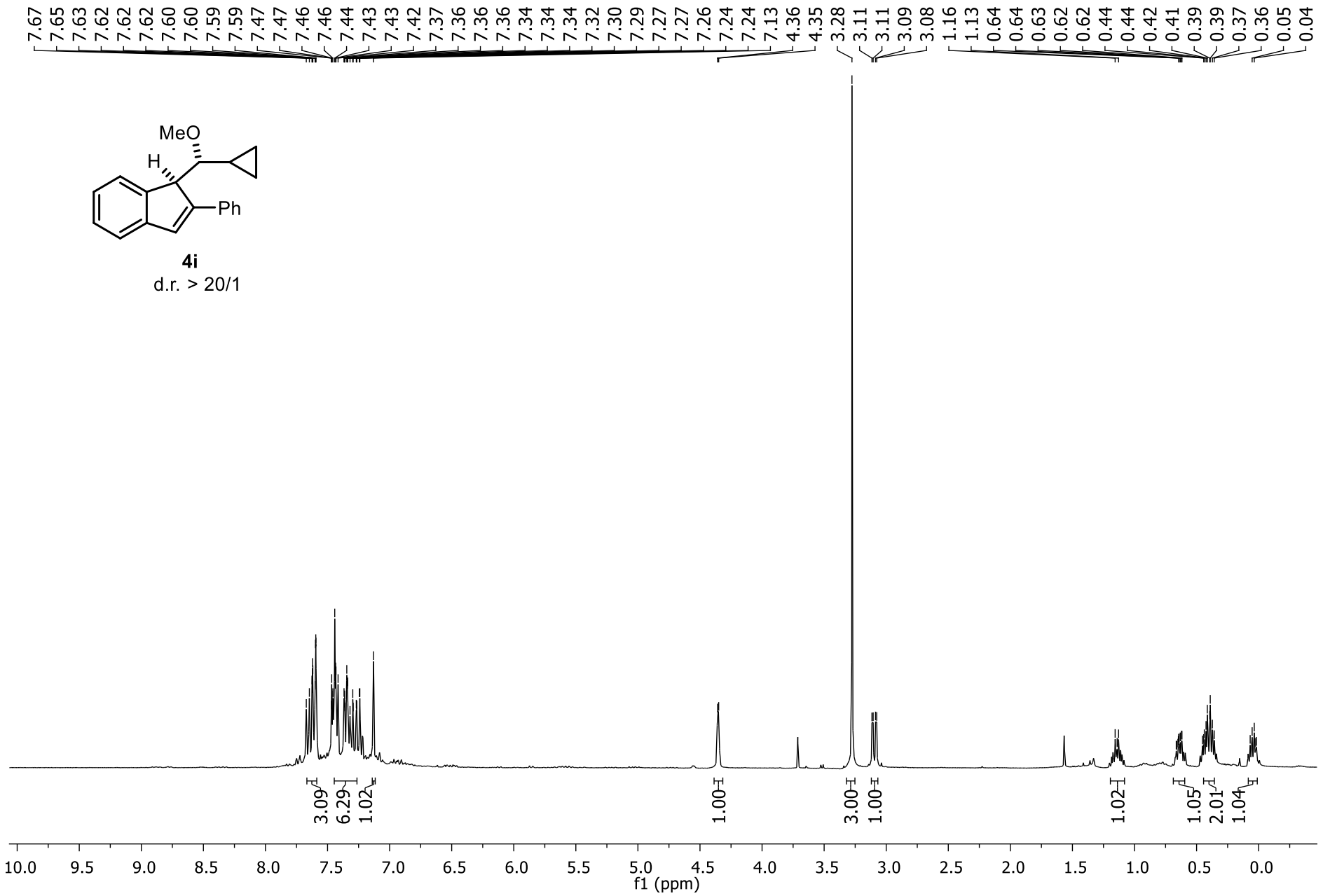
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

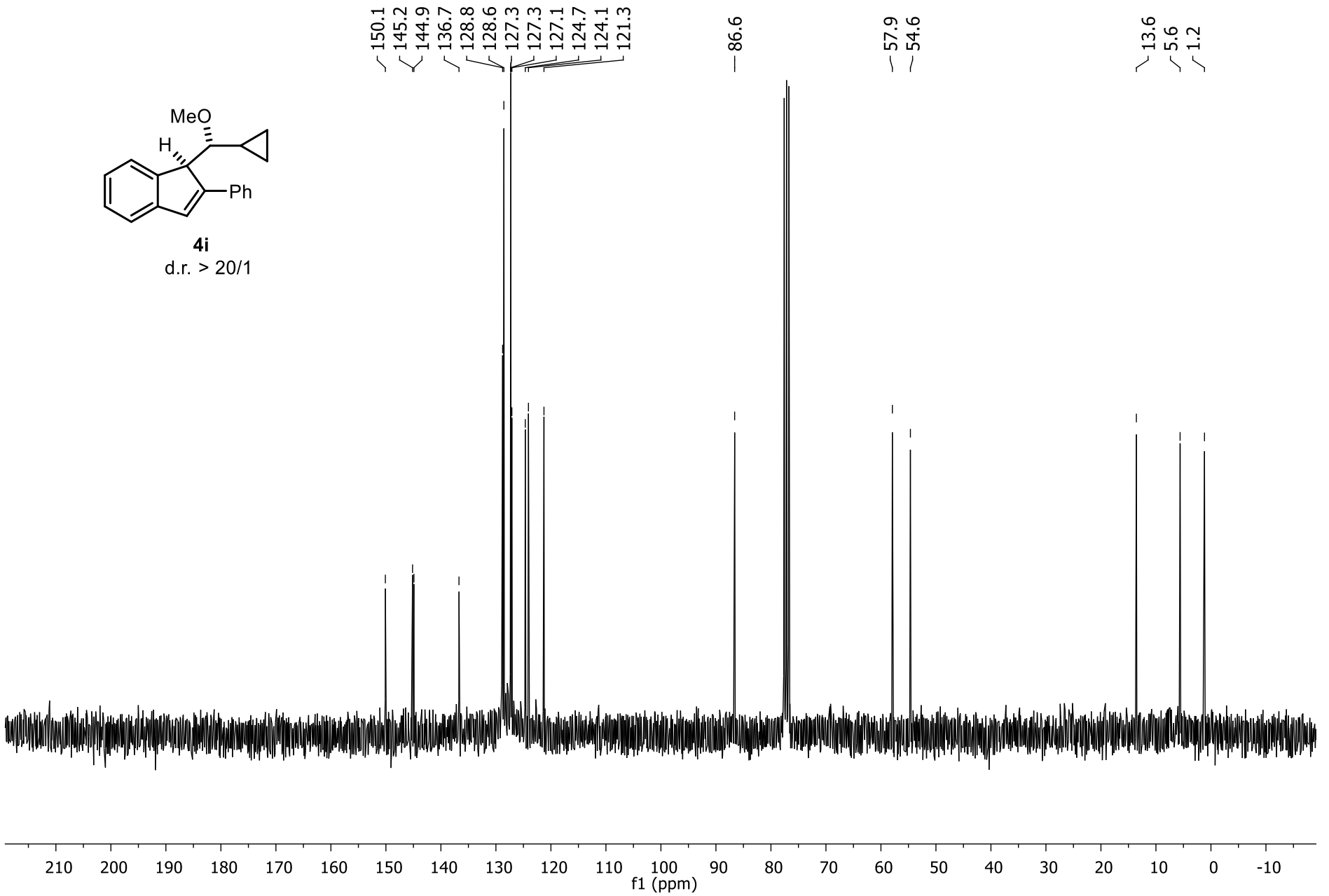


^{1}H NMR (300 MHz, $CDCl_3$)

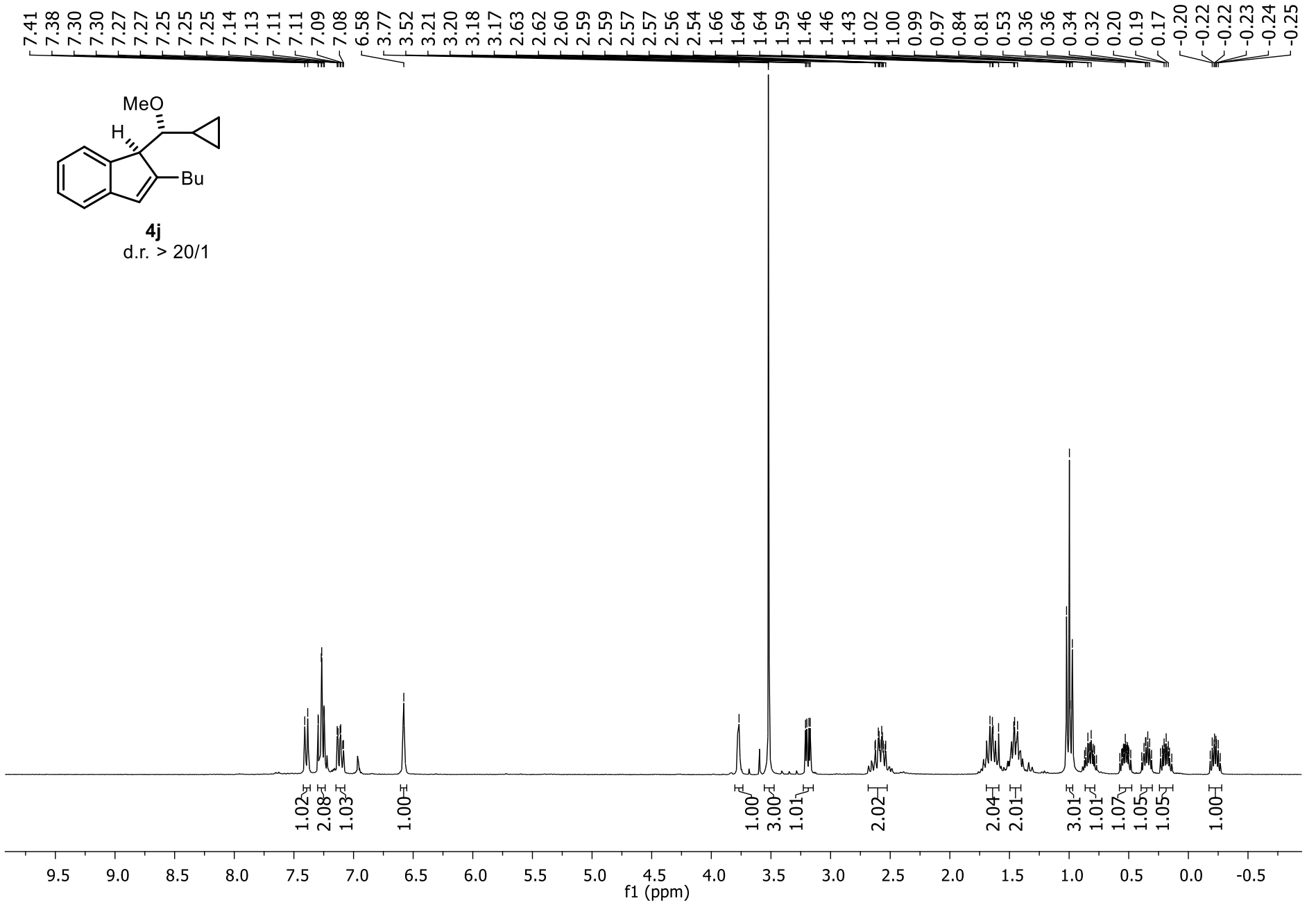


4i
d.r. > 20/1

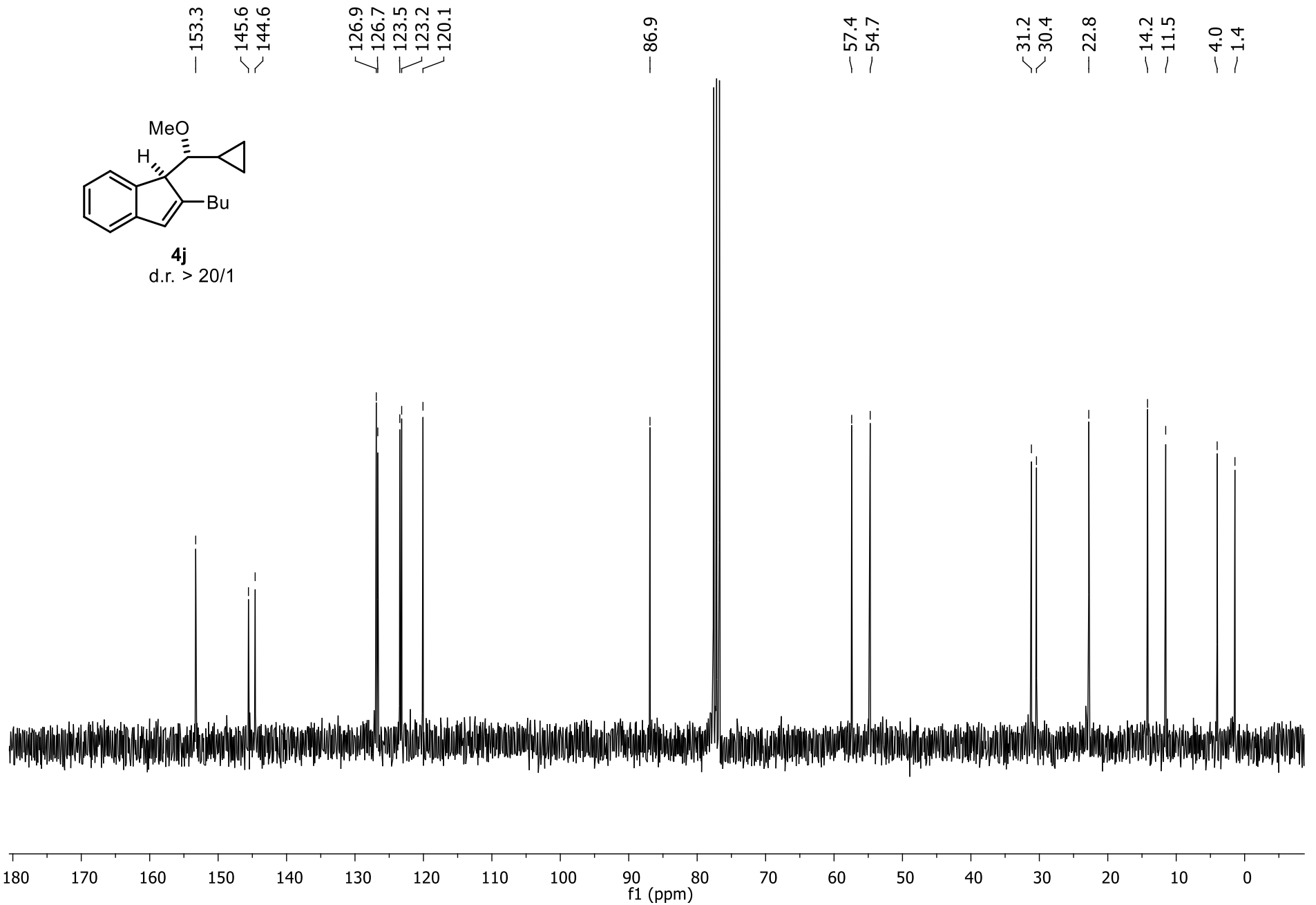
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



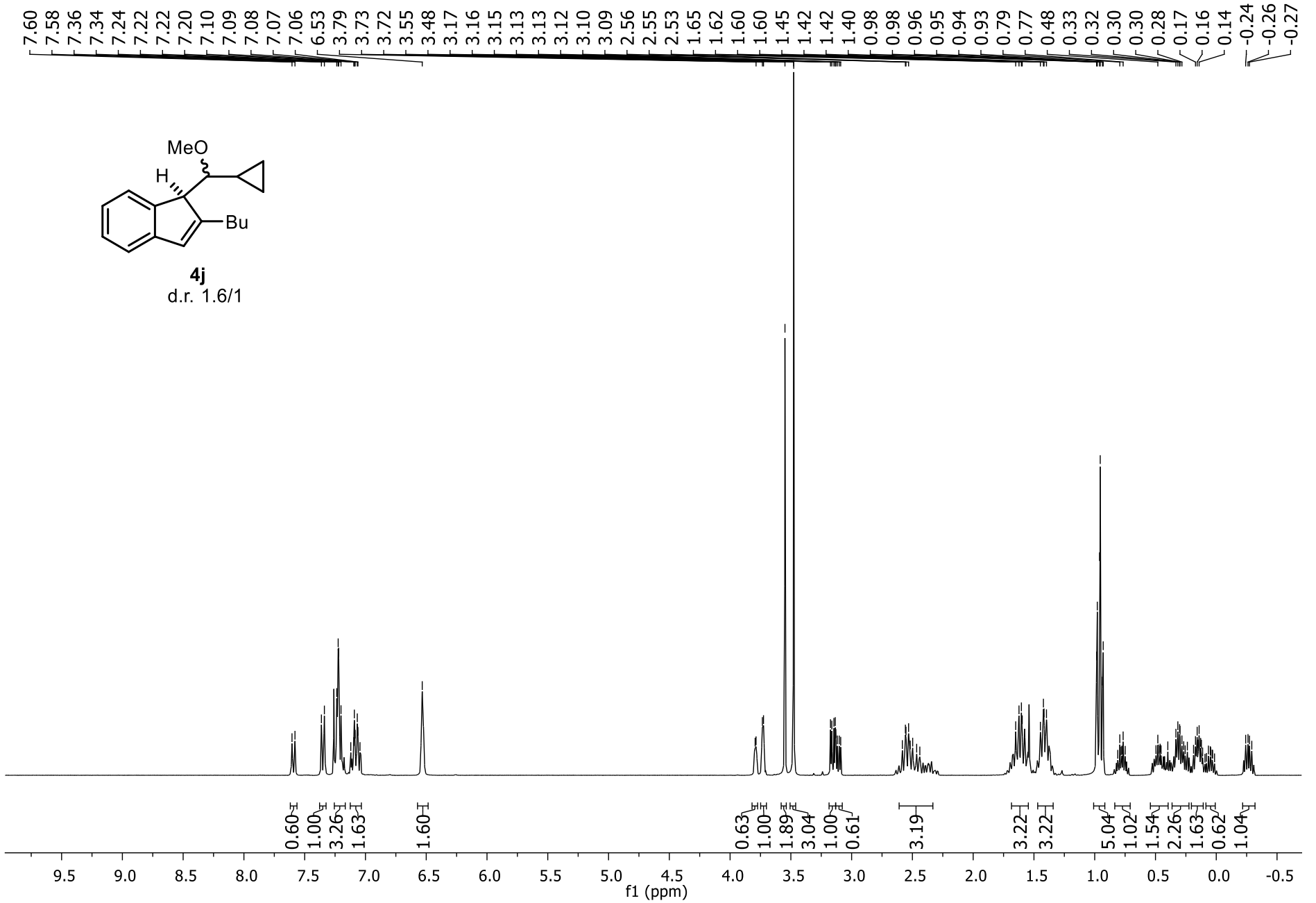
^{1}H NMR (300 MHz, $CDCl_3$)



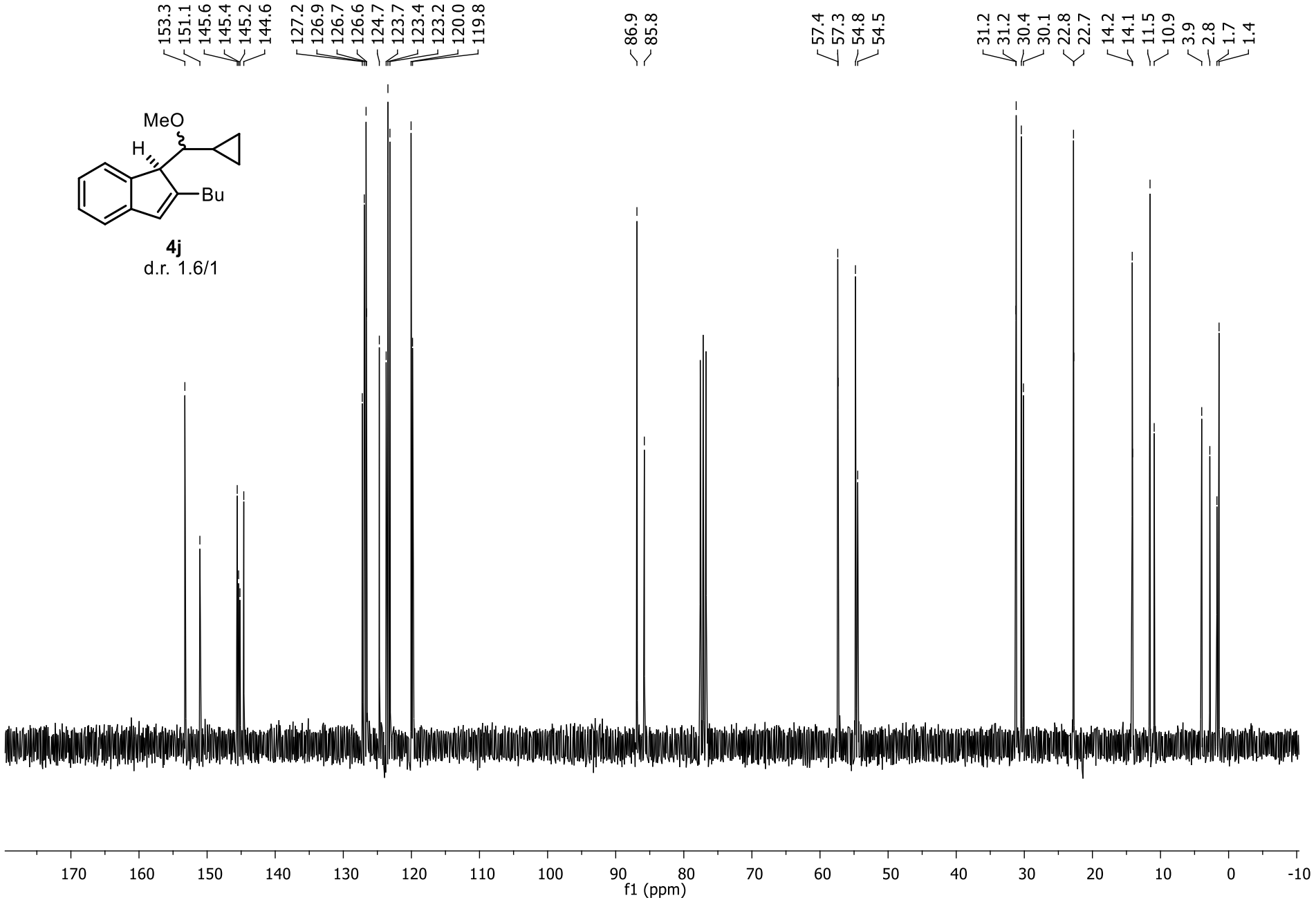
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



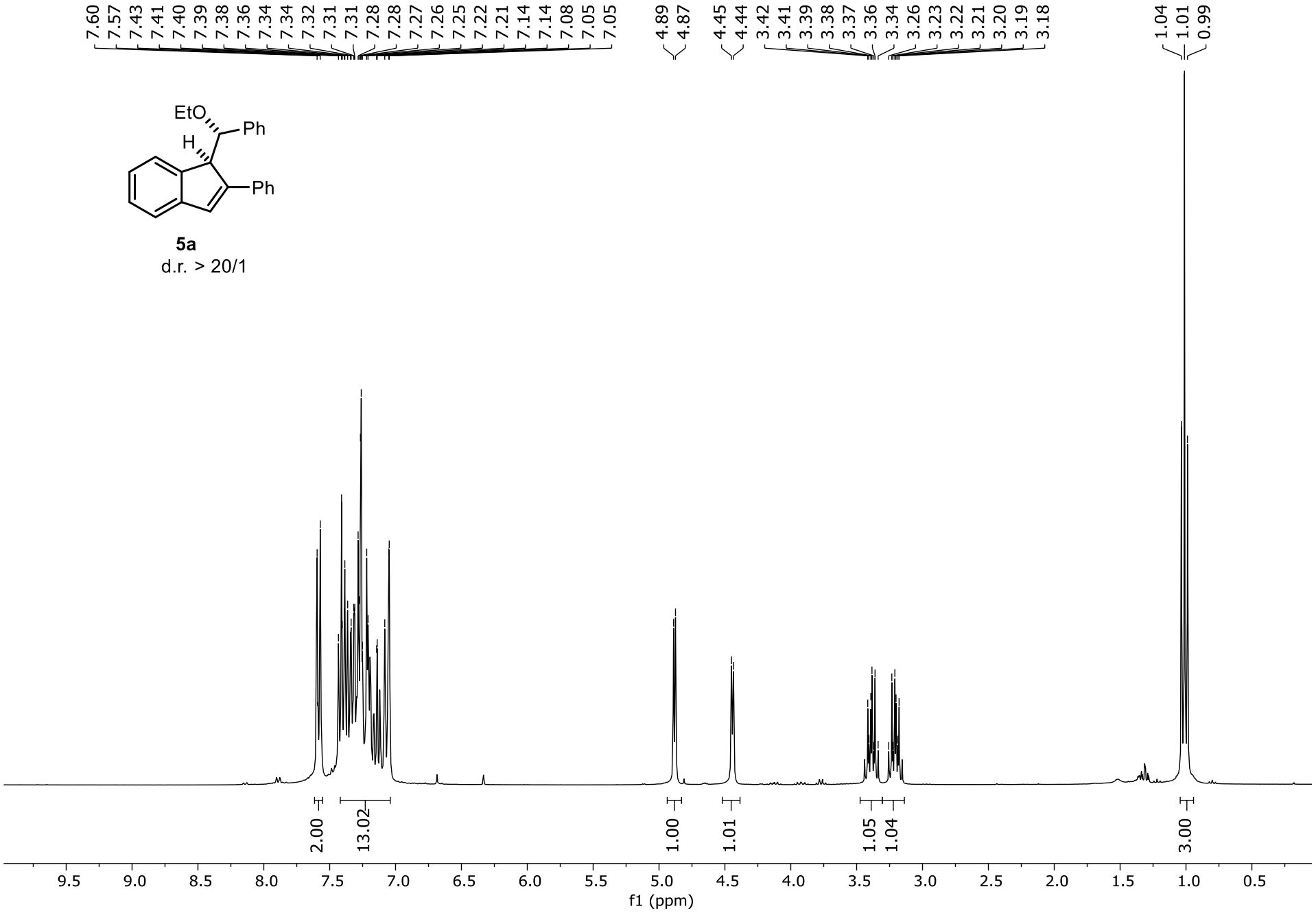
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

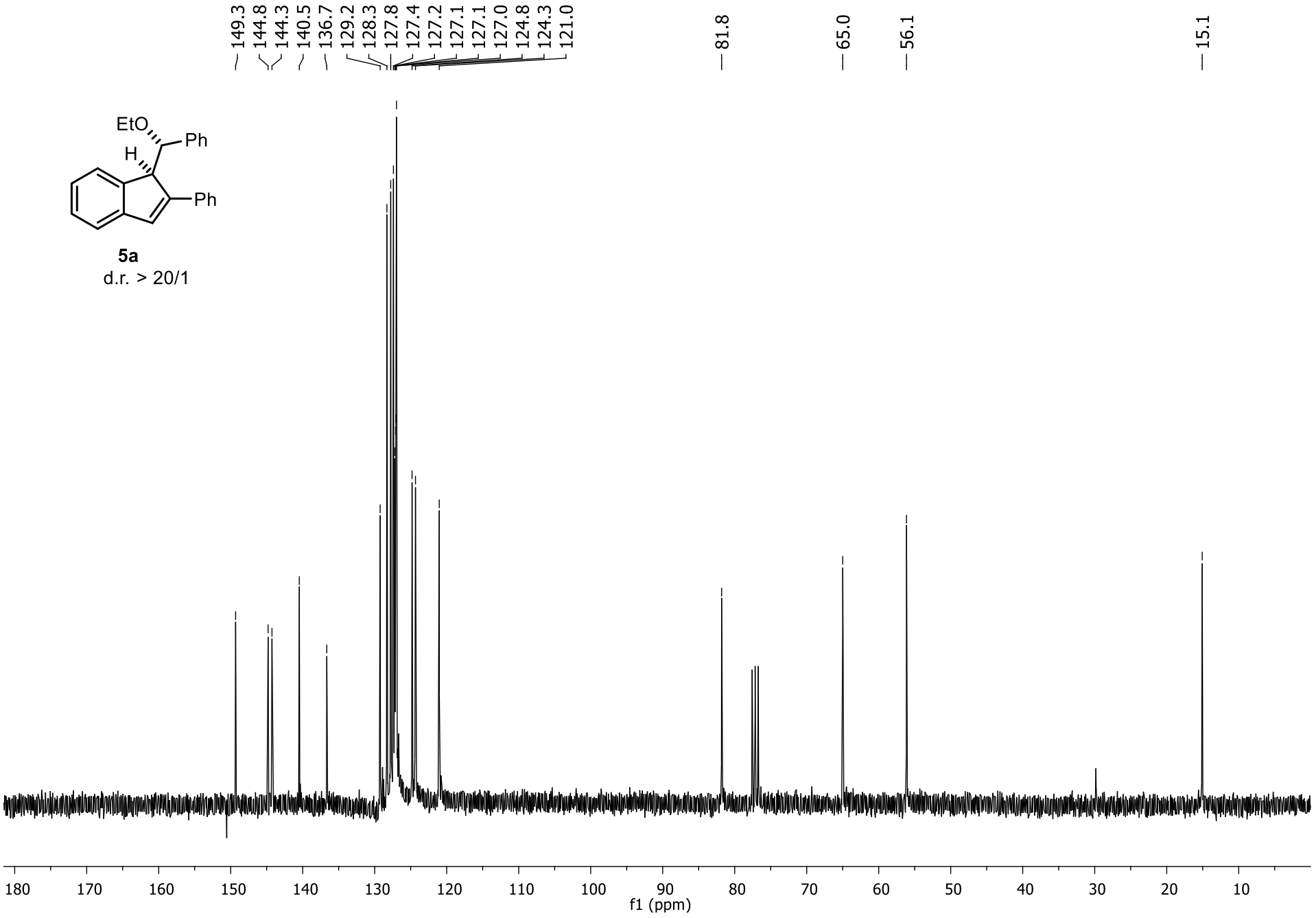


^{1}H NMR (300 MHz, $CDCl_3$)

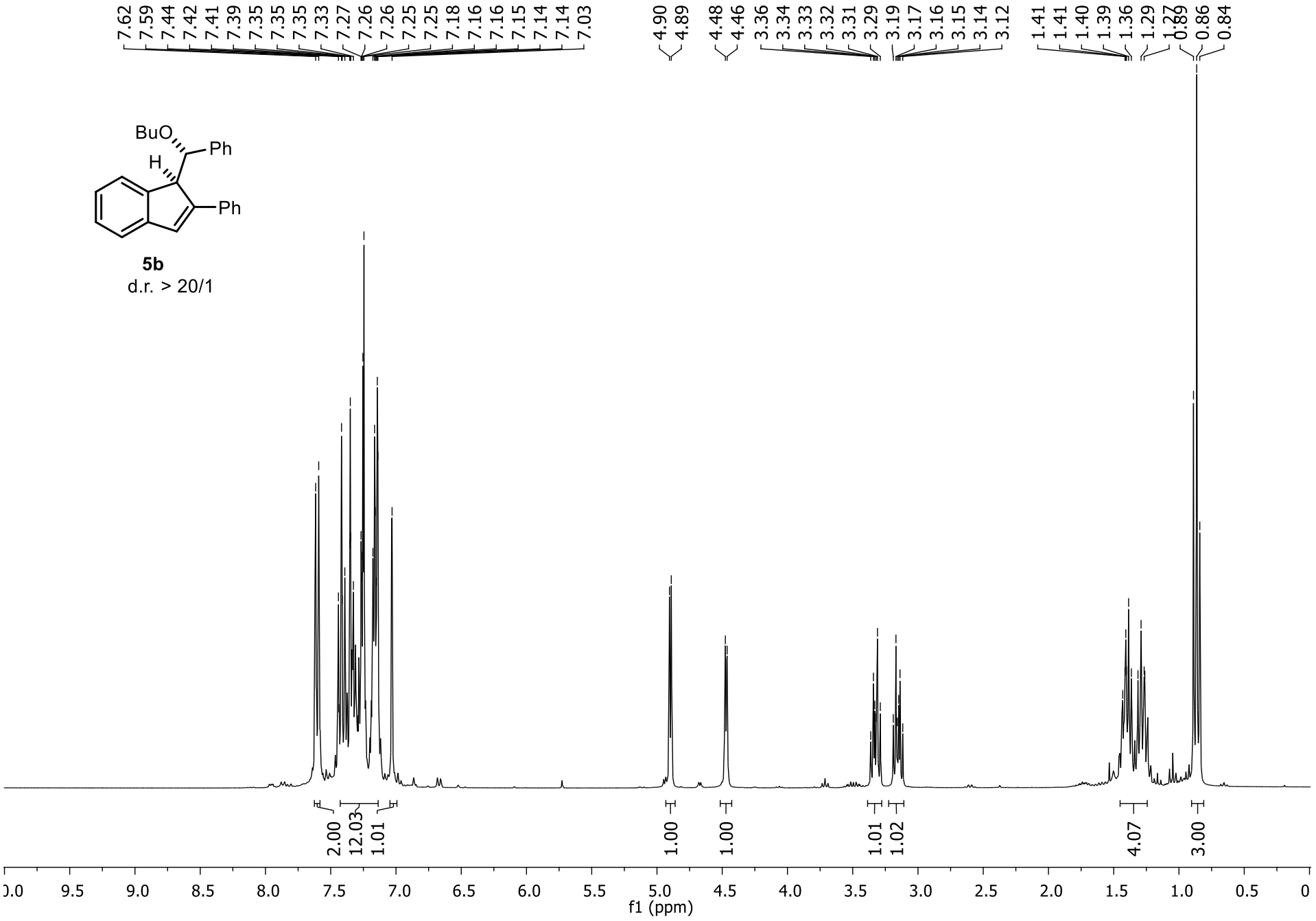


5a
d.r. > 20/1

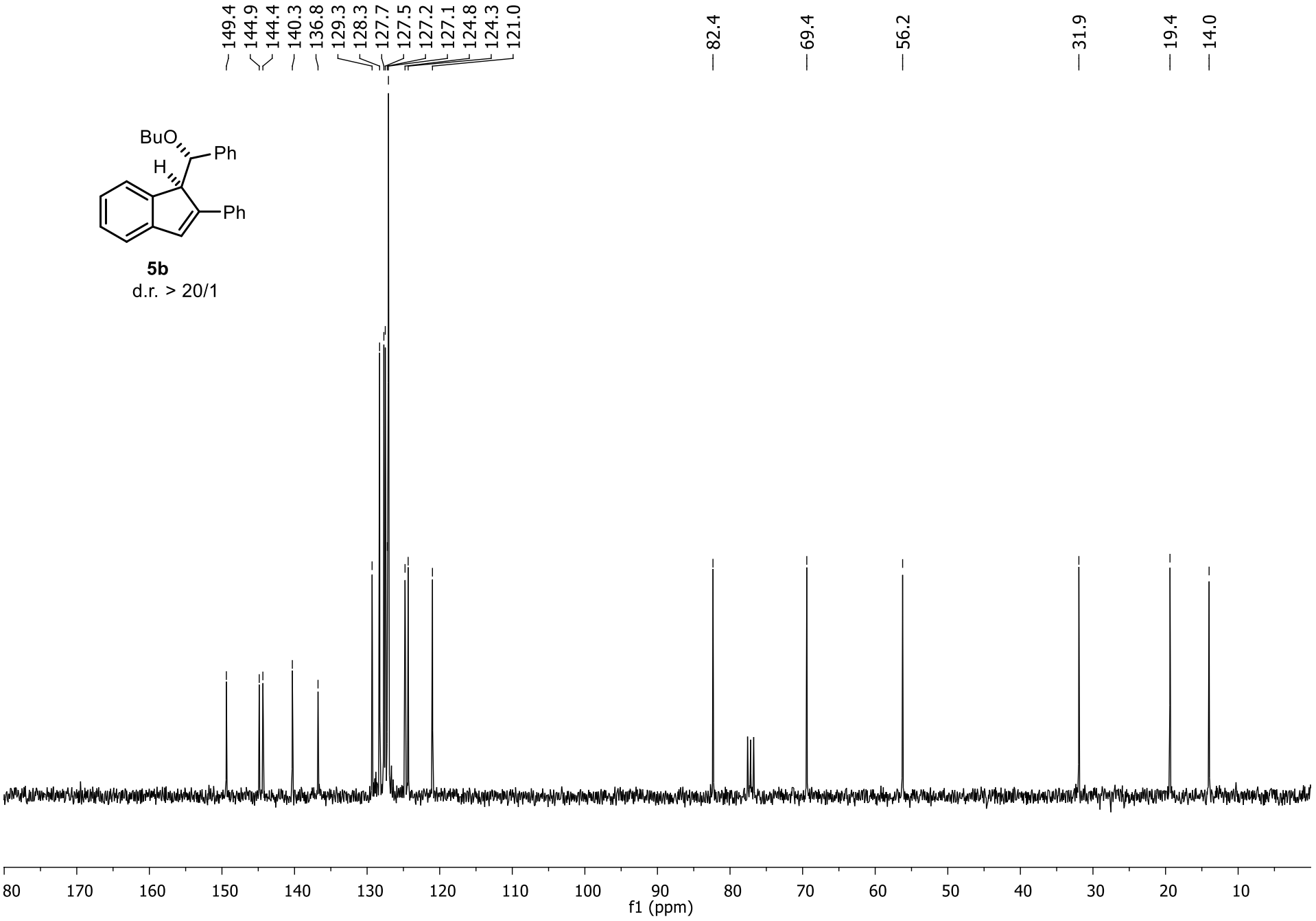
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



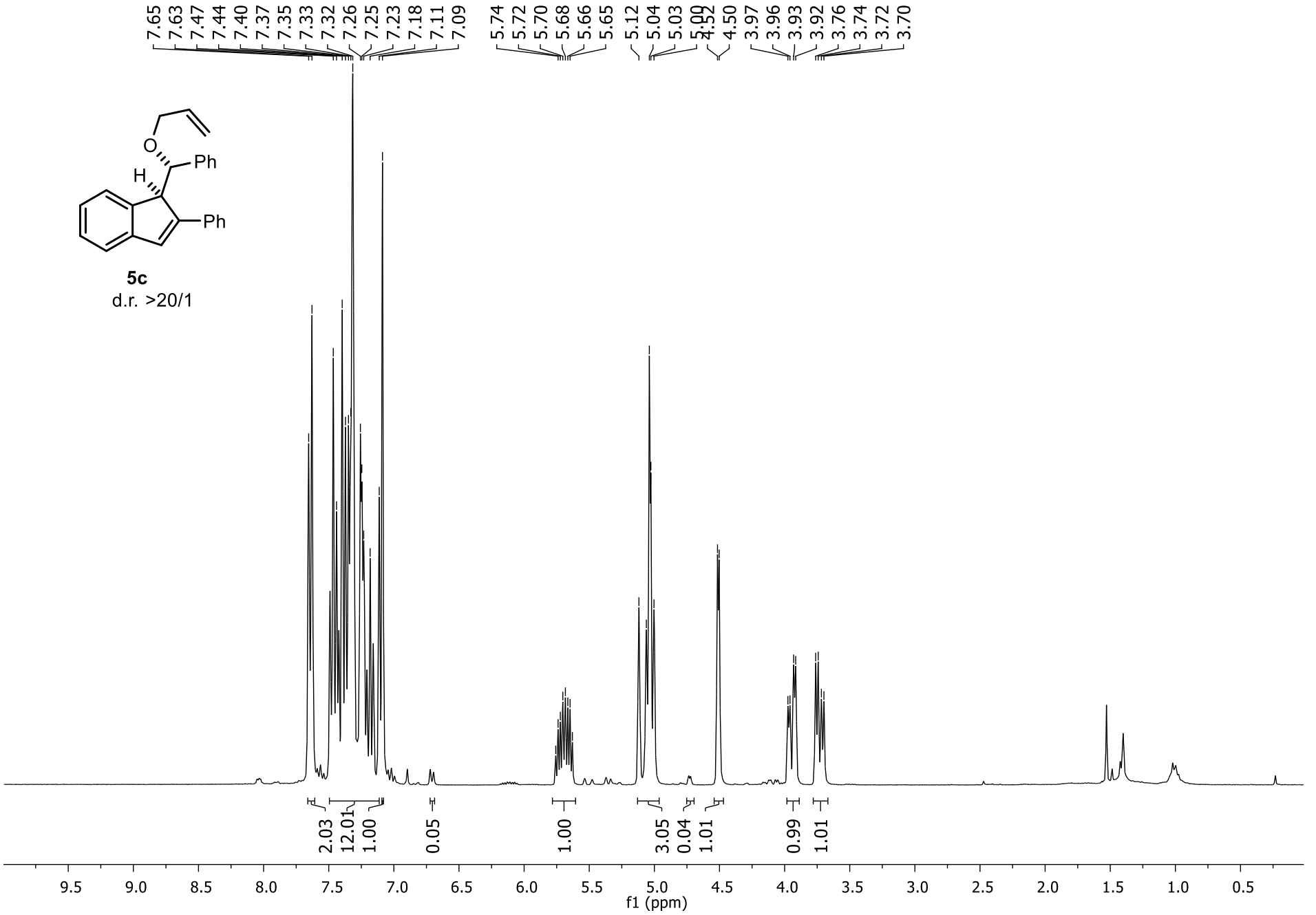
^{1}H NMR (300 MHz, $CDCl_3$)



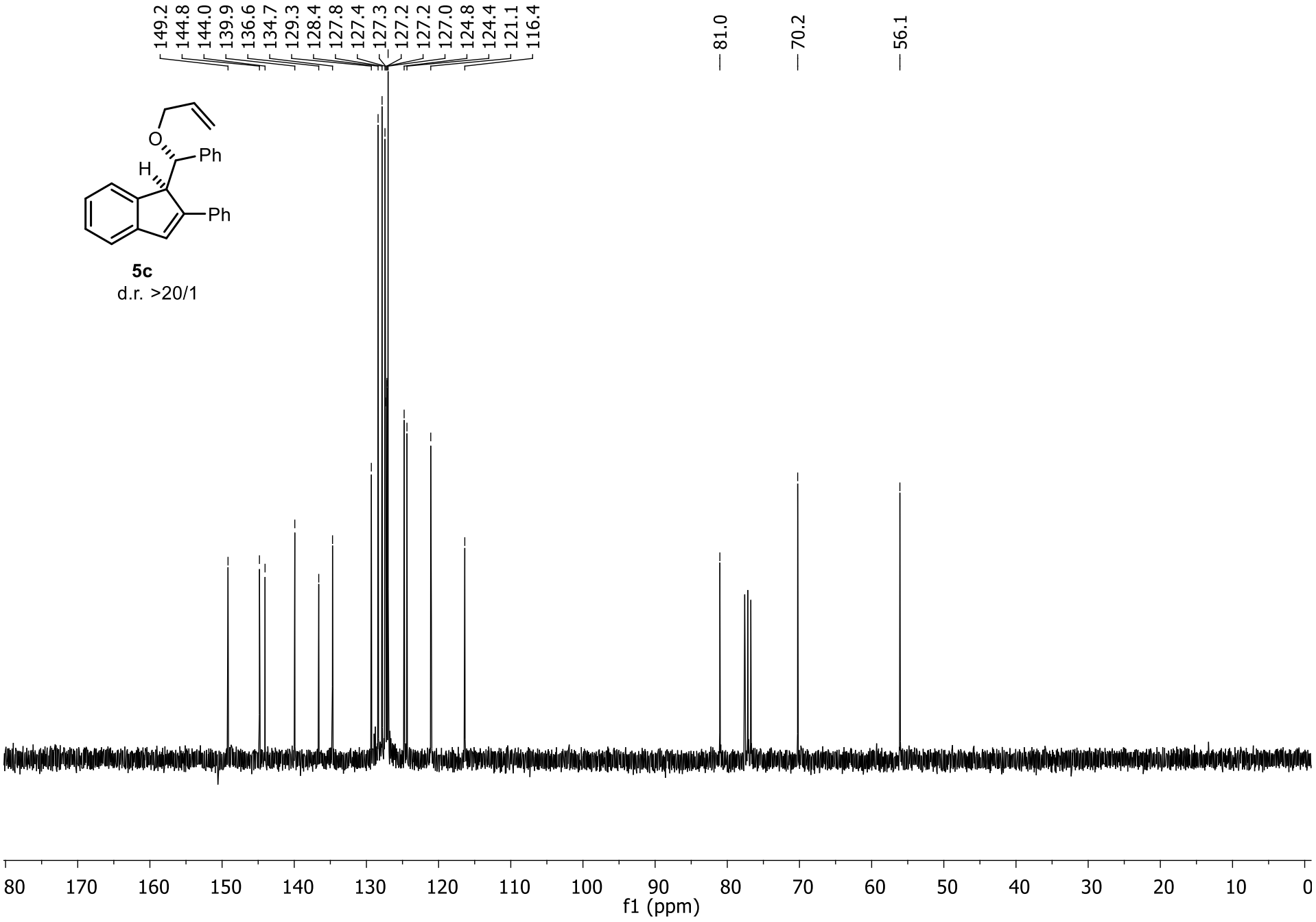
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



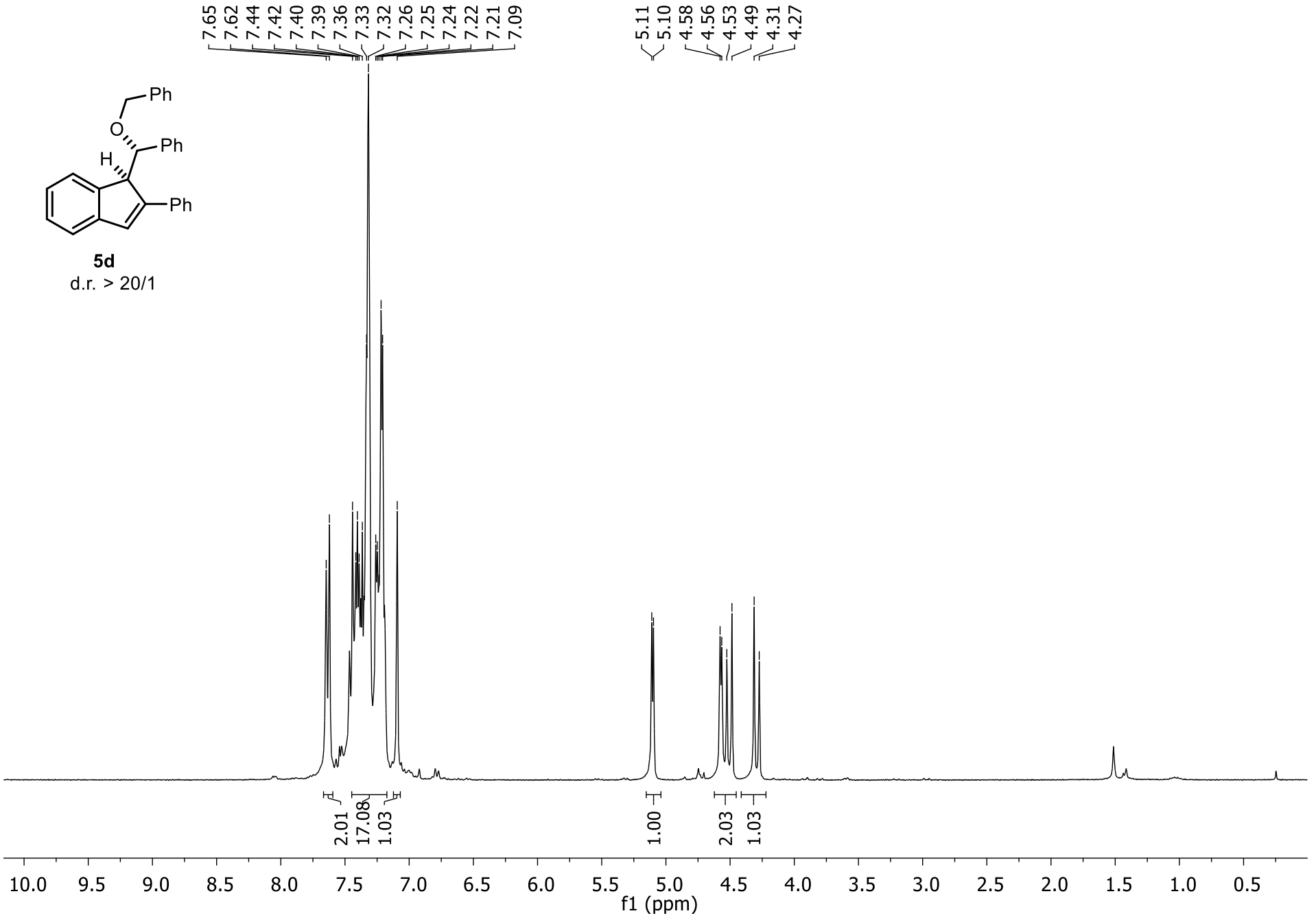
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

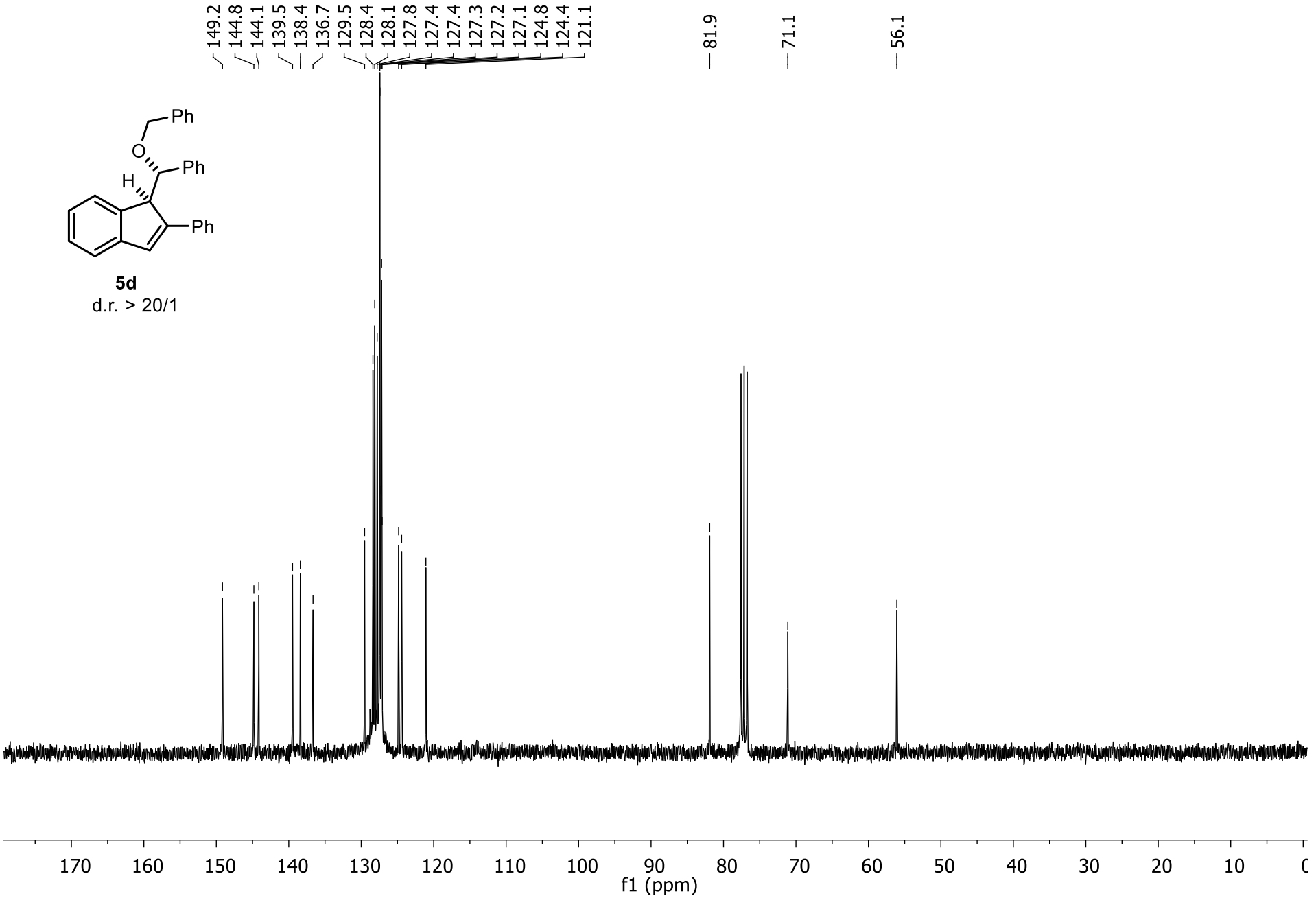


^{1}H NMR (300 MHz, $CDCl_3$)

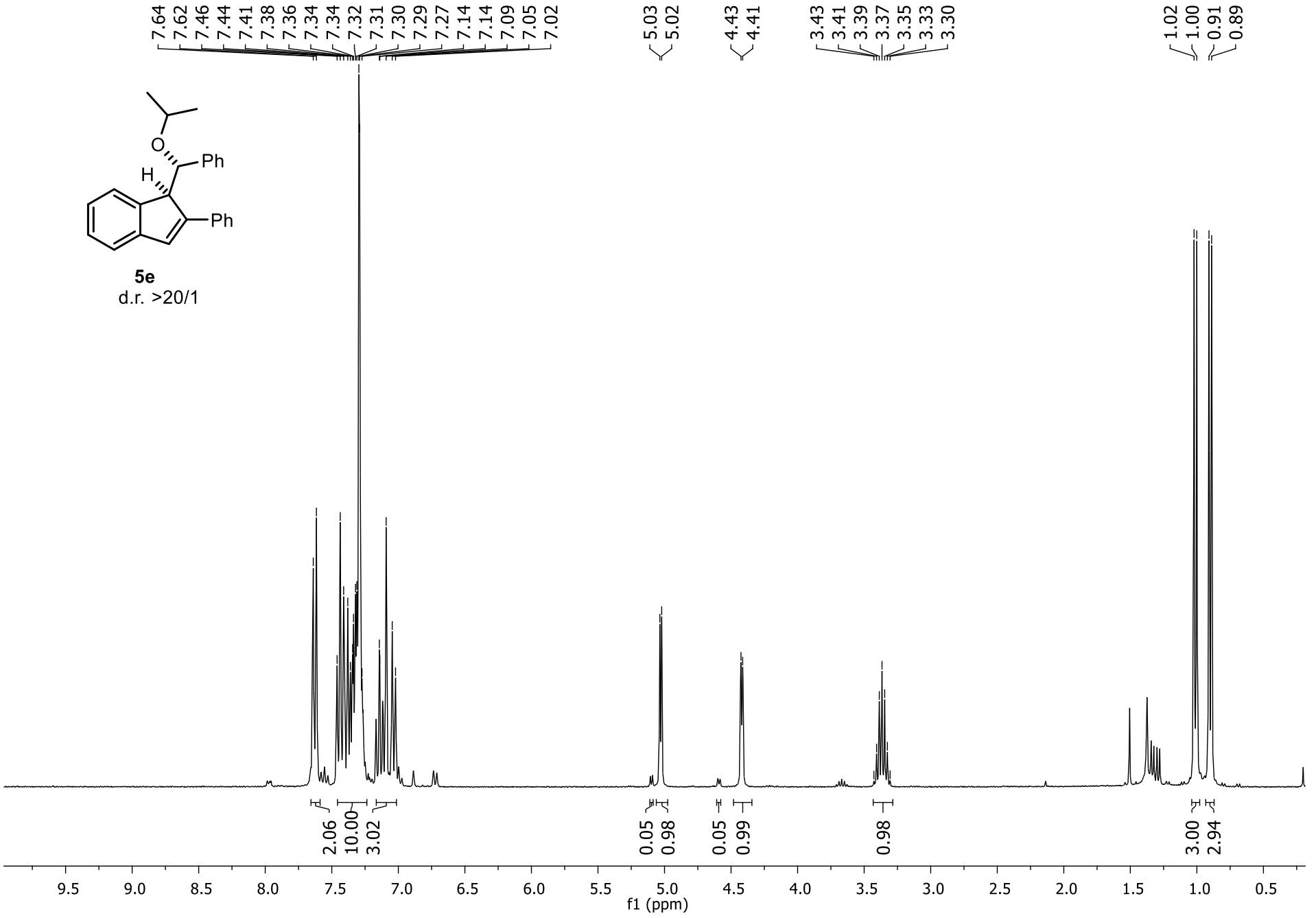


5d
d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

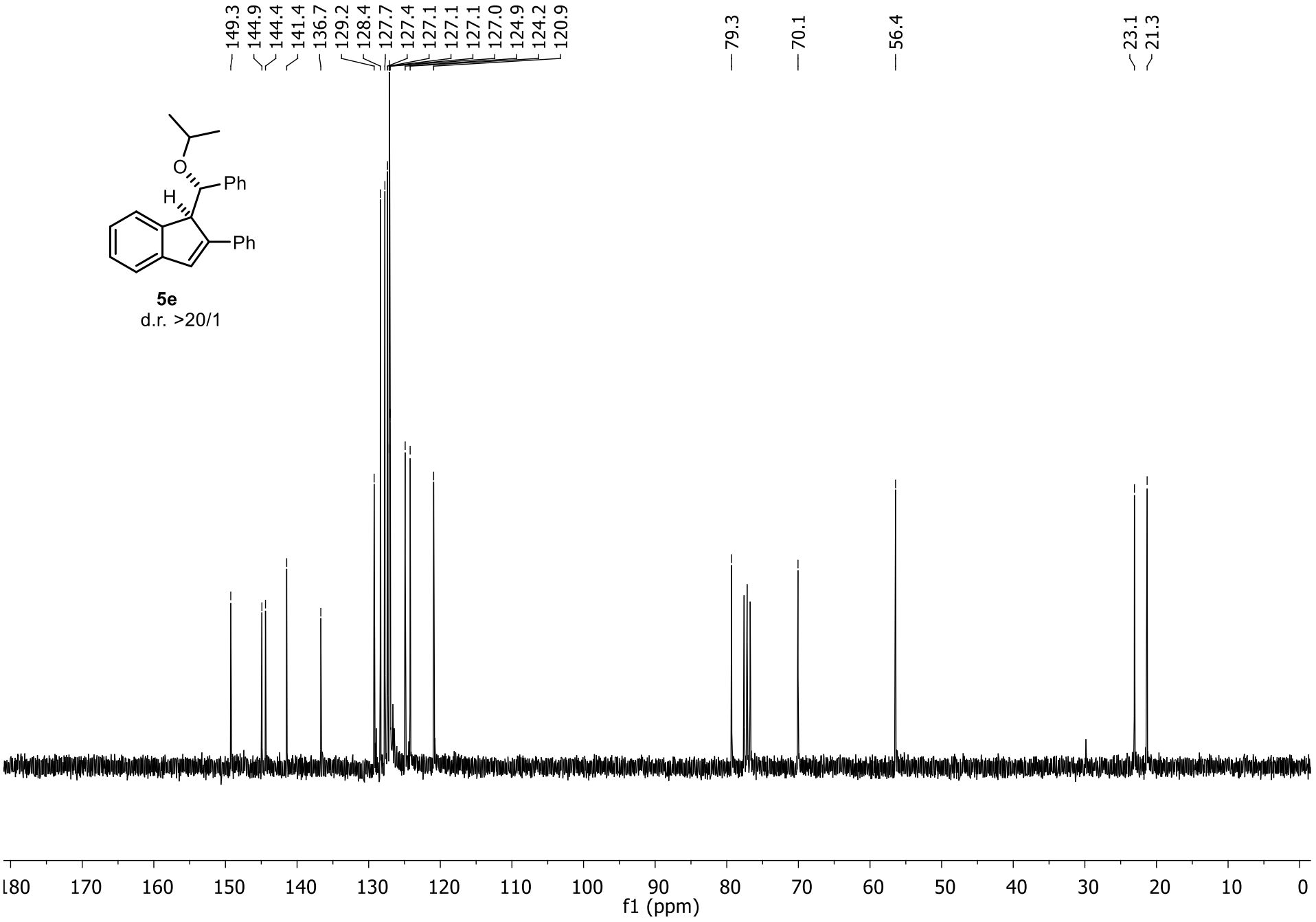


^{1}H NMR (300 MHz, $CDCl_3$)



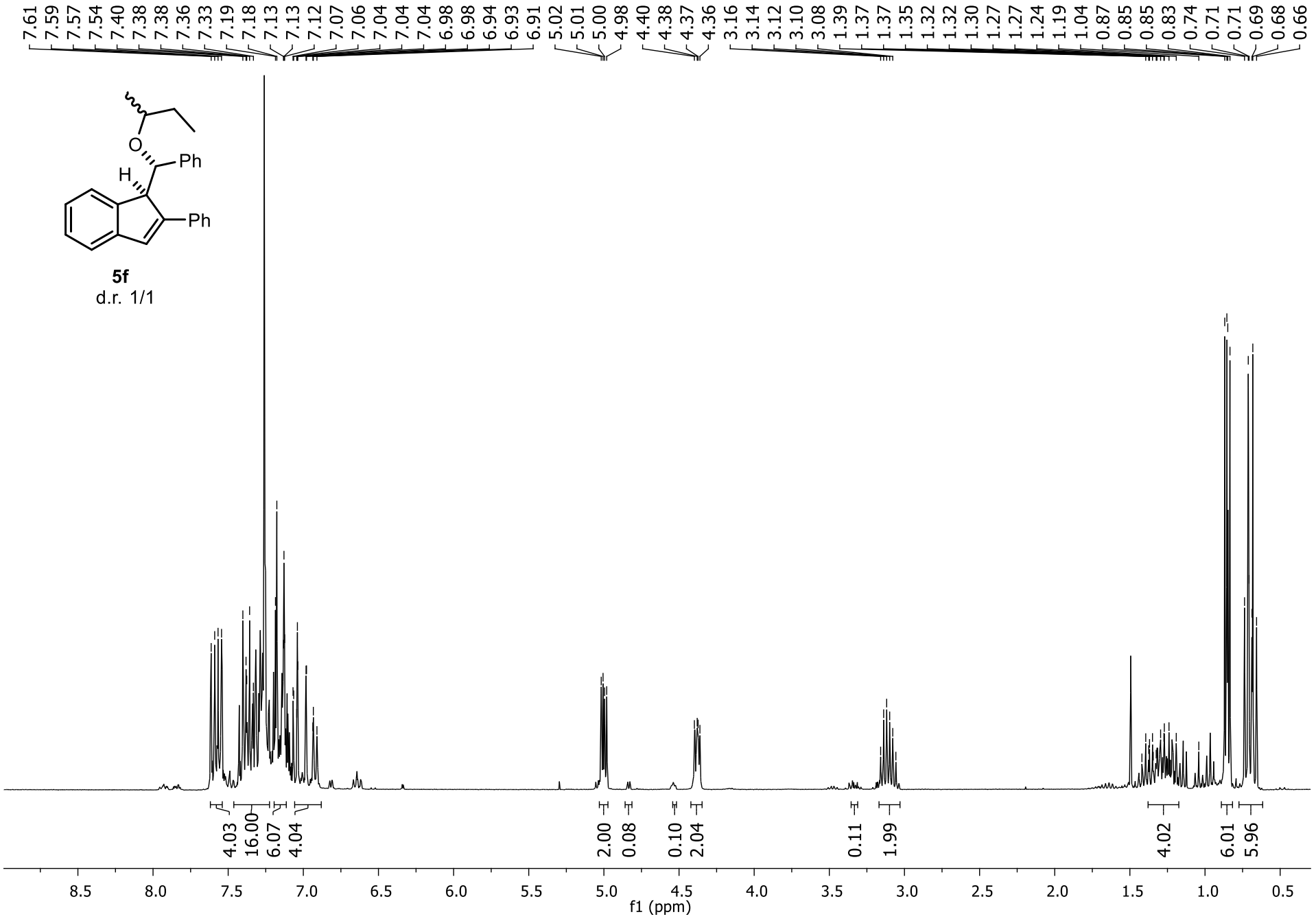
5e
d.r. >20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

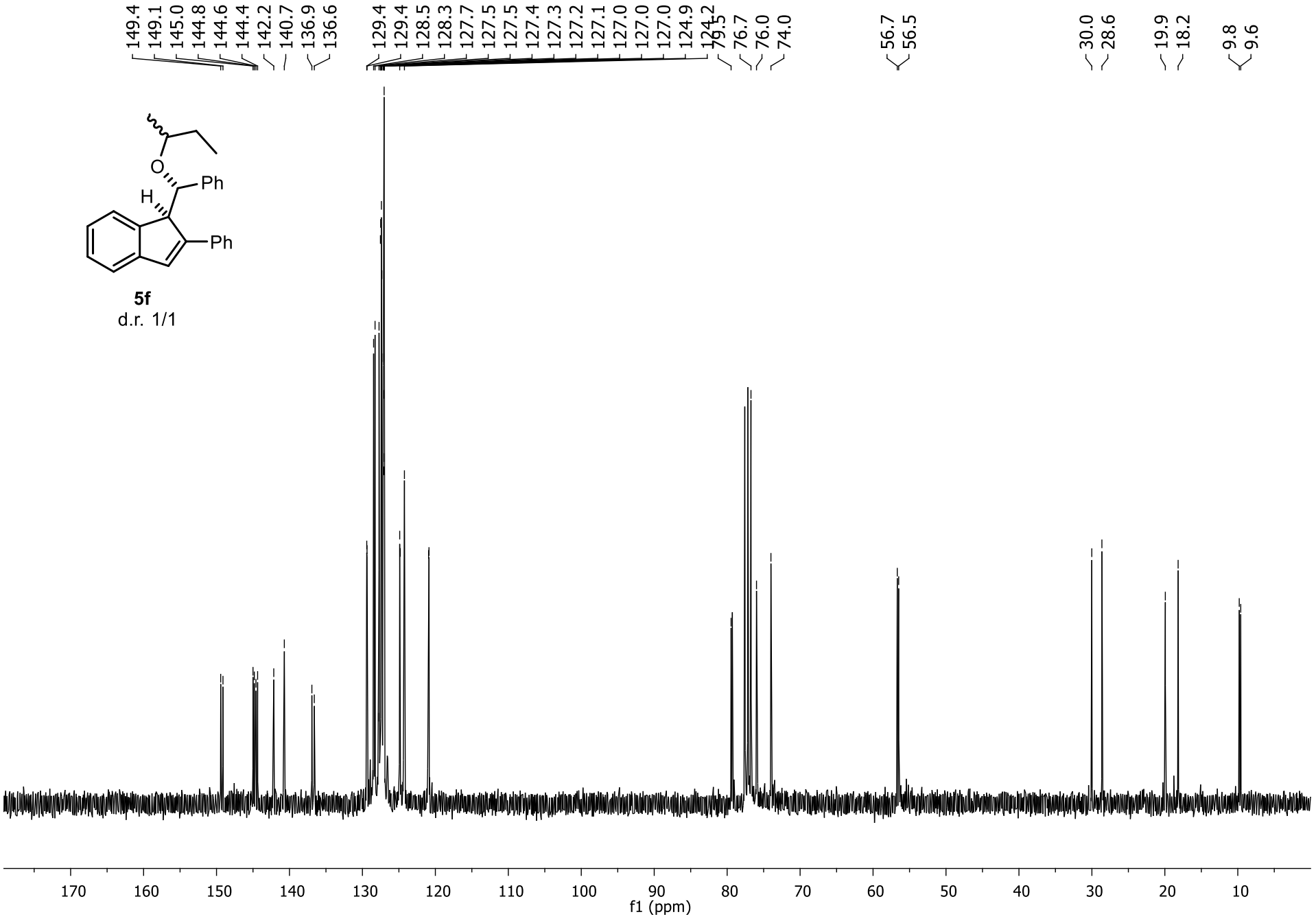


5e
d.r. >20/1

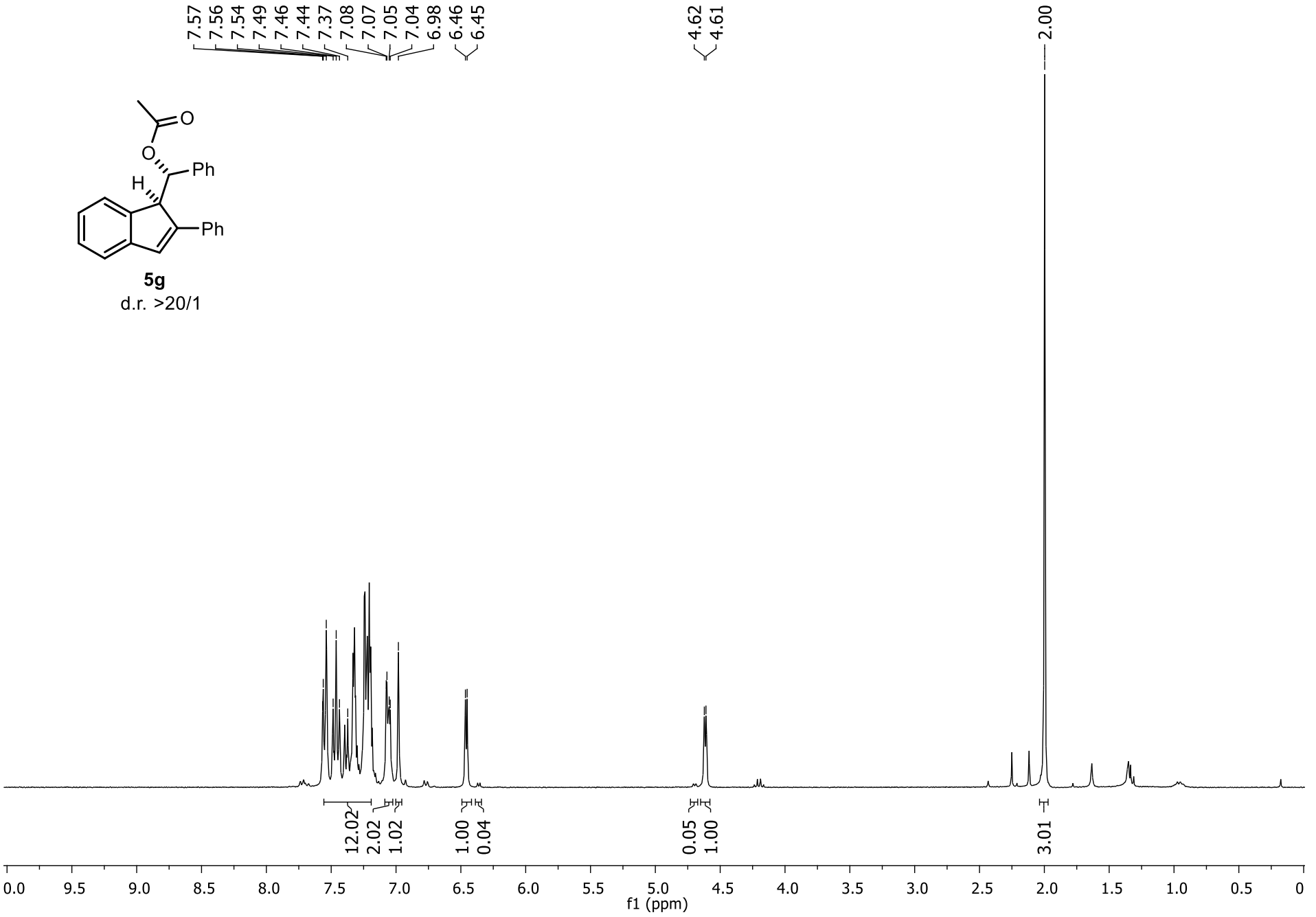
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

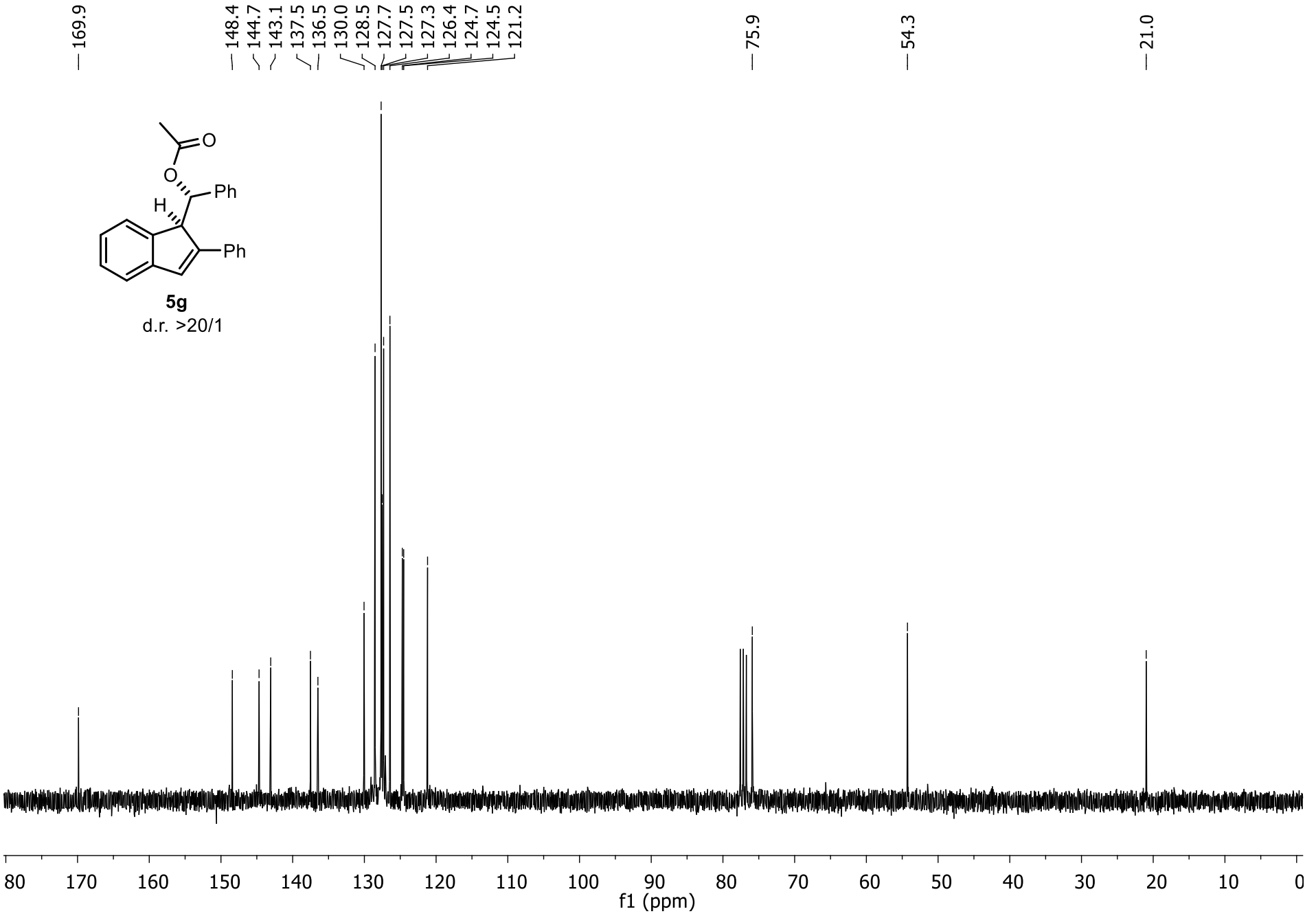


^{1}H NMR (300 MHz, $CDCl_3$)

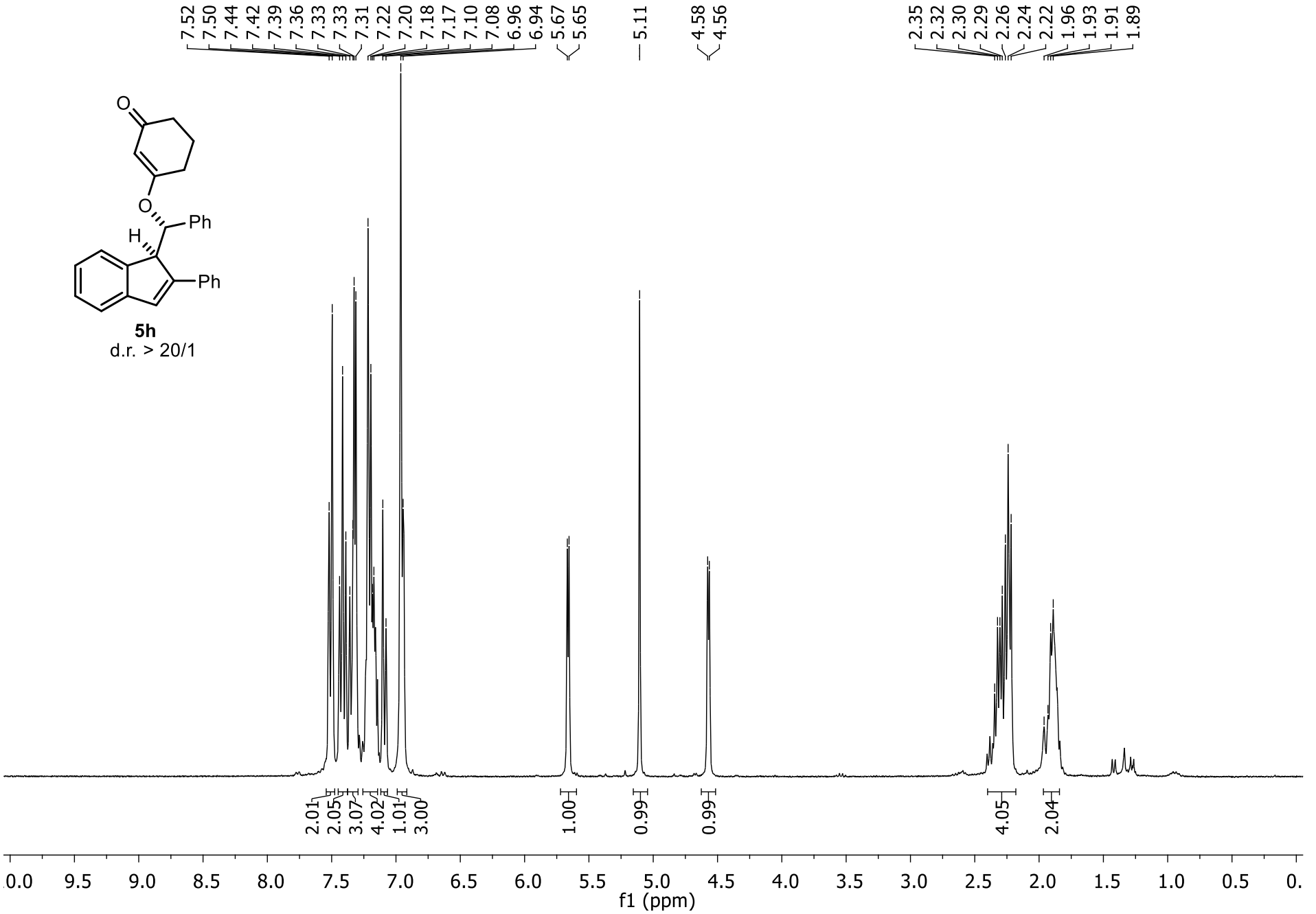


5g
d.r. >20/1

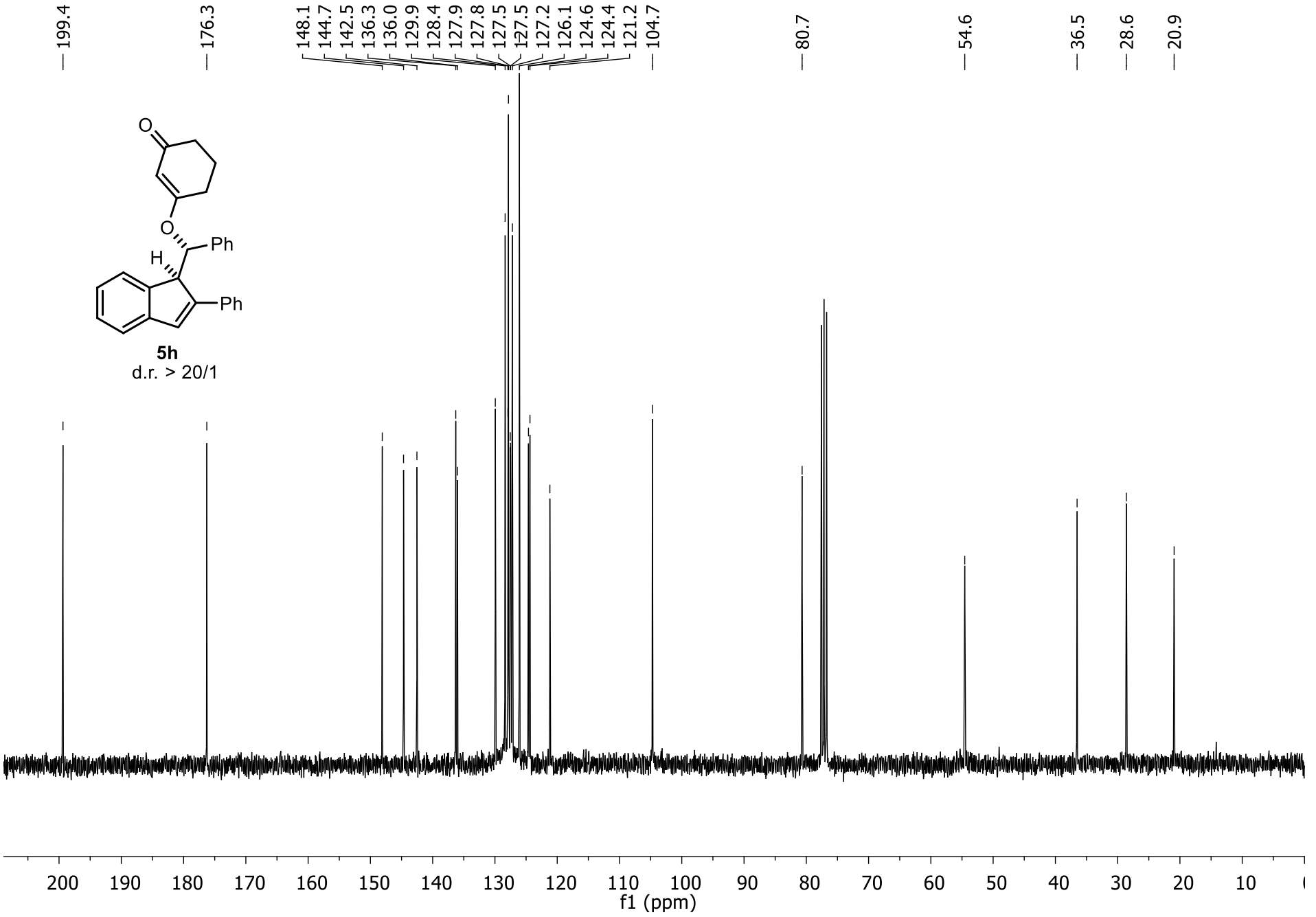
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



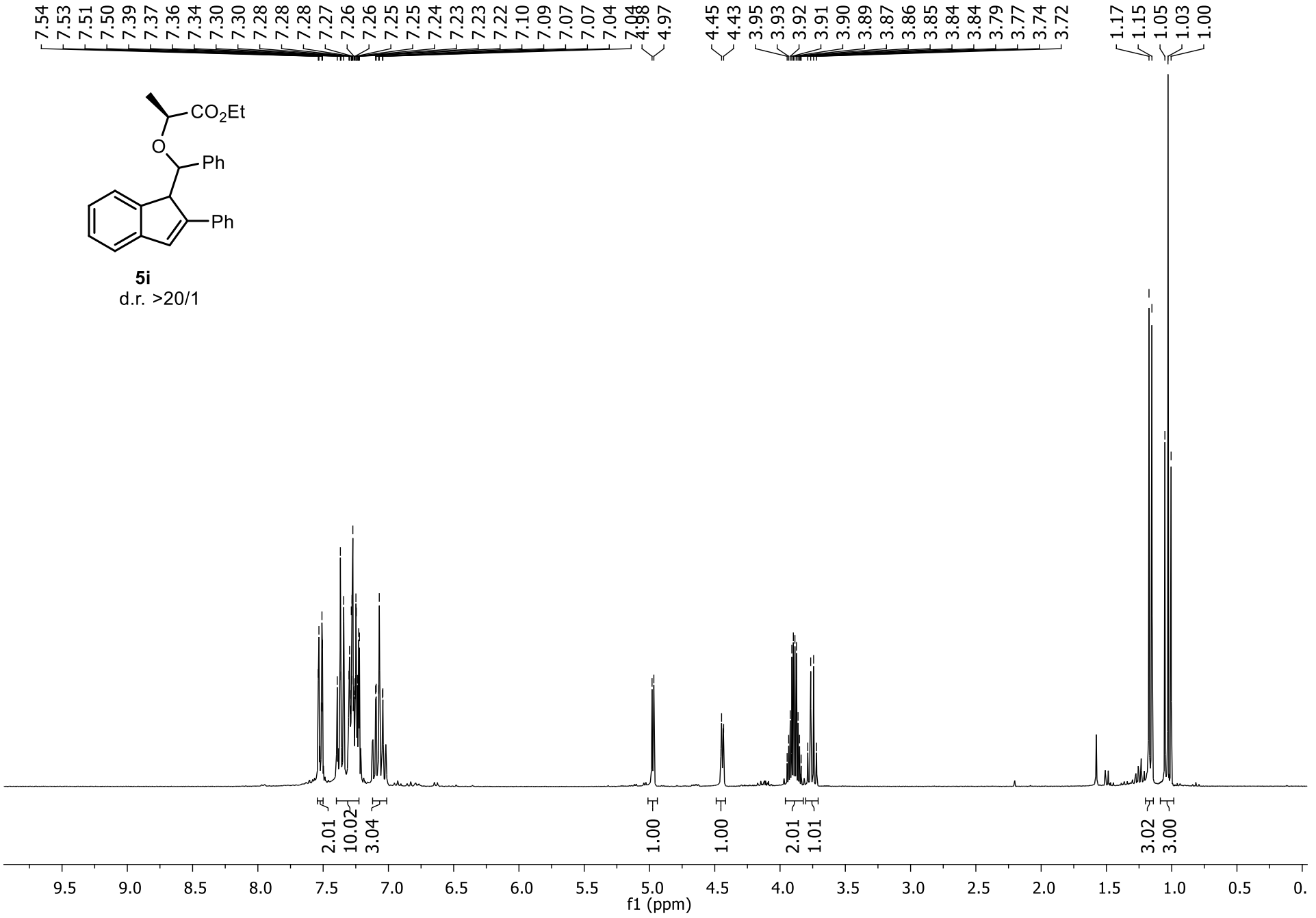
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

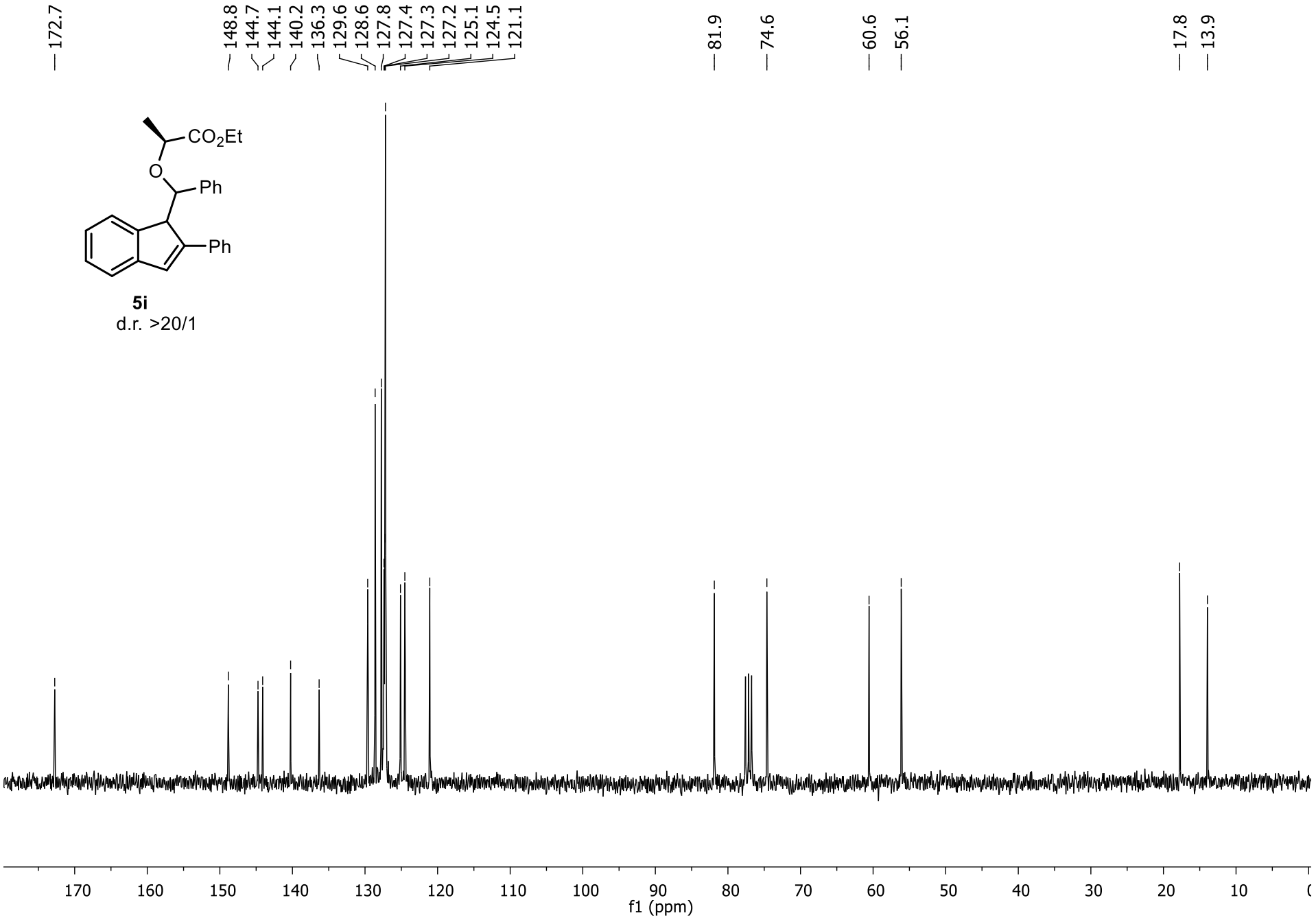


^{1}H NMR (300 MHz, $CDCl_3$)

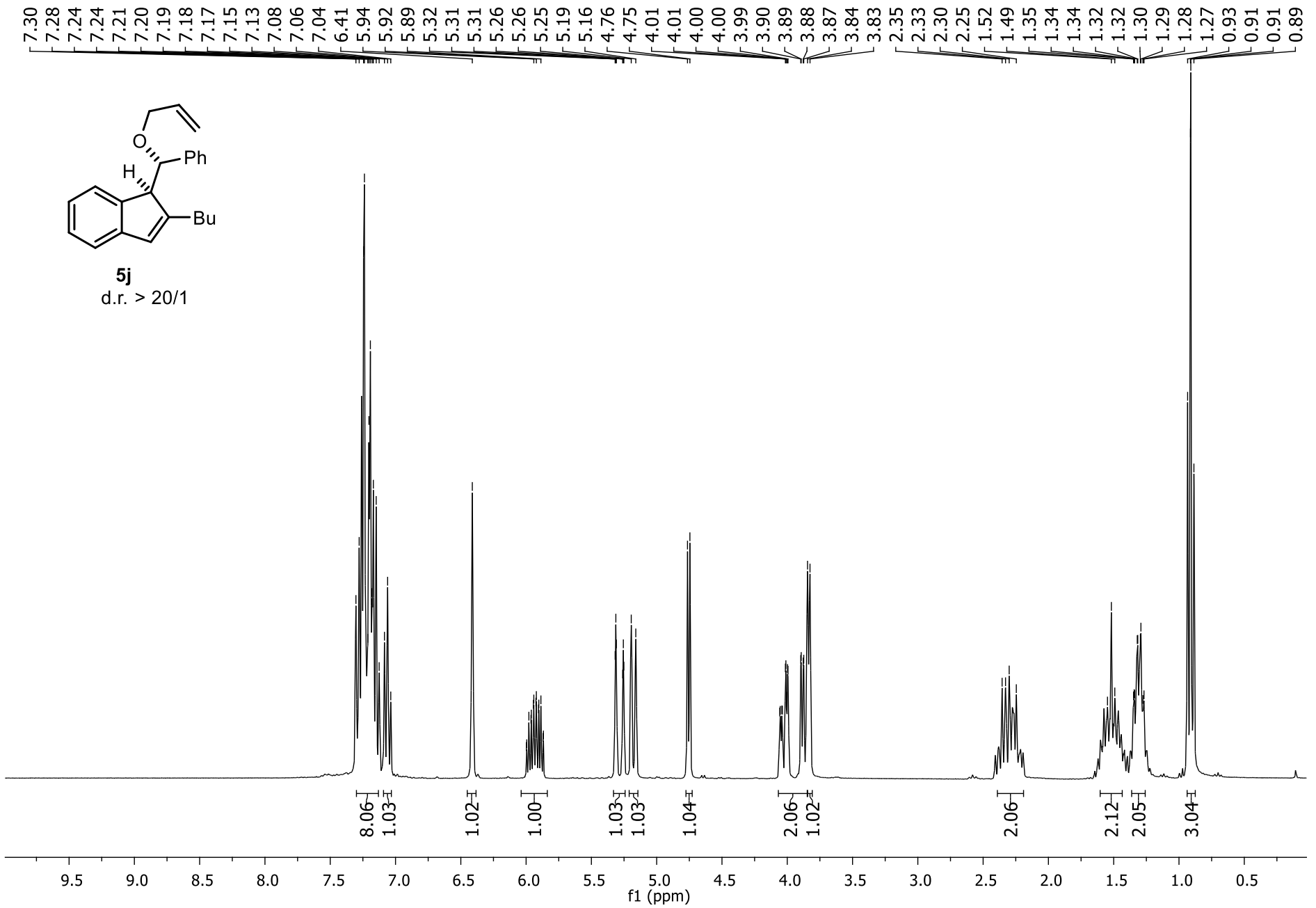


5i
d.r. >20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

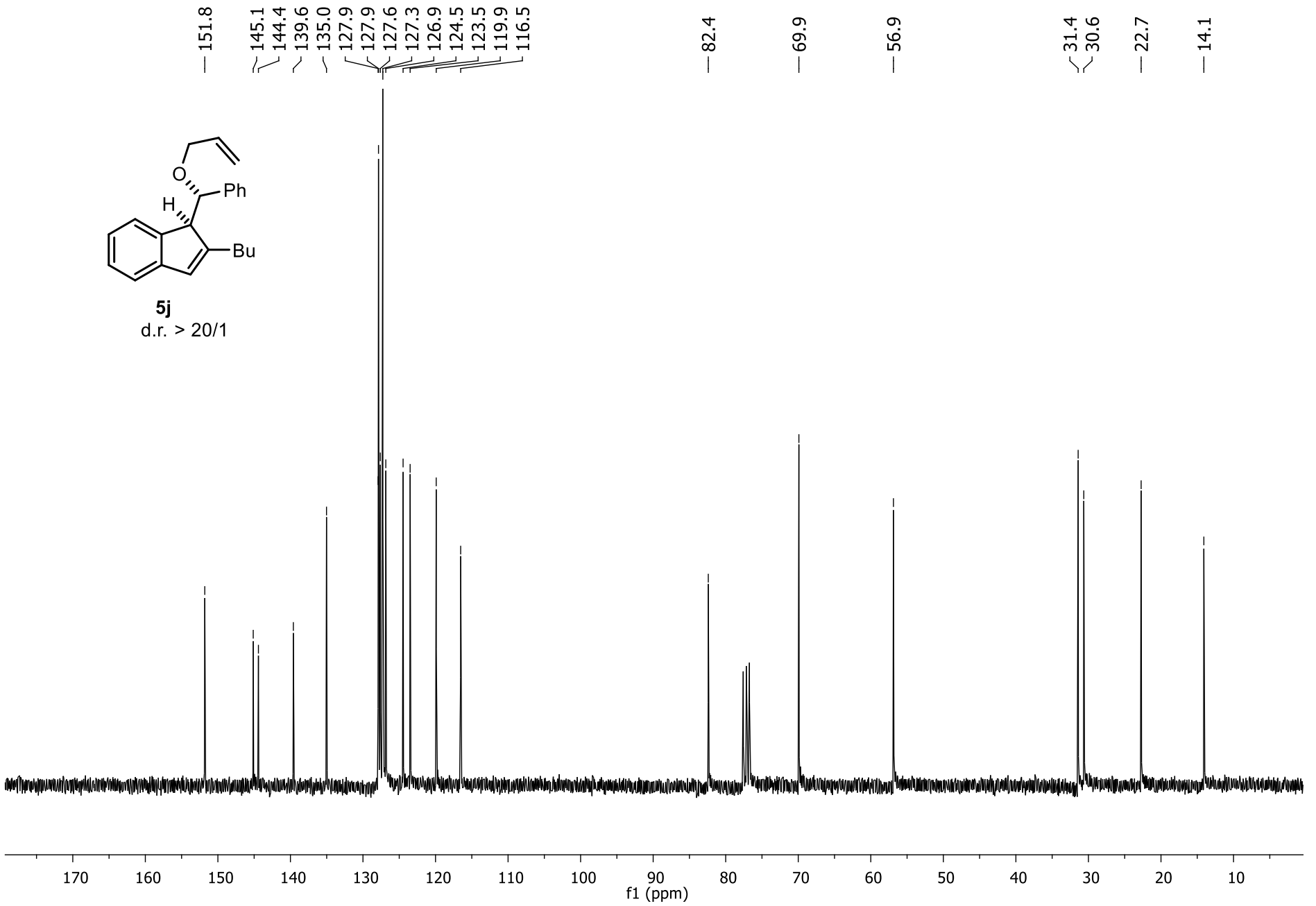


^{1}H NMR (300 MHz, $CDCl_3$)

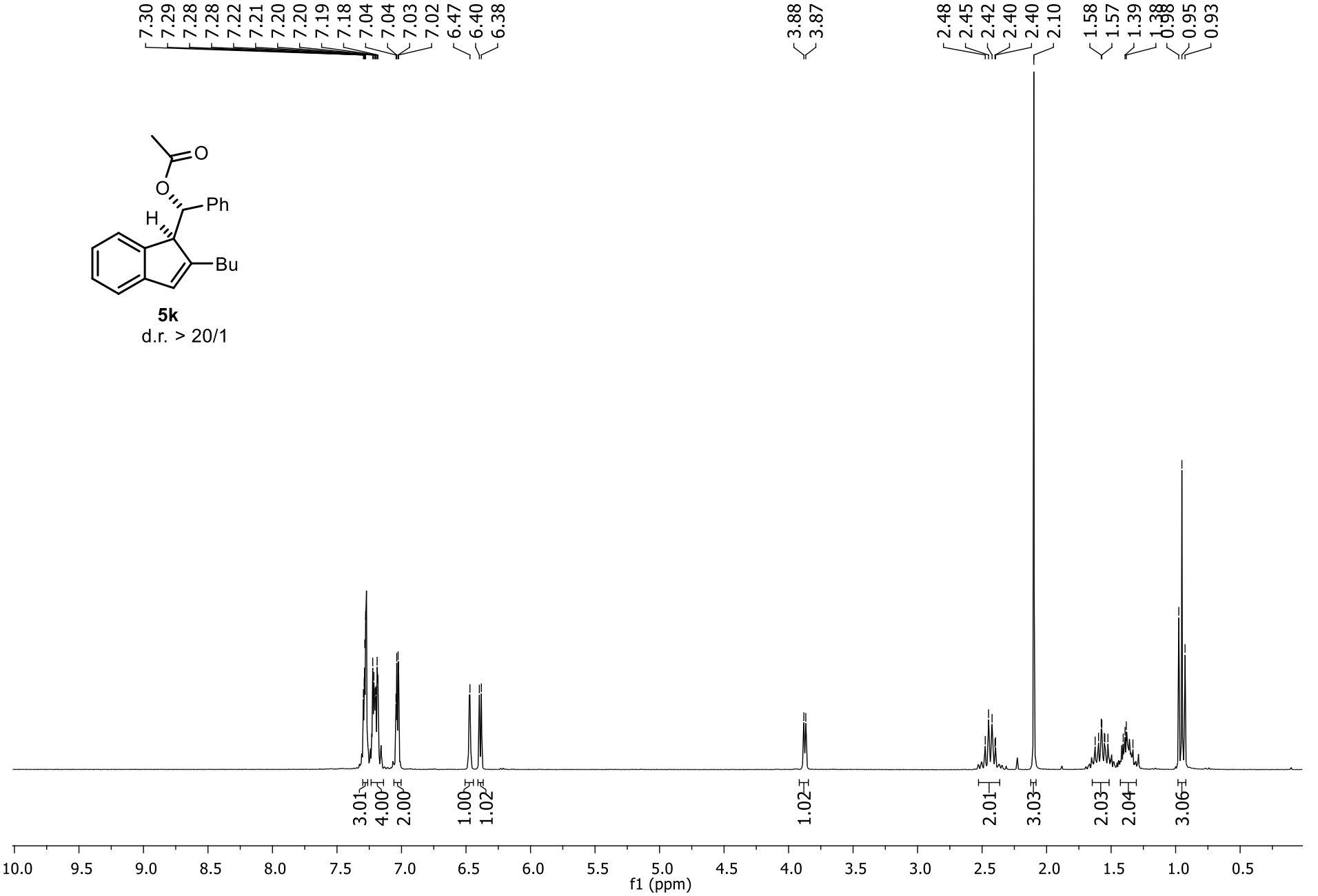


5j
d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

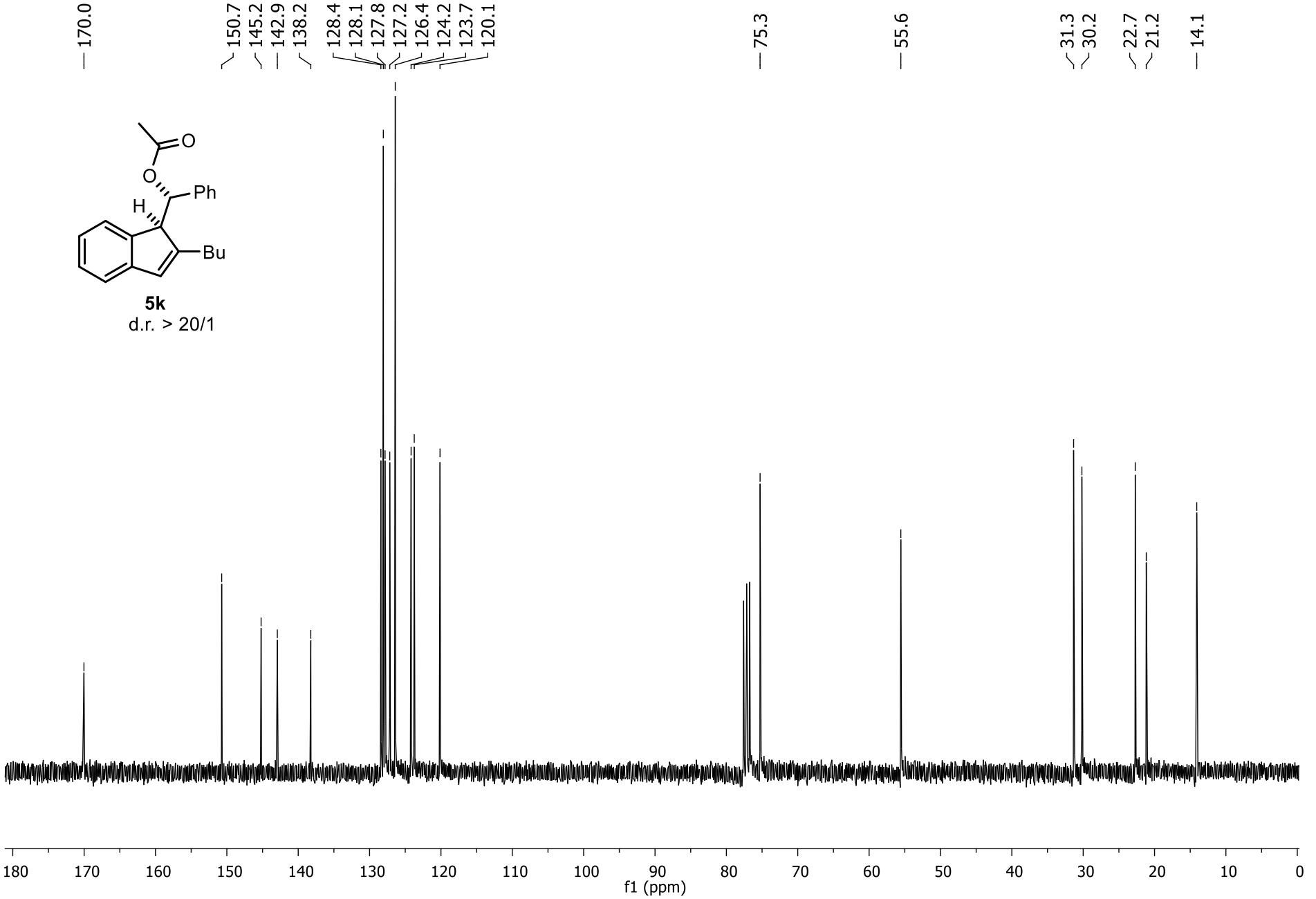


^{1}H NMR (300 MHz, $CDCl_3$)

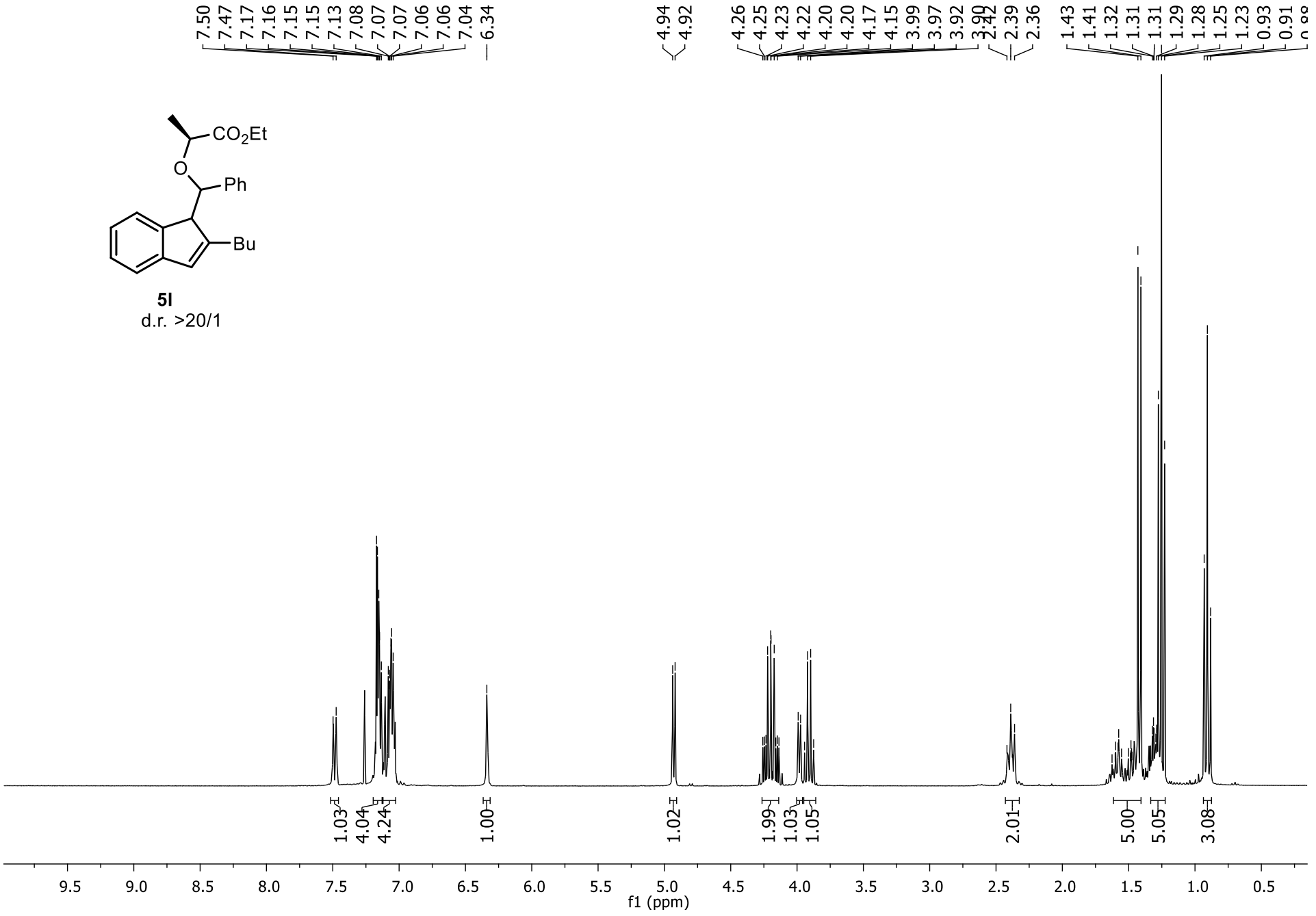


5k
d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

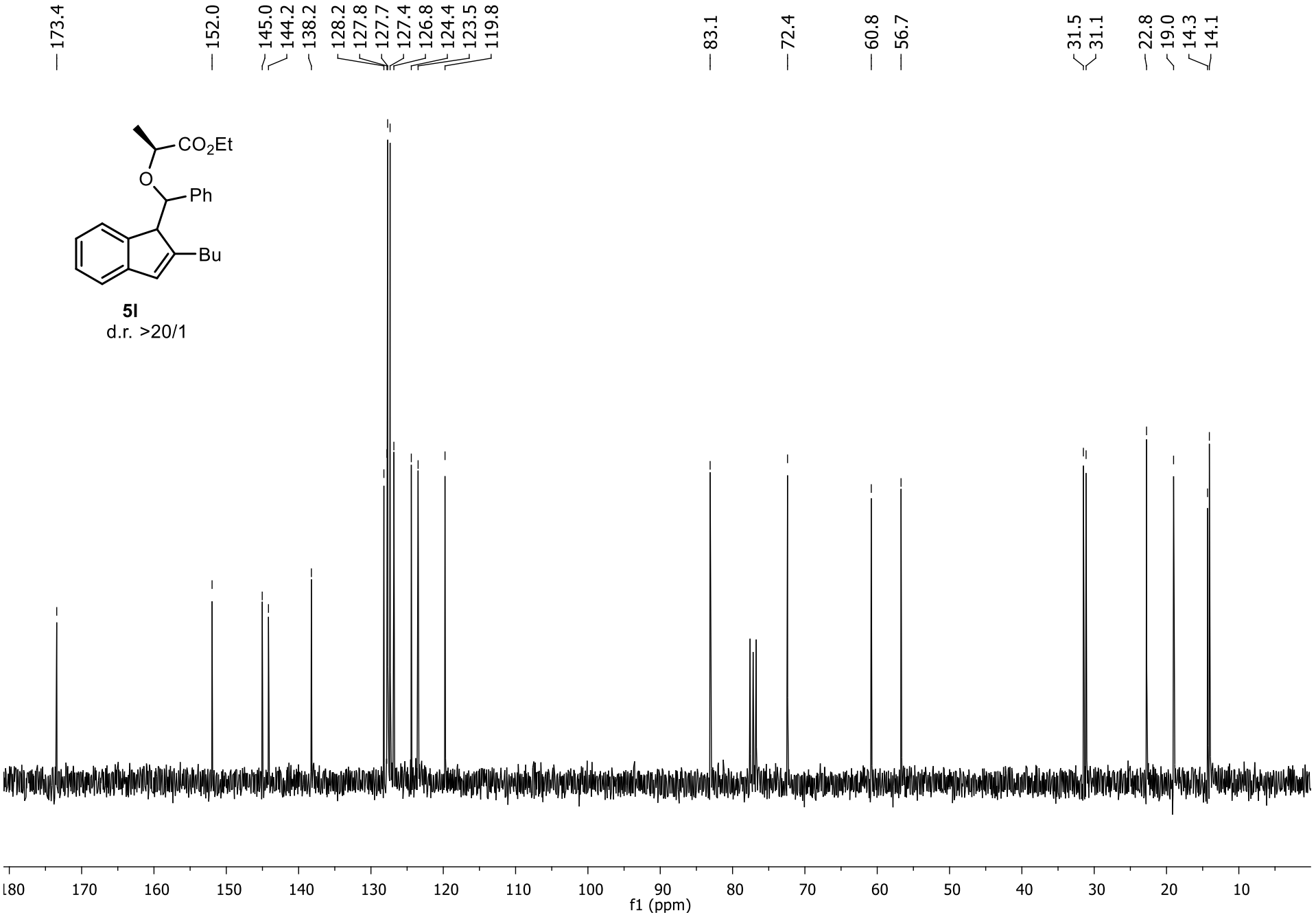


^{1}H NMR (300 MHz, $CDCl_3$)

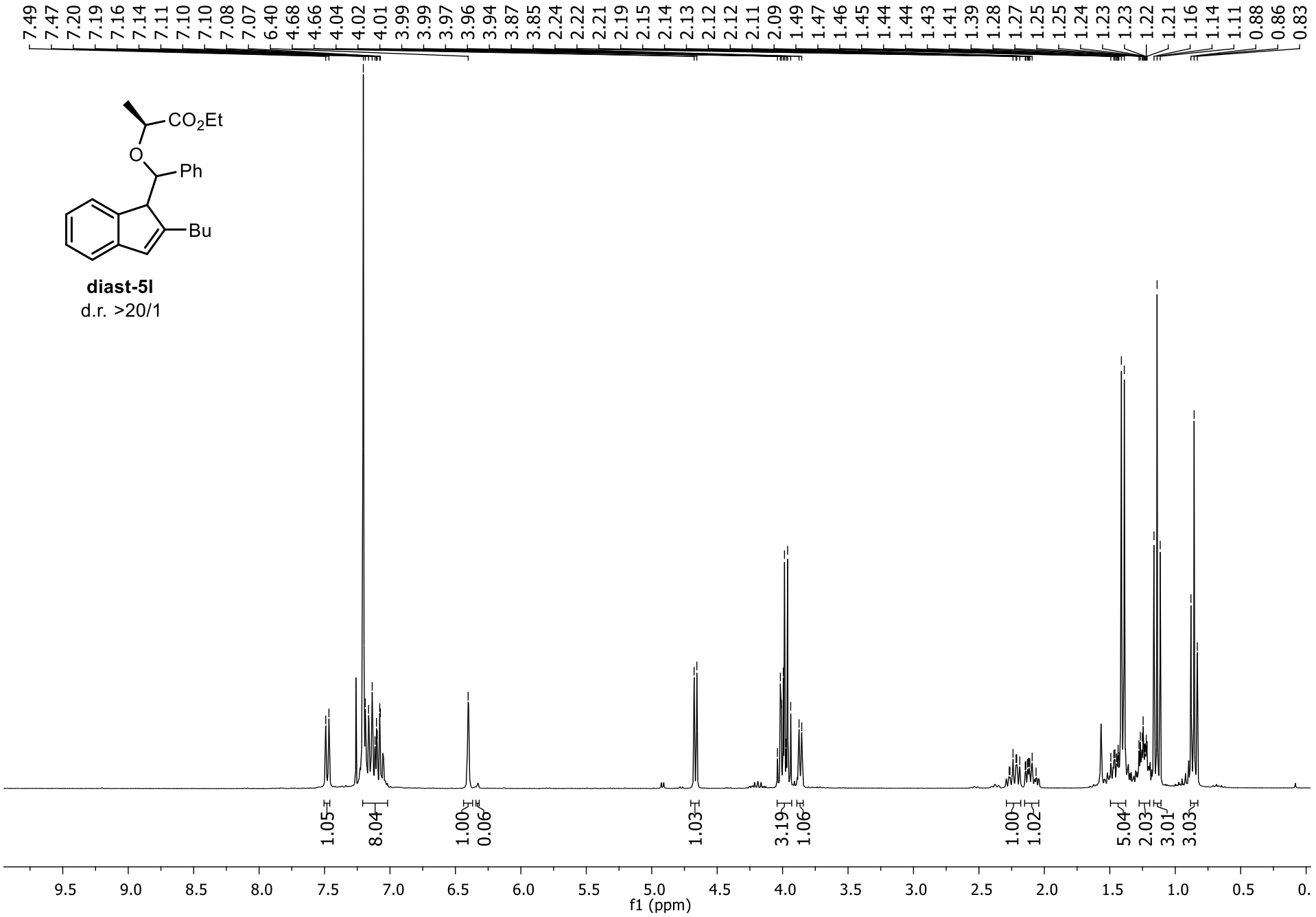


5l
d.r. >20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

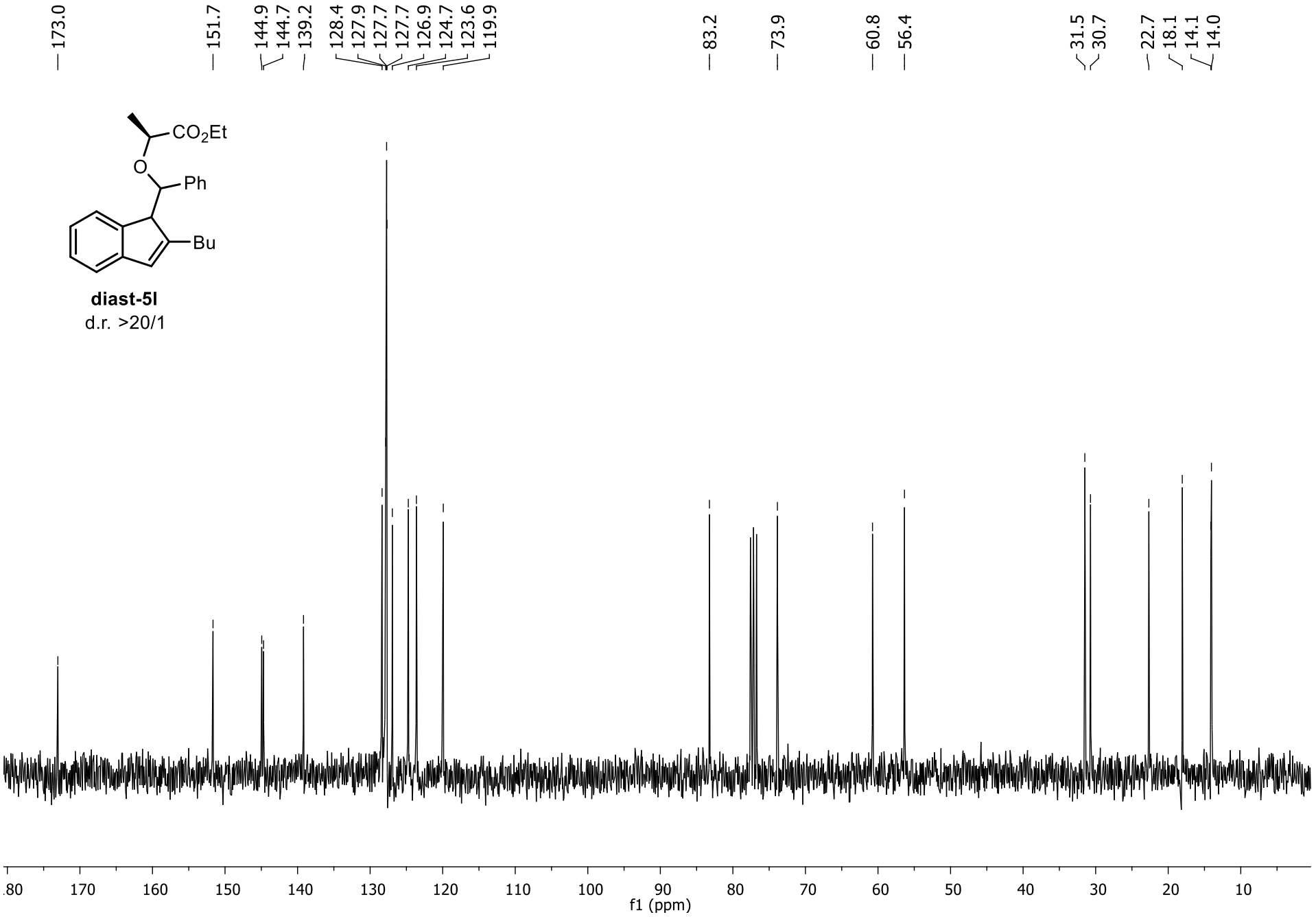


^{1}H NMR (300 MHz, $CDCl_3$)

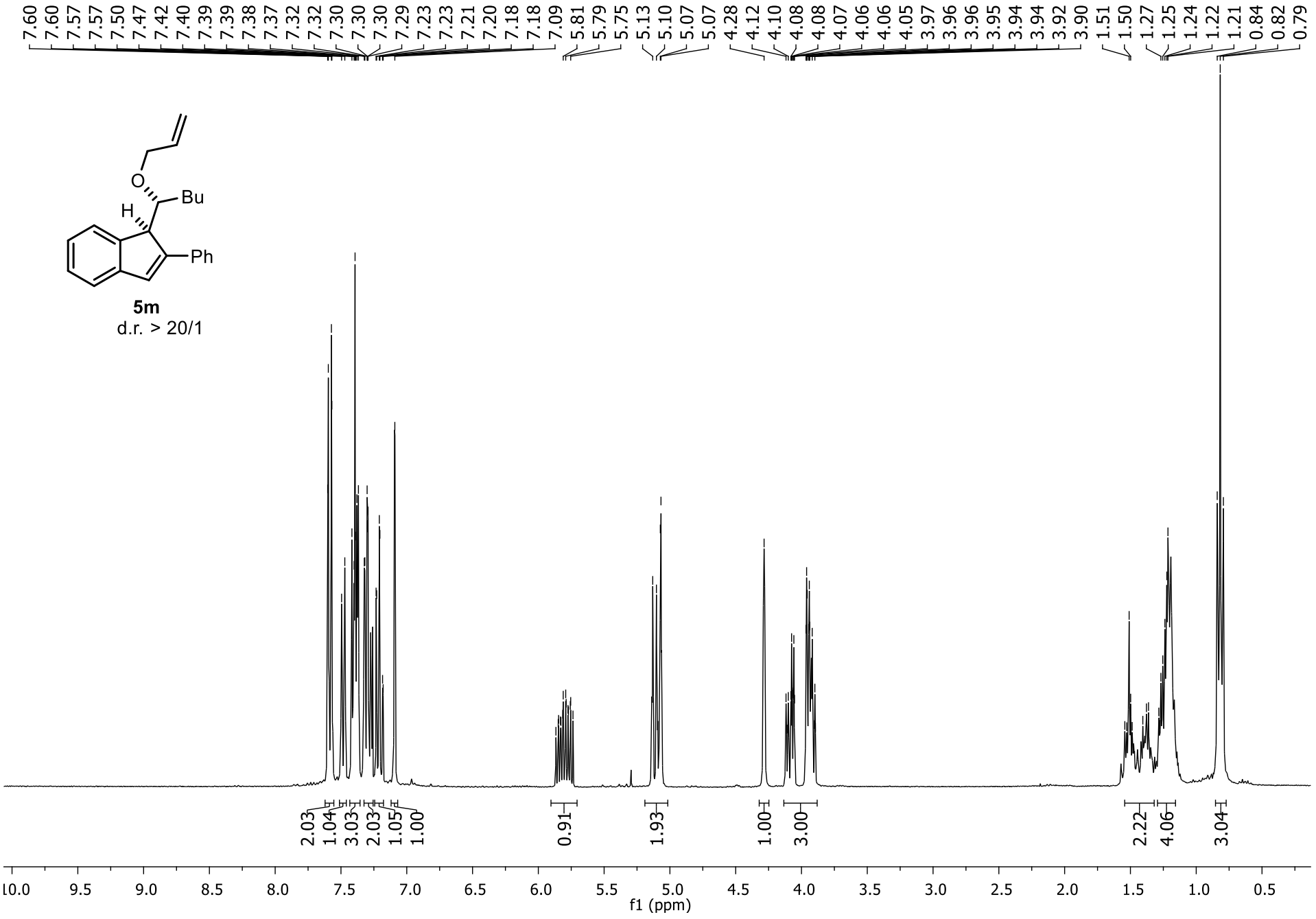


diast-5l
d.r. >20/1

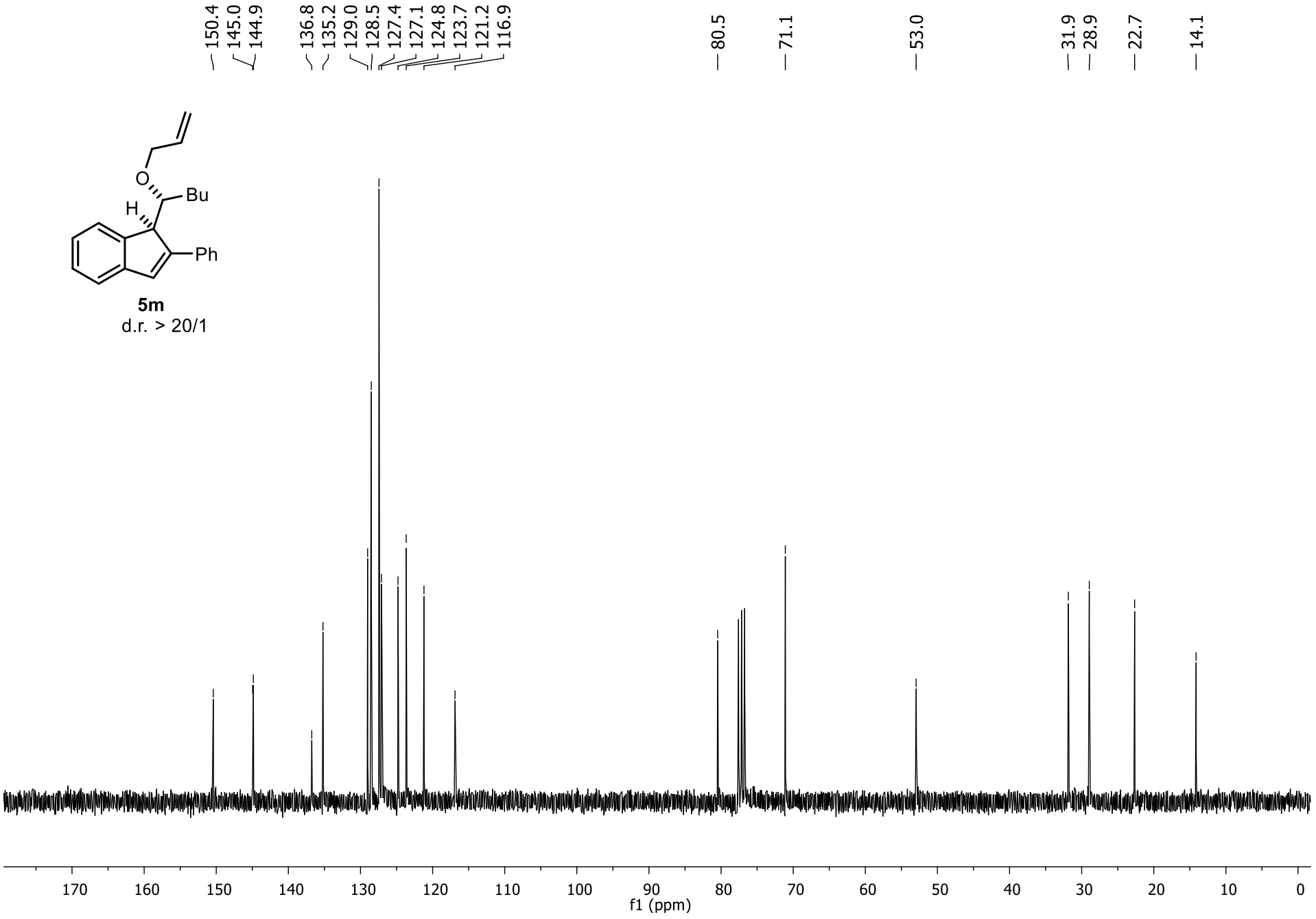
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



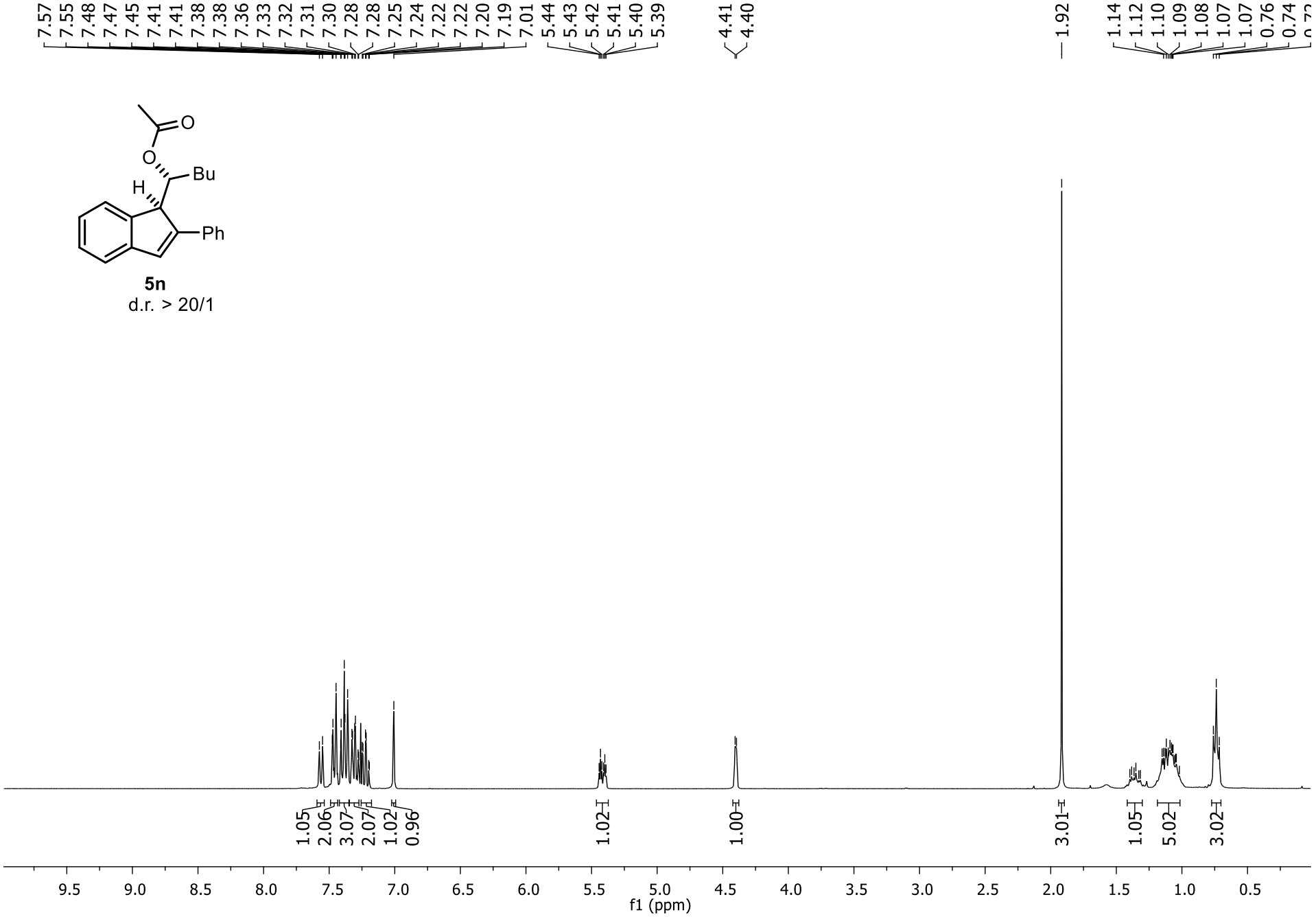
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

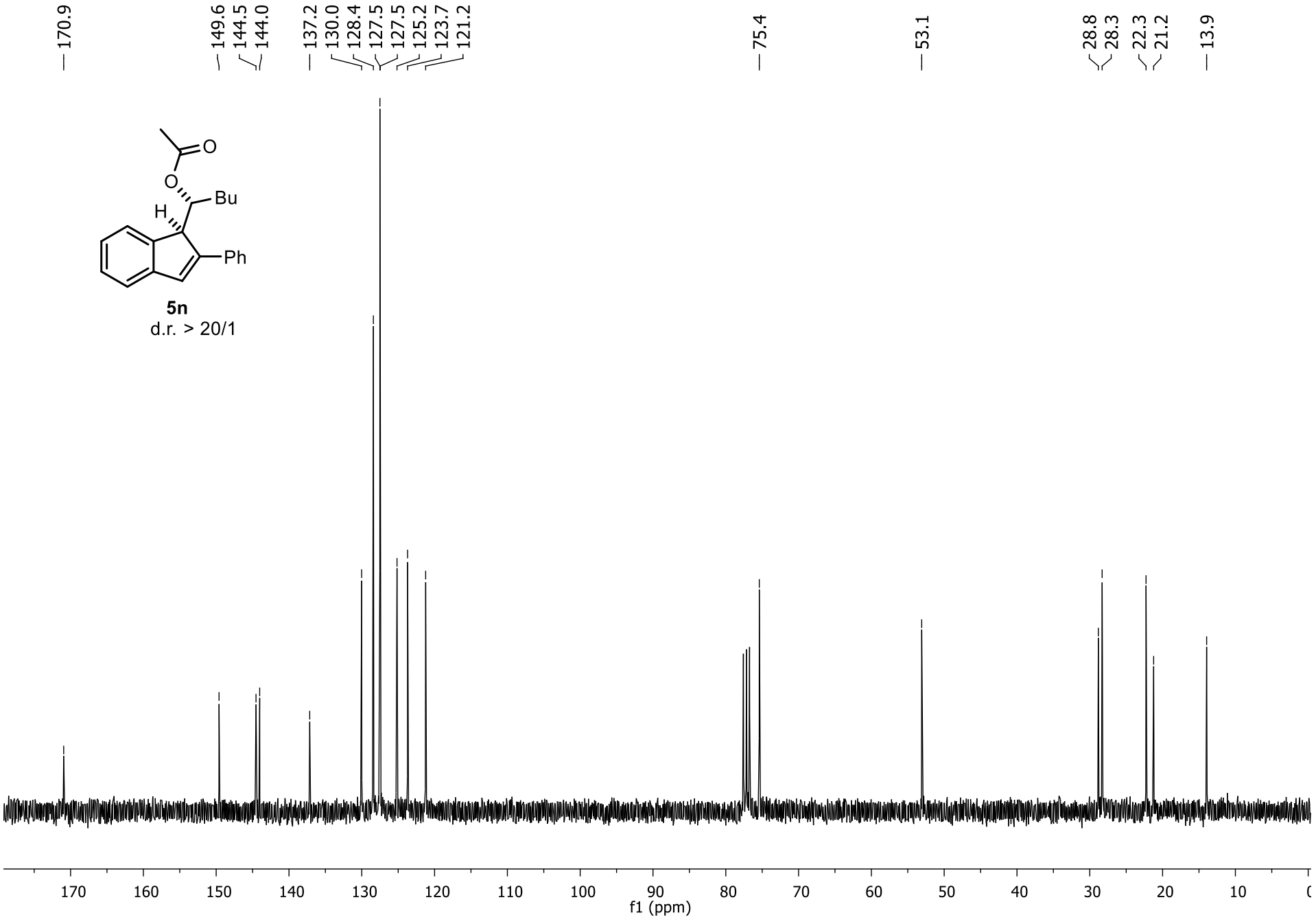


^{1}H NMR (300 MHz, $CDCl_3$)

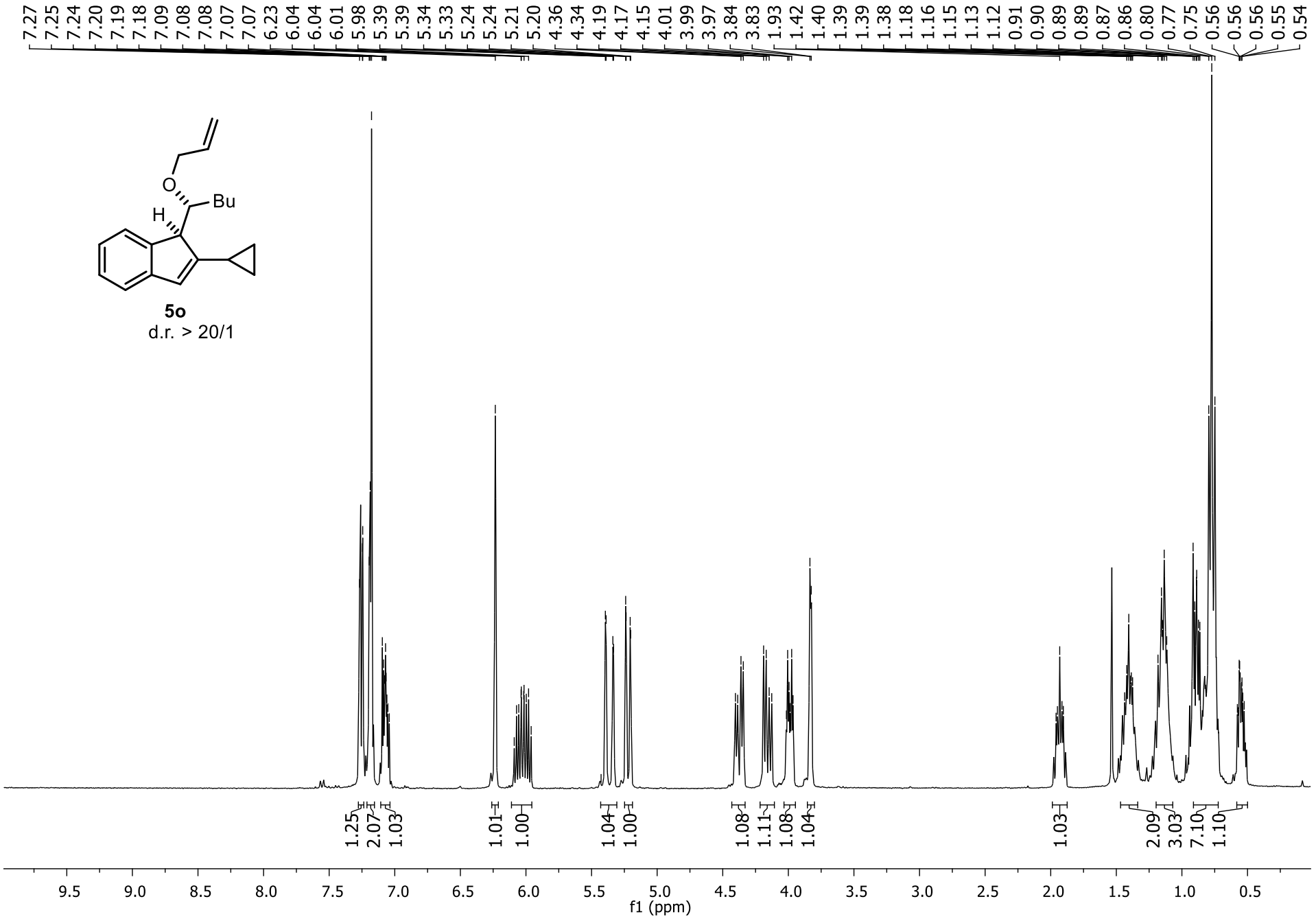


5n
d.r. > 20/1

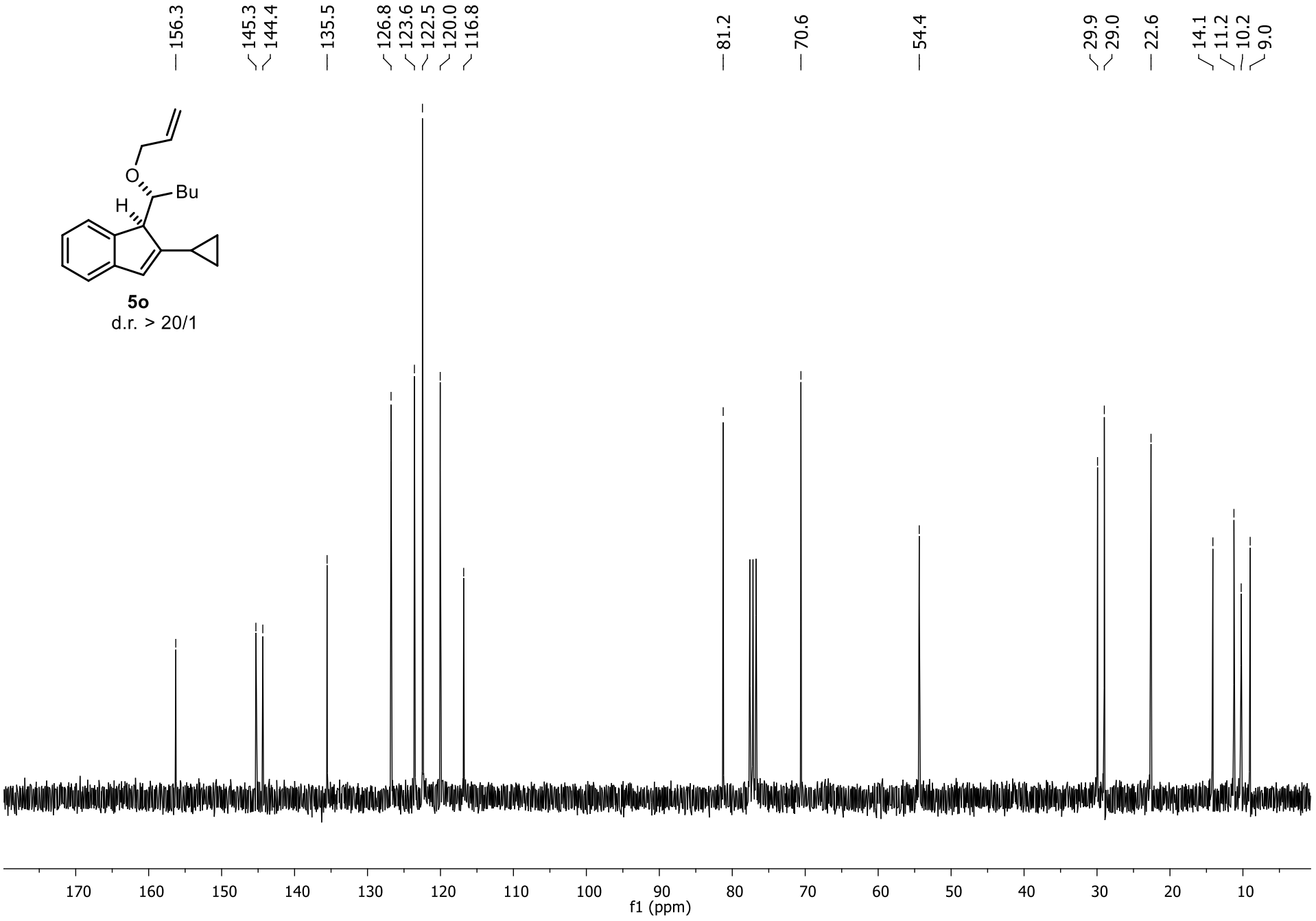
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



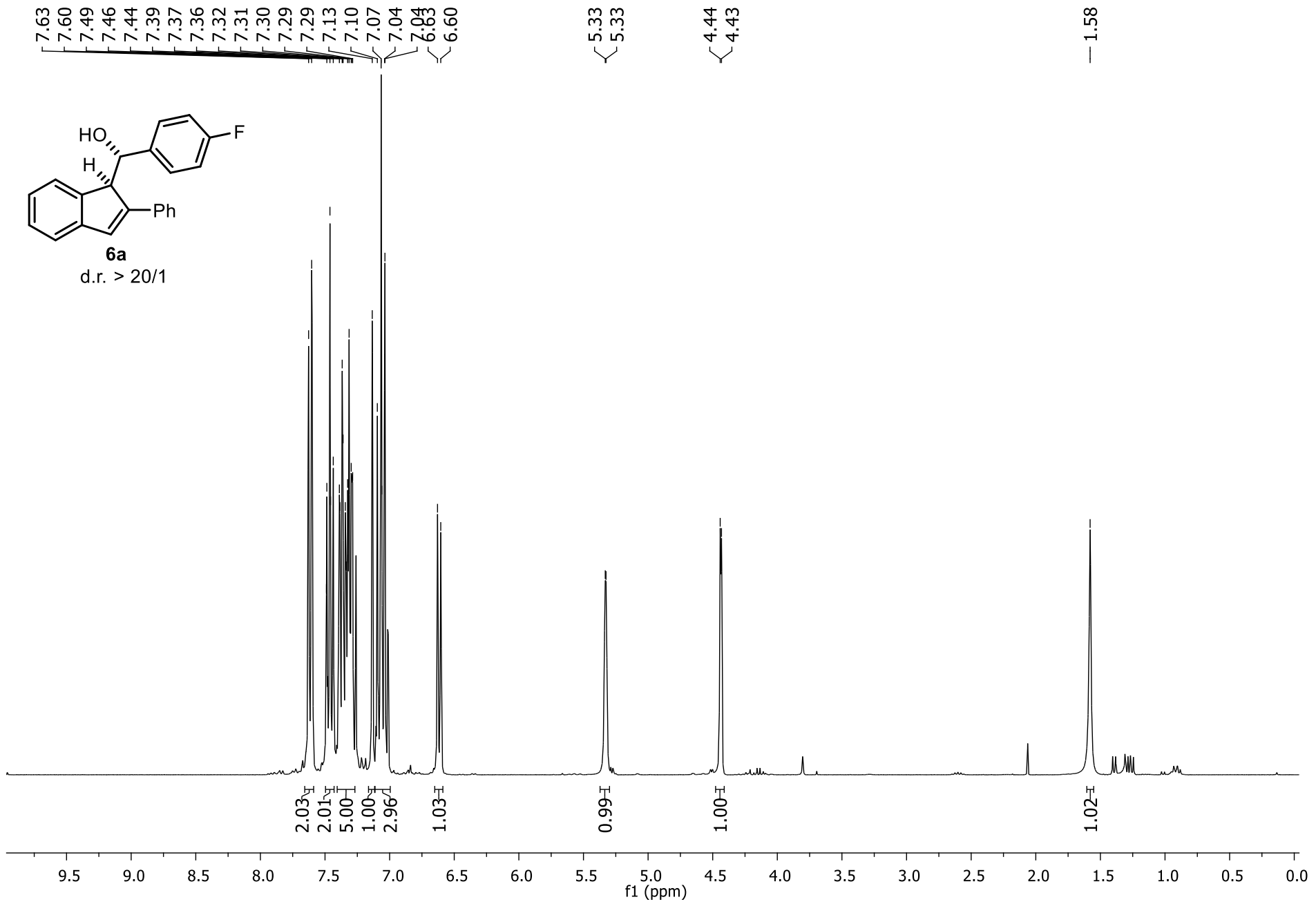
^{1}H NMR (300 MHz, $CDCl_3$)



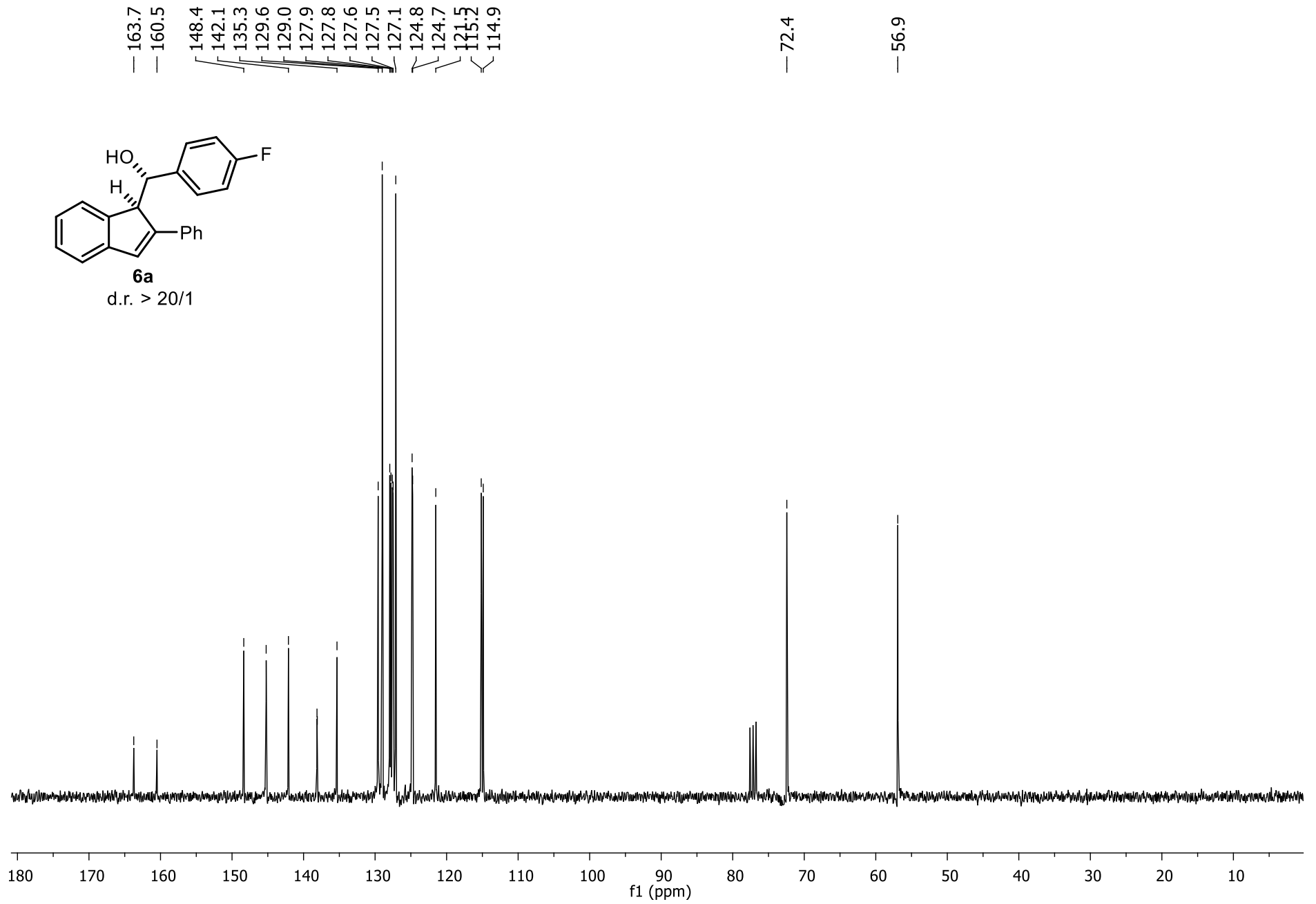
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



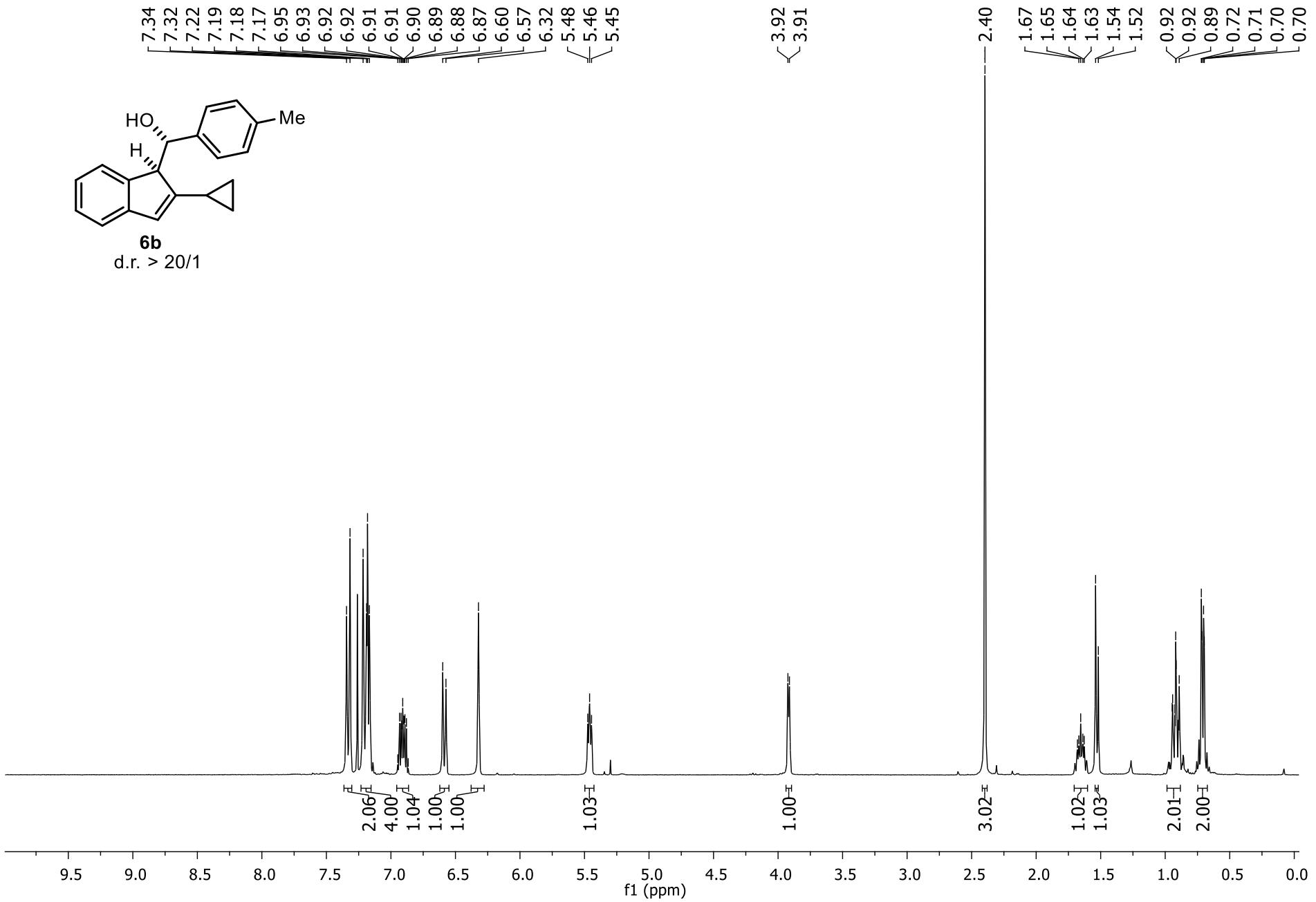
^{1}H NMR (300 MHz, $CDCl_3$)



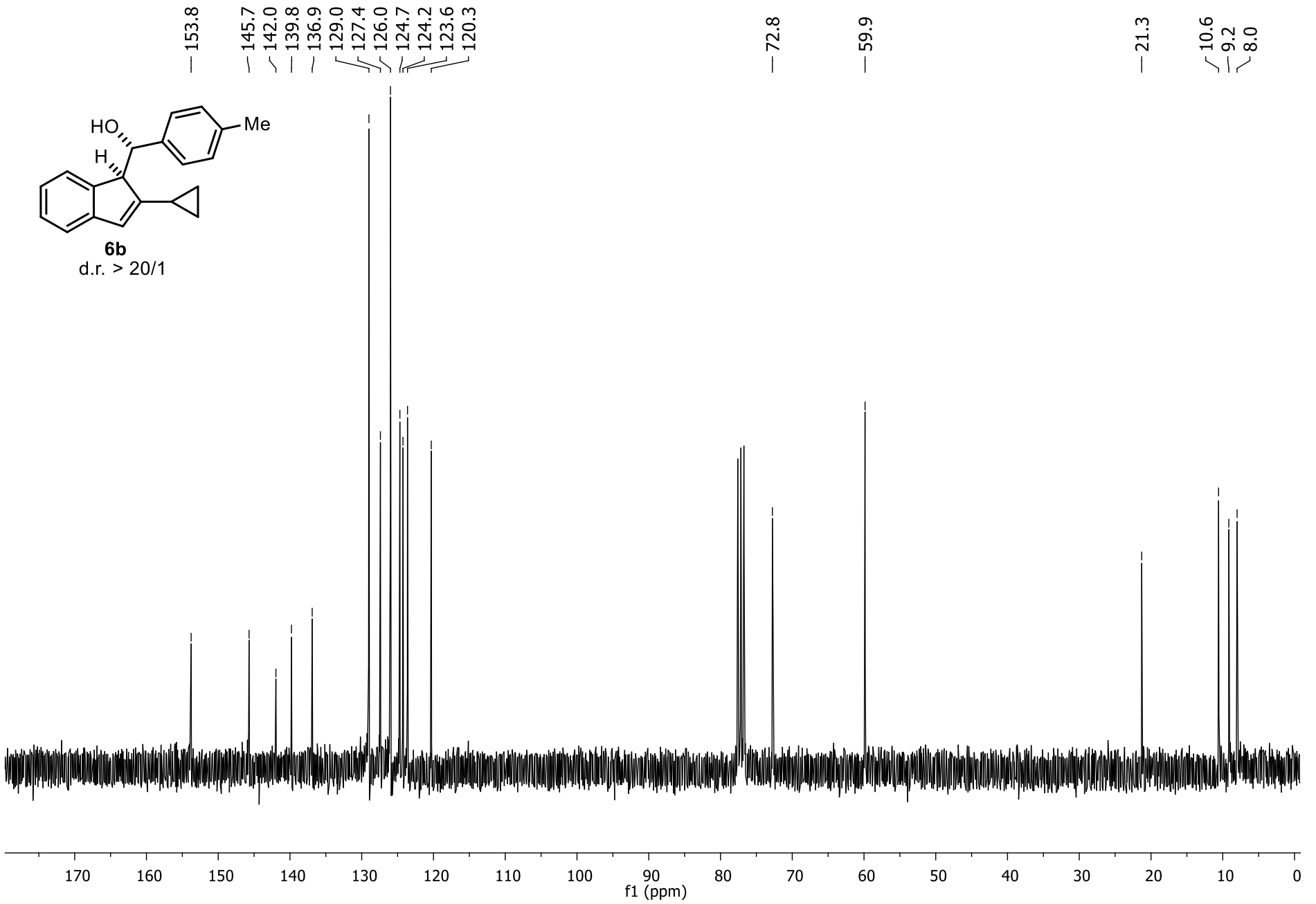
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



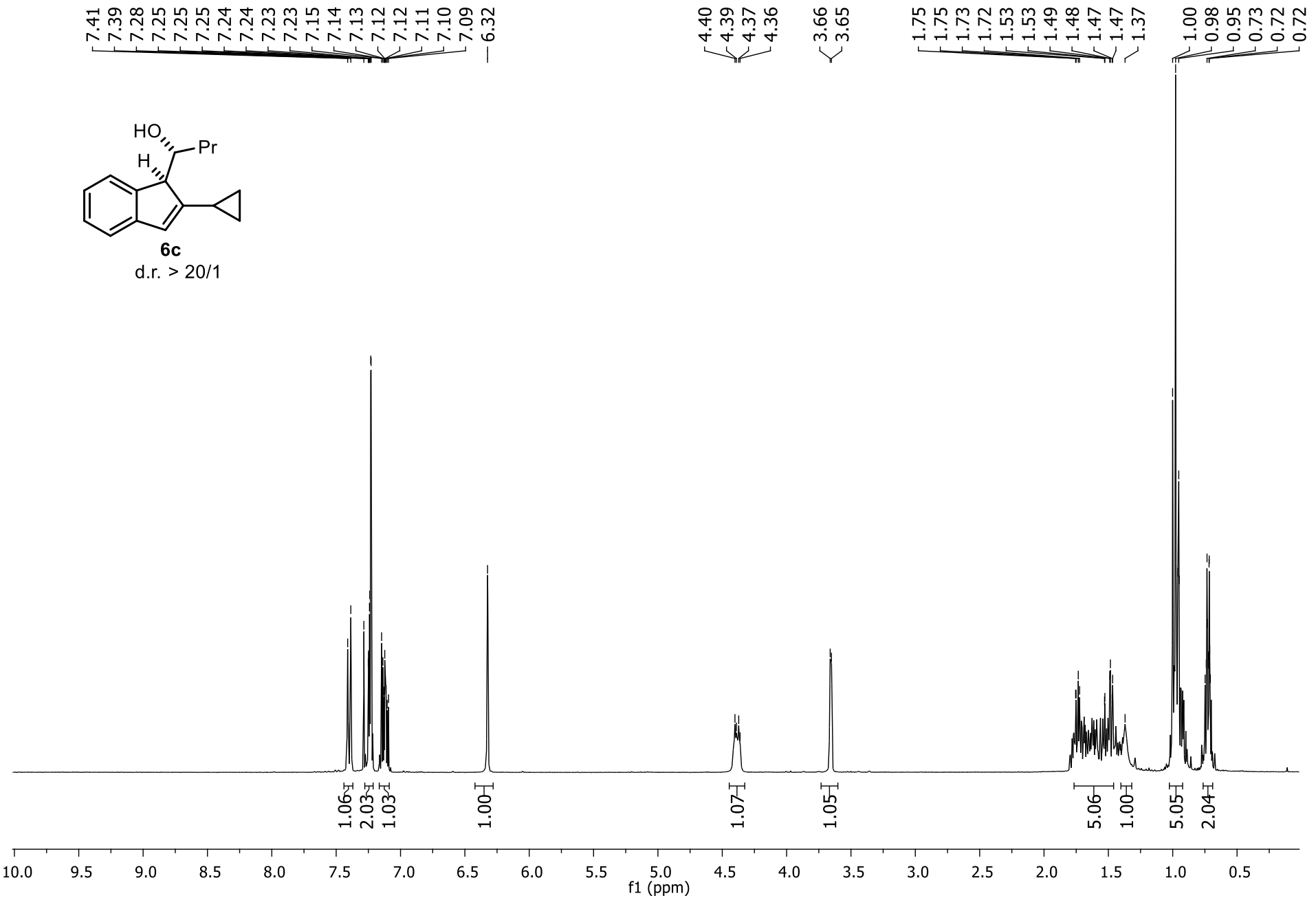
^{1}H NMR (300 MHz, $CDCl_3$)



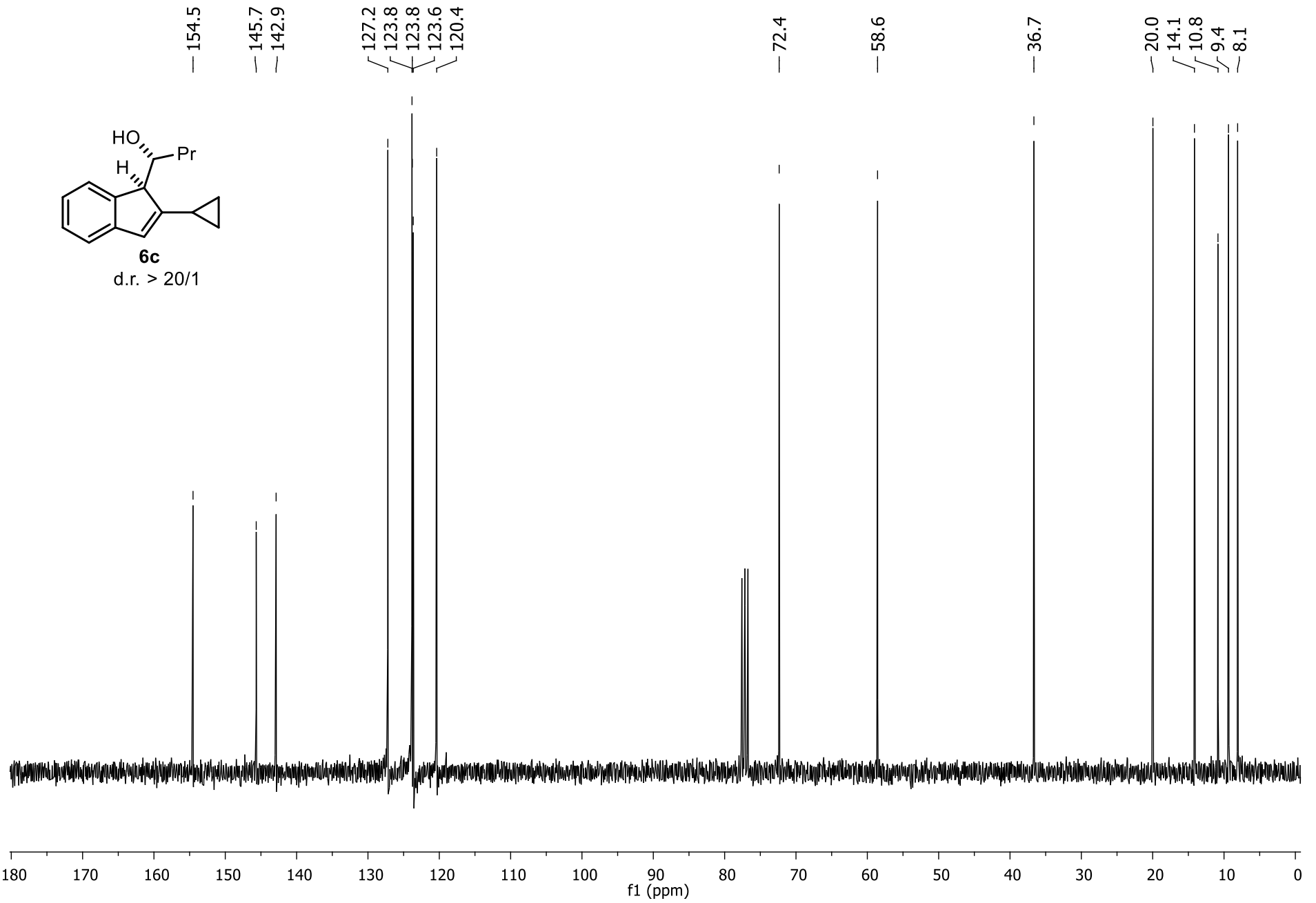
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



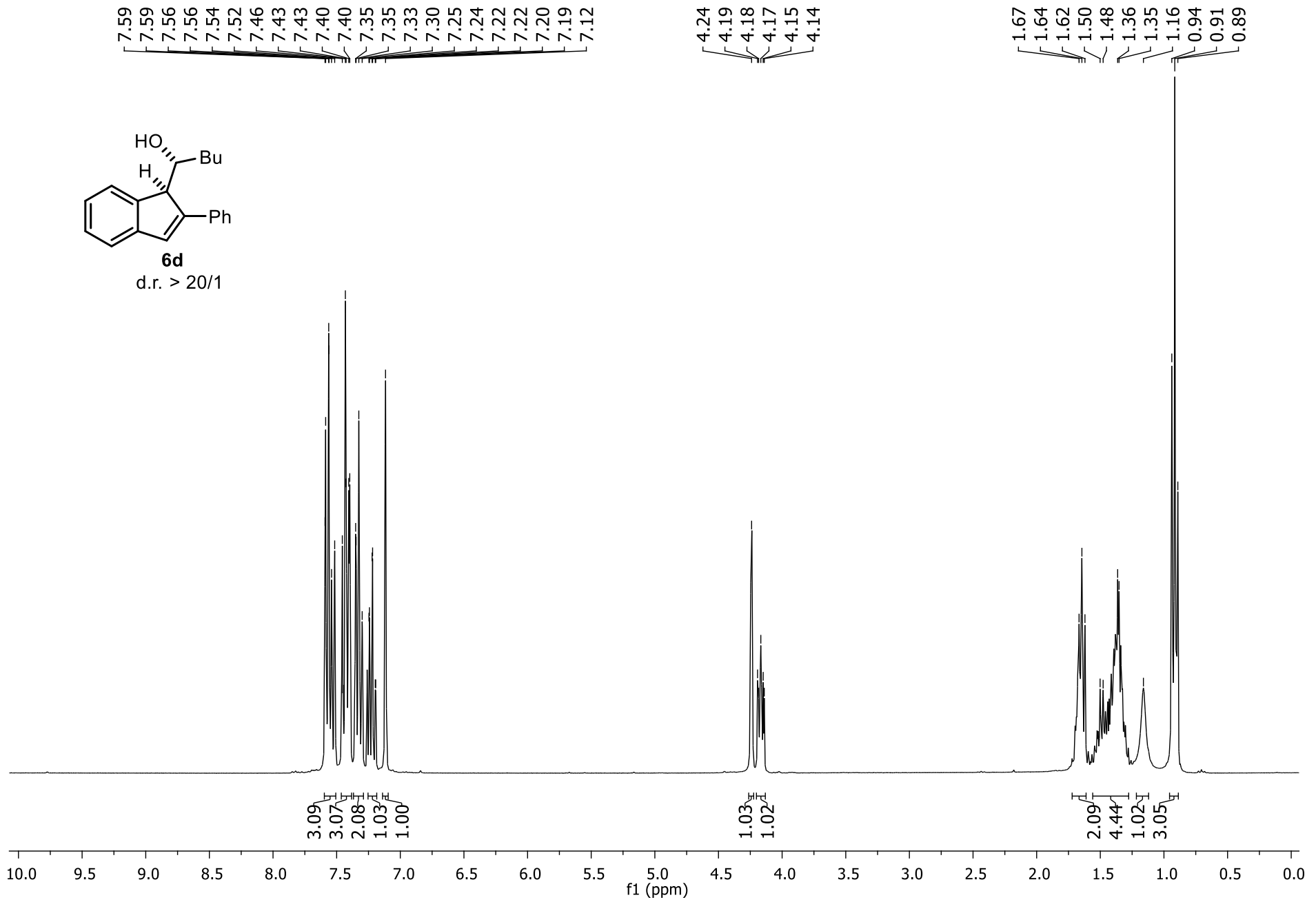
^{1}H NMR (300 MHz, $CDCl_3$)



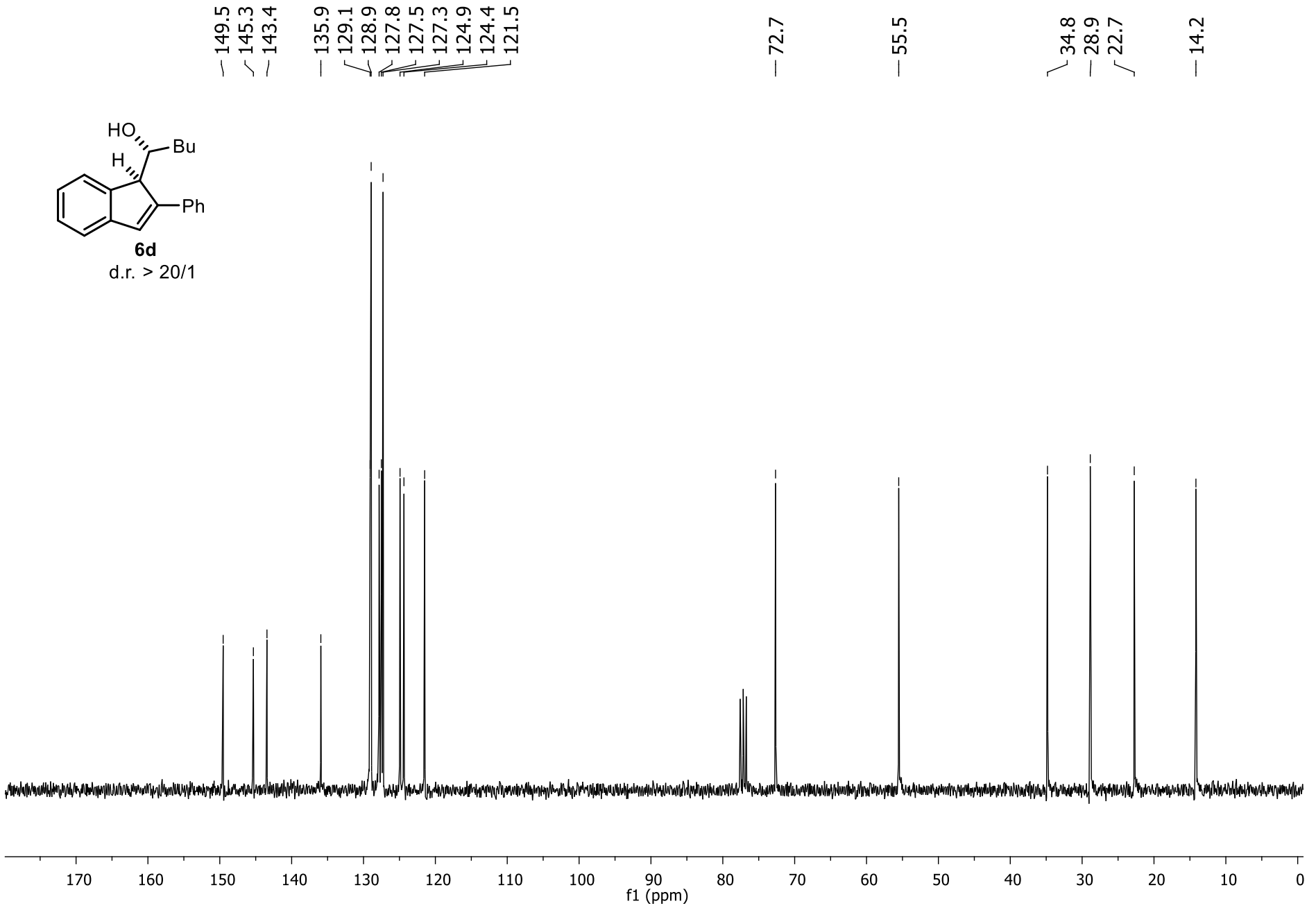
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



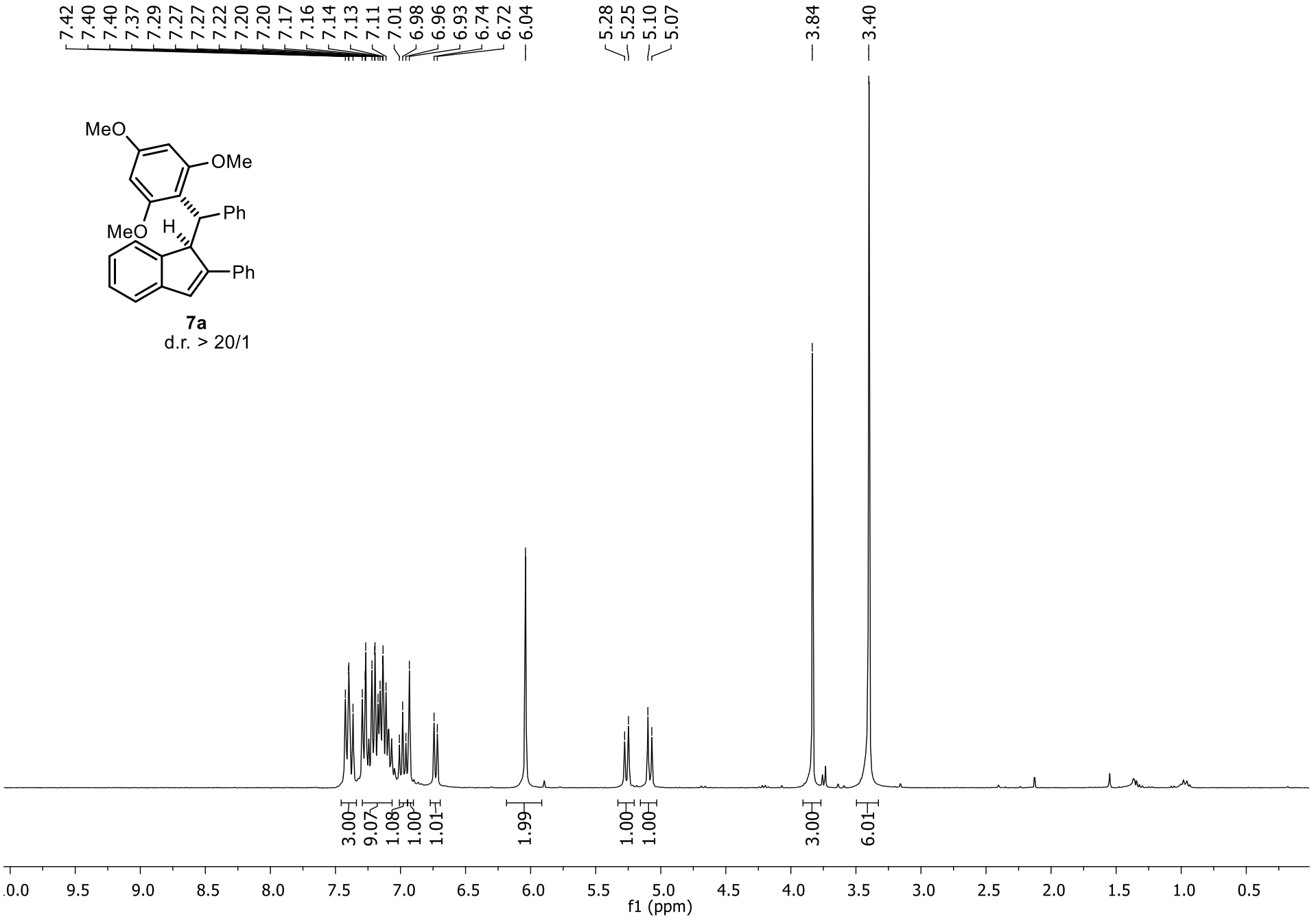
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

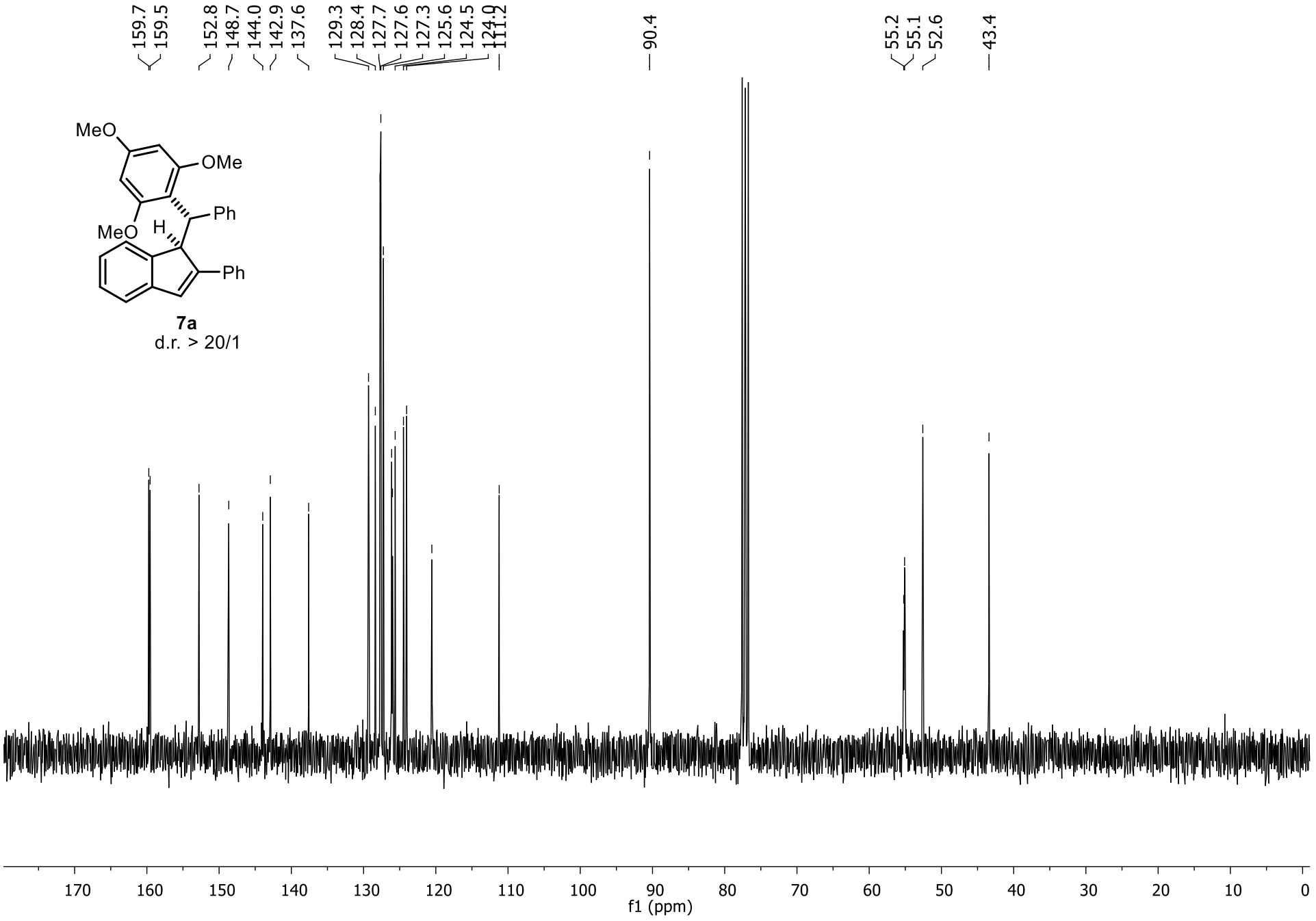


^{1}H NMR (300 MHz, $CDCl_3$)

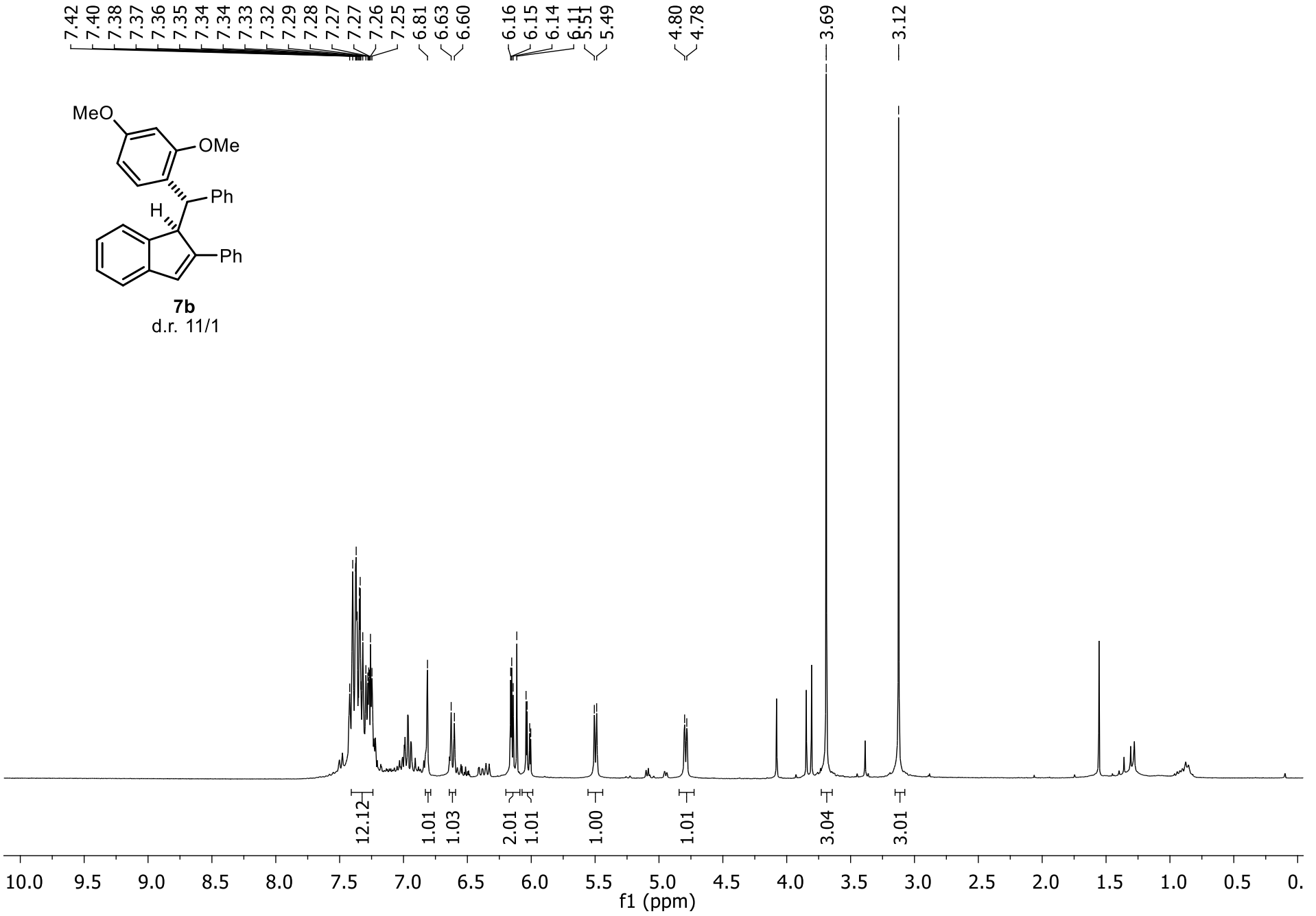


7a
d.r. > 20/1

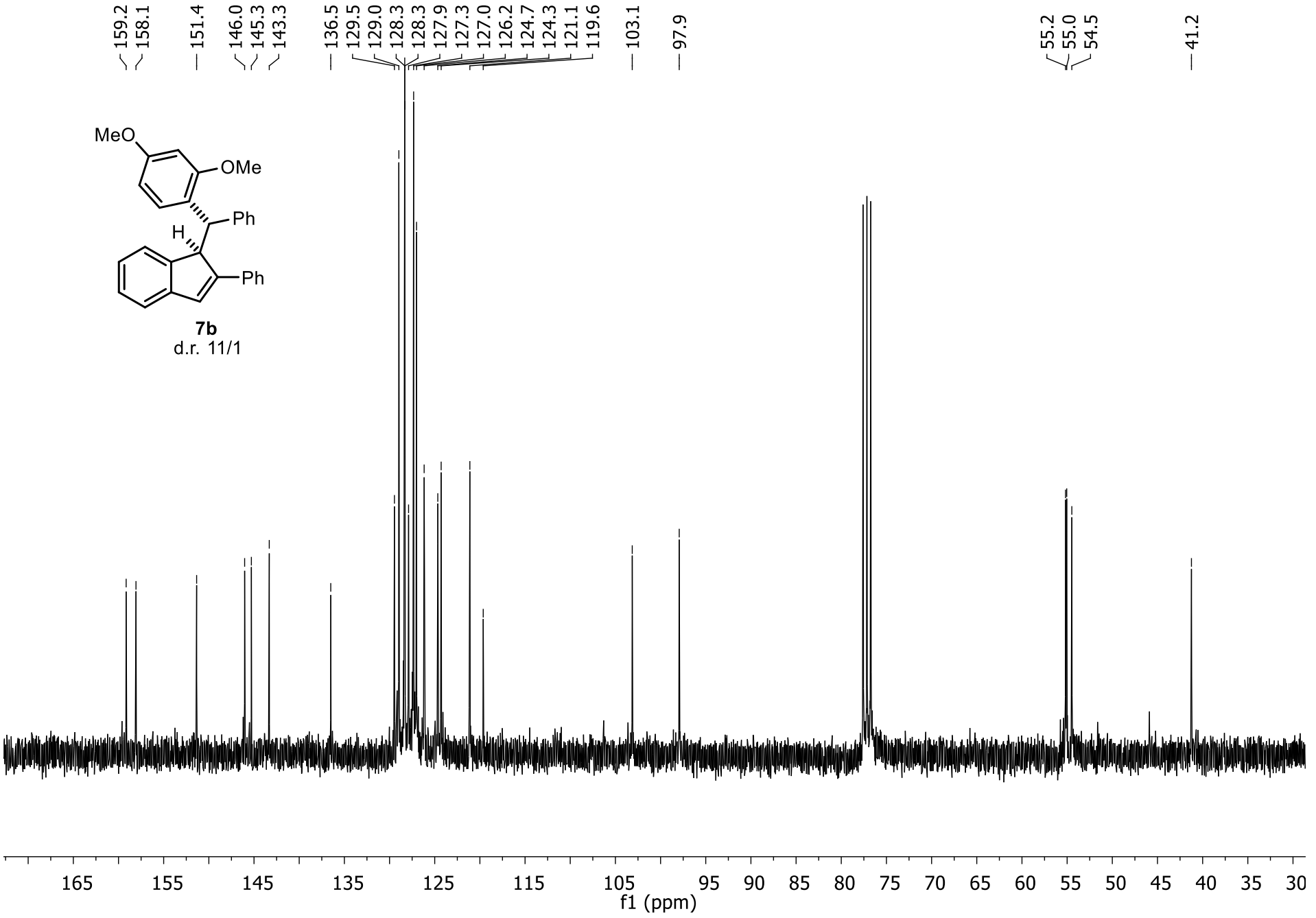
$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



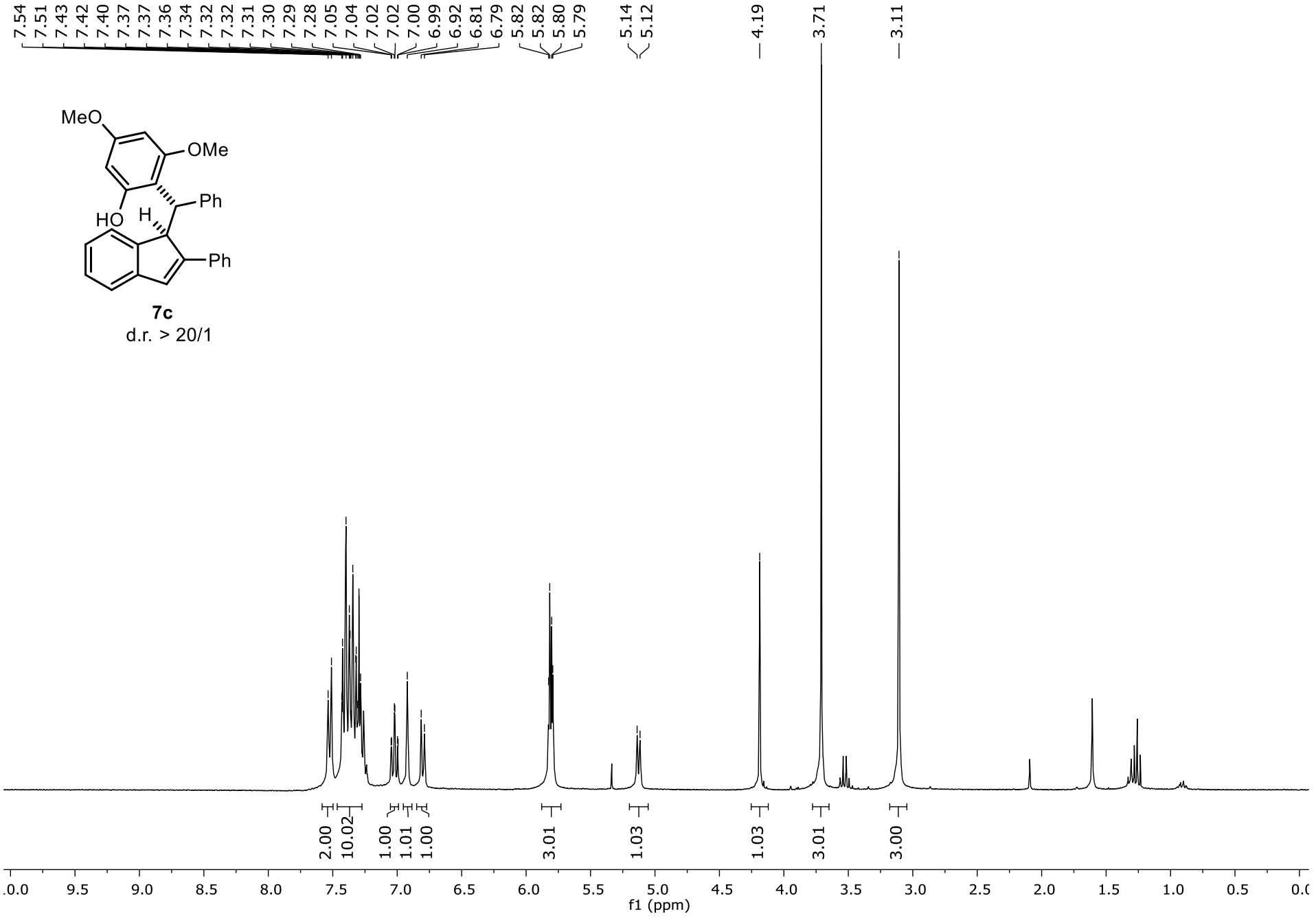
^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

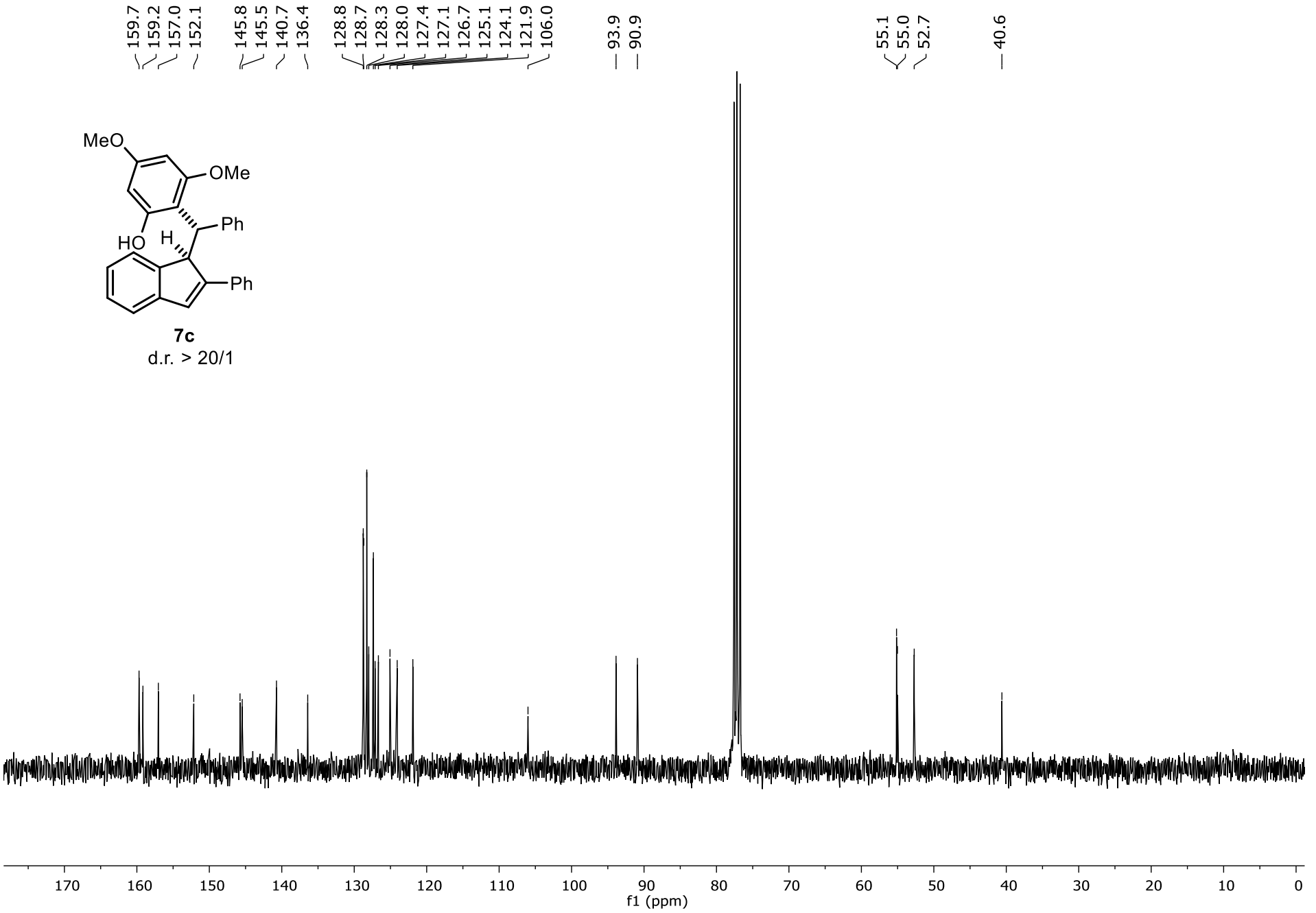


^{1}H NMR (300 MHz, $CDCl_3$)

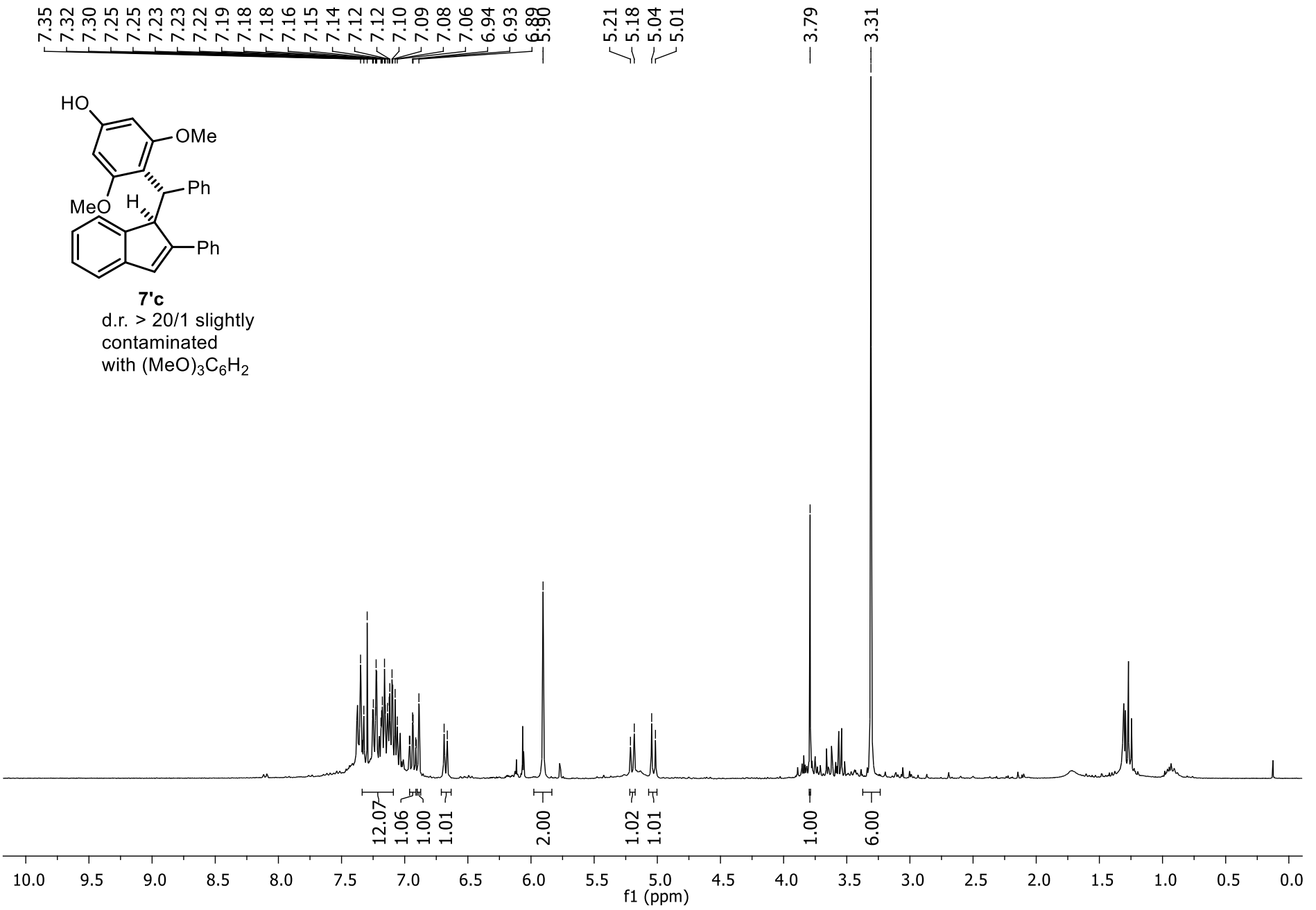


7c
d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

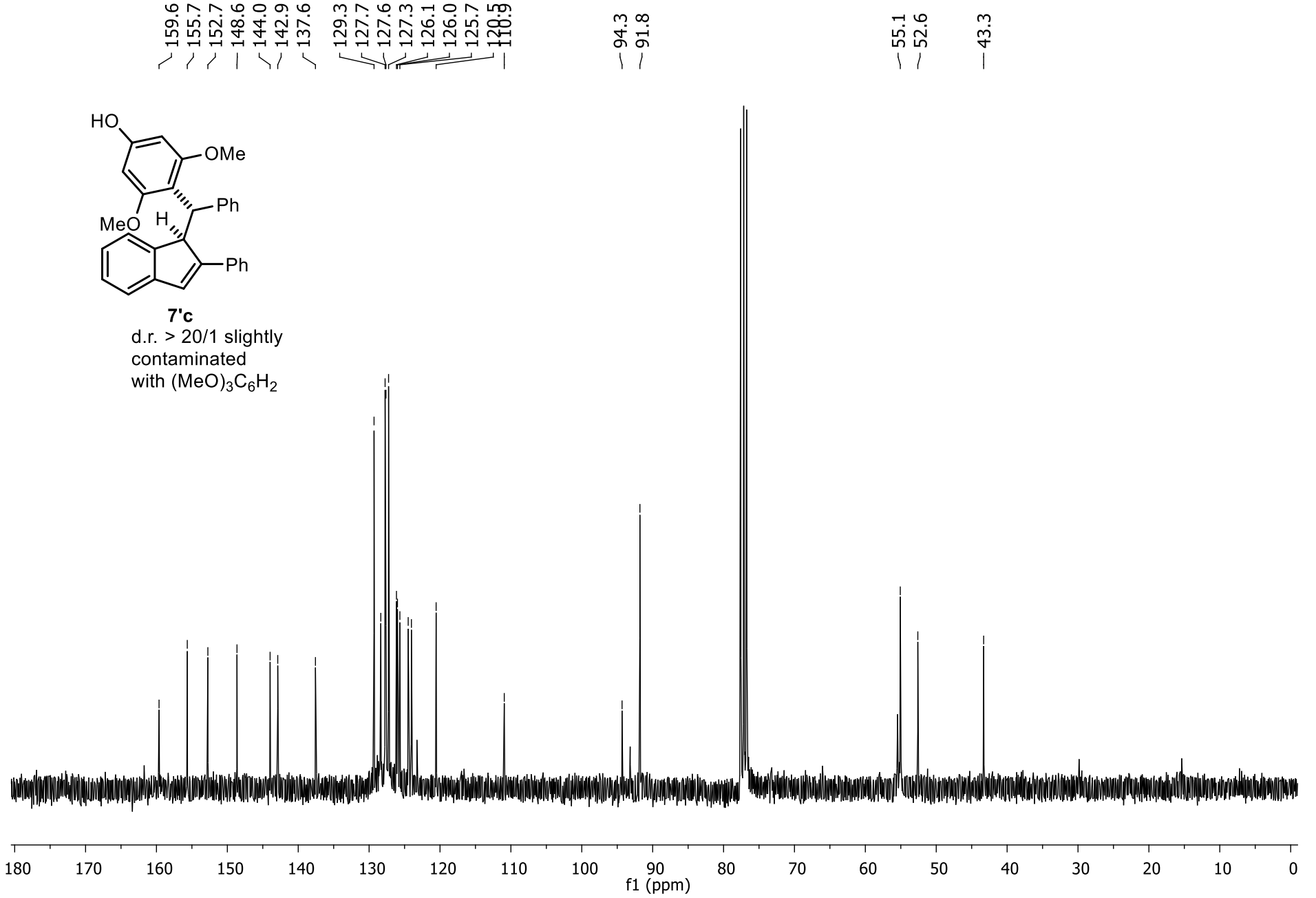


^{1}H NMR (300 MHz, $CDCl_3$)

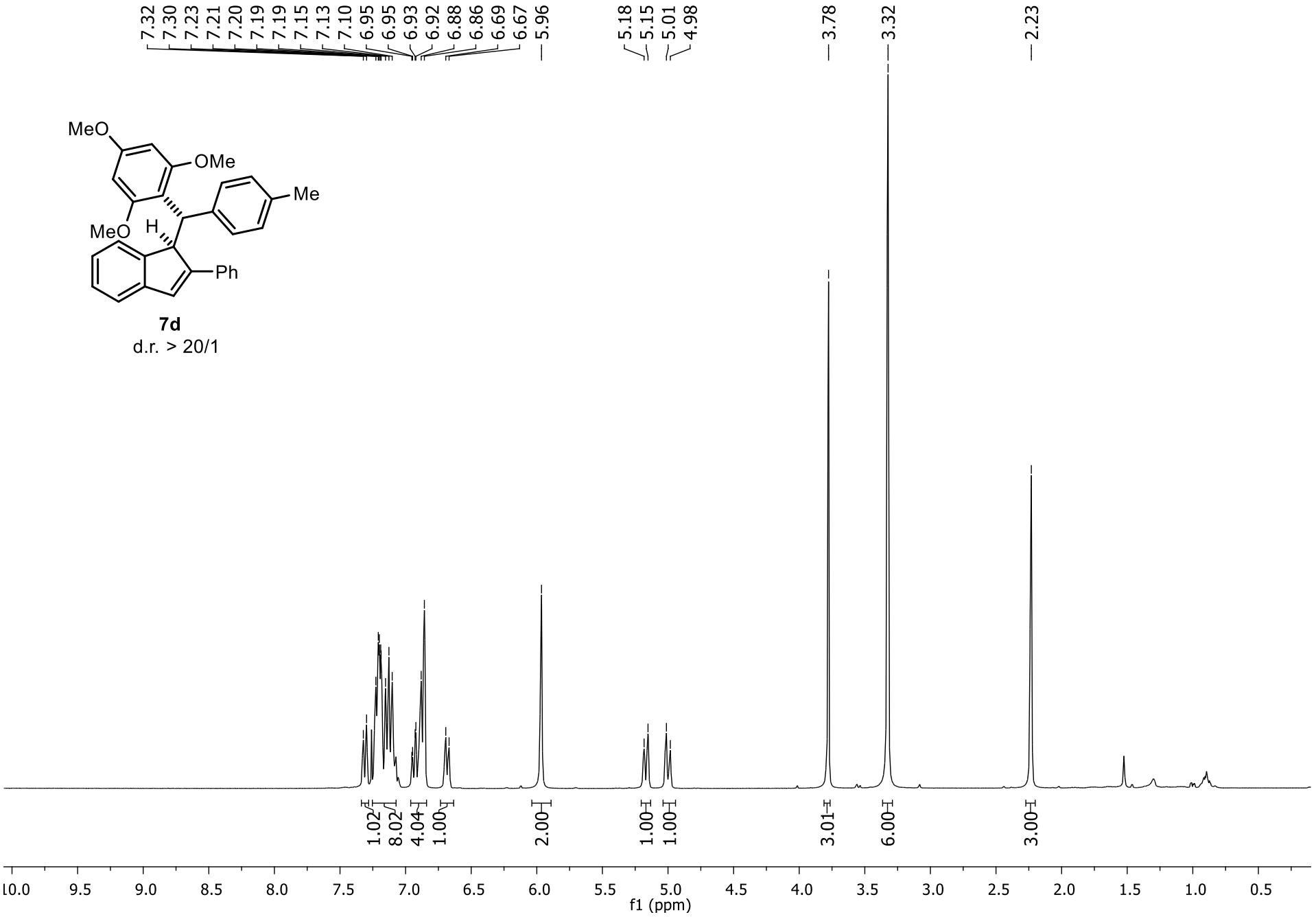


7'c
d.r. > 20/1 slightly contaminated with $(MeO)_3C_6H_2$

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)

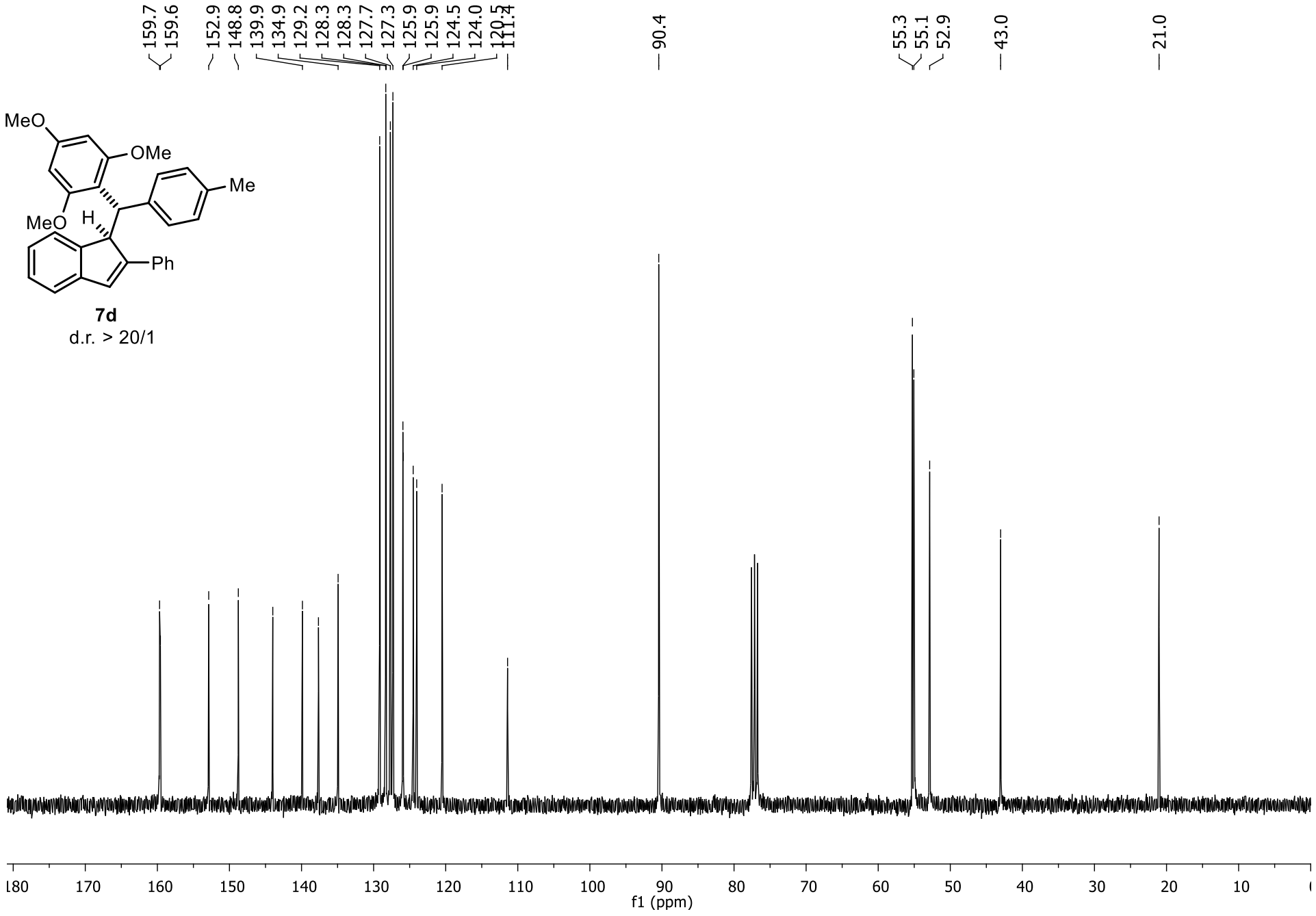


^{1}H NMR (300 MHz, $CDCl_3$)

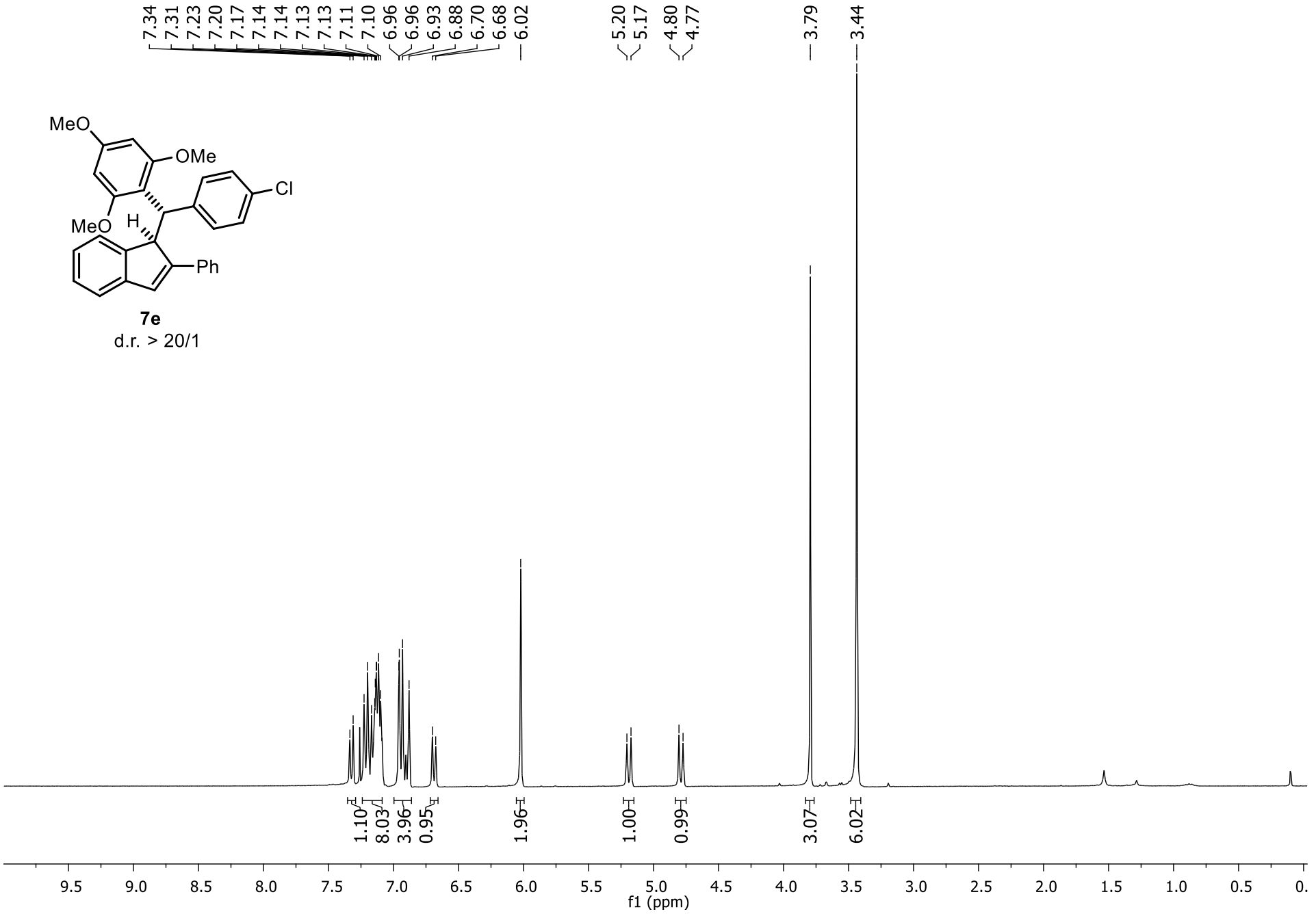


7d
d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



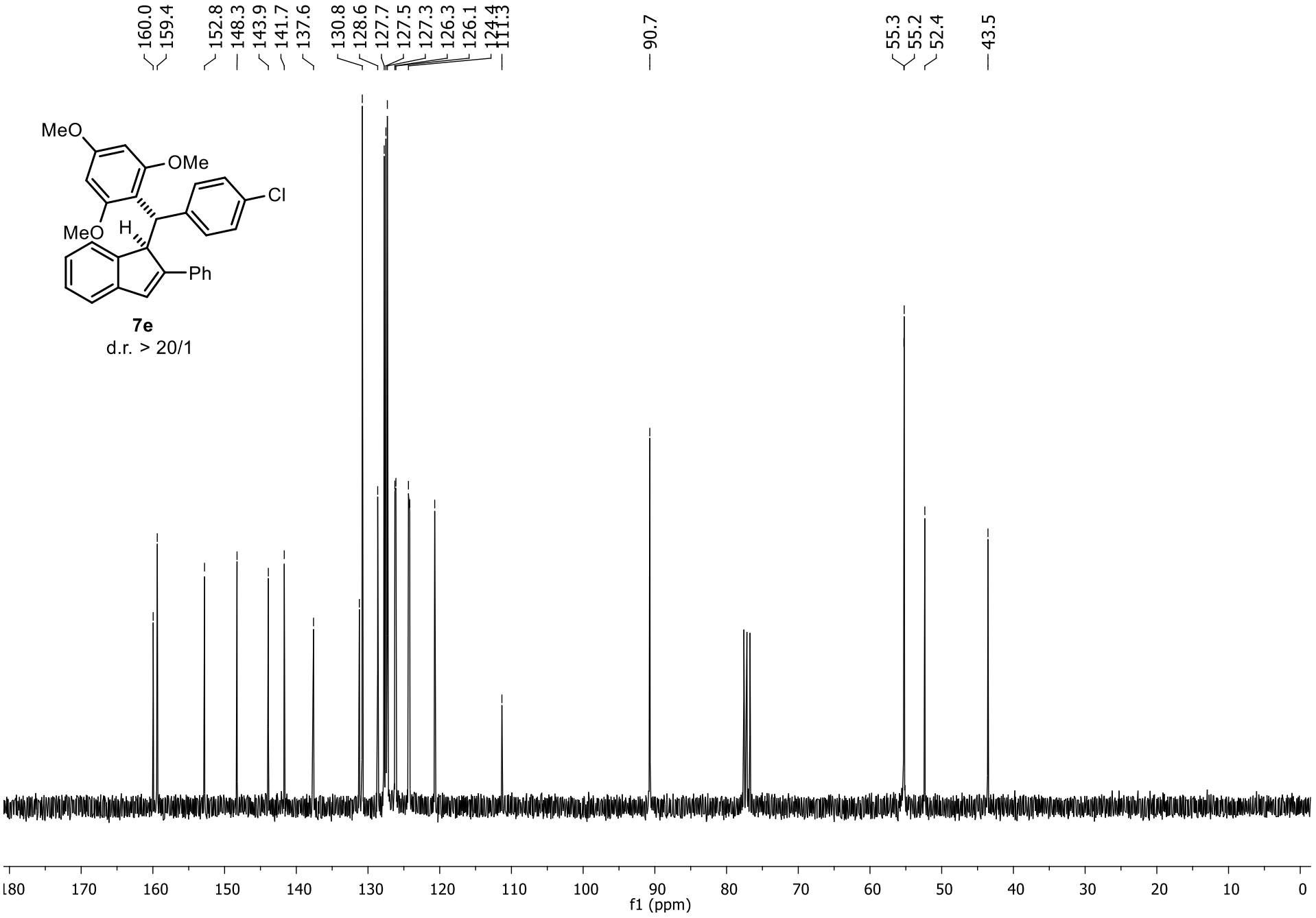
^{1}H NMR (300 MHz, $CDCl_3$)



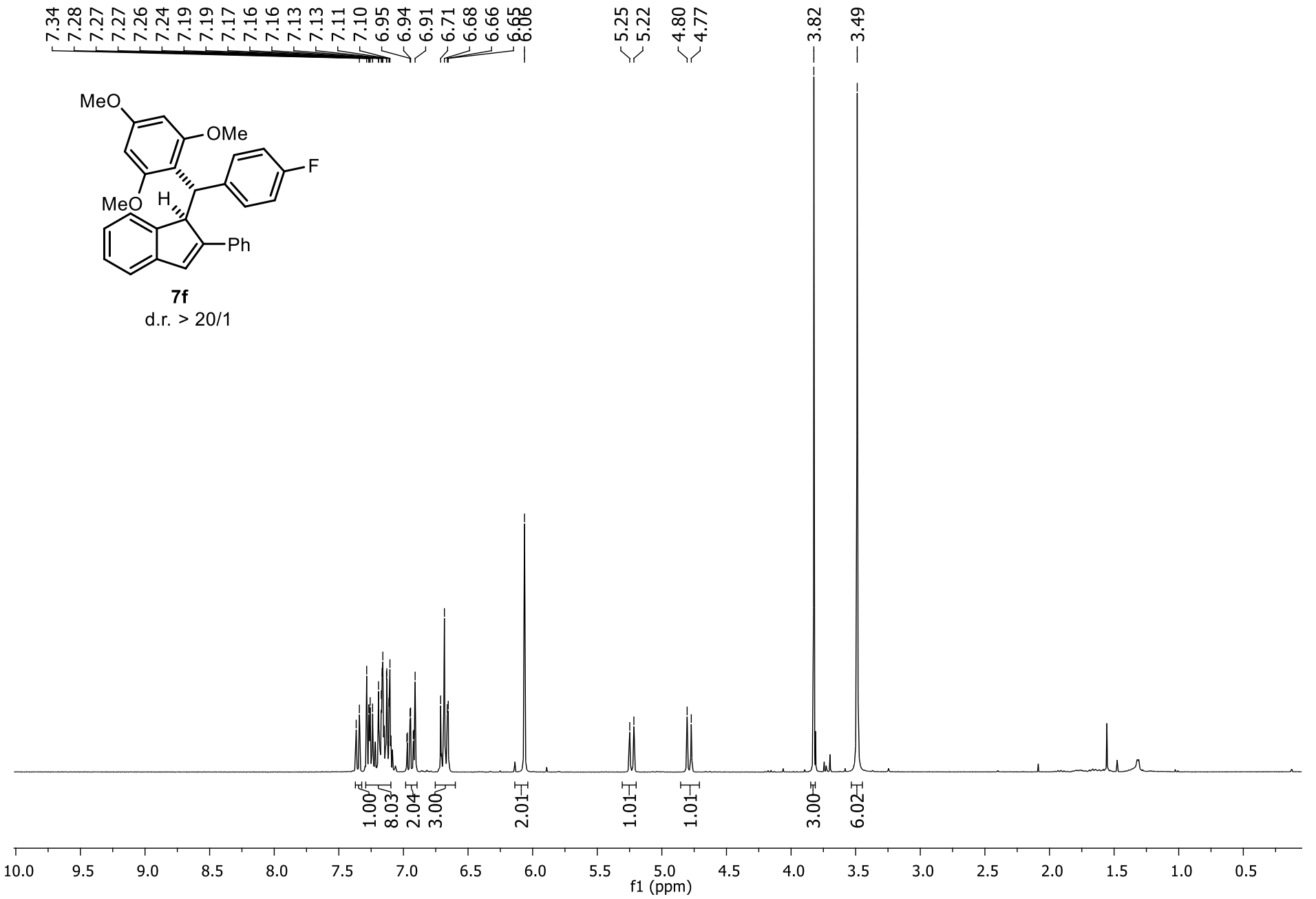
7e

d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



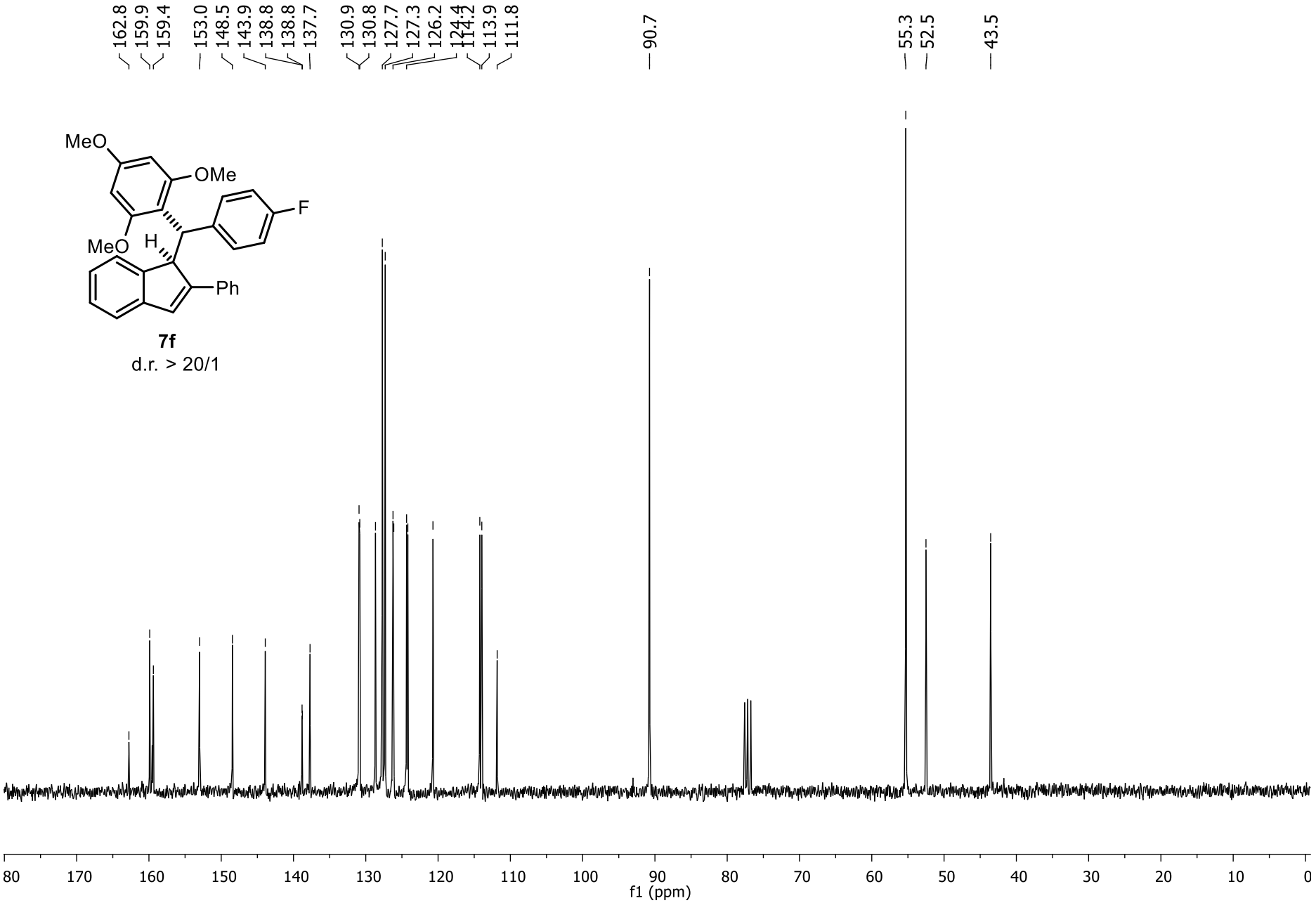
^{1}H NMR (300 MHz, $CDCl_3$)



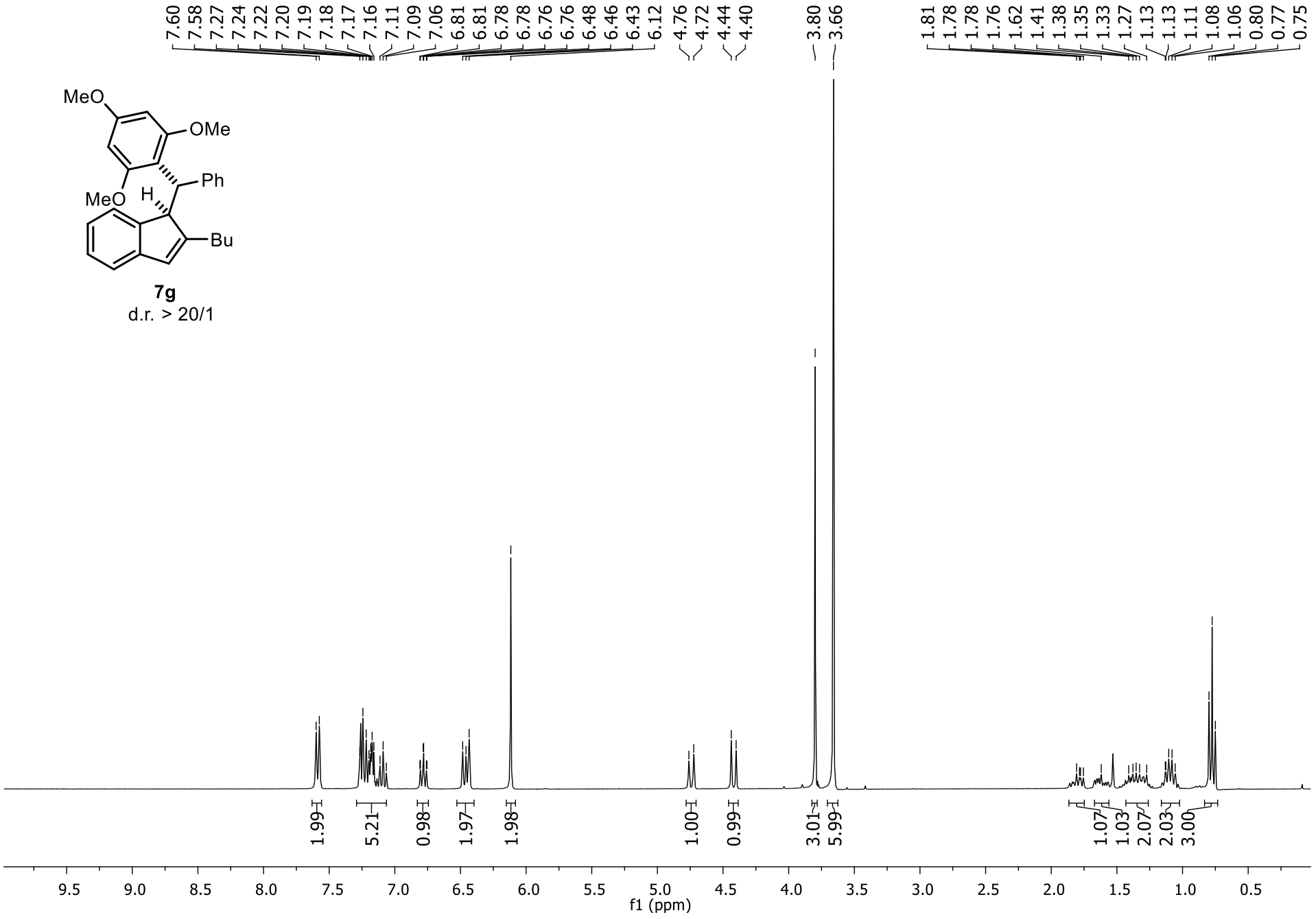
7f

d.r. > 20/1

$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)



^{1}H NMR (300 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR (75.4 MHz, $CDCl_3$)