Supporting Information

Dinuclear Iron Complex-Catalyzed Cross-Coupling of Primary Alkyl Fluorides with Aryl Grignard Reagents

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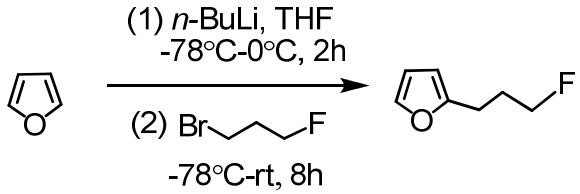
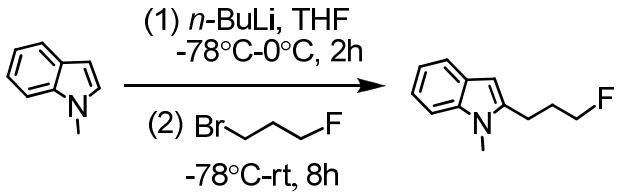
1. **Experimental Section**

General Procedures. All experiments were performed under an atmosphere of dry dinitrogen with the rigid exclusion of air and moisture using standard Schlenk or cannula techniques, or in a glovebox. All organic solvents were freshly distilled from sodium benzophenone ketyl immediately prior to use. 6-fluoro-1-phenyl-1-hexene,[1] 6-fluoro-1-hexene,[2] cyclopropylmethyl fluoride[3], cinnamyl fluoride[4], 6-difluorohexane[5] and phenyl Grignard reagents[6] were prepared according to literature methods. All other chemicals were purchased from either Strem or J&K Chemical Co. and used as received unless otherwise noted. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on a VARIAN Mercury 300 MHz or 400 MHz spectrometer. All chemical shifts were reported in units with references to the residual protons of the deuterated solvents for proton chemical shifts, the ^{13}C of deuterated solvents for carbon chemical shifts, and the ^{19}F of CF_3COOH for fluorine chemical shifts. Mass spectra were recorded with a HP-5989 instrument. GC/MS was performed on a Shimadzu GCMS-QP2010 Plus spectrometer. Atomic absorption spectroscopy (ICP) analyses were recorded with a LEEMAN LABS INC Prodige High Disportion ICP instrument.

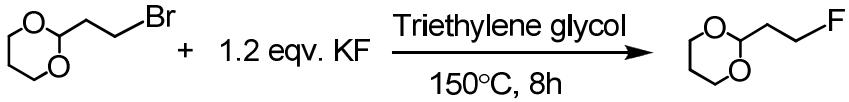
Synthesis of Organofluorine Substrates



Preparation of 2-(3'-fluoropropyl)furan. *n*-BuLi (30.0 mmol) in hexanes was added to a solution of furan (2.04 g, 30.0 mmol) in anhydrous THF (50 mL) cooled at −78°C. The solution was stirred at 0°C for 2 h, and then l-bromo-3-fluoropropane (30.0 mmol) was added. The solution was allowed to warm to room temperature, and then stirred for 8 h to give a light yellow solution. The reaction mixture was then quenched with a saturated aqueous NH_4Cl solution. After extraction with Et_2O (20 mL × 3), the combined organic portions were dried over anhydrous Na_2SO_4. 2-(3-fluoropropyl)furan was obtained as a colorless oil (1.60 g, 42% yield) by distillation. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.32 (s, 1H), 6.30 (m, 1H), 6.04 (m, 1H), 4.57 (t, J = 6.0 Hz, 2H), 4.41 (t, J = 6.0 Hz, 2H), 2.78 (t, J = 7.5 Hz, 2H), 2.11-1.98 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 154.7, 141.1, 110.1, 105.3, 82.97 (d, J = 163.8 Hz), 28.89 (d, J = 20.0 Hz), 23.67 (d, J = 5.0 Hz). ^{19}F NMR (282MHz, $CDCl_3$, 25°C): δ 220.8 (m). HRMS: calcd for $[C_7H_9FO]^+$: 128.0637; Found: 128.0636.



Preparation of 2-(3'-fluoropropyl)-1-methyl-1*H*-indole. *n*-BuLi (30.0 mmol) in hexanes was added to a solution of 1-methyl-1*H*-indole (3.94 g, 30.0 mmol) in anhydrous THF (50 mL) cooled at −78°C. The solution was stirred at 0°C for 2 h, and then l-bromo-3-fluoropropane (30.0 mmol) was added. The solution was allowed to warm to room temperature, and stirred for 8 h to give a light yellow solution. The reaction mixture was then quenched with a saturated aqueous NH_4Cl solution. After extraction with Et_2O (20 mL × 3), the combined organic portions were dried over anhydrous Na_2SO_4. Removal of the solvent gave a brown residue, which was subjected to column chromatographic separation (SiO_2, 300-400 mesh) to give 2-(3-fluoropropyl)-1-methyl-1*H*-indole as a pale yellow oil (1.70 g, 30% yield). ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.64 (d, *J* = 7.8 Hz,1H), 7.37 (d, *J* = 7.8 Hz,1H), 7.30-7.24 (m, 1H), 7.20-7.15 (m, 1H), 6.36 (s, 1H), 4.72 (t, *J* = 5.7 Hz, 1H), 4.56 (t, *J* = 5.7 Hz, 1H), 3.75 (s, 3H), 2.97 (t, *J* = 7.5 Hz, 2H), 2.29-2.11 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 139.6, 137.3, 127.7, 120.7, 119.8, 119.3, 108.8, 98.88, 83.01 (d, *J* = 164.1 Hz), 29.37 (d, *J* = 20.0 Hz), 29.32, 22.40 (d, *J* = 5.3 Hz). ^{19}F NMR (282MHz, $CDCl_3$, 25°C): δ 220.4 (m). HRMS: calcd for $[C_{12}H_{14}FN]^+$: 191.1110; Found: 191.1109.

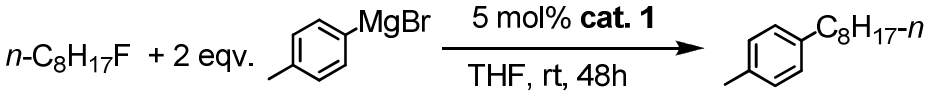


Preparation of 2-(2'-fluoroethyl)-1,3-dioxane. A mixture of anhydrous potassium fluoride (2.10 g, 36.2 mmol), triethylene glycol (60 ml) and 2-(2-bromoethyl)-1,3-dioxane (5.80 g, 30.0 mmol) was heated at 150°C for 8h with vigorous stirring. 2-(2'-fluoroethyl)-1,3-dioxane was obtained as a colorless oil (1.20 g, 30% yield) by distillation. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 4.71 (t, *J* = 5.4 Hz, 1H), 4.62 (t, *J* = 6.0 Hz, 1H), 4.47 (t, *J* = 6.0 Hz, 1H), 4.13-4.07 (m, 2H), 3.82-3.73 (m, 2H), 2.10-1.91 (m, 3H), 1.37-1.33 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 98.79 (d, *J* = 5.9 Hz), 79.77 (d, *J* = 162.2 Hz), 66.78, 36.09 (d, *J* = 19.5 Hz), 25.61. ^{19}F NMR (282MHz, $CDCl_3$, 25°C): δ 220.0 (m). HRMS: calcd for $[C_6H_{10}FO_2]^+$: 133.0665; Found: 133.0664.

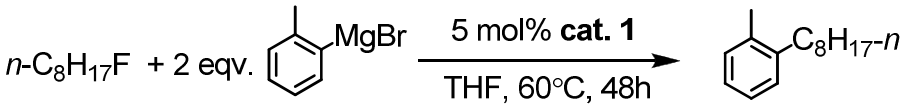
Studies on the performance of some iron complexes as catalysts for cross-coupling reaction of *n*-$C_8H_{17}F$ with *p*-Me-PhMgBr. To a solution of iron complex (0.050 mmol) in THF (10 mL) was added *p*-Me-PhMgBr (2.00 mmol), and *n*-$C_8H_{17}F$ (1.00 mmol) at room temperature and further stirred at room temperature for 48h. A 1.0 M aqueous HCl solution (5 mL) was added to quench the reaction. After extraction with Et_2O (5 mL × 3), the combined organic portions were dried over anhydrous Na_2SO_4. The

yields of 1-C_8H_{16}, 2-C_8H_{16}, *n*-C_8H_{18}, *n*-C_8H_{18}-Ph-*p*-Me and *p*-Me-Ph-Ph-*p*-Me were determined by GC-MS.

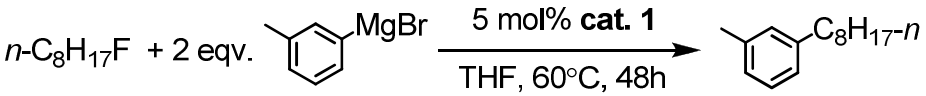
General procedure for [(IPr_2Me_2)Fe(μ_2-NDipp)$_2$(IPr_2Me_2)]-catalyzed C-F bond arylation reactions. To a solution of iron complex [(IPr_2Me_2)Fe(μ_2-NDipp)$_2$(IPr_2Me_2)] (41 mg, 0.050 mmol) in THF (10 mL) was added the aryl Grignard reagent (2.00 mmol), and organic fluoride (1.00 mmol) at -116°C. The mixture was then warmed up to room temperature and further stirred at room temperature or 60°C for 48h. The reaction mixture was then quenched with a 1.0 M aqueous HCl solution (5 mL). After extraction with Et_2O (5 mL × 3), the combined organic portions were dried over anhydrous Na_2SO_4. Removal of the solvent gave a brown residue, which was subjected to column chromatographic separation (SiO_2, 300-400 mesh) to give the arylation products. The yields indicated are referred to the fluoride.



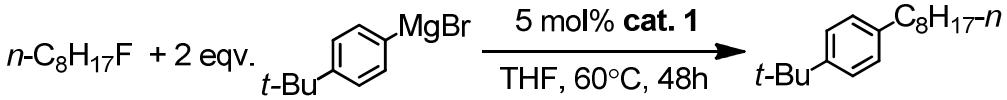
4-Methyl-1-octylbenzene:[7a] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of *p*-TolMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (163 mg, 80% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.08 (m, 4H), 2.57 (t, *J* = 7.8 Hz, 2H), 2.32 (s, 3H), 1.60 (m, 2H), 1.30-1.28 (m, 10H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 139.8, 134.8, 128.8, 128.2, 35.51, 31.88, 31.67, 29.49, 29.34, 29.26, 22.66, 20.95, 14.09. Besides 4-methyl-1-octylbenzene, GC-MS analysis showed the retention of *n*-octyl fluoride in 7% yield and the formation of *n*-C_8H_{18} and 1-octene in 3% and 2% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 12% yield.



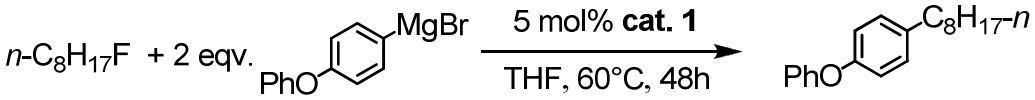
2-Methyl-1-octylbenzene:[7b] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of *o*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (153 mg, 75% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.20 (m, 4H), 2.66 (t, *J* = 7.8 Hz, 2H), 2.38 (s, 3H), 1.65 (m, 2H), 1.42-1.36 (m, 10H), 0.97 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 141.2, 135.8, 130.1, 128.8, 125.8, 125.7, 33.40, 31.96, 30.36, 29.80, 29.60, 29.36, 22.74, 19.33, 14.17. Besides 2-methyl-1-octylbenzene, GC-MS analysis showed the retention of *n*-octyl fluoride in 18% yield, respectively.



3-Methyl-1-octylbenzene:[7c] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of *m*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (169 mg, 83% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.18 (t, *J* = 7.5 Hz, 1H), 7.00 (m, 3H), 2.57 (t, *J* = 7.8 Hz, 2H), 2.34 (s, 3H), 1.61 (m, 2H), 1.31-1.28 (m, 10H), 0.89 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 142.8, 137.6, 129.2, 128.0, 126.2, 125.3, 35.91, 31.88, 31.57, 29.48, 29.40, 29.25, 22.65, 21.35, 14.07. Besides 3-methyl-1-octylbenzene, GC-MS analysis showed the formation of *n*-C_8H_{18}, 1-octene and 2-octene in 2%, 3% and 8% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 3,3'-dimethylbiphenyl in 19% yield.

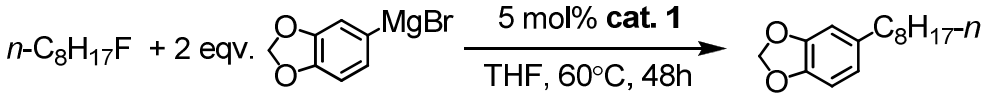


4-*tert*-butyl-1-octylbenzene:[7d] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 4-Bu^t-PhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (222 mg, 90% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.35 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 2.62 (t, *J* = 7.5 Hz, 2H), 1.66 (m, 2H), 1.38-1.33 (m, 19H), 0.93 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 148.3, 139.9, 128.1, 125.1, 35.53, 34.36, 31.99, 31.61, 31.49, 29.60, 29.57, 29.37, 22.76, 14.19. Besides 4-*tert*-butyl-1-octylbenzene, GC-MS analysis showed the formation of 2-octene in 6% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-di-tert-butylbiphenyl in 8% yield.

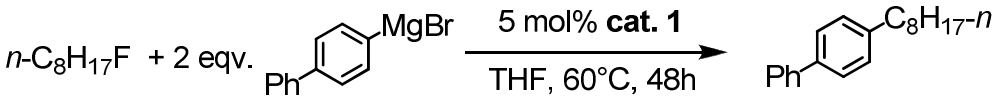


4-Octyl-1-phenoxybenzene: The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of *p*-PhO-PhMgBr (2.00 mmol). Purification by silica gel chromatography (hexane) and further purified by Kugelrohr distillation afforded the title compound as a white solid (240 mg, 85% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.34 (t, *J* = 7.5 Hz, 2H), 7.18-6.95 (m, 7H), 2.61 (t, *J* = 7.5 Hz, 2H), 1.64 (m, 2H), 1.34-1.31 (m, 10H), 0.92 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 157.7, 154.8, 138.0, 129.6, 129.5, 122.8, 118.9, 118.4, 35.22, 31.87, 31.63, 29.46, 29.28, 29.26, 22.66, 14.10. HRMS: calcd for $[C_{20}H_{26}O]^+$: 282.1984; Found: 282.1986.

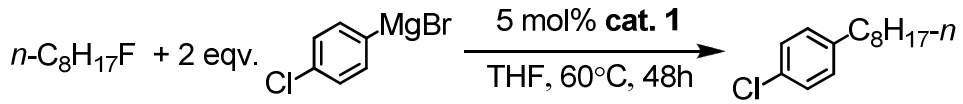
Besides 4-octyl-1-phenoxybenzene, GC-MS analysis showed the formation of 2-octene in 7% yield, respectively.



4-Octyl-1,2-methylenedioxybenzene: The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 1,2-methylenedioxybenzyl-4-magnesium bromide (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (200 mg, 85% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 6.74-6.61 (m, 3H), 5.92 (s, 2H), 2.52 (t, *J* = 7.5 Hz, 2H), 1.57 (m, 2H), 1.31-1.28 (m, 10H), 0.89 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 147.3, 145.3, 136.8, 120.9, 108.8, 107.9, 100.6, 35.64, 31.83, 31.74, 29.42, 29.22, 29.15, 22.62, 14.06. HRMS: calcd for $[C_{15}H_{22}O_2]^+$: 234.1620; Found: 234.1616. Besides 4-octyl-1,2-methylenedioxybenzene, GC-MS analysis showed the formation of 1-octene and 2-octene in 4% and 9% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product biaryl in 5% yield.

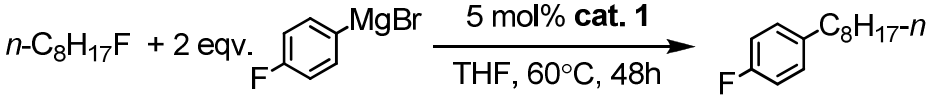


4-Phenyl-1-octylbenzene: The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 4-biphenylmagnesium bromide (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) and further purified by Kugelrohr distillation afforded the title compound as a white solid (190 mg, 71% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.61-7.26 (m, 9H), 2.66 (t, *J* = 7.5 Hz, 2H), 1.66 (m, 2H), 1.34-1.28 (m, 10H), 0.90 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 142.1, 141.2, 138.5, 128.8, 128.7, 127.0, 126.9, 35.63, 31.92, 31.55, 29.53, 29.42, 29.31, 22.71, 14.15. HRMS: calcd for $[C_{20}H_{26}]^+$: 266.2035; Found: 266.2032. Besides 4-phenyl-1-octylbenzene, GC-MS analysis showed the formation of *n*-octane and 2-octene in 4% and 12% yield, respectively.

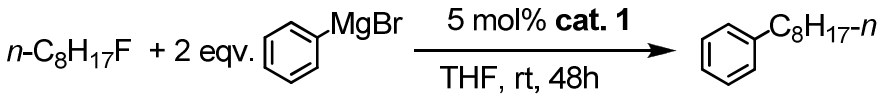


4-Chloro-1-octylbenzene:[7e] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 4-ClPhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (180 mg, 80% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.25 (d, *J* = 8.4 Hz, 2H), 7.12 (d, *J* = 8.1 Hz, 2H), 2.59 (t, *J* = 7.5

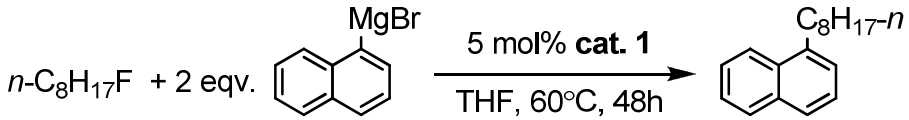
Hz, 2H), 1.60 (m, 2H), 1.32-1.29 (m, 10H), 0.91 (t, J = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 141.2, 131.1, 129.7, 128.2, 35.25, 32.83, 32.37, 29.40, 29.21, 29.16, 22.63, 14.06. Besides 4-chloro-1-octylbenzene, GC-MS analysis showed the formation of 1-octene in 4% yield, and the retention of *n*-octyl fluoride in 8% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dichlorobiphenyl in 8% yield.



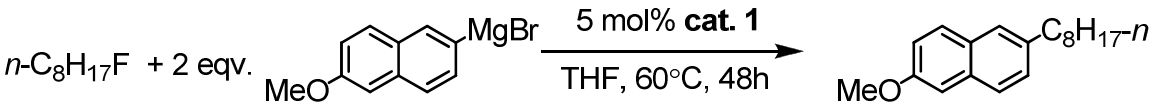
4-Fluoro-1-octylbenzene:[7f] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 4-FPhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (157 mg, 75% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.17-7.12 (m, 2H), 7.02-6.95 (m, 2H), 2.60 (t, J = 7.8 Hz, 2H), 1.62 (m, 2H), 1.34-1.30 (m, 10H), 0.92 (t, J = 6.9 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 161.1 (d, J = 241.3 Hz), 138.4 (d, J = 3.1 Hz), 129.6 (d, J = 7.7 Hz), 114.9 (d, J = 20.9 Hz), 35.13, 31.88, 31.64, 29.46, 29.27, 29.22, 22.67, 14.08. Besides 4-fluoro-1-octylbenzene, GC-MS analysis showed the formation of 1-octene in 8% yields, and the retention of *n*-octyl fluoride in 4% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-difluorobiphenyl in 24% yield.



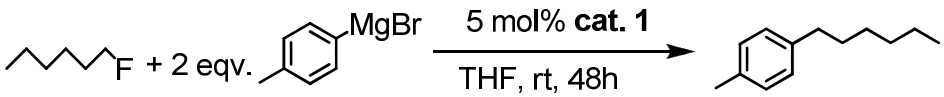
***n*-Octylbenzene:**[7g] The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of PhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (124 mg, 65% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.36-7.23 (m, 5H), 2.67 (t, J = 7.8 Hz, 2H), 1.68 (m, 2H), 1.38-1.34 (m, 10H), 0.96 (t, J = 6.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 142.9, 128.4, 128.2, 125.5, 36.01, 31.91, 31.57, 29.51, 29.38, 29.29, 22.69, 14.12. Besides *n*-octylbenzene, GC-MS analysis showed the formation of *n*-octane and 1-octene in 14% and 6% yields, and the retention of *n*-octyl fluoride in 11% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product biphenyl in 20% yield.



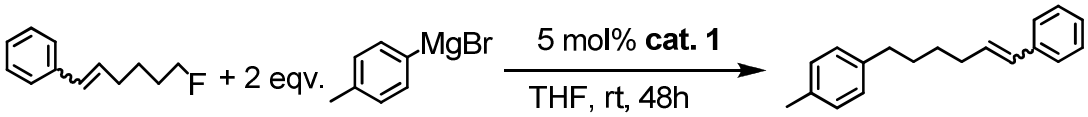
1-Octylnaphthalene： The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 1-naphthylmagnesium bromide (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (154 mg, 64% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 8.09 (d, *J* = 8.1 Hz, 1H), 7.89 (d, *J* = 7.2 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.56-7.34 (m, 4H), 3.10 (t, *J* = 7.8 Hz, 2H), 1.79 (m, 2H), 1.50-1.32 (m, 10H), 0.93 (t, *J* = 6.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 139.0, 133.8, 131.8, 128.6, 126.3, 125.7, 125.5, 125.4, 125.2, 123.8, 33.07, 31.85, 30.81, 29.80, 29.46, 29.26, 22.62, 14.07. HRMS: calcd for $[C_{18}H_{24}]^+$: 240.1878; Found: 240.1882. Besides 1-octylnaphthalene, GC-MS analysis showed the formation of 1-octene in 8% yields, and the retention of *n*-octyl fluoride in 24% yield, respectively.



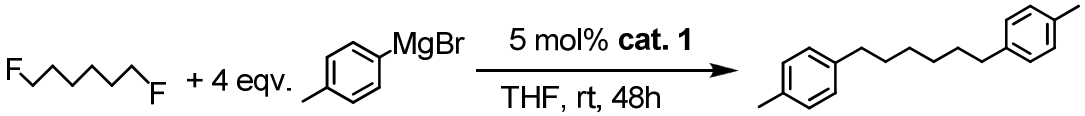
2-Methoxy-6-octylnaphthalene： The reaction was carried out according to the typical procedure by using *n*-octyl fluoride (132 mg, 1.00 mmol) and a THF solution of 6-methoxynaphthyl-2-magnesium bromide (2.00 mmol). Purification by silica gel chromatography (hexane) and further purified by Kugelrohr distillation afforded the title compound as a white solid (200 mg, 74% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.70-7.66 (m, 2H), 7.55 (s, 1H), 7.33-7.26 (m, 1H), 7.15-7.12 (m, 2H), 3.92 (s, 3H), 2.74 (t, *J* = 7.8 Hz, 2H), 1.70 (m, 2H), 1.34-1.29 (m, 10H), 0.90 (t, *J* = 6.6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 157.0, 138.1, 132.8, 129.0, 128.8, 127.9, 126.5, 126.1, 118.5, 101.5, 55.23, 35.88, 31.87, 31.48, 29.50, 29.33, 29.26, 22.65, 14.10. HRMS: calcd for $[C_{19}H_{26}O]^+$: 270.1984; Found: 270.1983. Besides 2-methoxy-6-octylnaphthalene, GC-MS analysis showed the formation of 2-octene in 20% yield, respectively.



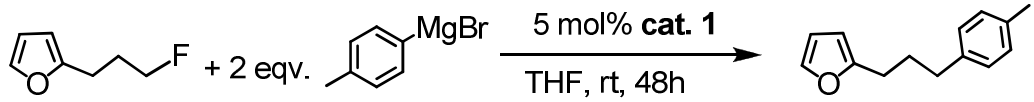
4-Methyl-1-hexylbenzene:[7h] The reaction was carried out according to the typical procedure by using *n*-fluorohexane (104 mg, 1.00 mmol) and a THF solution of *p*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (173 mg, 98% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C)：δ 7.17 (m, 4H), 2.66 (t, *J* = 7.5 Hz, 2H), 2.41 (s, 3H), 1.69 (m, 2H), 1.40-1.37 (m, 6H), 0.99 (t, *J* = 6.1 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C)：δ 139.8, 134.9, 128.9, 128.3, 35.55, 31.79, 31.67, 29.05, 22.65, 20.98, 14.13. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 18% yield.



1-Phenyl-6-*p*-tolyl-1-hexene: The reaction was carried out according to the typical procedure by using a mixture of *cis*- and *trans*-isomers (3:7) of 6-fluoro-1-phenyl-1-hexene (178 mg, 1.00 mmol) and a THF solution of *p*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane) afforded the title compound as a colorless oil (160 mg, 64% yields); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.43-7.13 (m, 9H), 6.51-6.42 (m, 1H), 6.33-6.23 (m, 1H x 7/10), 5.77-5.68 (m, 1H x 3/10), 2.68 (t, *J* = 7.5 Hz, 2H), 2.46-2.42 (m, 2H x 3/10), 2.39(s, 3H), 2.34-2.27 (m, 2H x 7/10), 1.79-1.67 (m, 2H), 1.63-1.52 (m, 2H) . ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 139.6, 139.5, 137.9, 137.7, 135.1, 133.0, 130.9, 129.9, 129.0, 128.9, 128.8, 128.5, 128.3, 128.1, 126.8, 126.5, 125.9, 35.40, 35.31, 32.96, 31.22, 29.56, 29.01, 28.46, 21.04. HRMS: calcd for $C_{19}H_{22}^{+}$: 250.1722; Found: 250.1724. Besides 1-phenyl-6-p-tolyl-1-hexene, GC-MS analysis showed the formation of hex-1-enylbenzene in 16% yield, and the retention of 6-fluoro-1-phenyl-1-hexene in 17% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 22% yield.

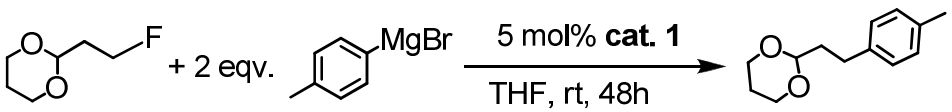


1,6-Di(*p*-tolyl)hexane: Under the standard protocol, the reaction conducted with four equivalents of *p*-MePhMgBr (4.00 mmol), one equivalent of 1,6-difluorohexane (1.00 mmol), and catalytic amount of **1** (41 mg, 0.050 mmol) gave the product as a colorless oil (190 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$, 25°C): *δ* 7.15-7.10 (m, 8H), 2.61 (t, *J* = 7.6 Hz, 4H), 2.37 (s, 6H), 1.65 (m, 4H), 1.41 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$, 25°C): δ 139.7, 134.9, 128.9, 128.3, 35.50, 31.56, 29.17, 21.00. HRMS: calcd for $[C_{20}H_{26}]^{+}$: 266.2035; Found: 266.2032. Besides 1,6-di(*p*-tolyl)hexane, GC-MS analysis showed the formation of 4-methyl-1-hexylbenzene in 18% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 21% yield.

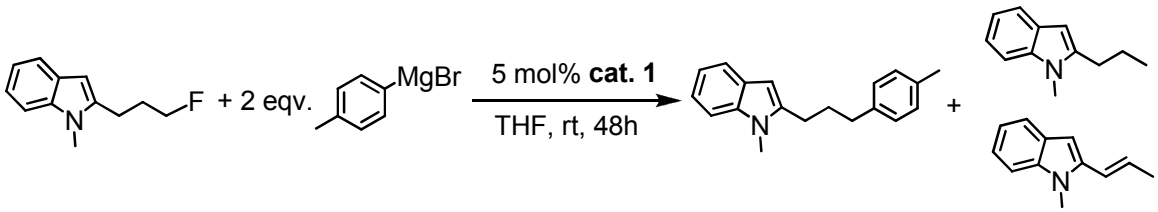


2-(3-*p*-Tolylpropyl)furan: The reaction was carried out according to the typical procedure by using 2-(3'-fluoropropyl)furan (128 mg, 1.00 mmol) and a THF solution of *p*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (hexane/CH_2Cl_2 = 9:1) afforded the title compound as a white solid (172 mg, 86% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.36 (m, 1H), 7.14 (m, 4H), 6.33 (m, 1H), 6.04 (m, 1H), 2.70 (m, 4H), 2.38 (s, 2H), 2.00 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 156.0,

140.8, 138.8, 135.2, 129.0, 128.3, 110.0, 104.8, 34.76, 29.74, 27.41, 20.99. HRMS: calcd for $[C_{14}H_{16}O]^+$: 200.1201; Found: 200.1204. Besides 2-(3-*p*-tolylpropyl)furan, GC-MS analysis showed the formation of 2-propylfuran in 8% yields, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 37% yield.

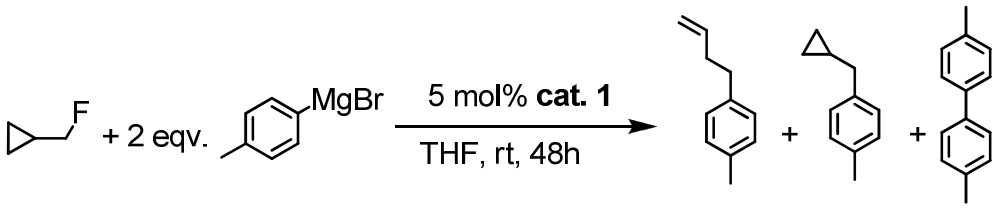


2-(4-Methylphenethyl)-1,3-dioxane: The reaction was carried out according to the typical procedure by using 2-(2'-fluoroethyl)-1,3-dioxane (134 mg, 1.00 mmol) and a THF solution of *p*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (hexane/Et_2O = 9:1) afforded the title compound as a colorless oil (148 mg, 72% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): 7.19 (m, 4H), 4.61 (t, J = 5.3 Hz, 1H), 4.22 (dd, J_1 =11.1 Hz, J_2 = 5.1 Hz, 2H), 3.85 (m, 2H), 2.78 (m, 2H), 2.42 (s, 3H), 2.20 (m, 1H), 2.00 (m, 2H), 1.41 (m, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): 138.5, 135.2, 129.0, 128.3, 101.5, 66.83, 36.73, 29.62, 25.80, 20.97. HRMS: calcd for $[C_{13}H_{18}O_2]^+$: 206.1307; Found: 206.1309. Besides 2-(4-methylphenethyl)-1,3-dioxane, GC-MS analysis showed the formation of 2-ethyl-1,3-dioxane in 24% yield, respectively. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 42% yield.



1-Methyl-2-(3'-*p*-tolylpropyl)-1*H*-indole: The reaction was carried out according to the typical procedure by using 2-(3'-fluoropropyl)-1-methyl-1*H*-indole (191 mg, 1.00 mmol) and a THF solution of *p*-MePhMgBr (2.00 mmol). Purification by silica gel chromatography (*n*-hexane/CH_2Cl_2 = 6:1) afforded the title compound as a pale yellow oil (171 mg, 65% yield); ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.66 (m, 1H), 7.37-7.16 (m, 7H), 6.40 (s, 1H), 3.69 (s, 3H), 2.84 (m, 4H), 2.45 (s, 3H), 2.16 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 140.9, 138.8, 137.3, 135.4, 129.1, 128.9, 128.4, 120.5, 119.8, 119.2, 108.7, 98.80, 34.99, 30.18, 26.24, 21.08. HRMS: calcd for $[C_{19}H_{21}N]^+$: 263.1674; Found: 263.1671. Besides the cross-coupling product, 1-methyl-2-propyl-1*H*-indole[7i] and 1-methyl-2-(prop-1-enyl)-1*H*-indole[7j] have also been isolated as a mixture: Yield: 28%. Pale yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C): δ 7.64 (m, 1.4H), 7.35-7.14 (m, 4.5H), 6.65-6.38 (m, 1.4H), 6.34 (m, 1.0H), 3.76 (s, 1.4H), 3.76 (s, 3.0H), 2.78 (t, J = 7.5 Hz, 2.0H), 2.03 (d, J = 6.6 Hz, 1.4H), 1.84 (m, 2.0H), 1.14 (t, J = 7.5 Hz, 3.0H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C): δ 141.2, 138.8, 137.5, 137.3, 129.2, 128.0, 127.9, 121.1, 120.4, 120.1, 119.7, 119.6,

119.2, 109.0, 108.7, 98.69, 97.67, 29.73, 29.35, 28.91, 21.90, 18.98, 14.06. GC-MS analysis revealed the formation of the homo-coupling product 4,4'-dimethylbiphenyl in 50% yield.



[(IPr_2Me_2)Fe(μ_2-NDipp)$_2$(IPr_2Me_2)]-Catalyzed reaction of cyclopropylmethyl fluoride with *p*-tolylMgBr. To a solution of [(IPr_2Me_2)Fe(μ_2-NDipp)$_2$(IPr_2Me_2)] (41 mg, 0.05 mmol) in THF (10 mL) was added a solution of *p*-MePhMgBr (2.0 mmol) in THF at -116^{0}C, and then cyclopropylmethyl fluoride (0.40 ml, 2.5M in THF, 1.0 mmol) was added. The mixture was allowed to warm to room temperature. After stirred at room temperature for 48 hours, the solution was quenched with a 1.0 M aqueous HCl solution (5 mL). After extraction with Et_2O (5 mL × 3), the combined organic portions were dried over anhydrous Na_2SO_4. Removal of the solvent gave a yellow residue which was subjected to column chromatographic separation (SiO_2, 300-400 mesh, *n*-hexane as the elute). 4,4'-Dimethylbiphenyl (42 mg, 23%) and a mixture of 4-methyl-1-(3'-butenyl)benzene[7k] and 4-methyl-1-cyclopropylmethylbenzene[7l] (70 mg, 48%) were isolated as white solid and colorless oil, respectively. ^{1}H NMR (300 MHz, $CDCl_3$, 25°C) for the mixture: δ 7.27-7.19 (m, 7.2H), 6.03-5.90 (m, 1H), 5.18-5.06 (m, 2H), 2.78 (t, J = 7.5 Hz, 2H), 2.61 (d, J = 6.6 Hz, 1.6H), 2.50-2.44 (m, 2H), 2.42 (s, 5.4H) , 1.11-0.97 (m, 0.8H), 0.64-0.58 (m, 1.6H), 0.32-0.27 (m, 1.6H). ^{13}C NMR (75 MHz, $CDCl_3$, 25°C) for the mixture: δ 139.1, 138.8, 138.2, 135.3, 135.2, 129.0, 128.9, 128.3, 128.2, 114.8, 39.96, 35.70, 34.97, 29.77, 21.40, 12.07, 4.67. The integral ratio of the benzylic methylene protons suggests the corresponding yield of 27% for 4-methyl-1-(3'-butenyl)benzene, and 21% for 4-methyl-1-cyclopropylmethylbenzene.

2. References

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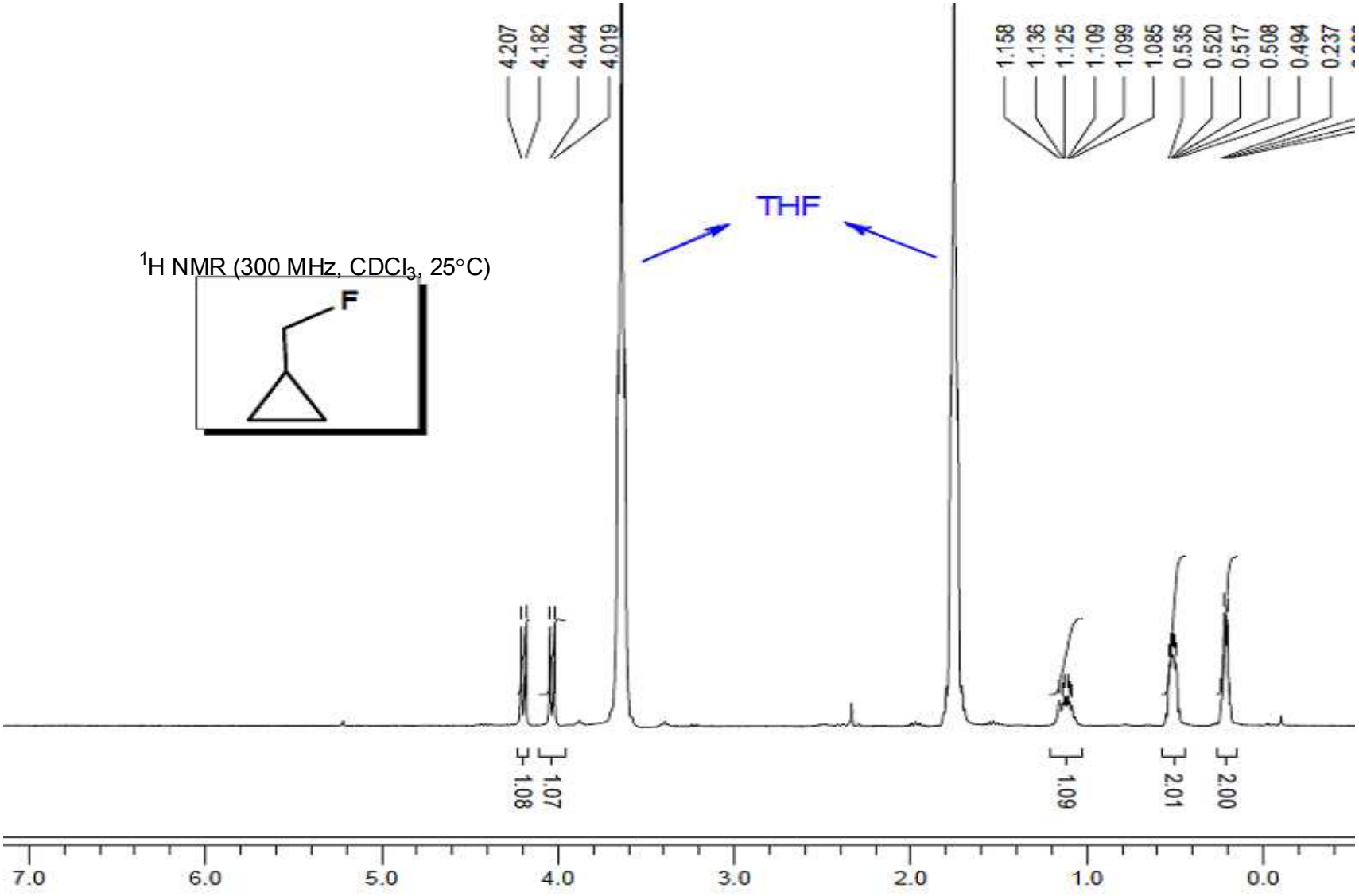
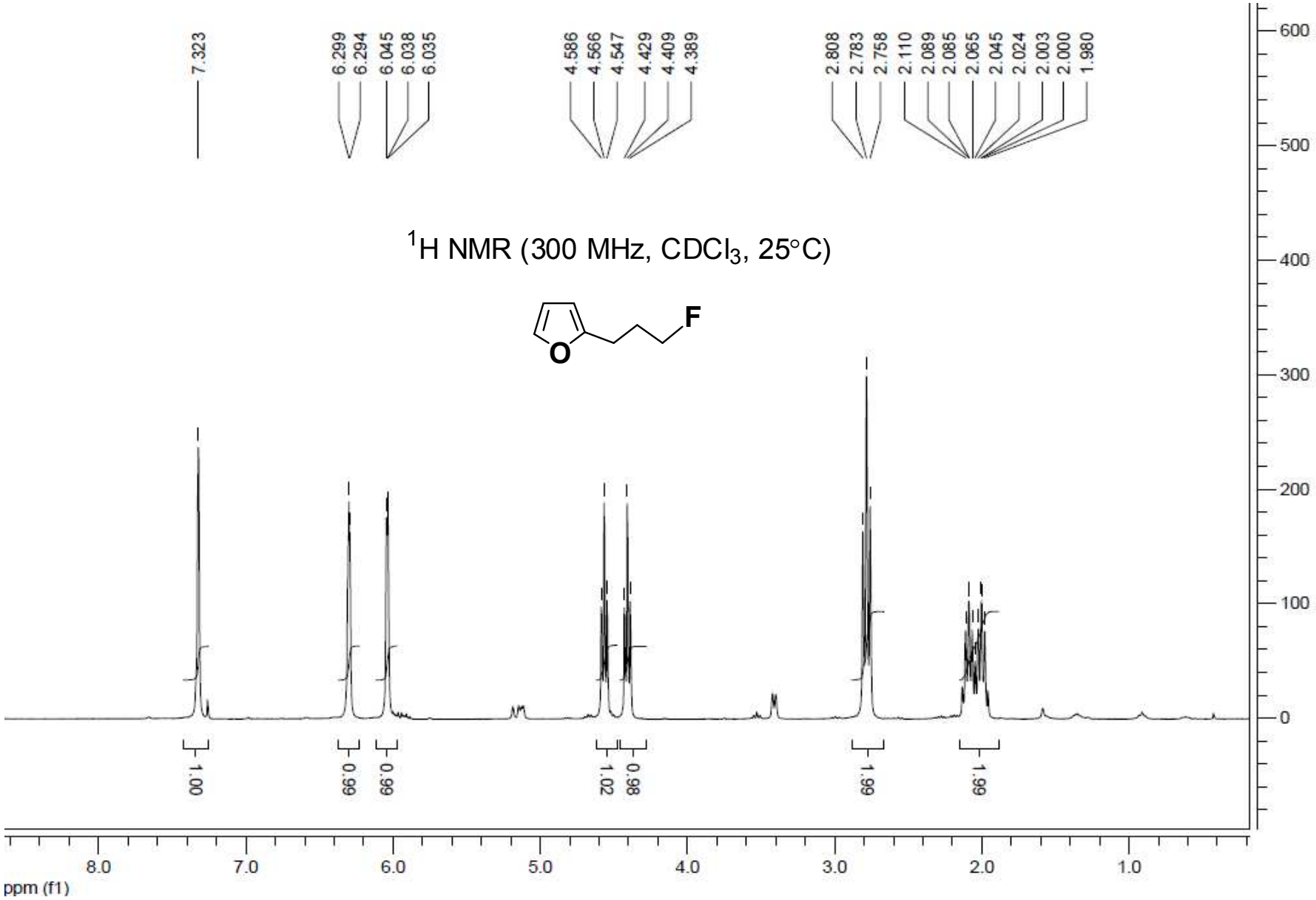
3. ^{1}H and ^{13}C NMR Spectra of Organofluorines and Arylation Products

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6.045
6.038
6.035
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4.566
4.547
4.429
4.409
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2.783
2.758
2.110
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2.085
2.065
2.045
2.024
2.003
2.000
1.980
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
F
O
1.00
0.99
0.99
1.02
0.98
1.99
1.99
600
500
400
300
200
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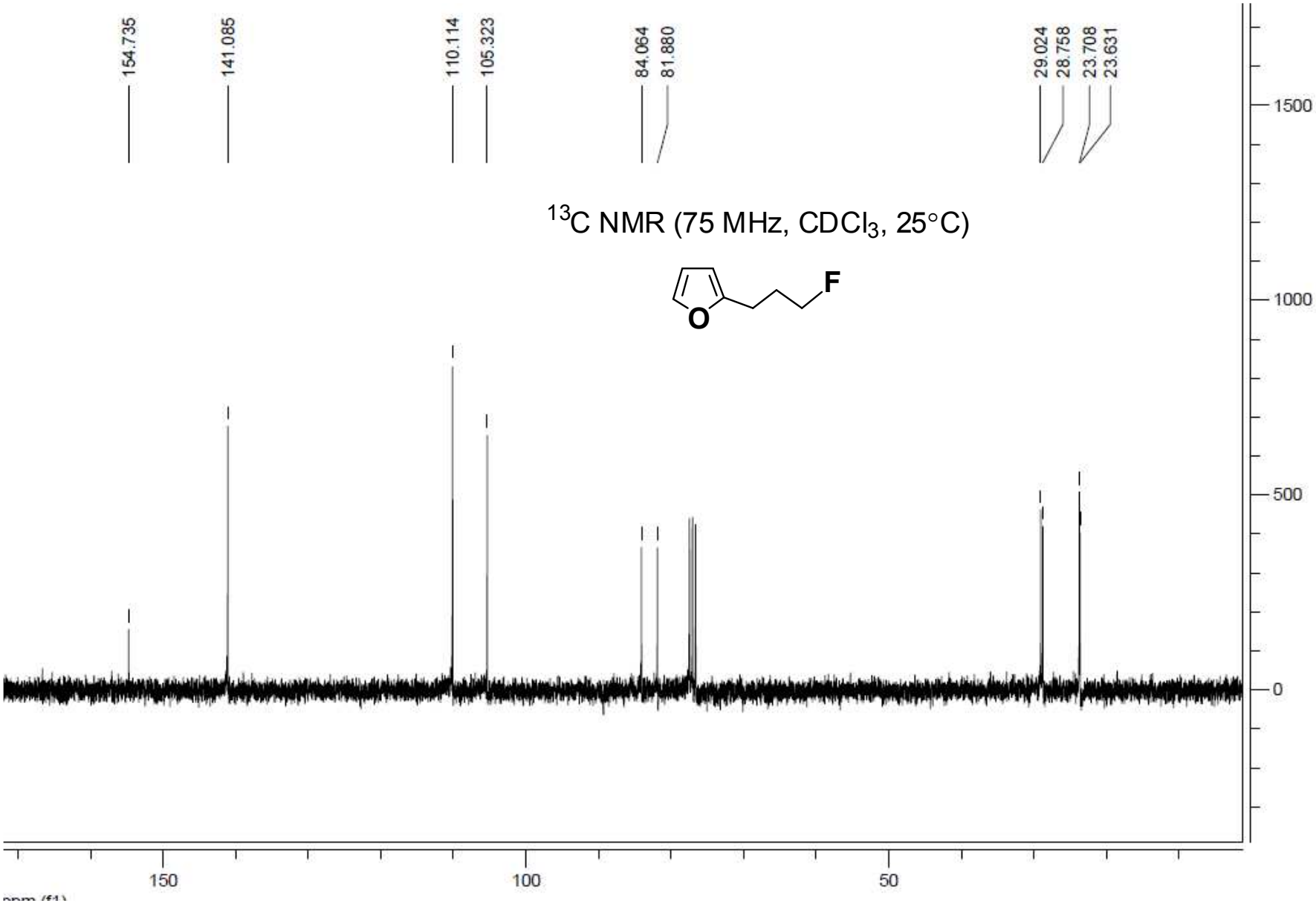
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)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81.880
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28.758
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O
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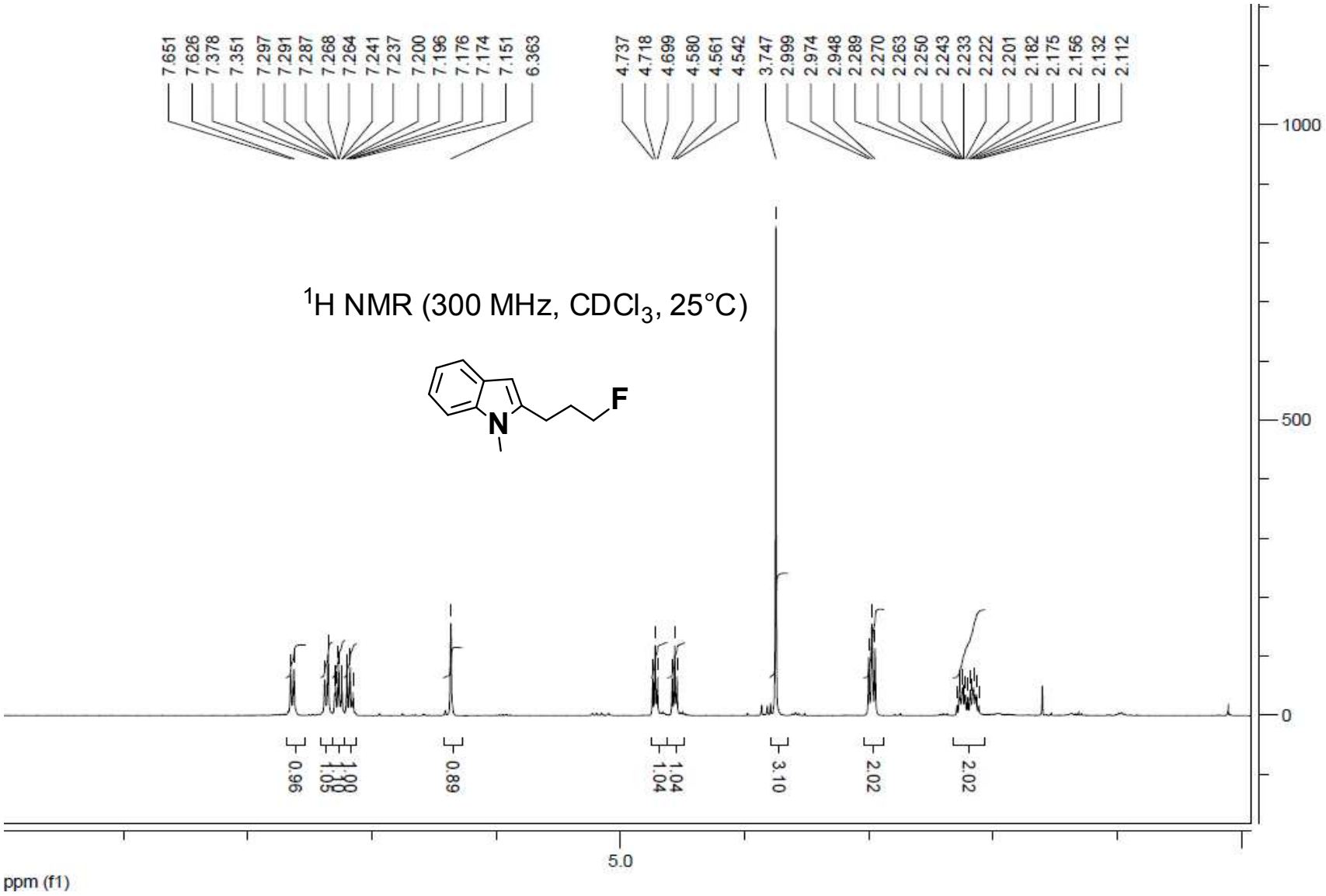
1000
500
0
150
100
50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7.351
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7.176
7.174
7.151
6.363
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2.289
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2.263
2.250
2.243
2.233
2.222
2.201
2.182
2.175
2.156
2.132
2.112
1H NMR (300 MHz, CDCl3, 25°C)
F
N
1000
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1.00
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2.02
2.02
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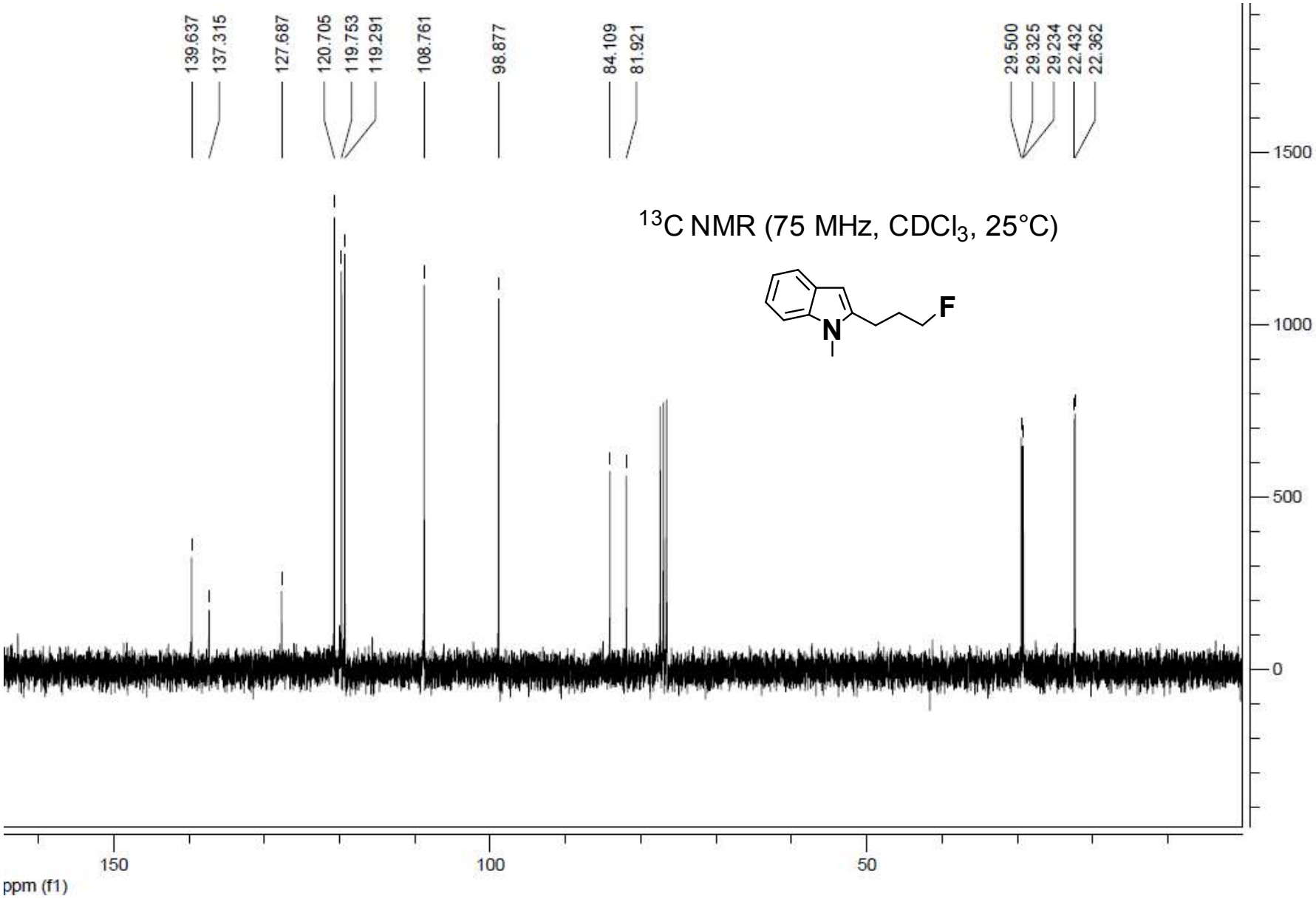
ppm (f1)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29.500
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29.234
22.432
22.362
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N
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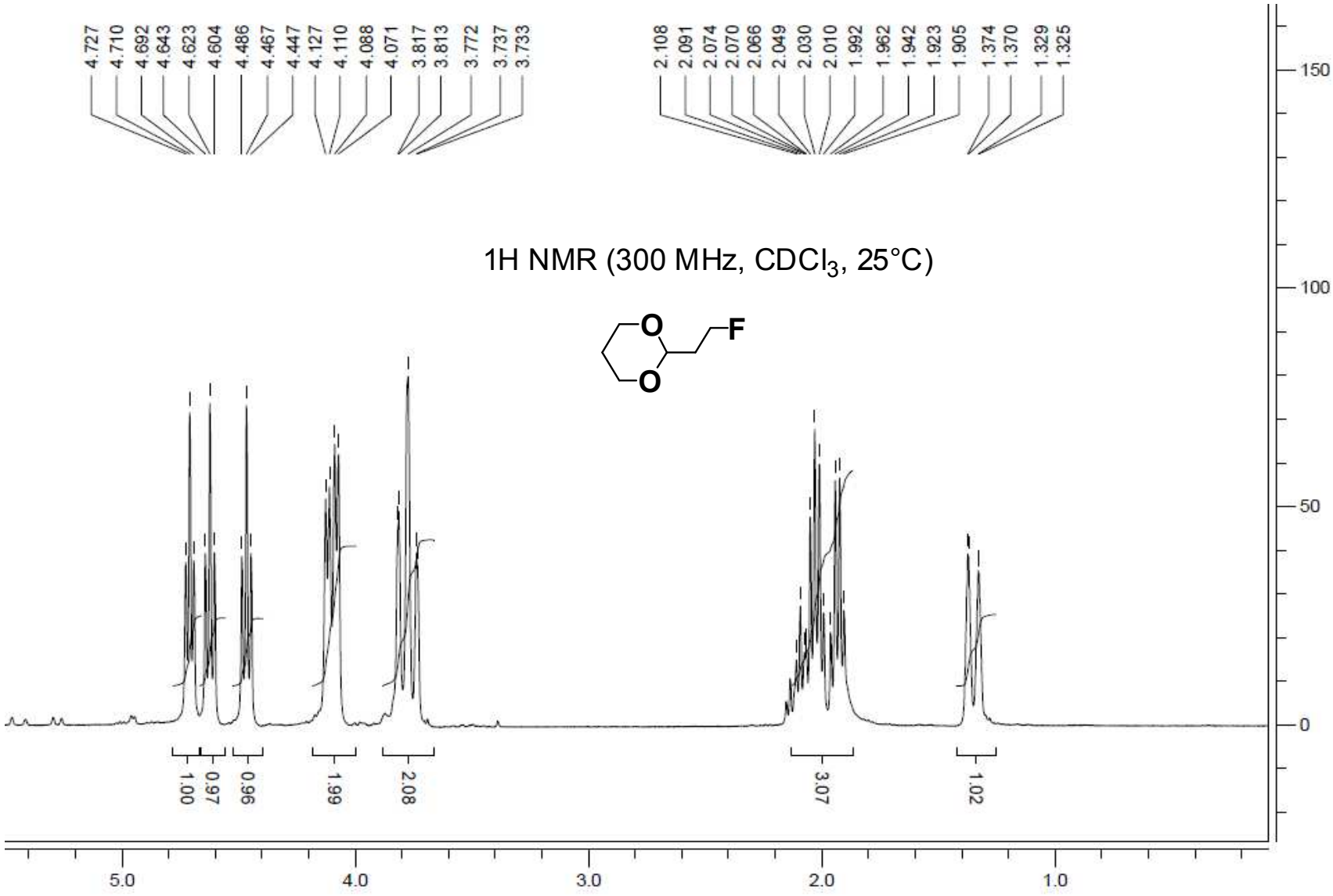
1000
500
0
150
100
50
ppm (f1)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1.370
1.329
1.325
1H NMR (300 MHz, CDCl3, 25°C)
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O
F
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50
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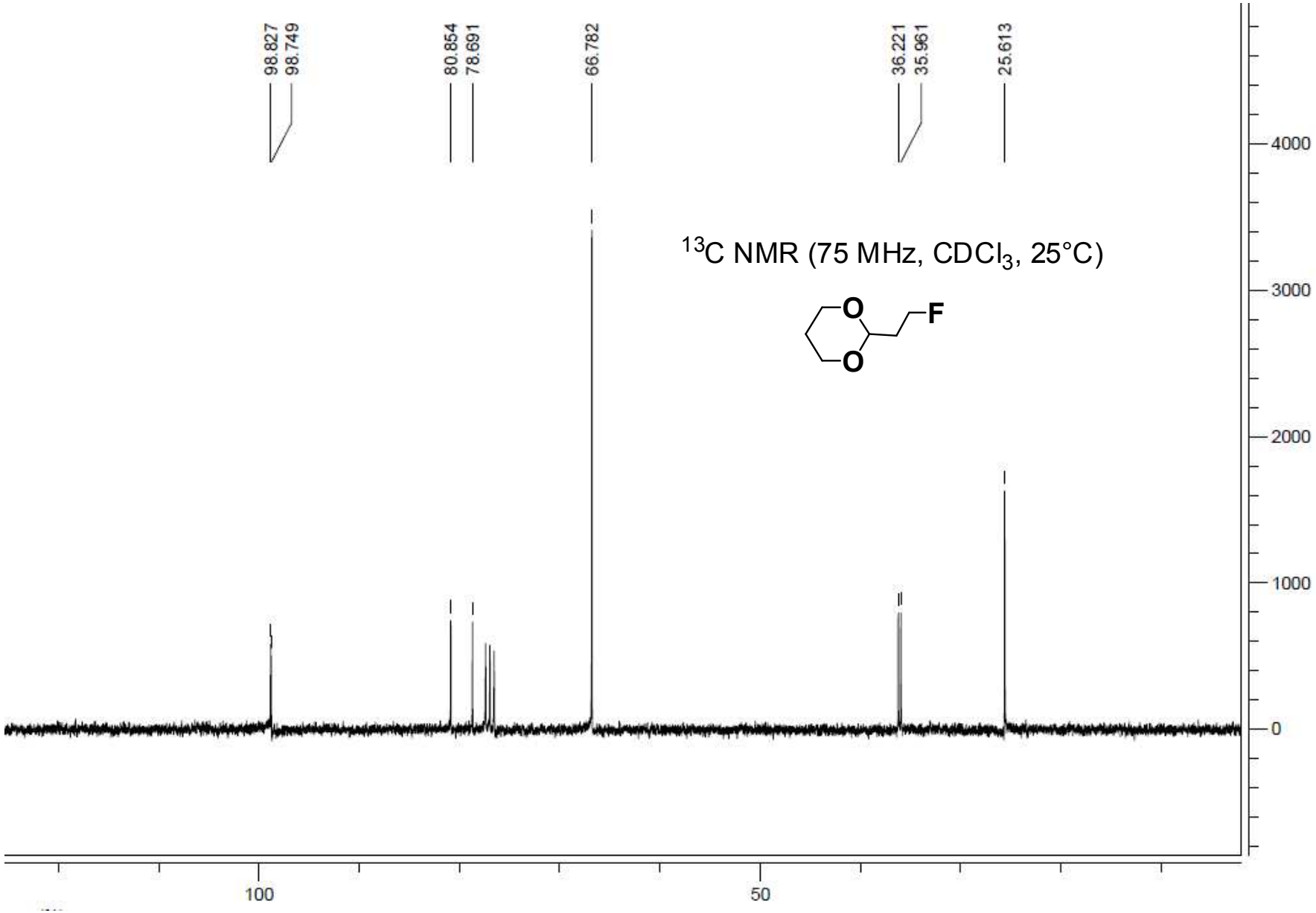
2.0
1.0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78.691
66.782
36.221
35.961
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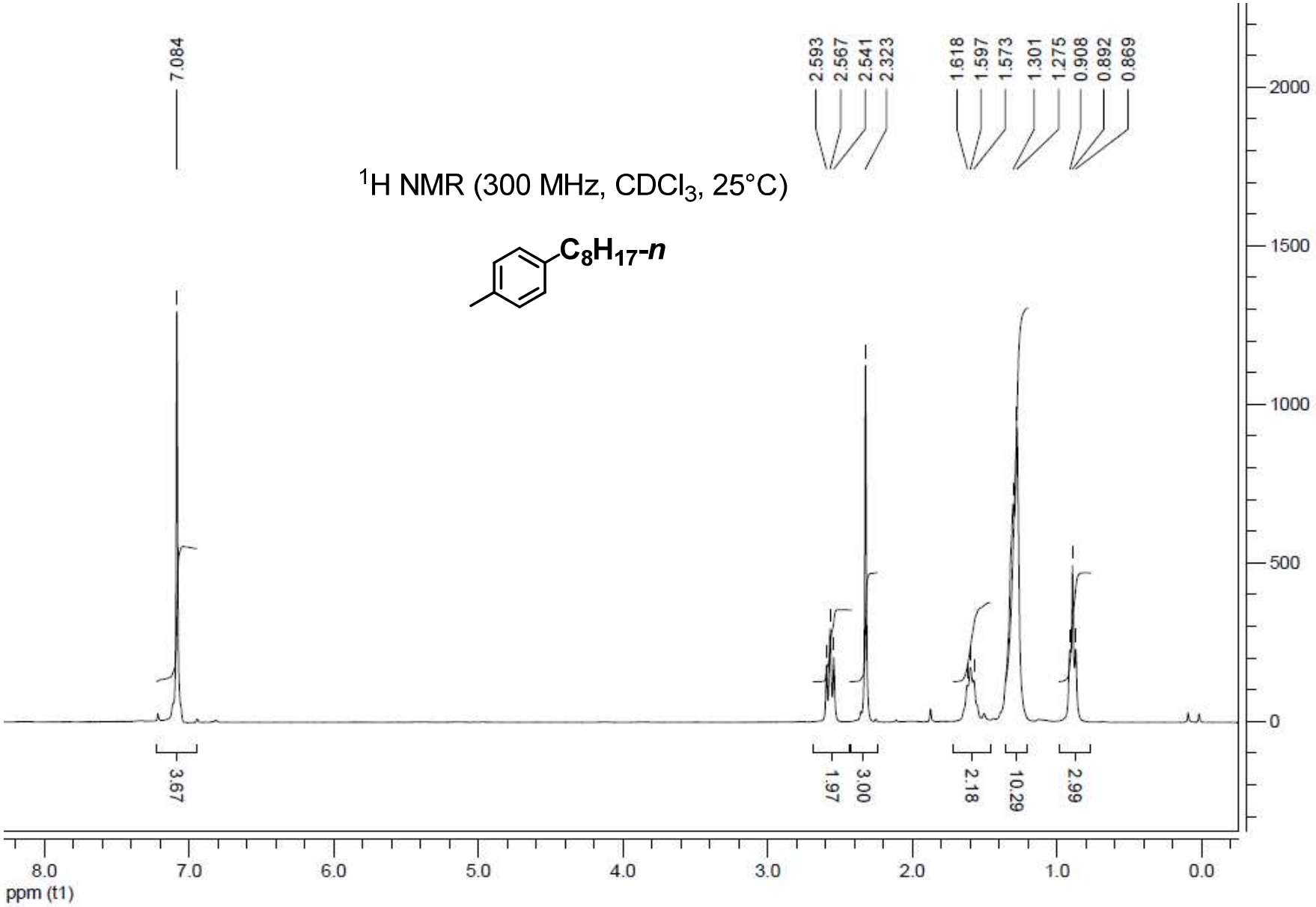
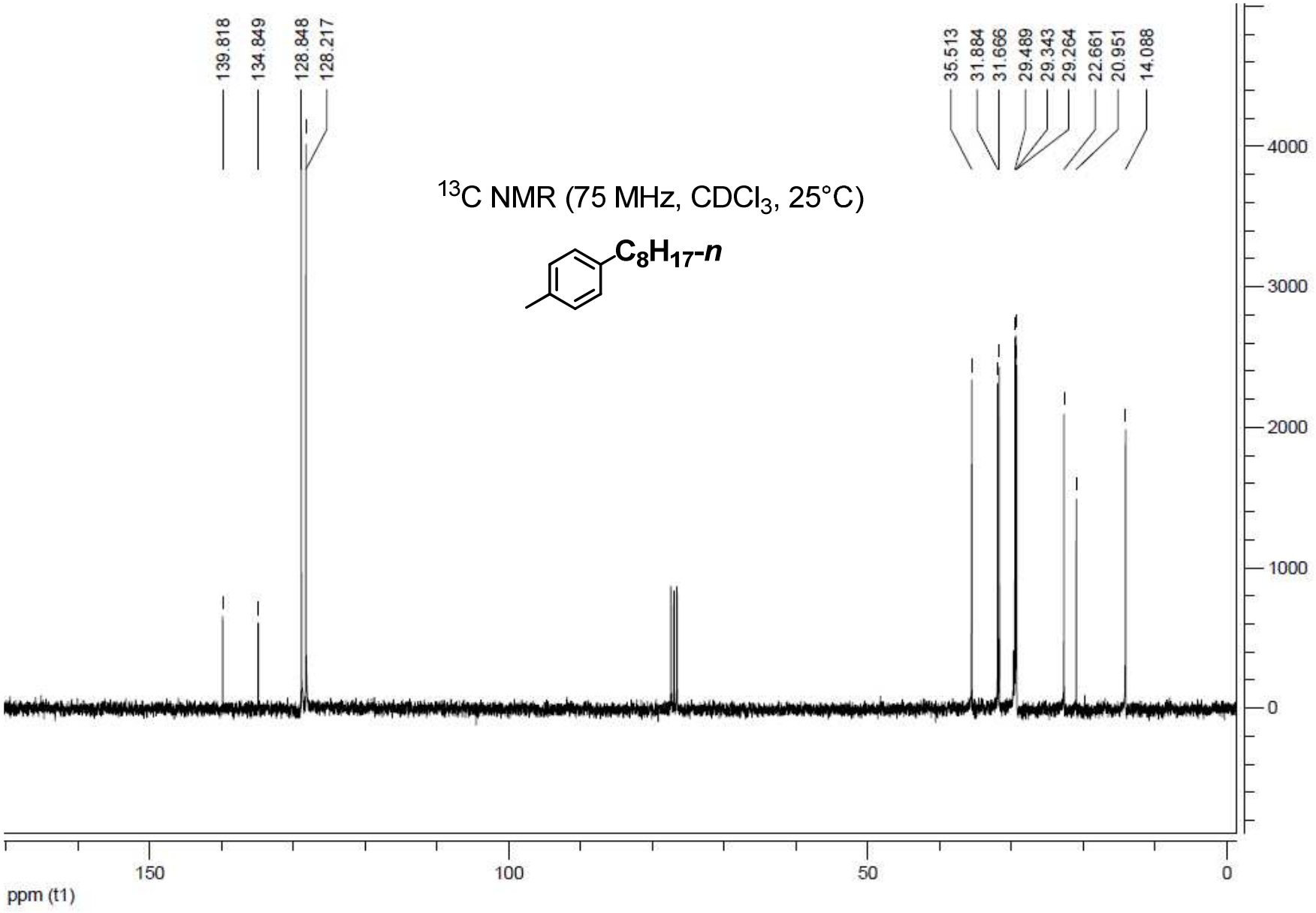
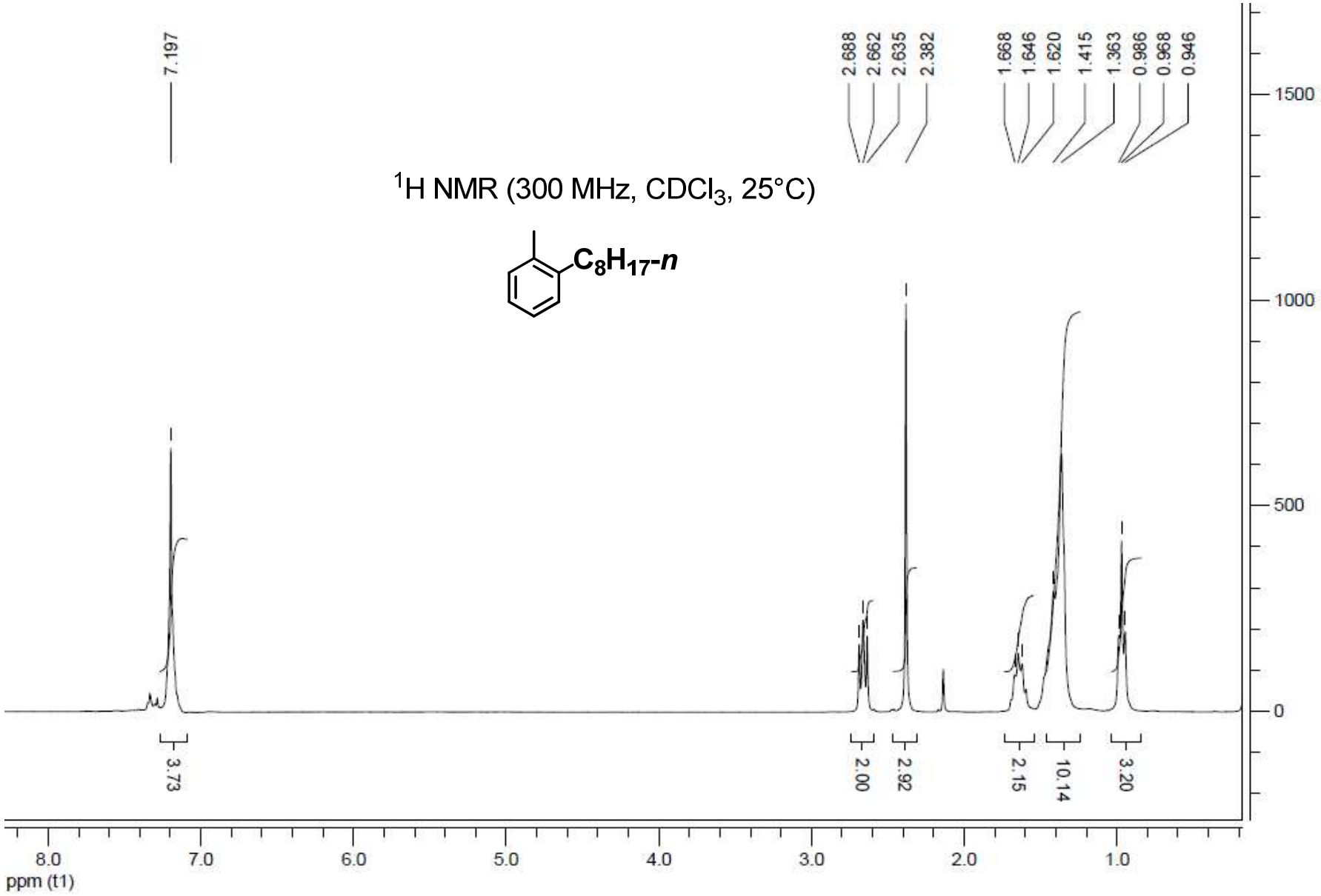
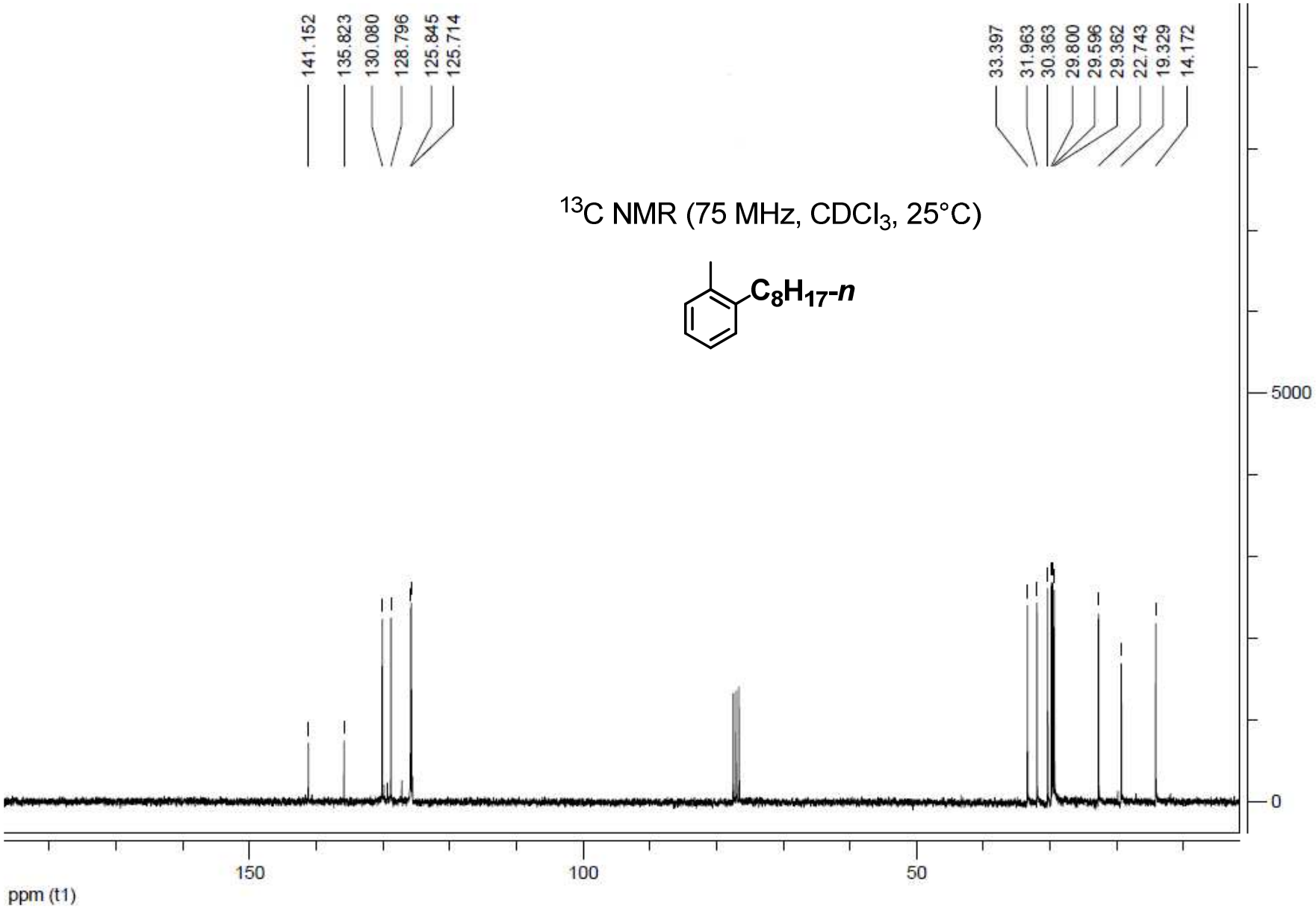
O
F
4000
3000
2000
1000
0
100
50

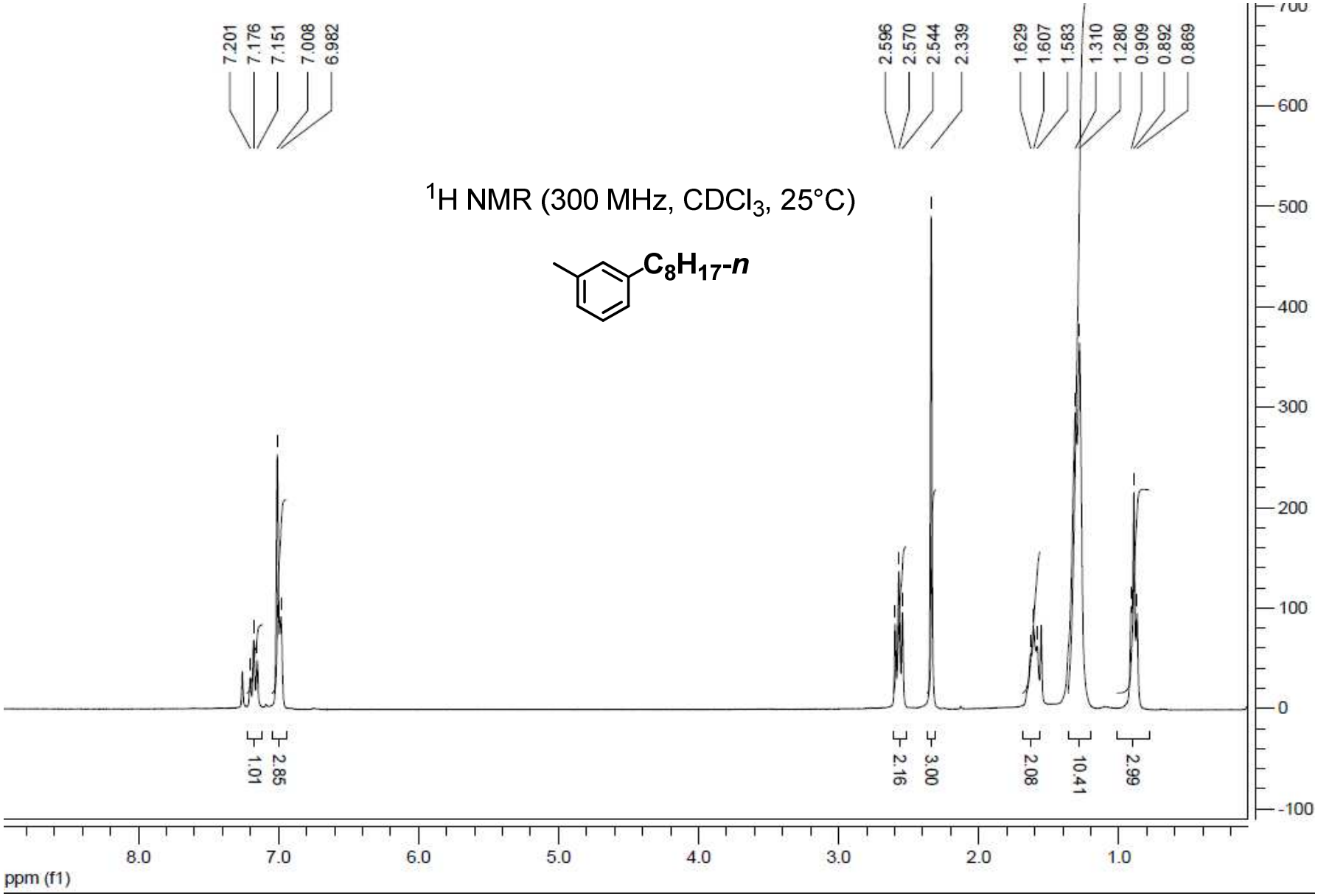

^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
7.084
2.593
2.567
2.541
2.323
1.618
1.597
1.573
1.301
1.275
0.908
0.892
0.869
3.67
1.97
3.00
2.18
10.29
2.99
2000
1500
1000
500
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


139.818
134.849
128.848
128.217
35.513
31.884
31.666
29.489
29.343
29.264
22.661
20.951
14.088
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
4000
3000
2000
1000
0
150
100
50
0
ppm (t1)

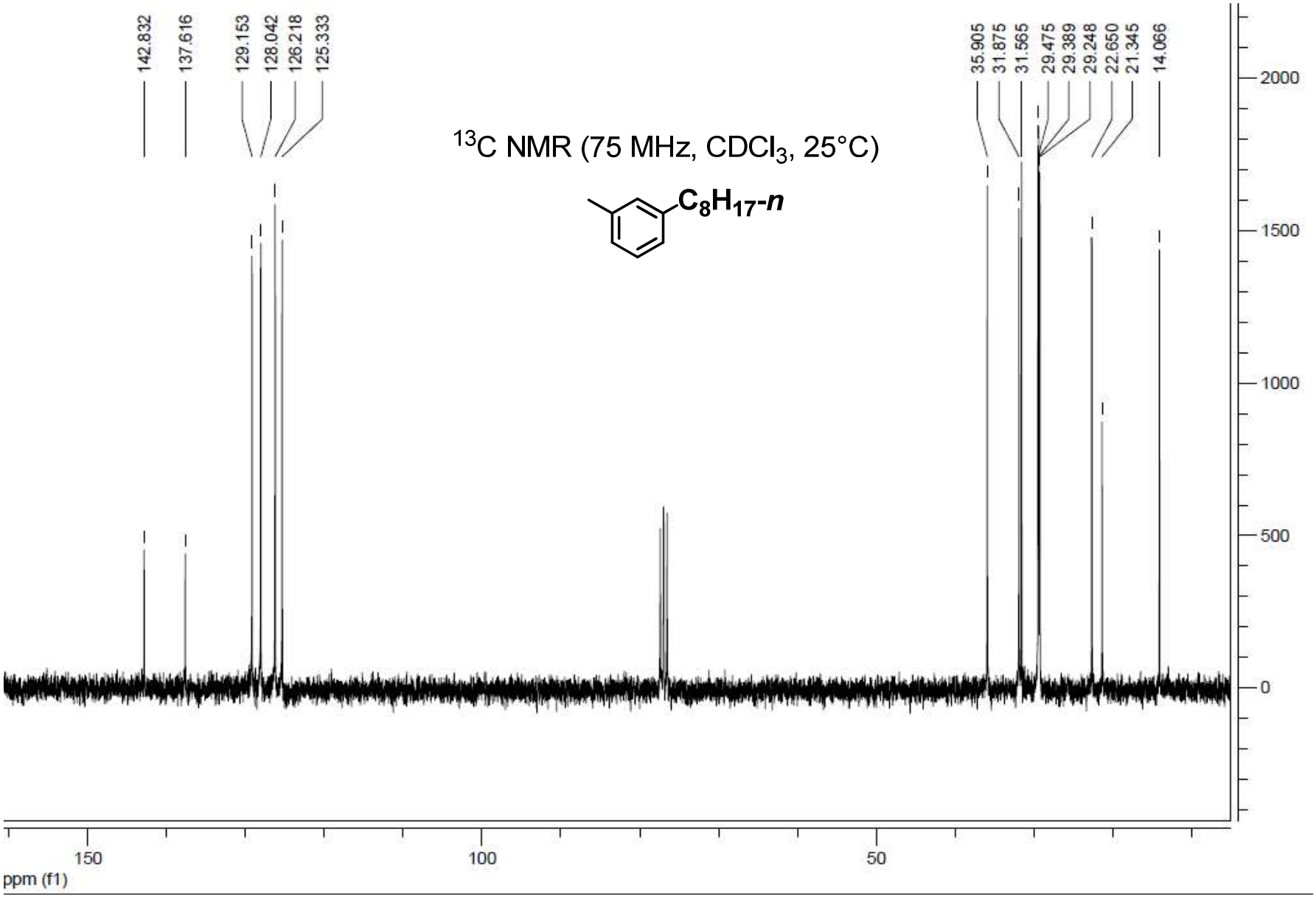


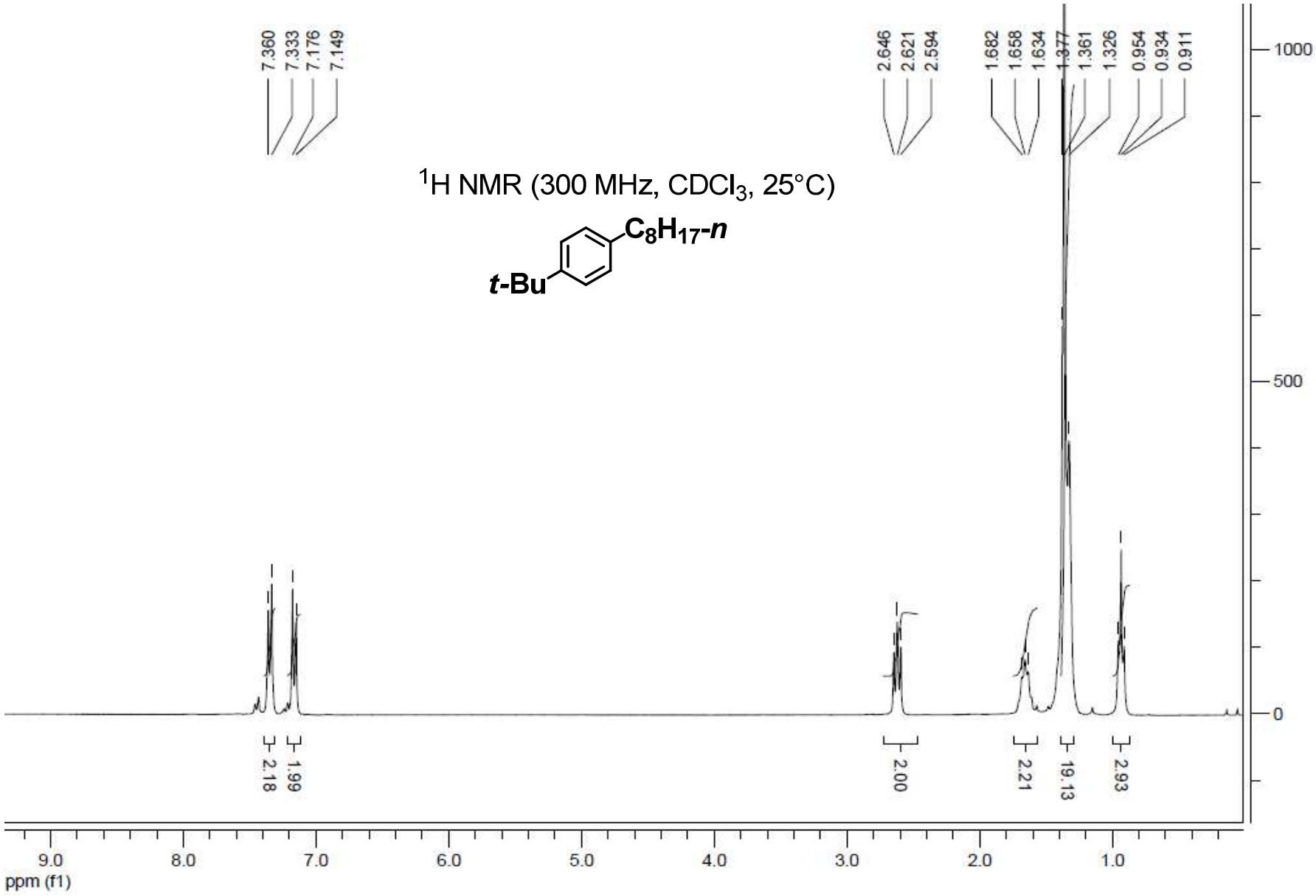
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)


141.152
135.823
130.080
128.796
125.845
125.714
33.397
31.963
30.363
29.800
29.596
29.362
22.743
19.329
14.172
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
5000
0
150
100
50
ppm (t1)

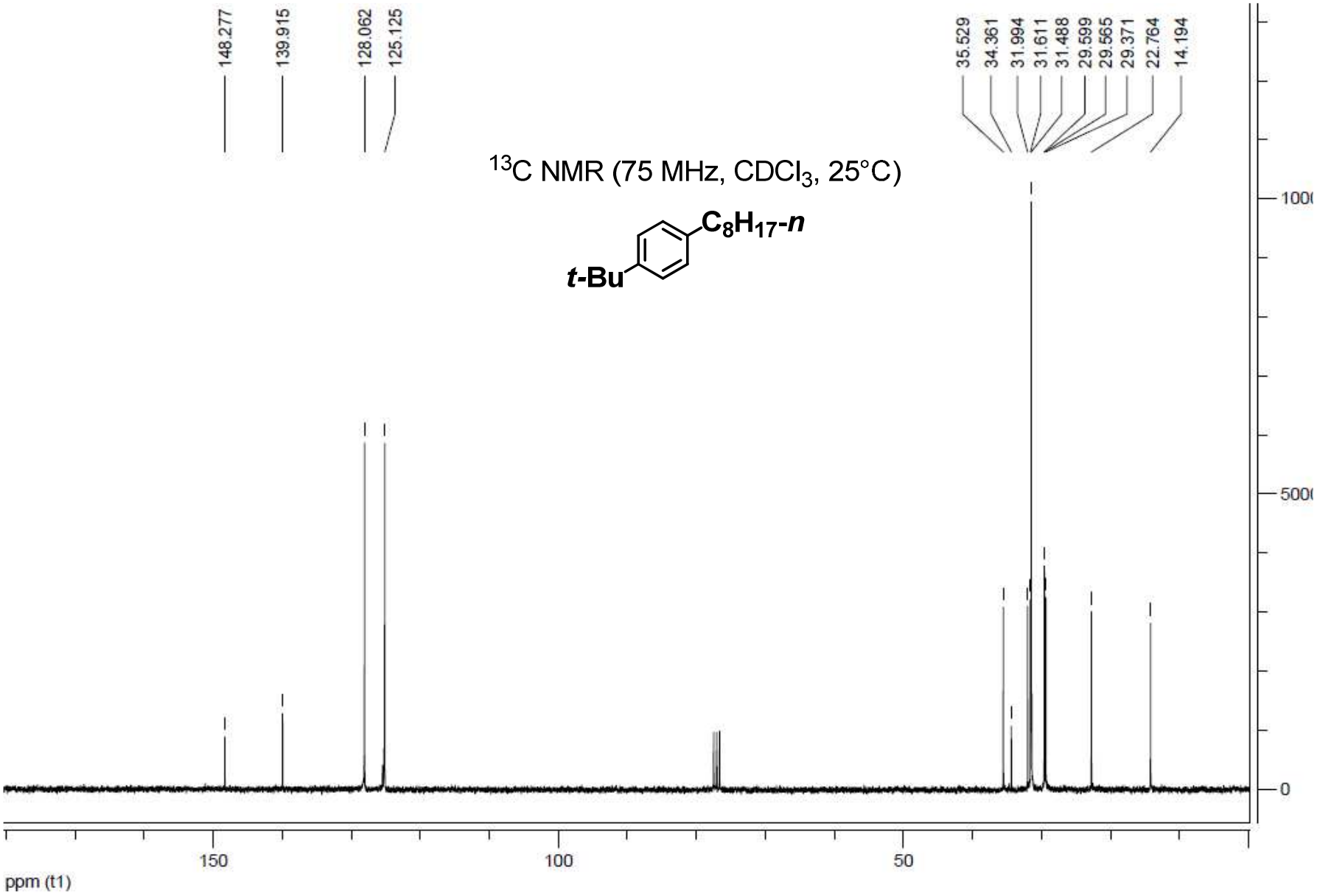


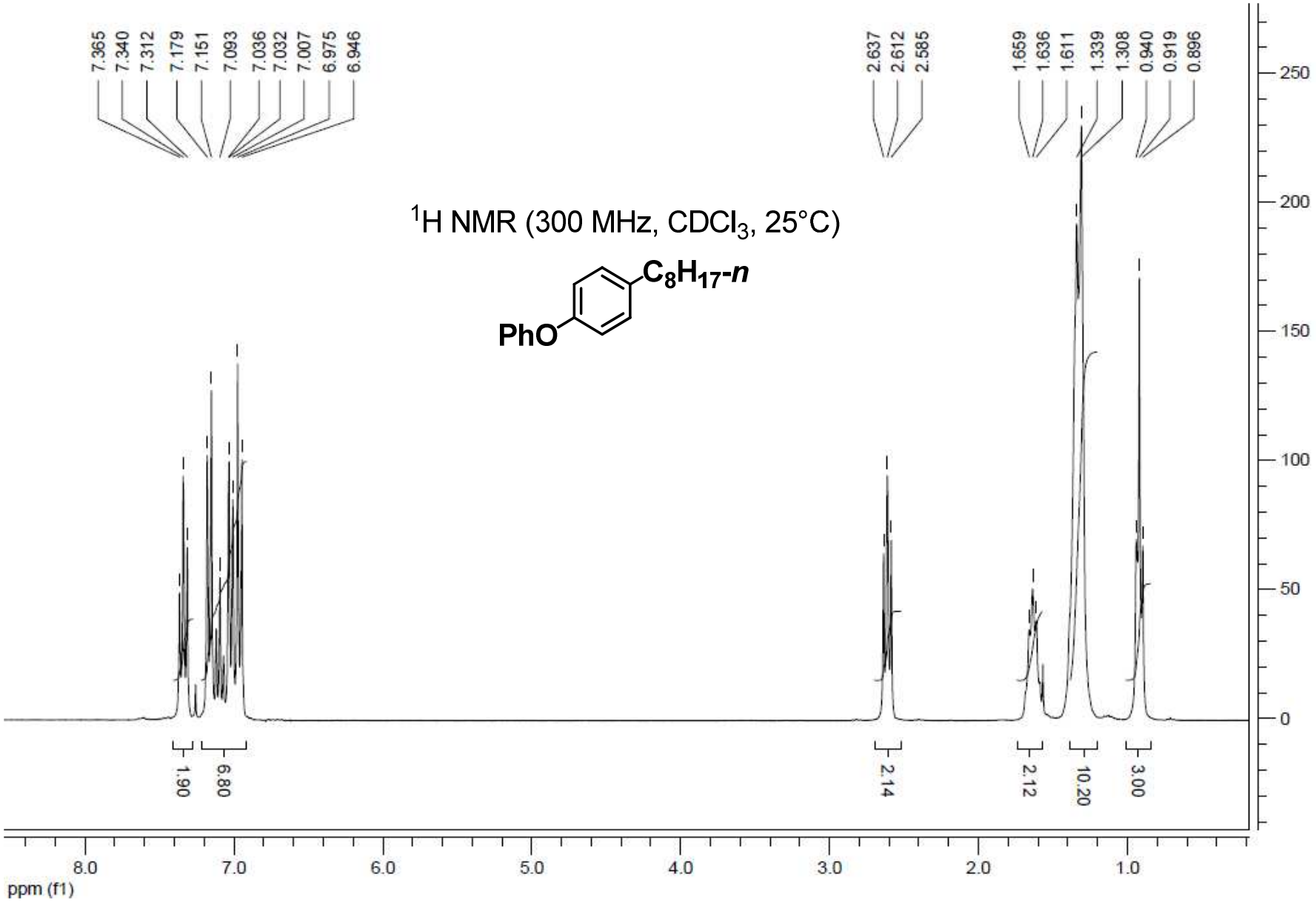
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)

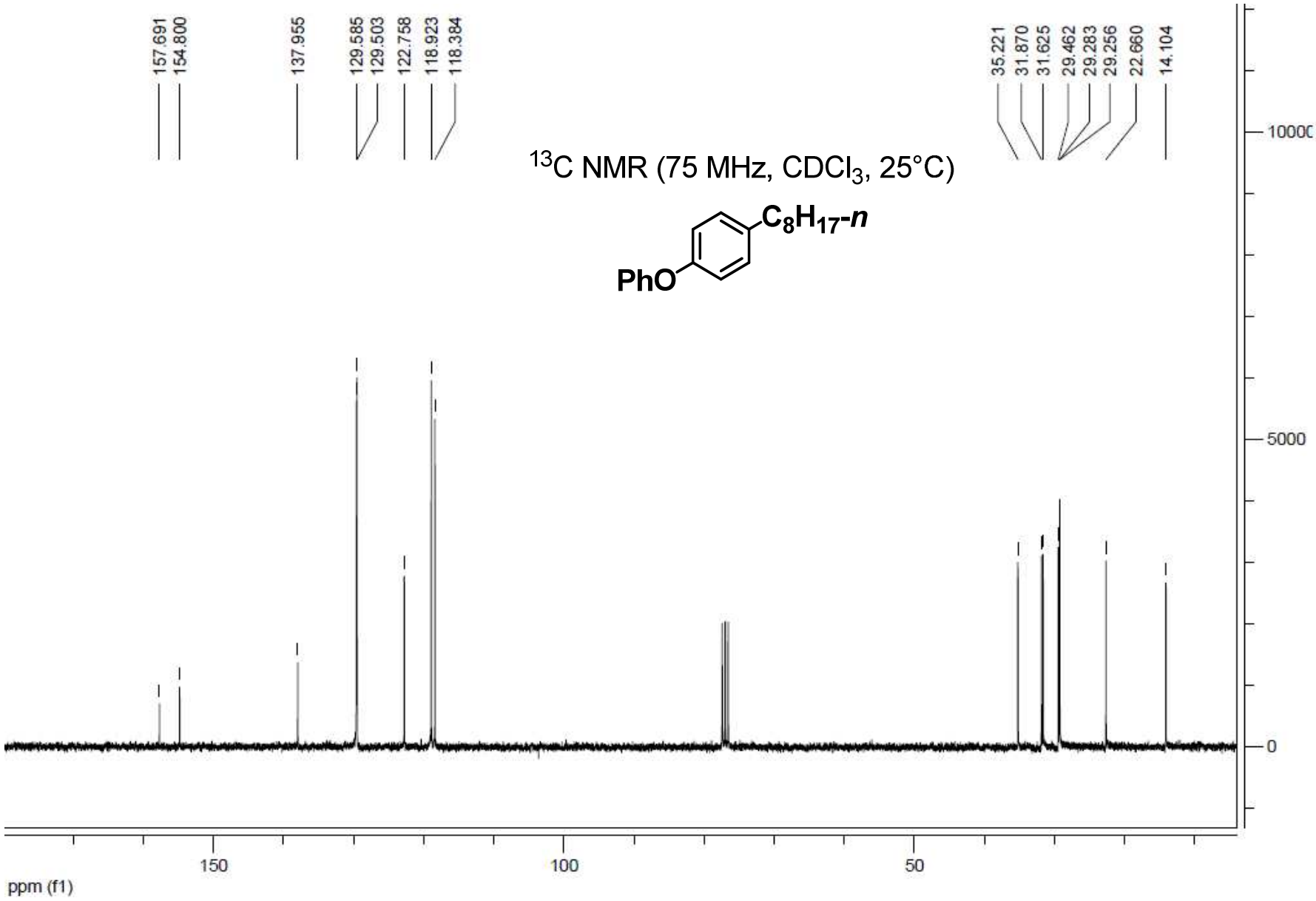

142.832
137.616
129.153
128.042
126.218
125.333
35.905
31.875
31.565
29.475
29.389
29.248
22.650
21.345
14.066
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
2000
1500
1000
500
0
150
100
50
ppm (f1)

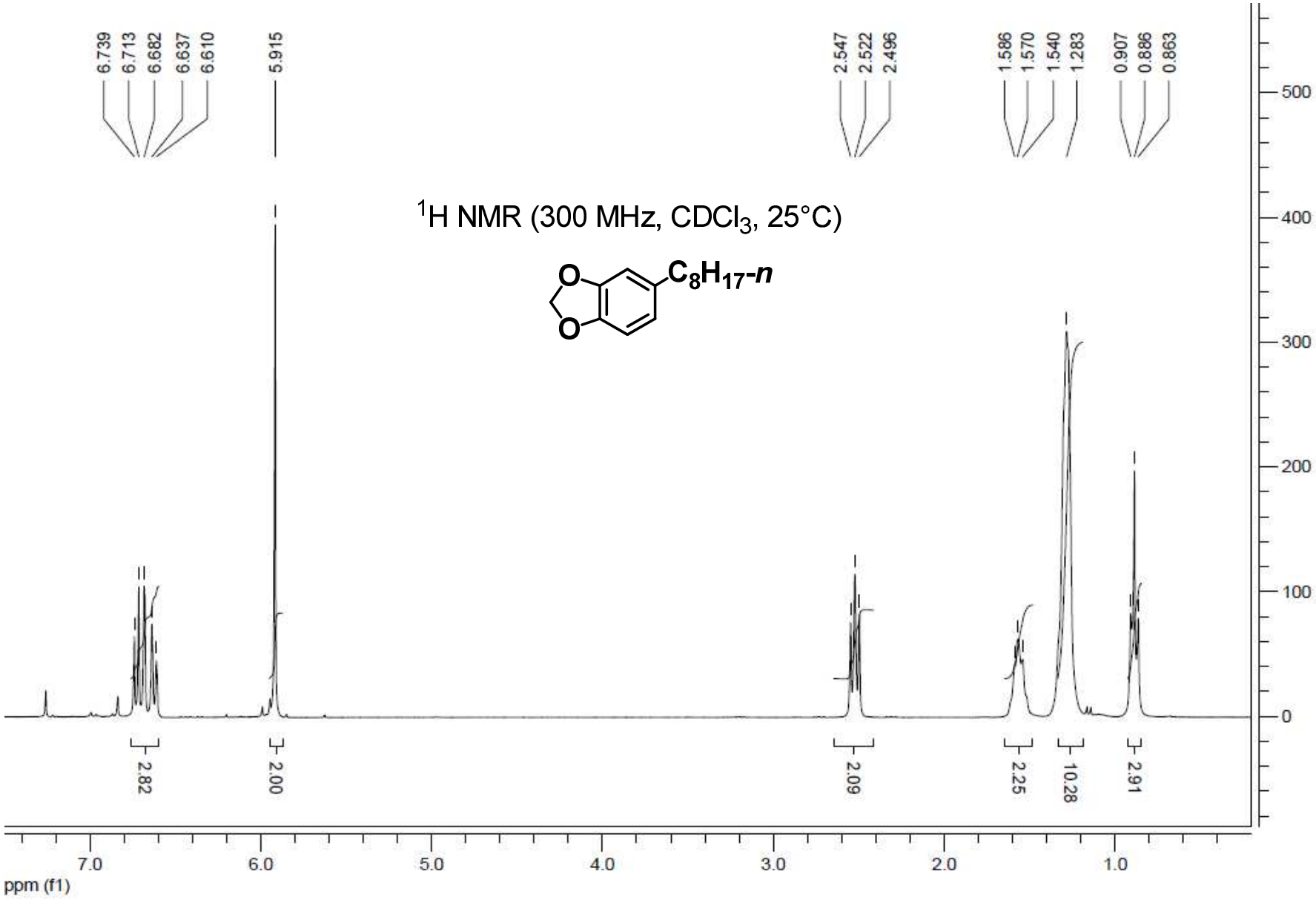


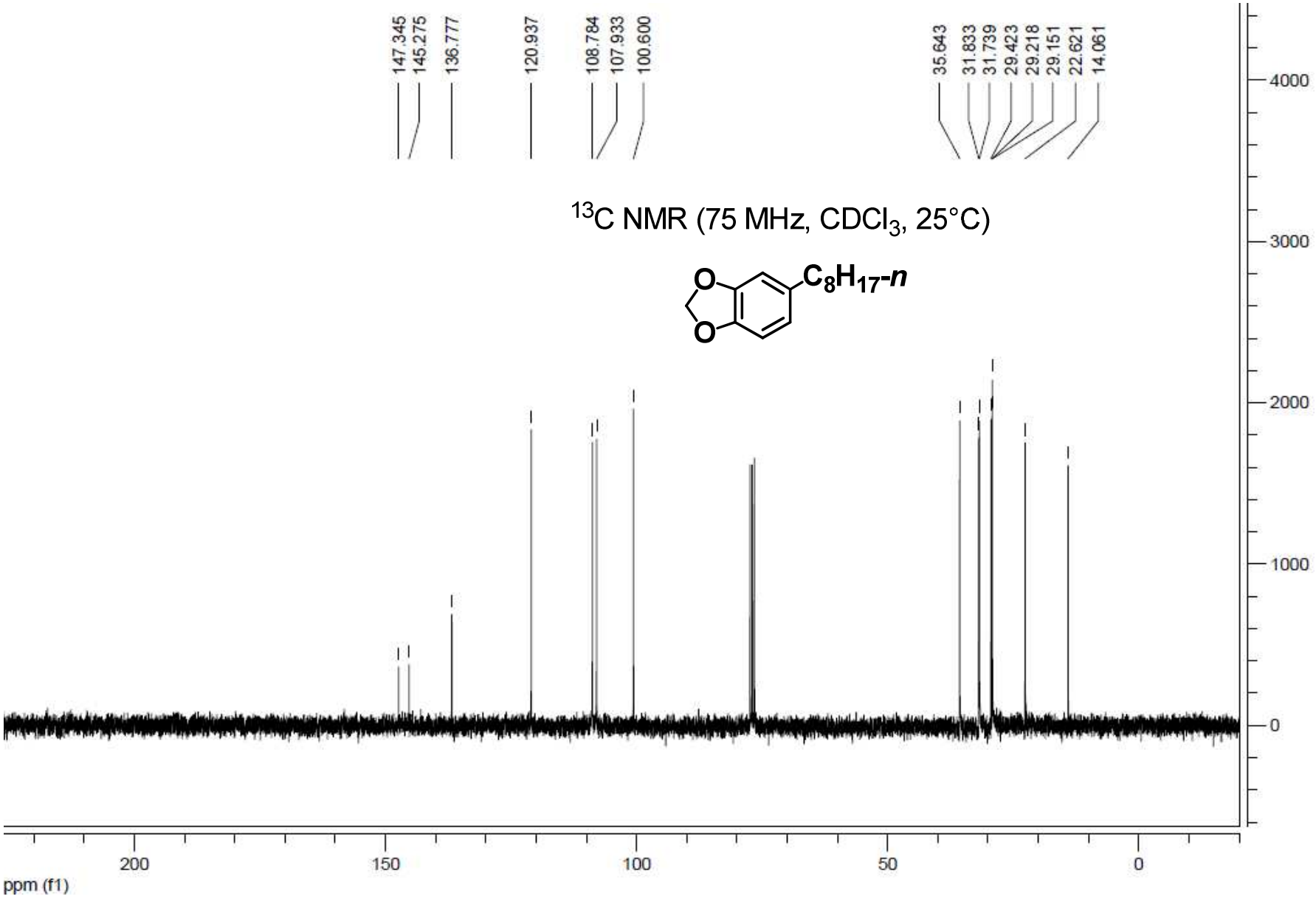
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)

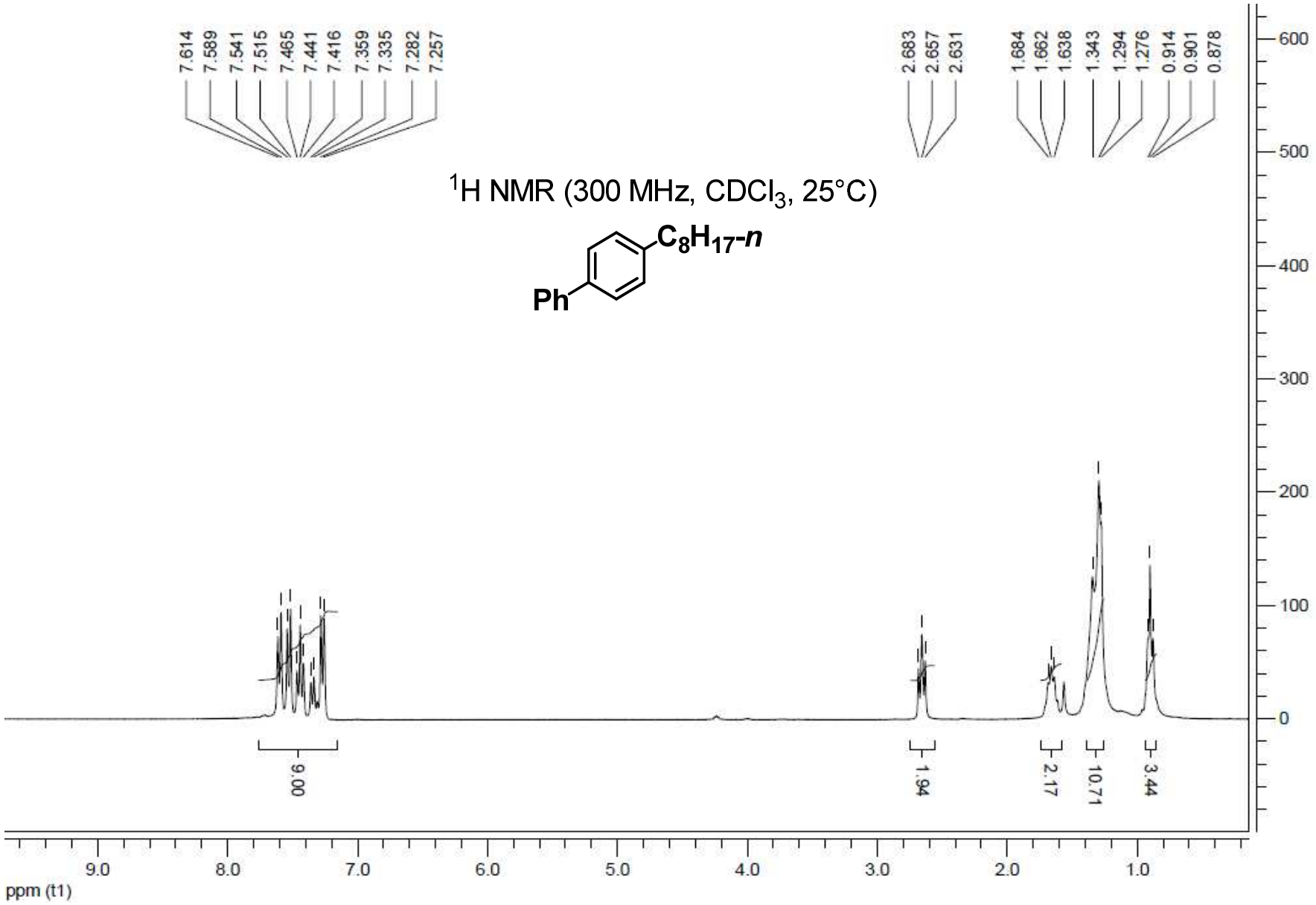

148.277
139.915
128.062
125.125
35.529
34.361
31.994
31.611
31.488
29.599
29.565
29.371
22.764
14.194
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
t-Bu
1000
500
0
150
100
50
ppm (t1)

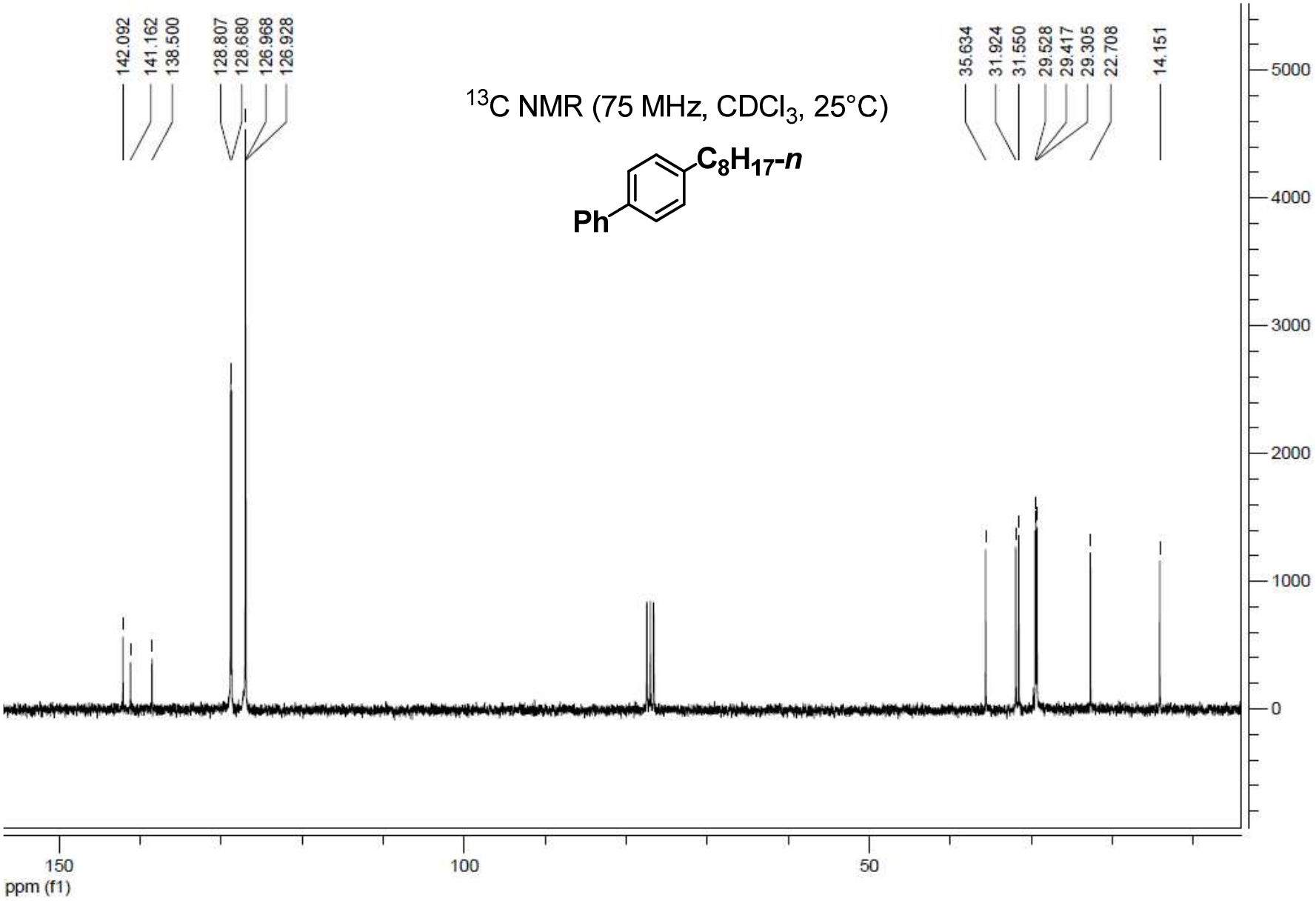

7.365
7.340
7.312
7.179
7.151
7.093
7.036
7.032
7.007
6.975
6.946
2.637
2.612
2.585
1.659
1.636
1.611
1.339
1.308
0.940
0.919
0.896
1H NMR (300 MHz, CDCl3, 25°C)
C8H17-n
PhO
1.90
6.80
2.14
2.12
10.20
3.00
250
200
150
100
50
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

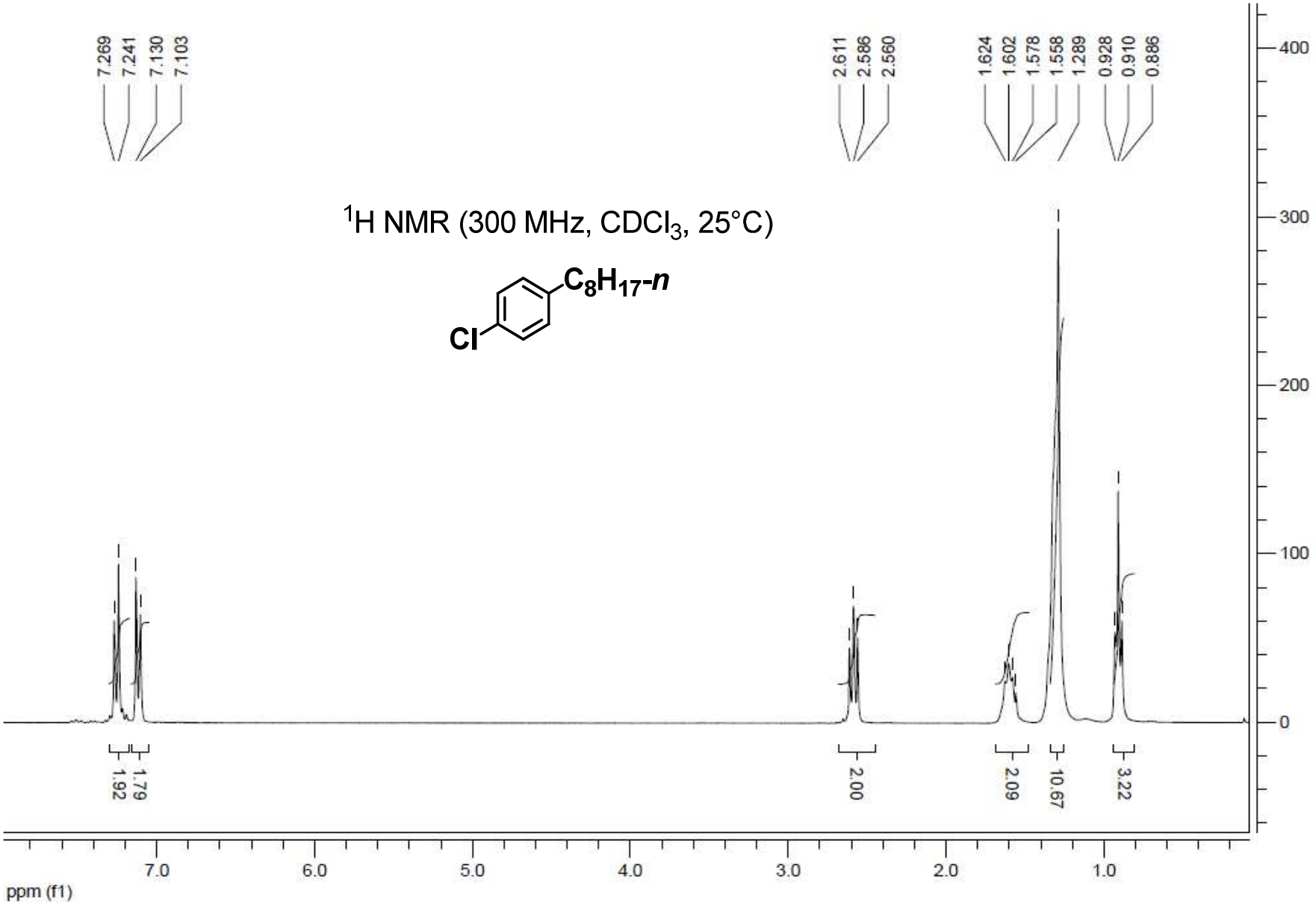

157.691
154.800
137.955
129.585
129.503
122.758
118.923
118.384
35.221
31.870
31.625
29.462
29.283
29.256
22.660
14.104
13C NMR (75 MHz, CDCl3, 25°C)
C8H17-n
PhO
10000
5000
0
150
100
50
ppm (f1)

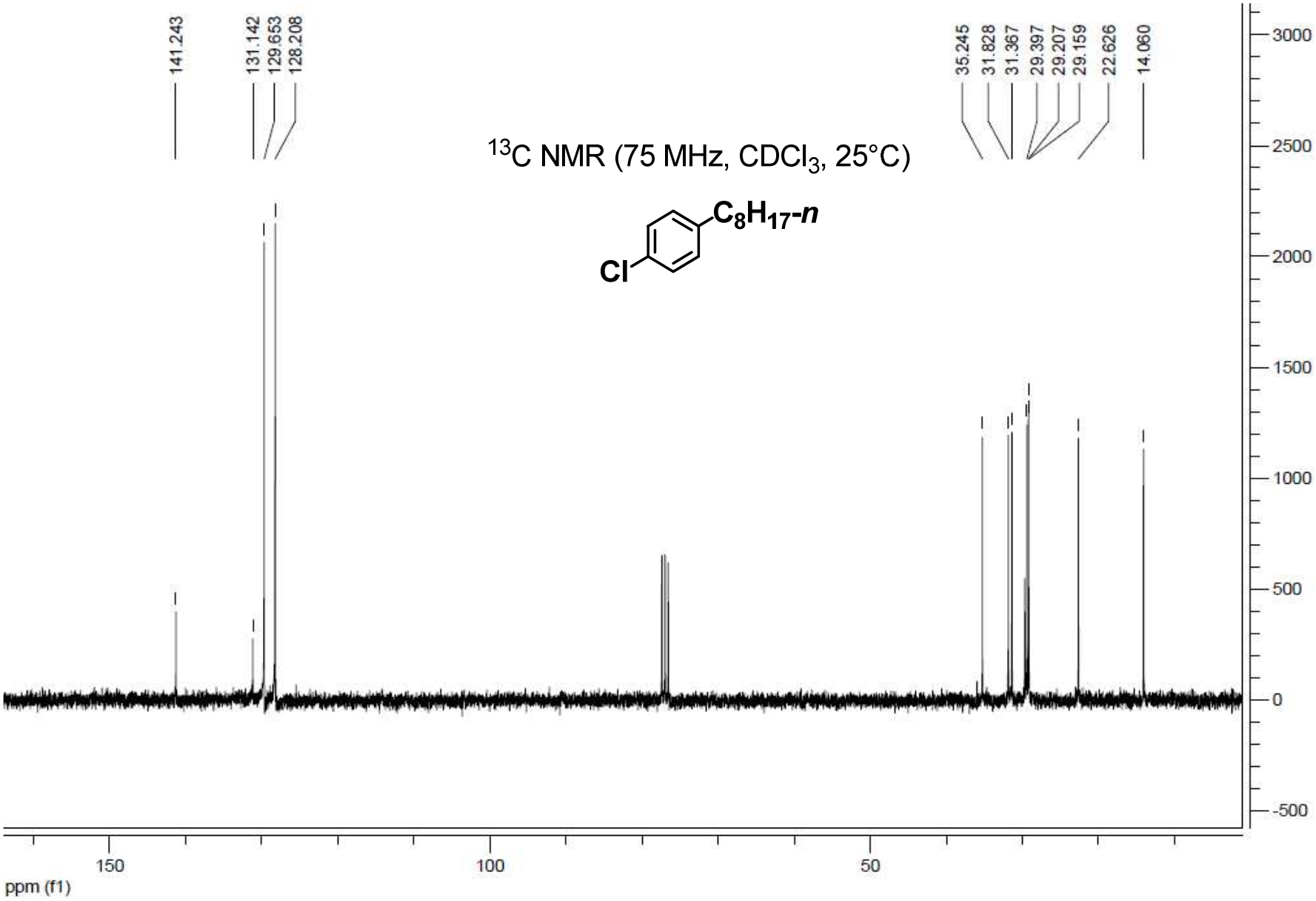

6.739
6.713
6.682
6.637
6.610
5.915
2.547
2.522
2.496
1.586
1.570
1.540
1.283
0.907
0.886
0.863
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
2.82
2.00
2.09
2.25
10.28
2.91
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)
500
400
300
200
100
0

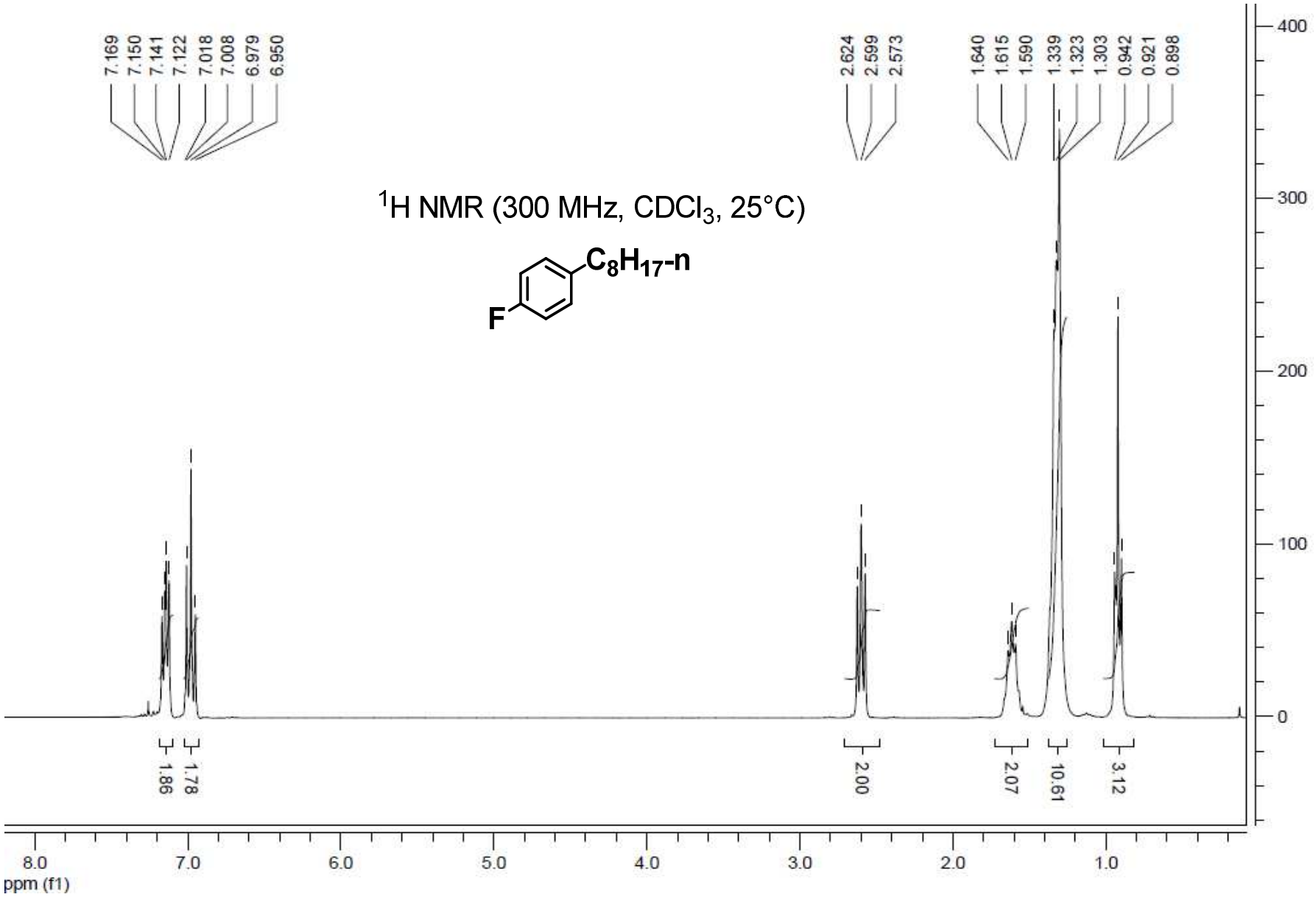

147.345
145.275
136.777
120.937
108.784
107.933
100.600
35.643
31.833
31.739
29.423
29.218
29.151
22.621
14.061
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
O
O
4000
3000
2000
1000
0
200
150
100
50
0
ppm (f1)

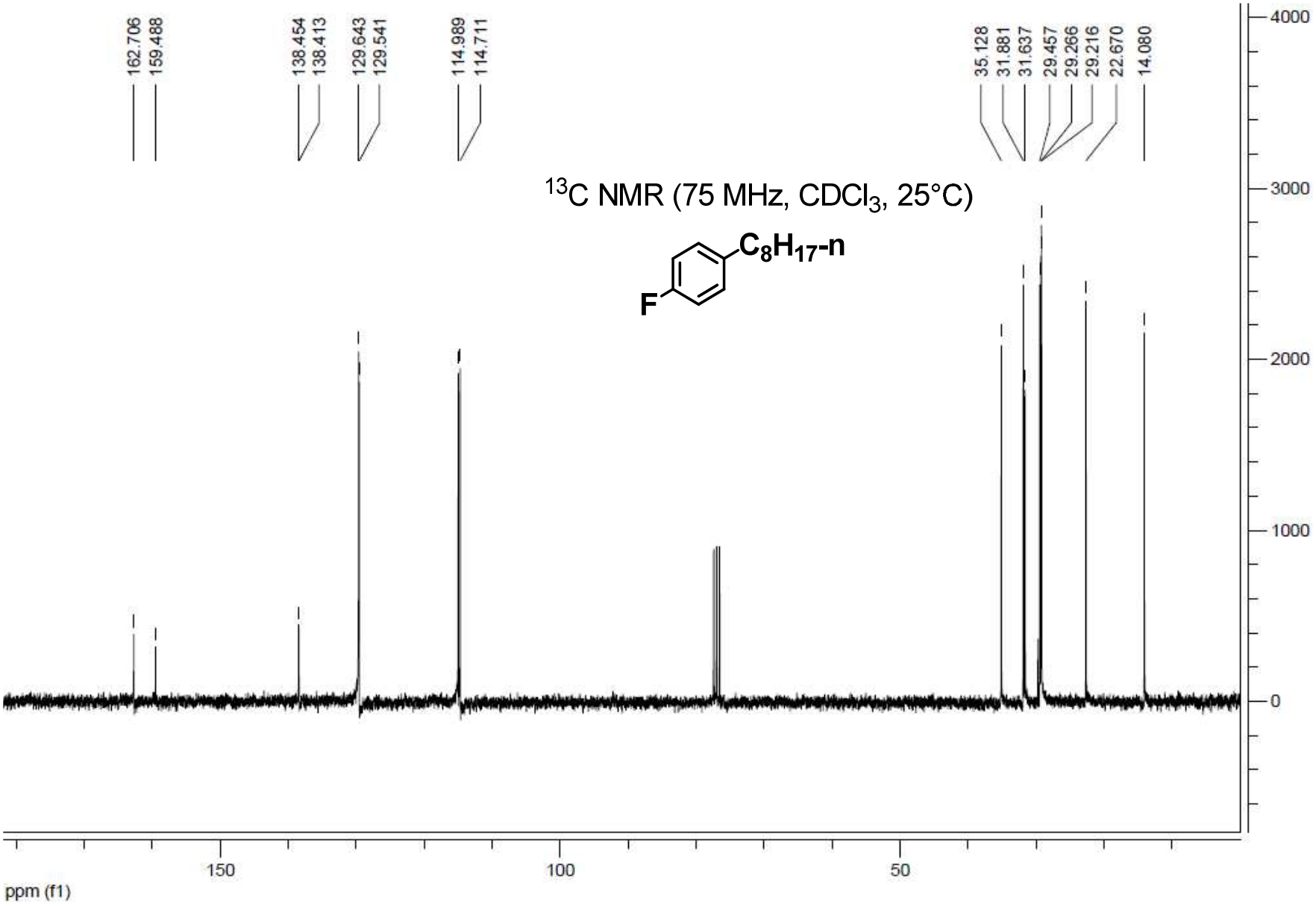

7.614
7.589
7.541
7.515
7.465
7.441
7.416
7.359
7.335
7.282
7.257
2.683
2.657
2.631
1.684
1.662
1.638
1.343
1.294
1.276
0.914
0.901
0.878
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
Ph
9.00
1.94
2.17
10.71
3.44
ppm (t1)

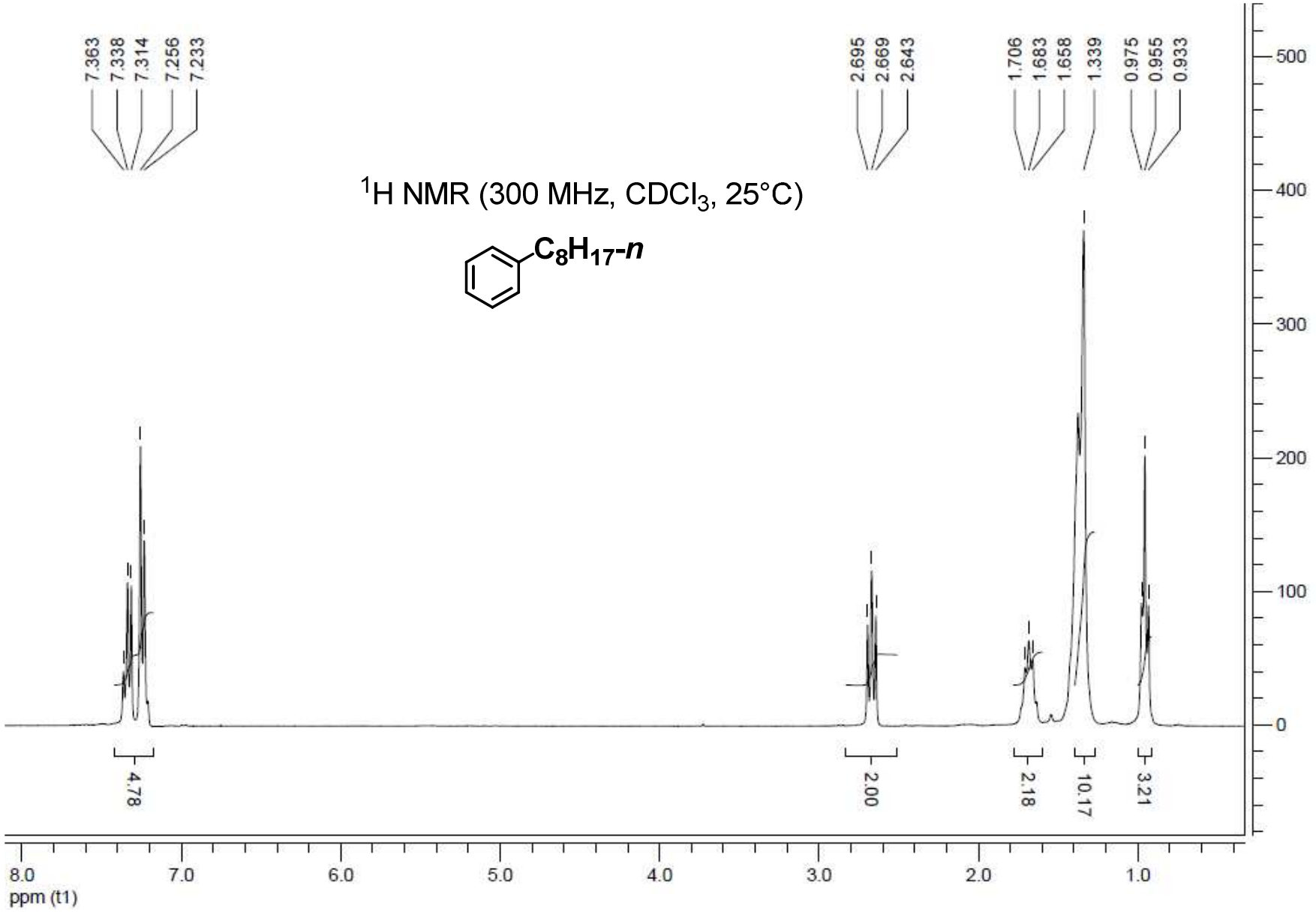

142.092
141.162
138.500
128.807
128.680
126.968
126.928
35.634
31.924
31.550
29.528
29.417
29.305
22.708
14.151
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
Ph
5000
4000
3000
2000
1000
0
150
100
50
ppm (f1)

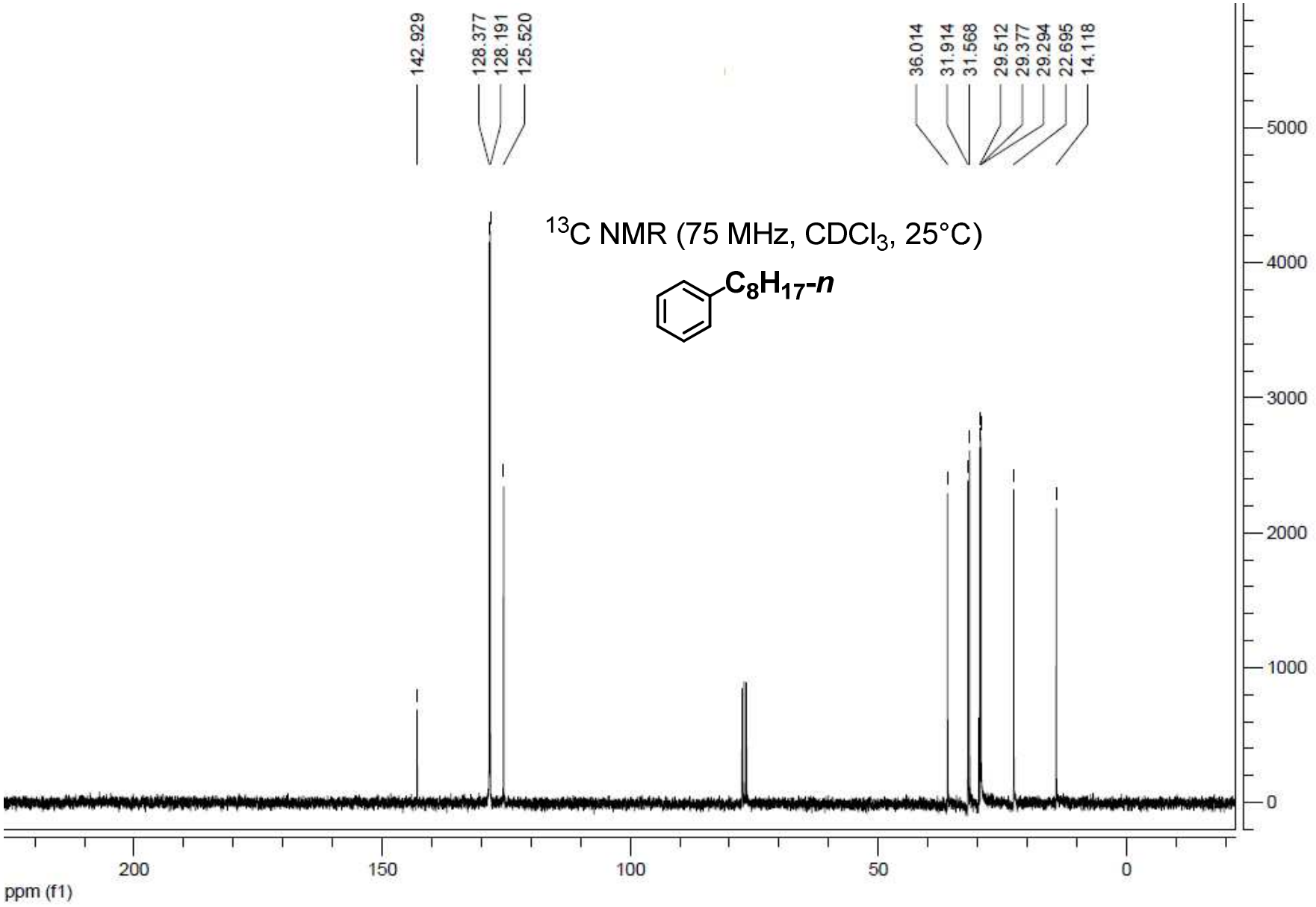

7.269
7.241
7.130
7.103
2.611
2.586
2.560
1.624
1.602
1.578
1.558
1.289
0.928
0.910
0.886
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
Cl
400
300
200
100
0
1.92
1.79
2.00
2.09
10.67
3.22
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

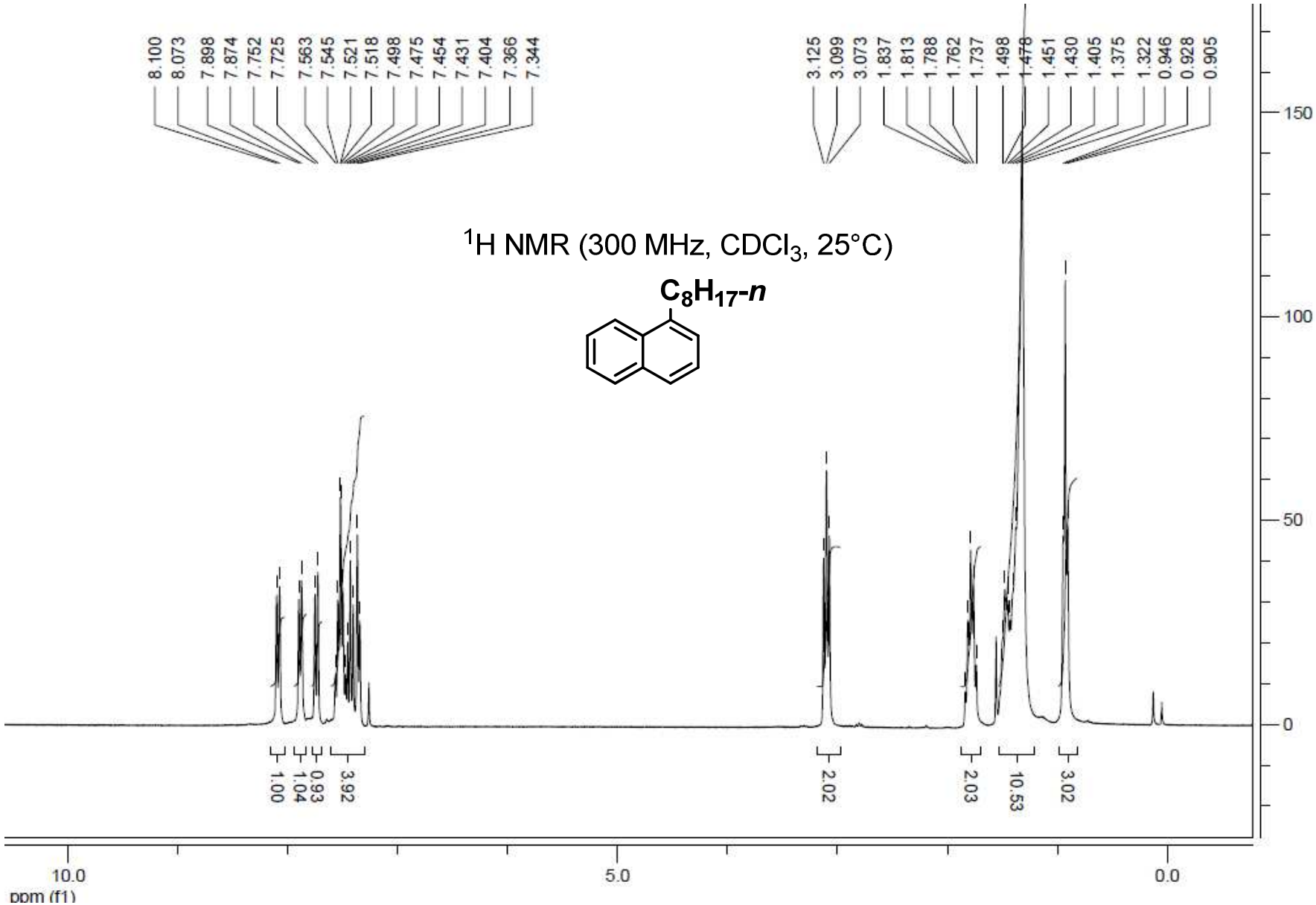

141.243
131.142
129.653
128.208
35.245
31.828
31.367
29.397
29.207
29.159
22.626
14.060
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
Cl
3000
2500
2000
1500
1000
500
0
-500
150
100
50
ppm (f1)

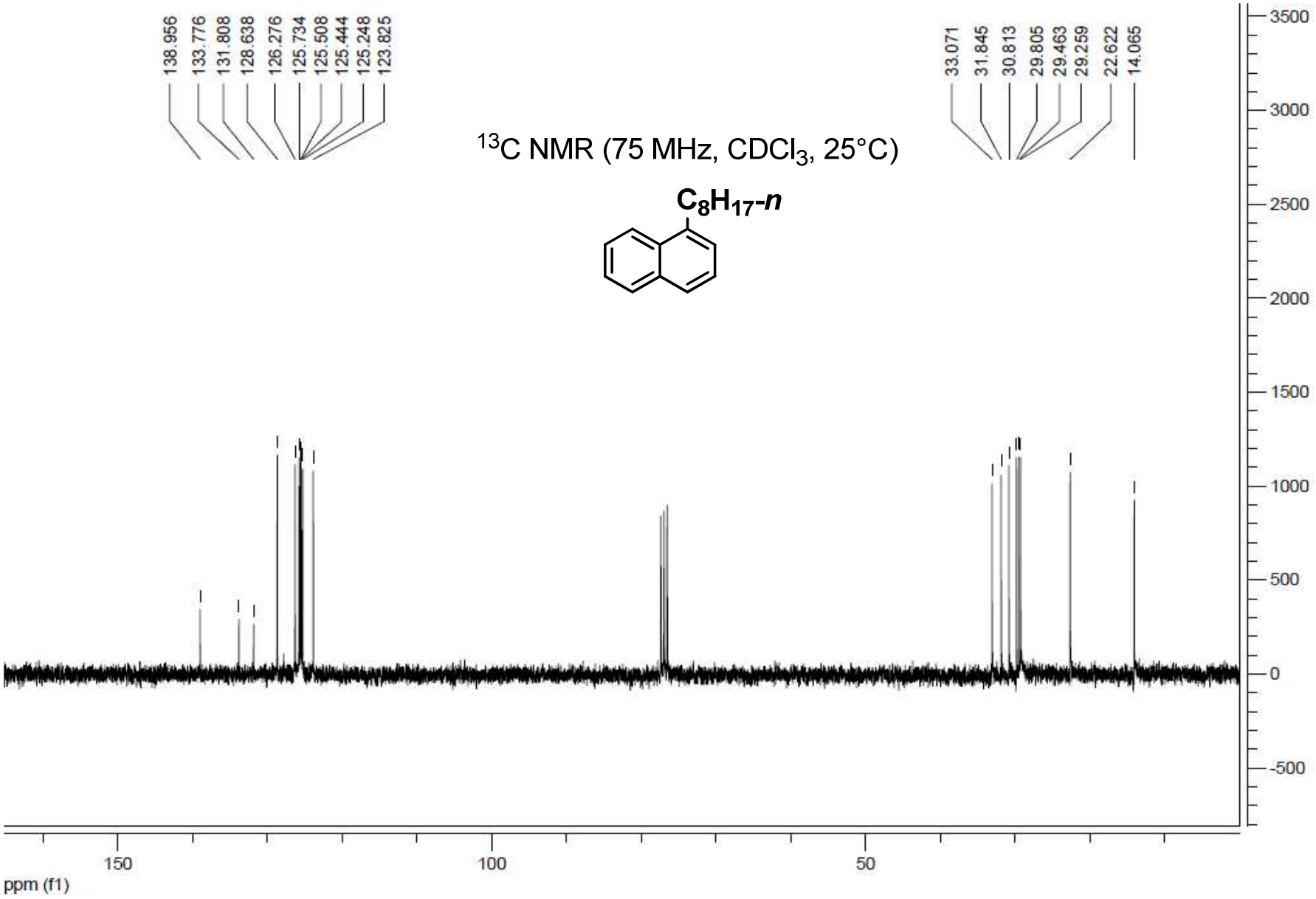

7.169
7.150
7.141
7.122
7.018
7.008
6.979
6.950
2.624
2.599
2.573
1.640
1.615
1.590
1.339
1.323
1.303
0.942
0.921
0.898
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-n
F
1.86
1.78
2.00
2.07
10.61
3.12
400
300
200
100
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

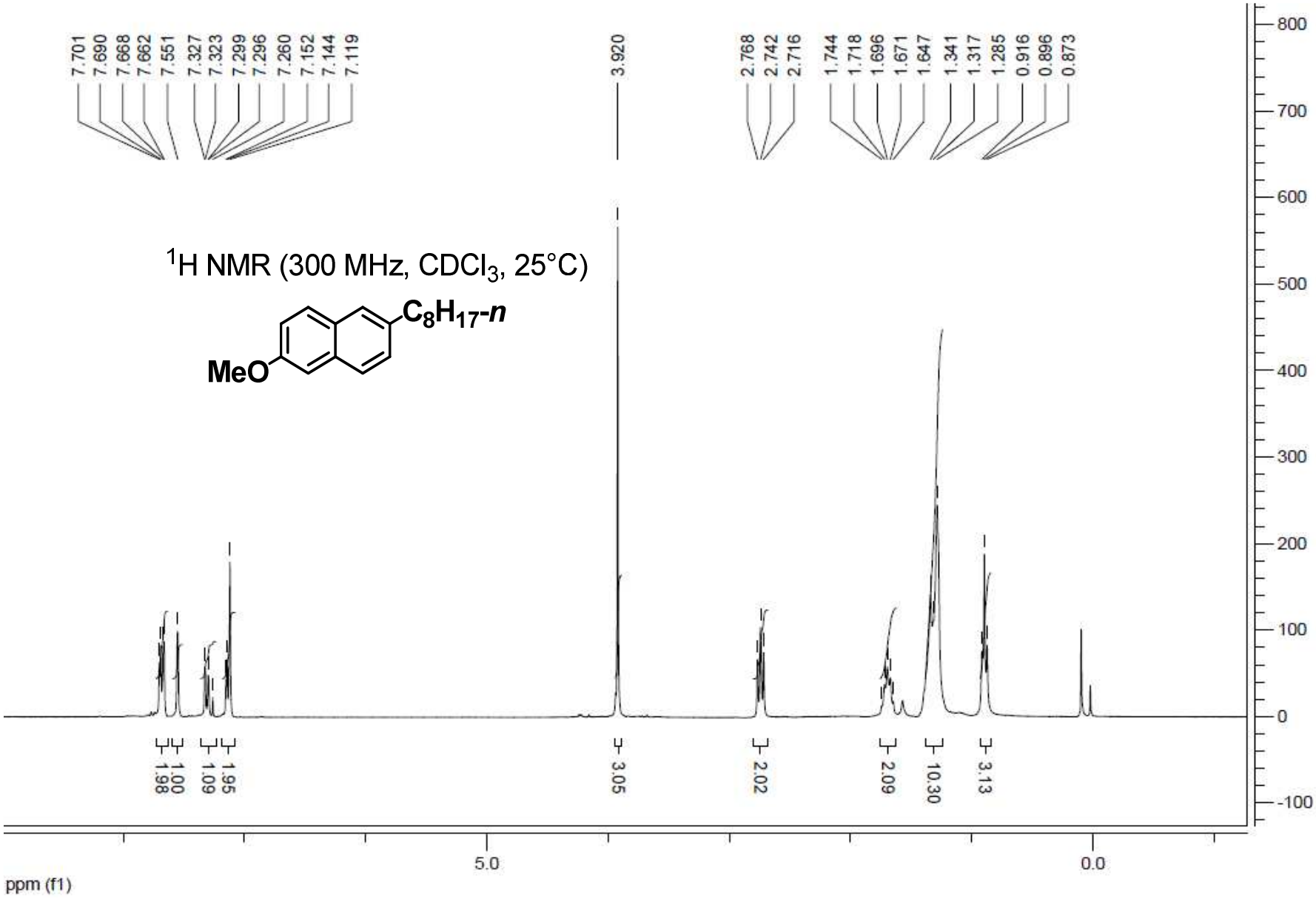

162.706
159.488
138.454
138.413
129.643
129.541
114.989
114.711
35.128
31.881
31.637
29.457
29.266
29.216
22.670
14.080
^{13}C NMR (75 MHz, CDCl$_3$, 25°C)
C_8H_{17}-n
F
4000
3000
2000
1000
0
150
100
50
ppm (f1)

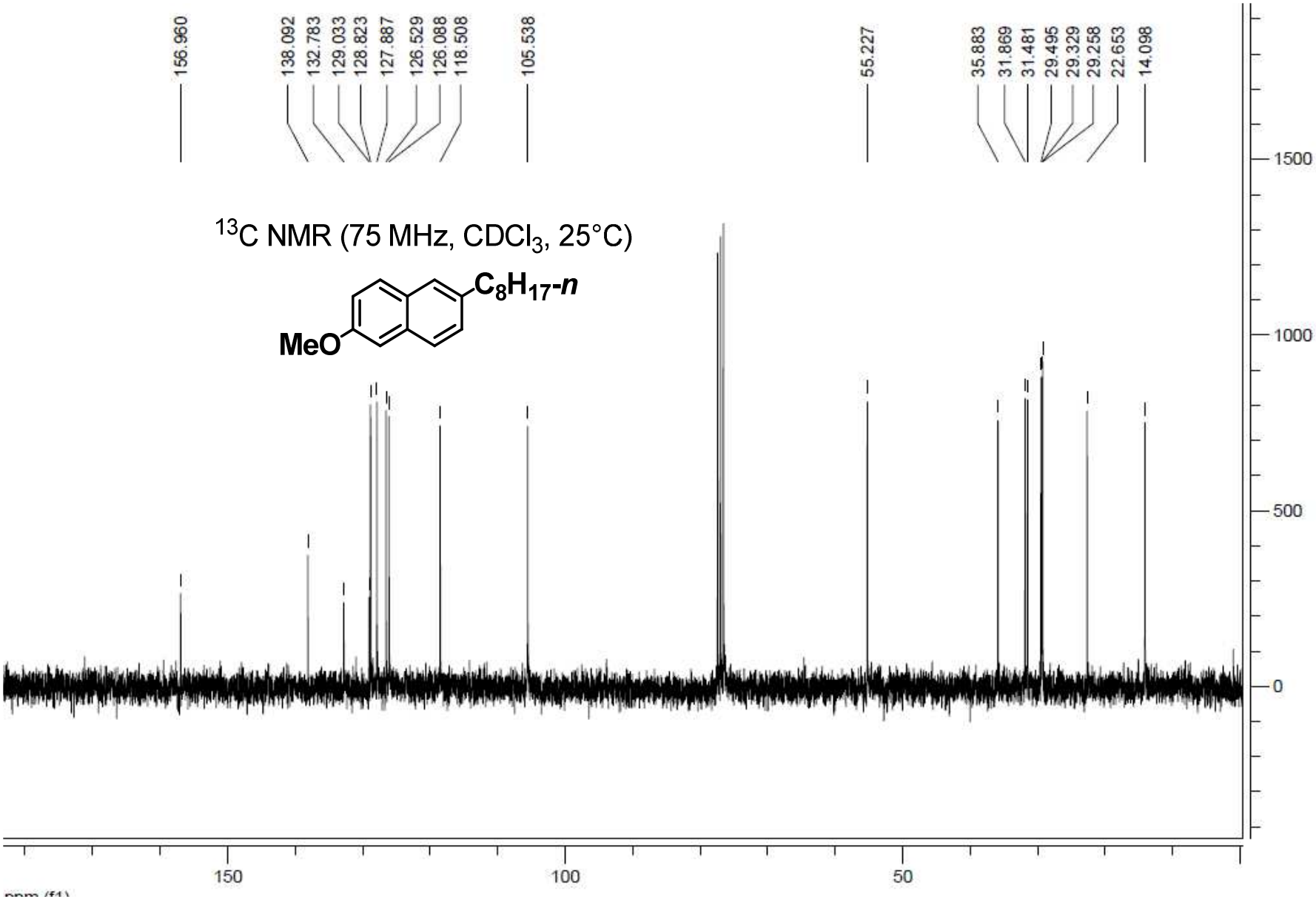

7.363
7.338
7.314
7.256
7.233
2.695
2.669
2.643
1.706
1.683
1.658
1.339
0.975
0.955
0.933
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
500
400
300
200
100
0
4.78
2.00
2.18
10.17
3.21
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (t1)

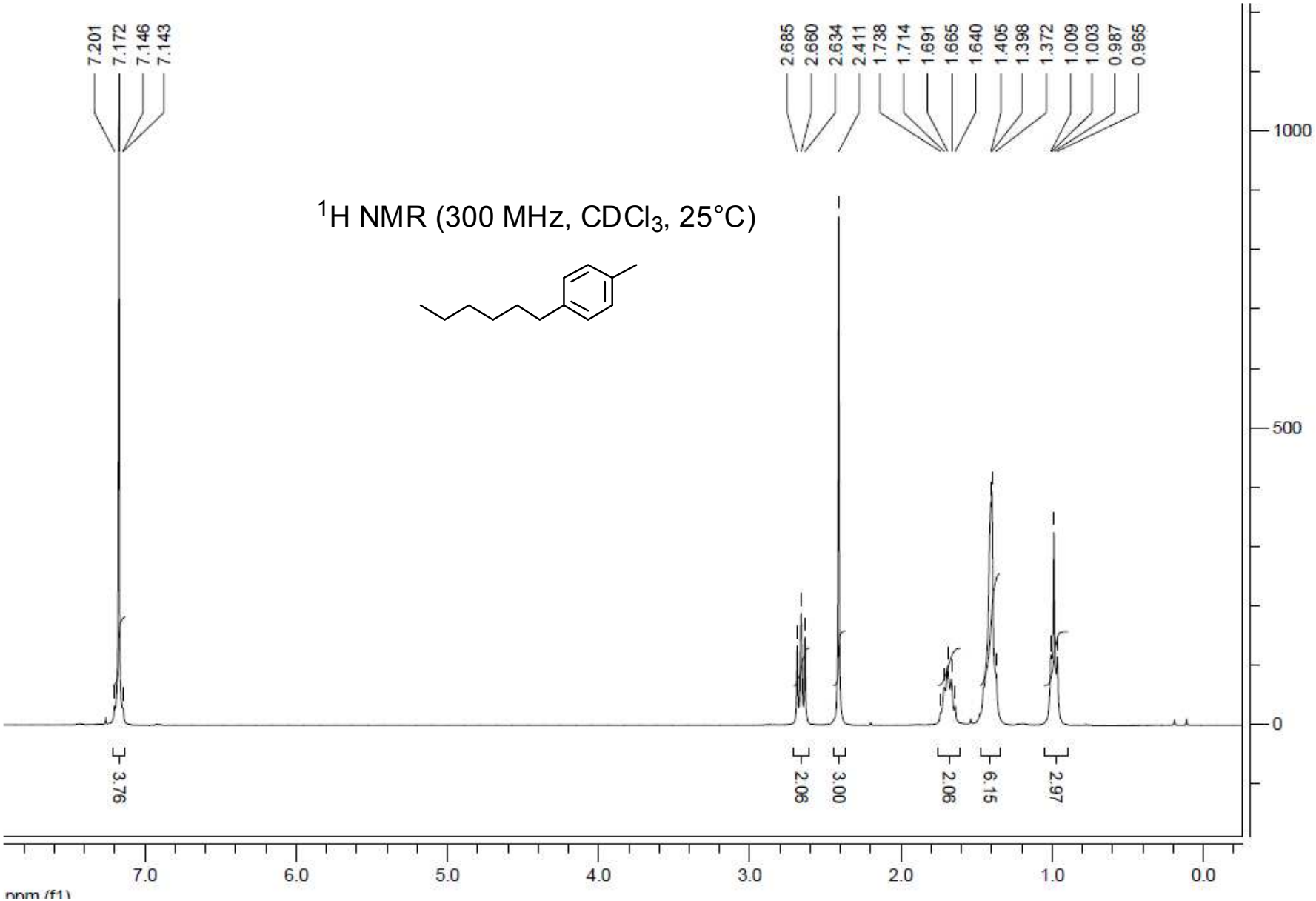

142.929
128.377
128.191
125.520
36.014
31.914
31.568
29.512
29.377
29.294
22.695
14.118
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
5000
4000
3000
2000
1000
0
200
150
100
50
0
ppm (f1)


8.100
8.073
7.898
7.874
7.752
7.725
7.563
7.545
7.521
7.518
7.498
7.475
7.454
7.431
7.404
7.366
7.344
3.125
3.099
3.073
1.837
1.813
1.788
1.762
1.737
1.498
1.478
1.451
1.430
1.405
1.375
1.322
0.946
0.928
0.905
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
150
100
50
0
1.00
1.04
0.93
3.92
2.02
2.03
10.53
3.02
10.0
5.0
0.0
ppm (f1)

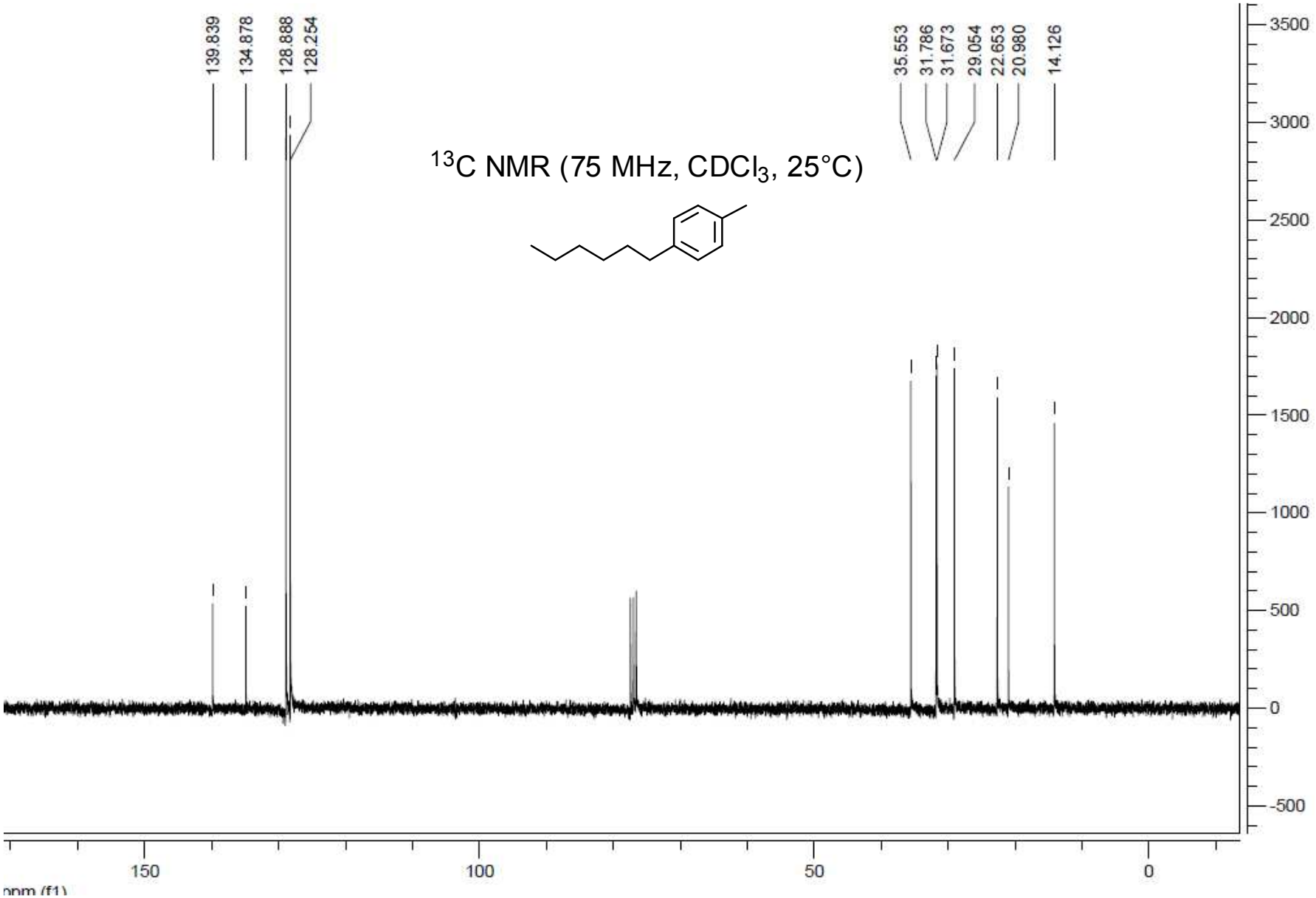

138.956
133.776
131.808
128.638
126.276
125.734
125.508
125.444
125.248
123.825
33.071
31.845
30.813
29.805
29.463
29.259
22.622
14.065
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
C_8H_{17}-*n*
3500
3000
2500
2000
1500
1000
500
0
-500
150
100
50
ppm (f1)

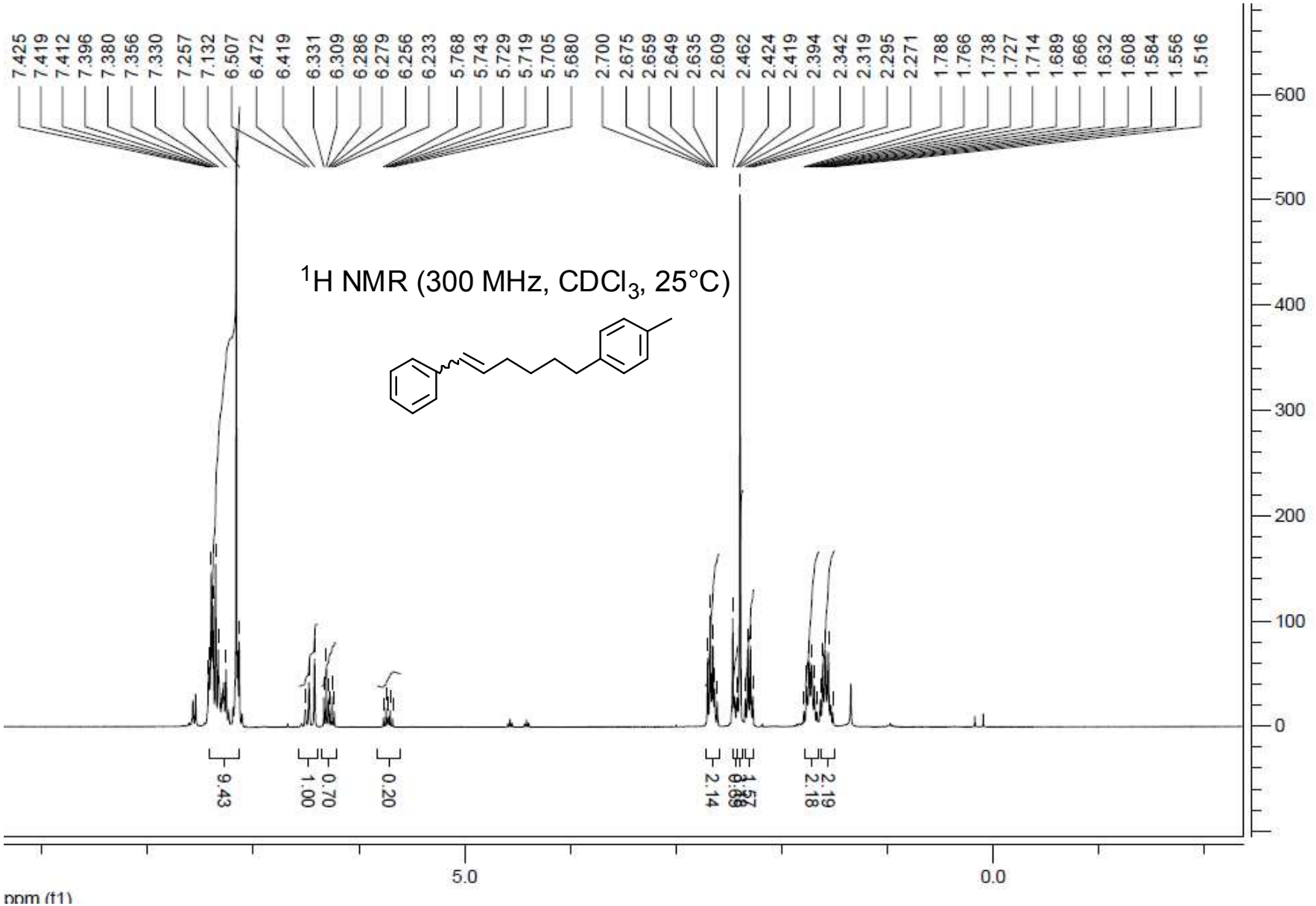

7.701
7.690
7.668
7.662
7.551
7.327
7.323
7.299
7.296
7.260
7.152
7.144
7.119
3.920
2.768
2.742
2.716
1.744
1.718
1.696
1.671
1.647
1.341
1.317
1.285
0.916
0.896
0.873
1H NMR (300 MHz, CDCl3, 25°C)
C8H17-n
MeO
1.98
1.00
1.09
1.95
3.05
2.02
2.09
10.30
3.13
800
700
600
500
400
300
200
100
0
-100
5.0
0.0
ppm (f1)

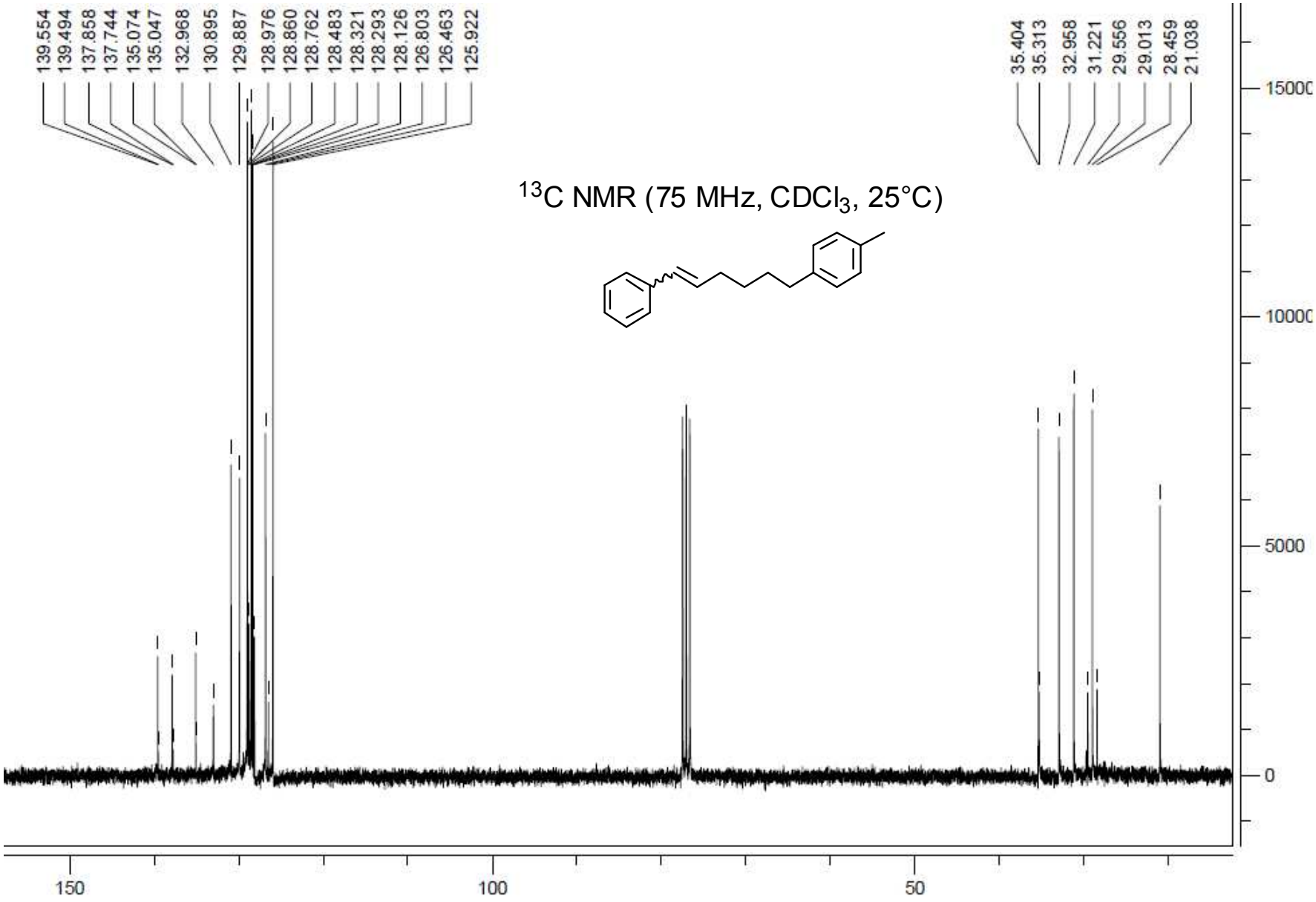

156.960
138.092
132.783
129.033
128.823
127.887
126.529
126.088
118.508
105.538
55.227
35.883
31.869
31.481
29.495
29.329
29.258
22.653
14.098
^{13}C NMR (75 MHz, CDCl$_3$, 25°C)
C$_8$H$_{17}$-*n*
MeO
1500
1000
500
0
150
100
50
ppm (f1)

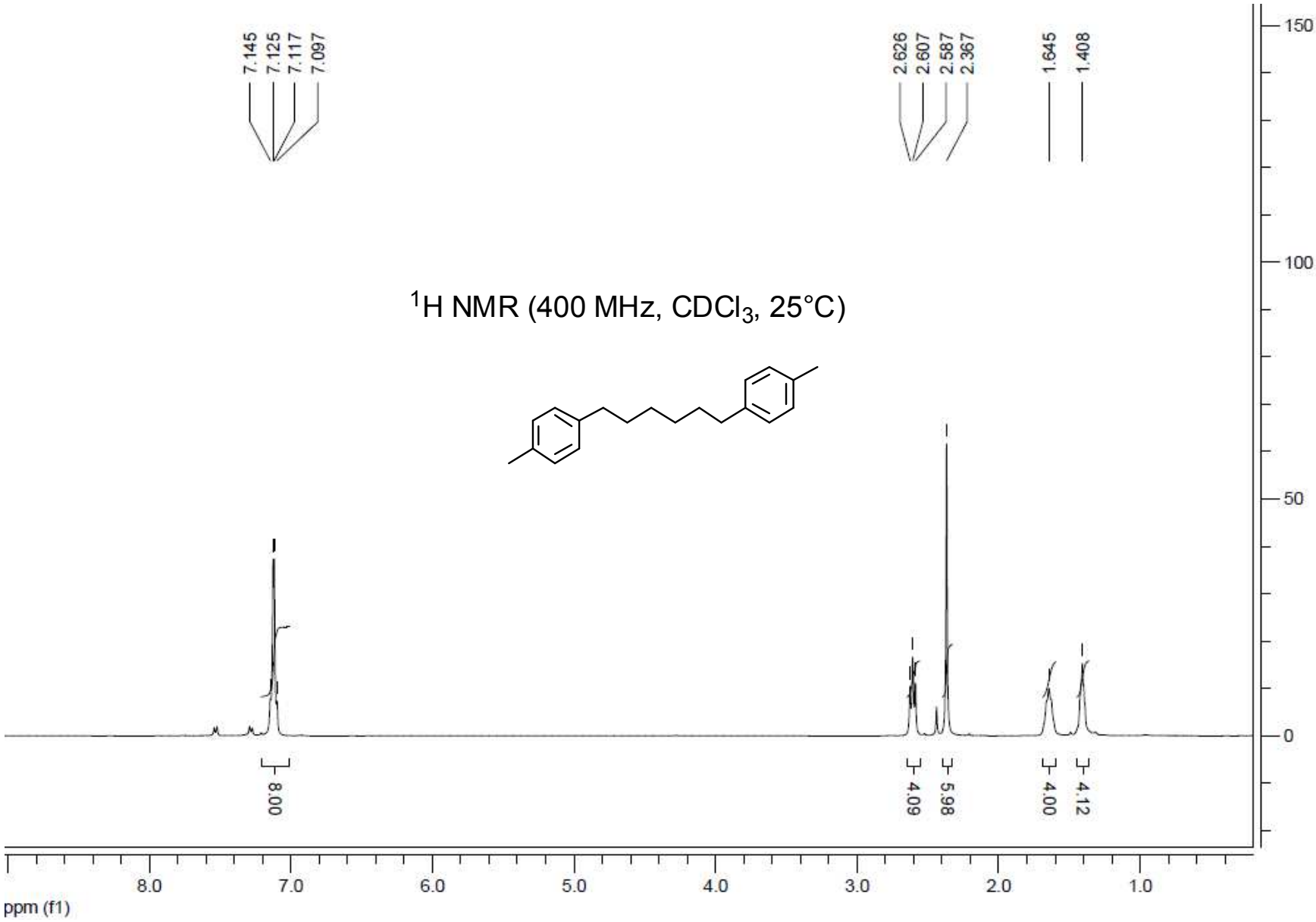


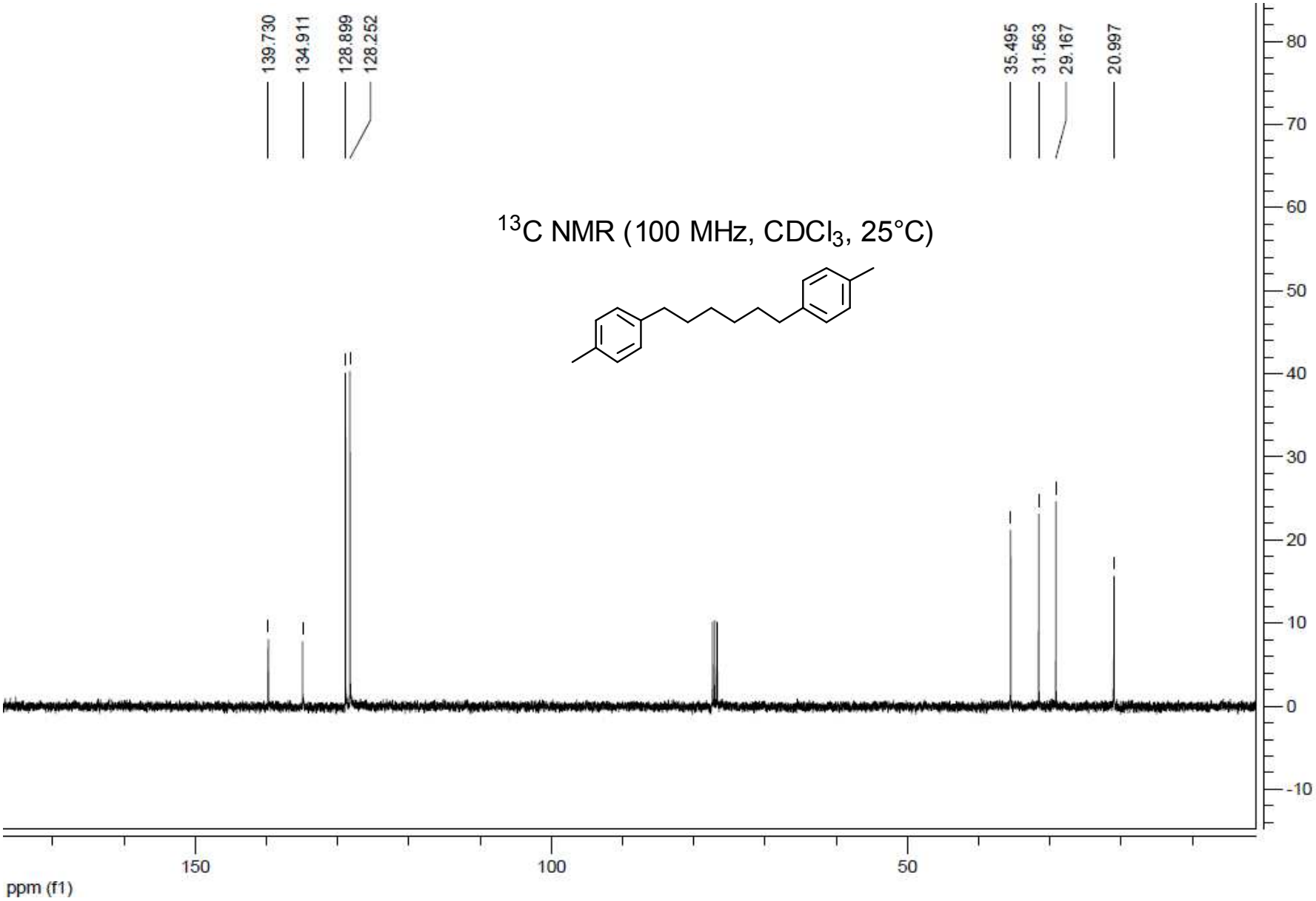
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)

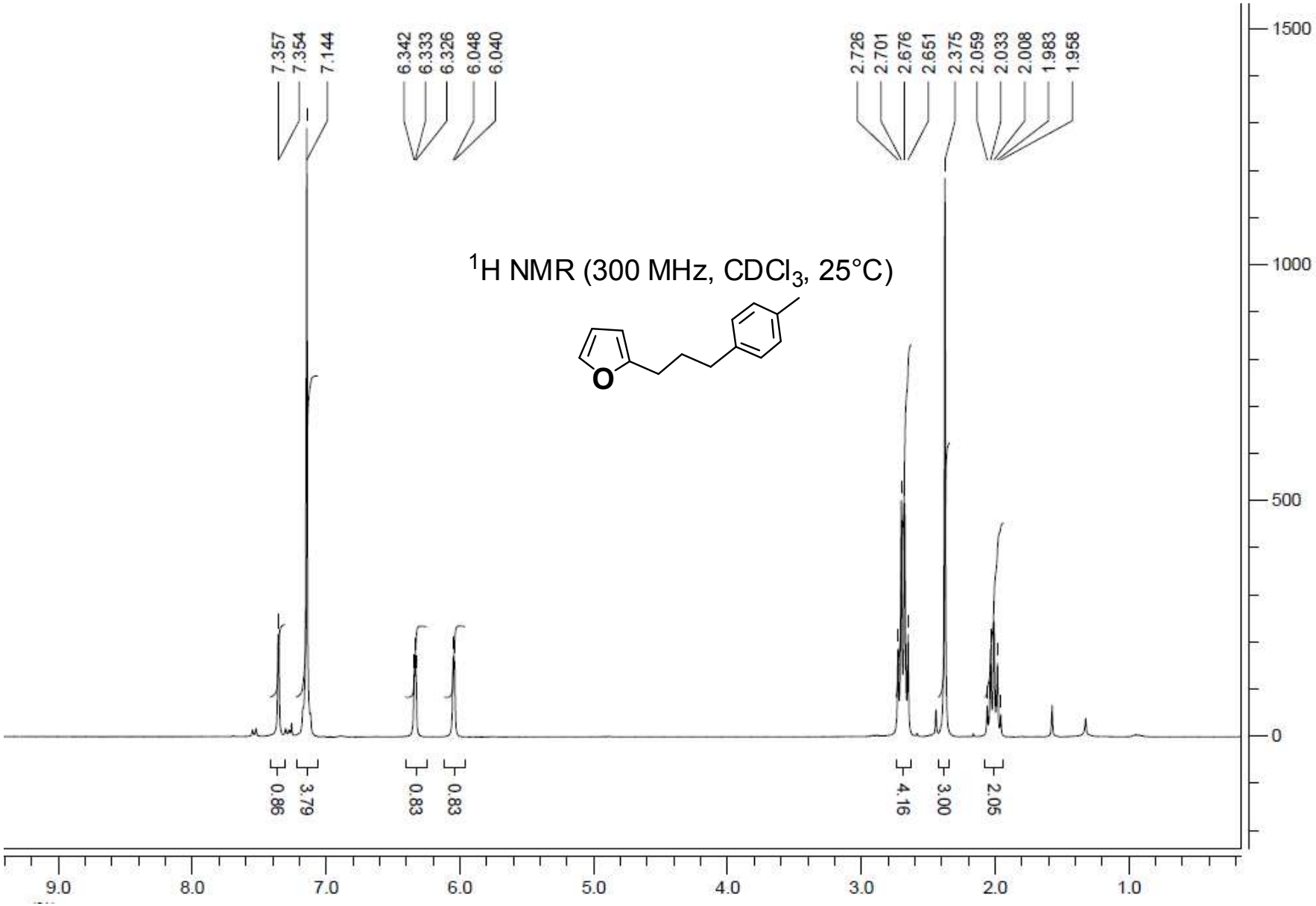

139.839
134.878
128.888
128.254
35.553
31.786
31.673
29.054
22.653
20.980
14.126
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
3500
3000
2500
2000
1500
1000
500
0
-500
150
100
50
0
ppm (f1)

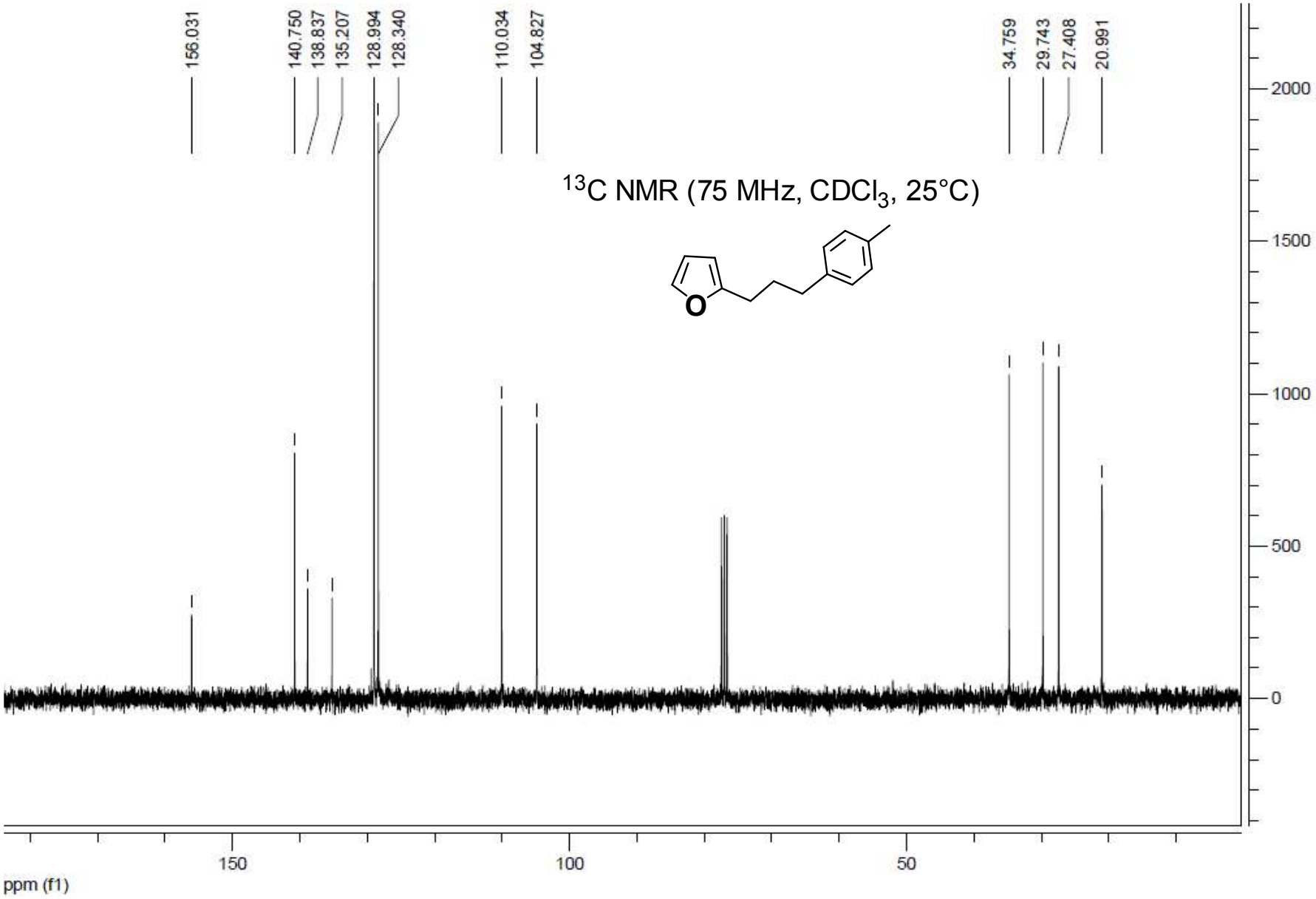

7.425
7.419
7.412
7.396
7.380
7.356
7.330
7.257
7.132
6.507
6.472
6.419
6.331
6.309
6.286
6.279
6.256
6.233
5.768
5.743
5.729
5.719
5.705
5.680
2.700
2.675
2.659
2.649
2.635
2.609
2.462
2.424
2.419
2.394
2.342
2.319
2.295
2.271
1.788
1.766
1.738
1.727
1.714
1.689
1.666
1.632
1.608
1.584
1.556
1.516
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
600
500
400
300
200
100
0
9.43
1.00
0.70
0.20
2.14
2.18
2.19
5.0
0.0
ppm (f1)


139.554
139.494
137.858
137.744
135.074
135.047
132.968
130.895
129.887
128.976
128.860
128.762
128.483
128.321
128.293
128.126
126.803
126.463
125.922
35.404
35.313
32.958
31.221
29.556
29.013
28.459
21.038
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
15000
10000
5000
0
150
100
50

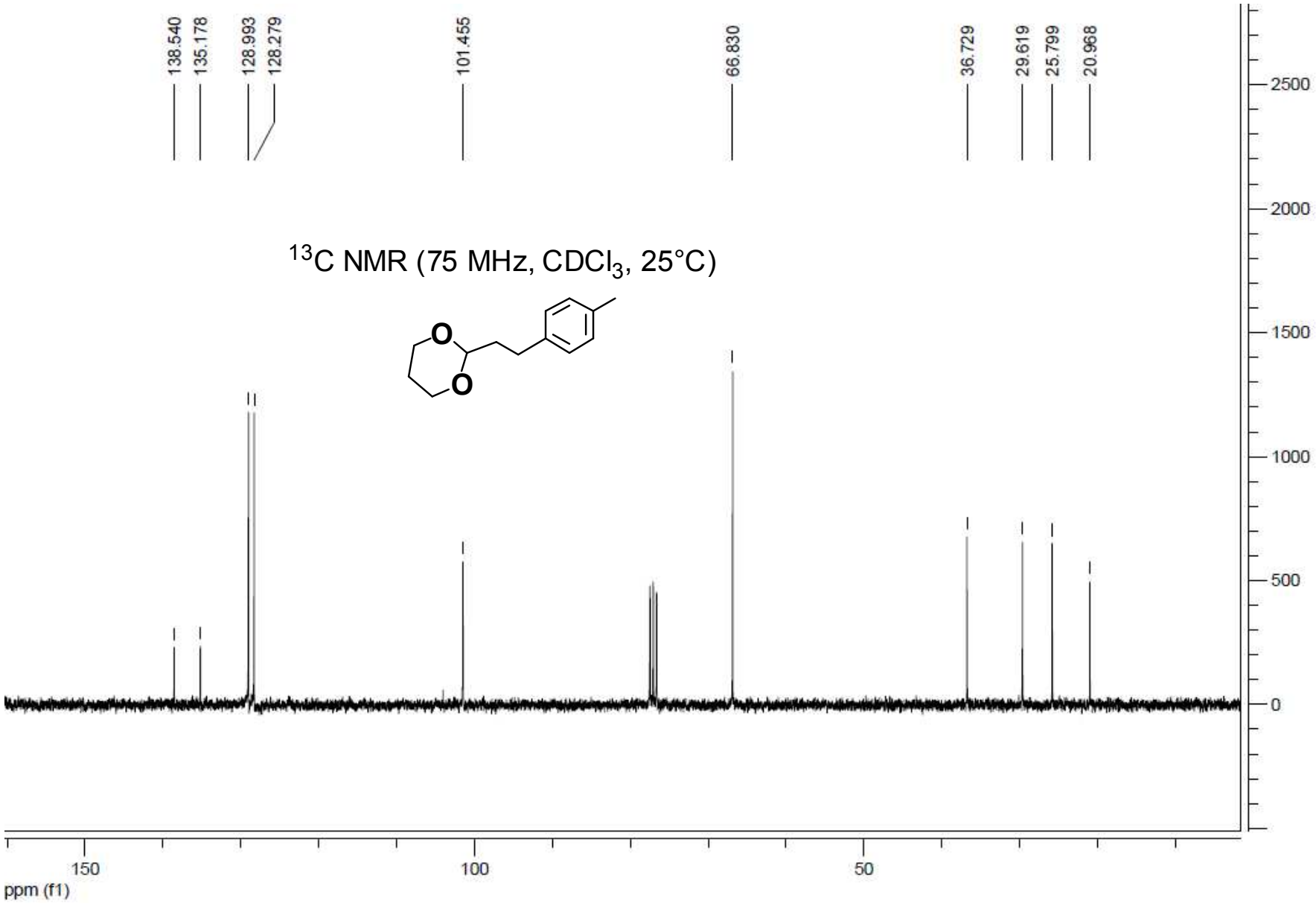

7.145
7.125
7.117
7.097
2.626
2.607
2.587
2.367
1.645
1.408
^{1}H NMR (400 MHz, $CDCl_3$, 25°C)
150
100
50
0
8.00
4.09
5.98
4.00
4.12
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)

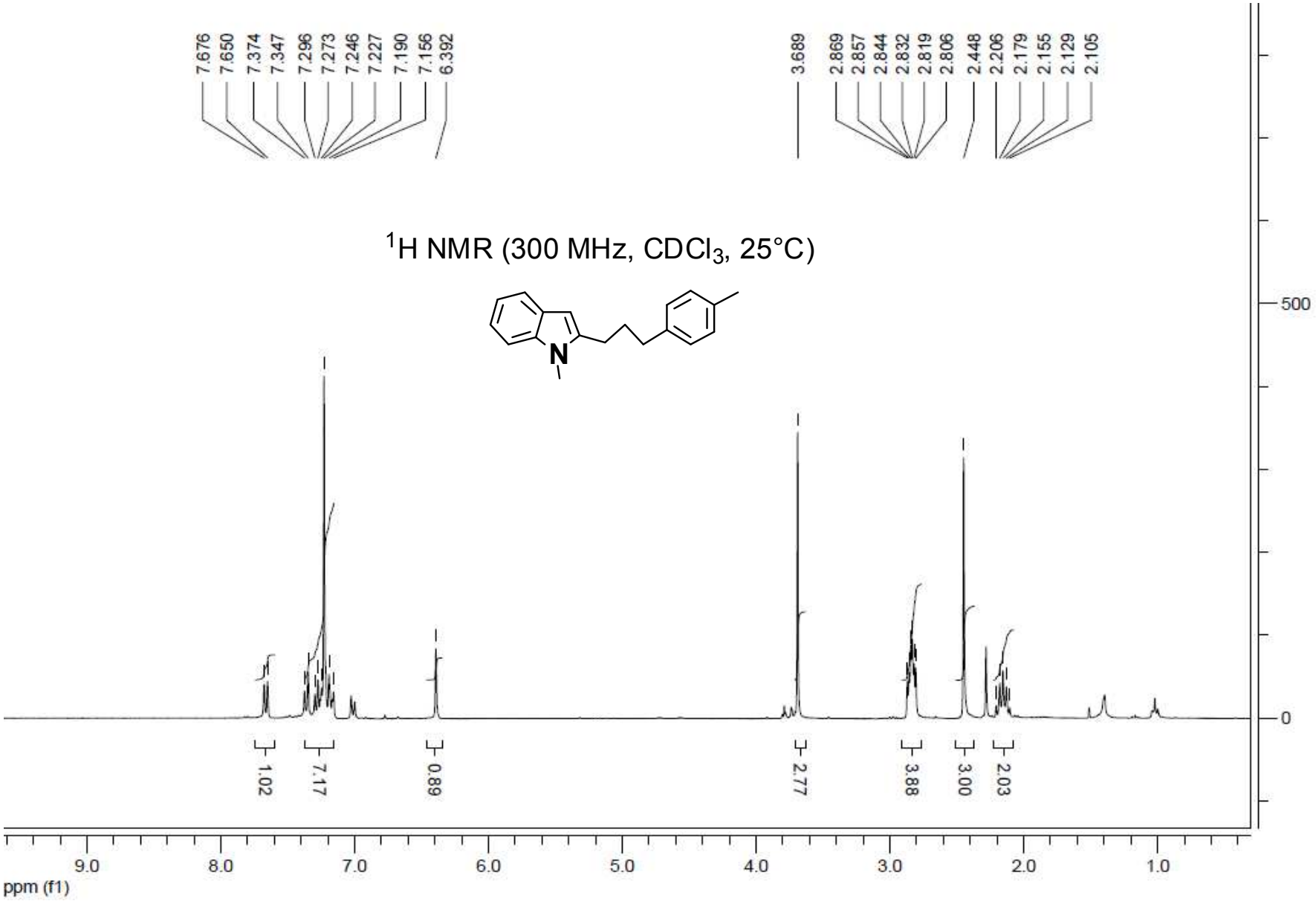

139.730
134.911
128.899
128.252
35.495
31.563
29.167
20.997
^{13}C NMR (100 MHz, $CDCl_3$, 25°C)
80
70
60
50
40
30
20
10
0
-10
150
100
50
ppm (f1)

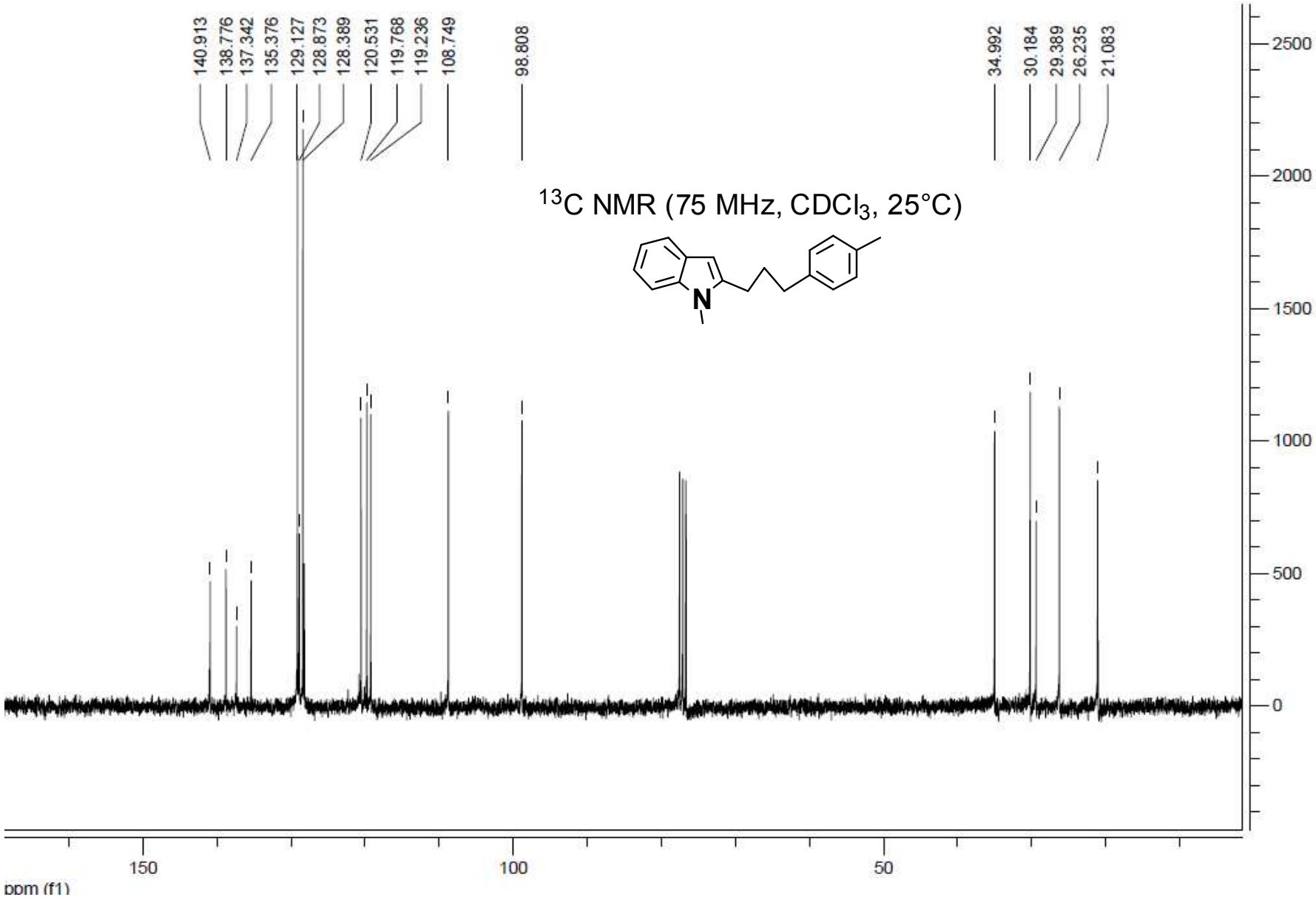

7.357
7.354
7.144
6.342
6.333
6.326
6.048
6.040
2.726
2.701
2.676
2.651
2.375
2.059
2.033
2.008
1.983
1.958
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
O
0.86
3.79
0.83
0.83
4.16
3.00
2.05
1500
1000
500
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0

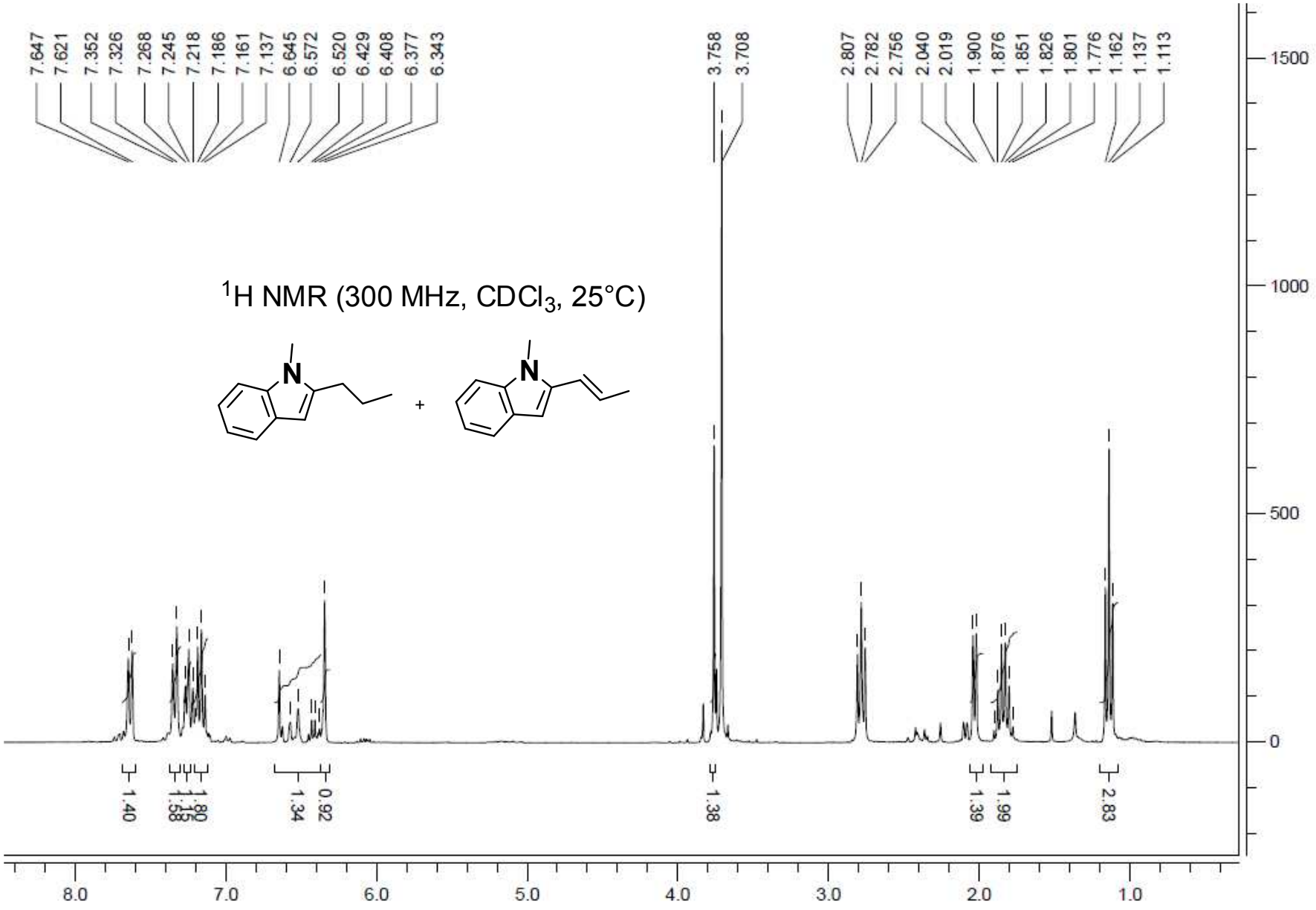

156.031
140.750
138.837
135.207
128.994
128.340
110.034
104.827
34.759
29.743
27.408
20.991
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
O
2000
1500
1000
500
0
150
100
50
ppm (f1)

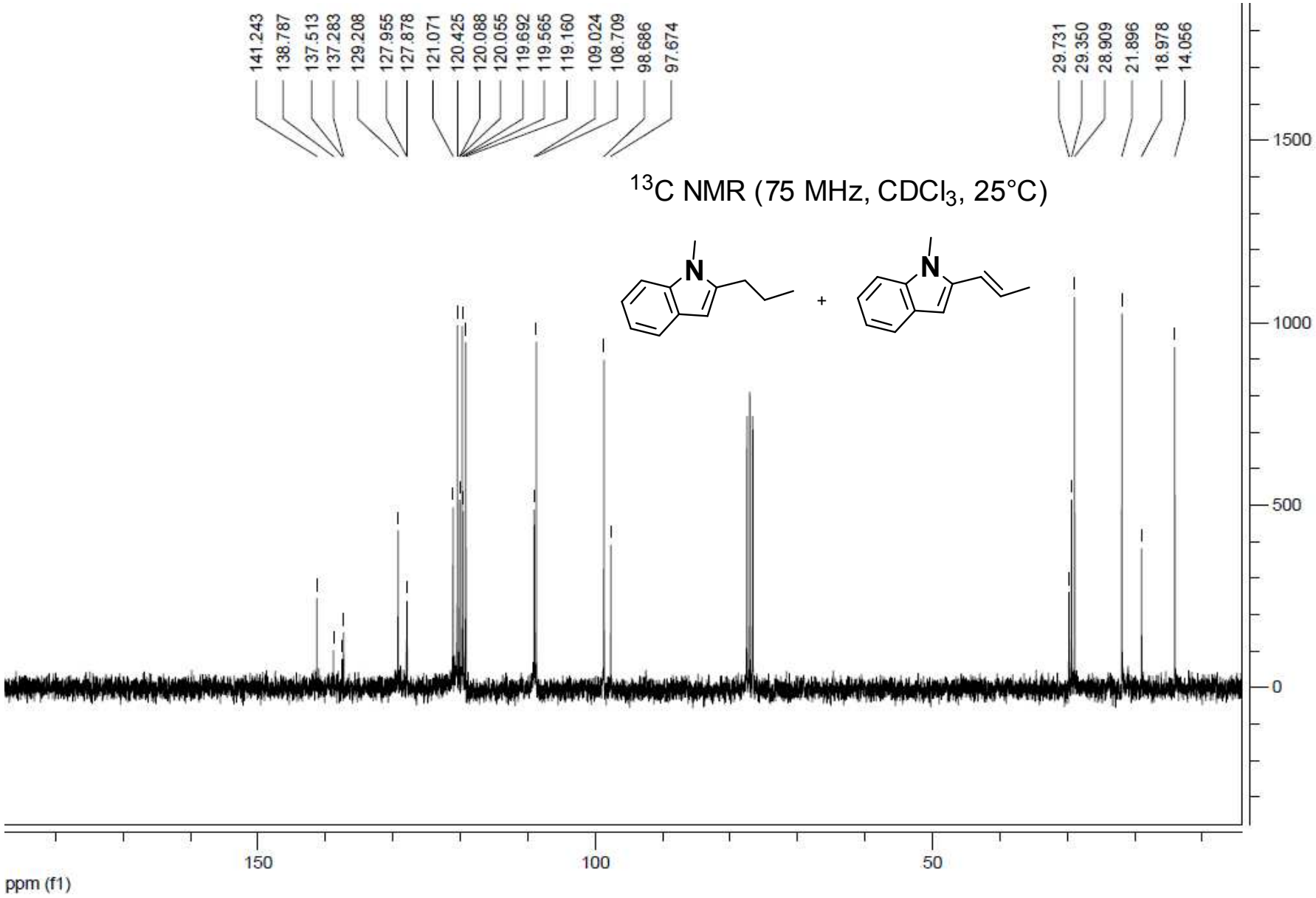

7.191
4.625
4.607
4.590
4.242
4.225
4.205
4.189
3.890
3.883
3.849
3.842
3.808
3.801
2.810
2.784
2.777
2.756
2.417
2.232
2.215
2.198
2.189
2.172
2.155
2.130
2.032
2.014
2.005
1.998
1.987
1.980
1.961
1.484
1.455
1.410
1.393
1.364
1H NMR (300 MHz, CDCl3, 25°C)
O
O
1500
1000
500
0
4.00
0.98
2.10
2.15
2.09
3.18
1.08
2.11
1.03
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm (f1)

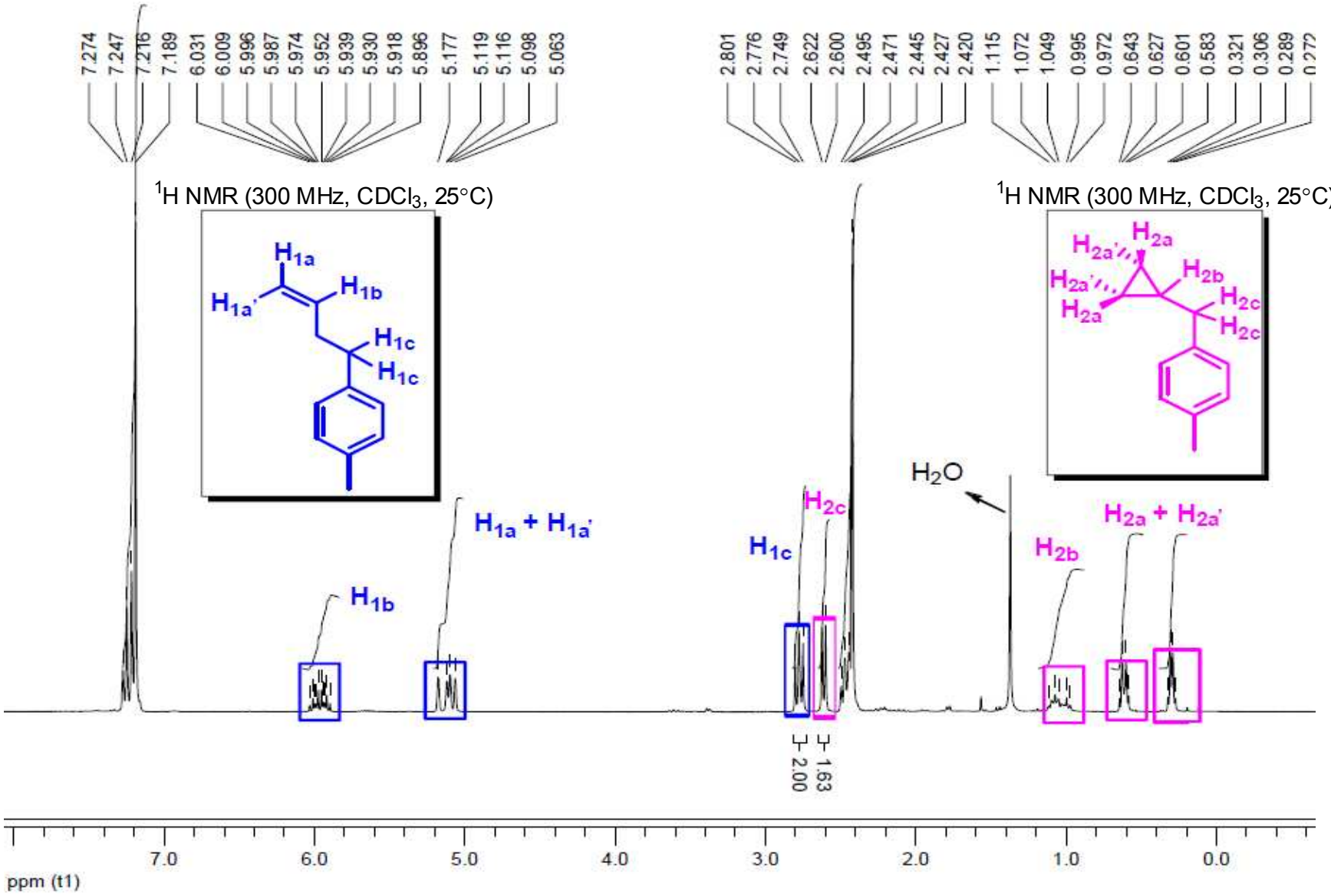

138.540
135.178
128.993
128.279
101.455
66.830
36.729
29.619
25.799
20.968
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
O
O
2500
2000
1500
1000
500
0
150
100
50
ppm (f1)

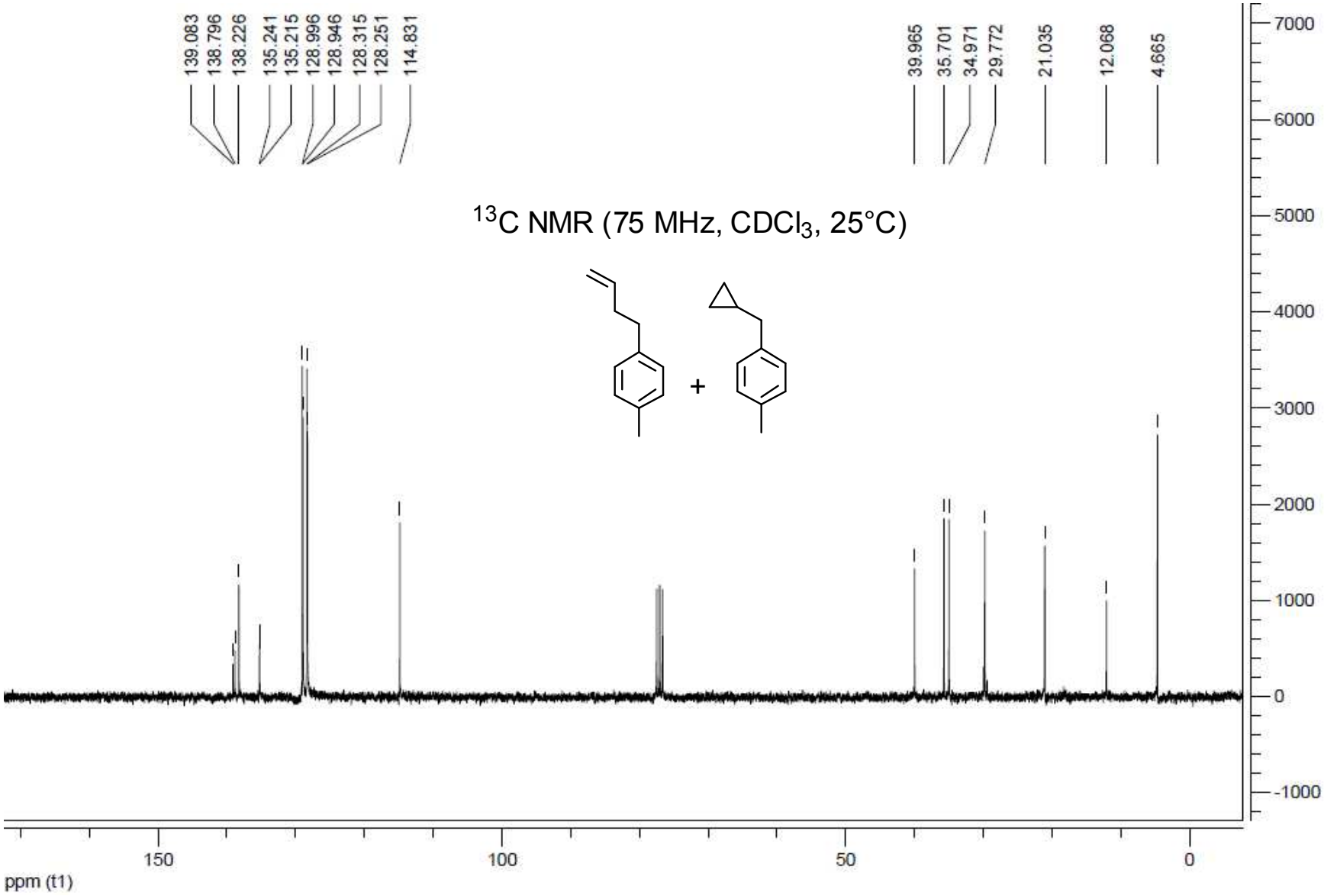

7.676
7.650
7.374
7.347
7.296
7.273
7.246
7.227
7.190
7.156
6.392
3.689
2.869
2.857
2.844
2.832
2.819
2.806
2.448
2.206
2.179
2.155
2.129
2.105
1H NMR (300 MHz, CDCl3, 25°C)
N
500
0
1.02
7.17
0.89
2.77
3.88
3.00
2.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
ppm (f1)


140.913
138.776
137.342
135.376
129.127
128.873
128.389
120.531
119.768
119.236
108.749
98.808
34.992
30.184
29.389
26.235
21.083
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
N
2500
2000
1500
1000
500
0
150
100
50
ppm (f1)


7.647
7.621
7.352
7.326
7.268
7.245
7.218
7.186
7.161
7.137
6.645
6.572
6.520
6.429
6.408
6.377
6.343
3.758
3.708
2.807
2.782
2.756
2.040
2.019
1.900
1.876
1.851
1.826
1.801
1.776
1.162
1.137
1.113
1H NMR (300 MHz, CDCl3, 25°C)
N
+
N
1.40
1.38
1.80
1.34
0.92
1.38
1.39
1.99
2.83
1500
1000
500
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0


141.243
138.787
137.513
137.283
129.208
127.955
127.878
121.071
120.425
120.088
120.055
119.692
119.565
119.160
109.024
108.709
98.686
97.674
29.731
29.350
28.909
21.896
18.978
14.056
13C NMR (75 MHz, CDCl3, 25°C)
N
+
N
1500
1000
500
0
150
100
50
ppm (f1)


7.274
7.247
7.216
7.189
6.031
6.009
5.996
5.987
5.974
5.952
5.939
5.930
5.918
5.896
5.177
5.119
5.116
5.098
5.063
2.801
2.776
2.749
2.622
2.600
2.495
2.471
2.445
2.427
2.420
1.115
1.072
1.049
0.995
0.972
0.643
0.627
0.601
0.583
0.321
0.306
0.289
0.272
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
^{1}H NMR (300 MHz, $CDCl_3$, 25°C)
H_{1a}
$H_{1a'}$
H_{1b}
H_{1c}
H_{1c}
H_{2a}
$H_{2a'}$
$H_{2a'}$
H_{2a}
H_{2b}
H_{2c}
H_{2c}
H_{1a} + $H_{1a'}$
H_{1b}
H_{1c}
H_{2c}
H_2O
H_{2b}
H_{2a} + $H_{2a'}$
2.00
1.63
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


139.083
138.796
138.226
135.241
135.215
128.996
128.946
128.315
128.251
114.831
39.965
35.701
34.971
29.772
21.035
12.068
4.665
^{13}C NMR (75 MHz, $CDCl_3$, 25°C)
+
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
100
50
0
ppm (t1)

2. HRMS of Organofluorines and Arylation Products

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

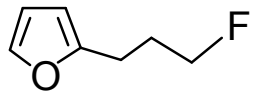
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-2609

Sample Serial Number: MZB-1

Operator: Li

Date: 2011/11/16



$[C_7H_9FO]^+$: 128.0637

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
192 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-4 F: 0-2 S: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
128.0636	128.0637	-0.1	-0.8	3.0	2773013.3	C7 H9 O F
	128.0635	0.1	0.8	-0.5	2773015.5	C2 H8 N3 O F2

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

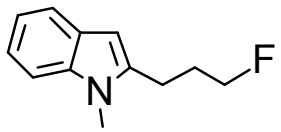
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-2721

Sample Serial Number: MZB-2

Operator: Li

Date: 2011/12/01



$[C_{12}H_{14}FN]^+$: 191.1110

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
606 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 F: 0-3 Cl: 0-2

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
191.1109	191.1110	-0.1	-0.5	6.0	9.3	C12 H14 N F
	191.1108	0.1	0.5	2.5	16.2	C7 H13 N4 F2

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

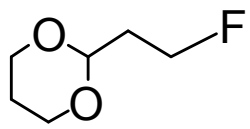
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-2722

Sample Serial Number: MZB-1

Operator: Li

Date: 2011/12/01



$[C_6H_{10}FO_2]^+$: 133.0665

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
256 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-3 F: 0-9 Cl: 0-2

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
133.0664	133.0665	-0.1	-0.8	1.5	2773014.8	C6 H10 O2 F
	133.0658	0.6	4.5	1.0	2773283.0	C6 H12 N Cl

$[M-H]^+$

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

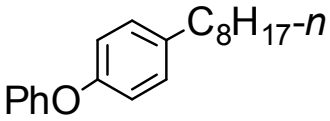
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-2614

Sample Serial Number: MZB-6

Operator: Li

Date: 2011/11/16



$[C_{20}H_{26}O]^+$: 282.1984

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
489 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-4 F: 0-2 S: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
282.1986	282.1984	0.2	0.7	8.0	0.3	C20 H26 O
	282.1982	0.4	1.4	4.5	7.6	C15 H25 N3 O F
	282.1993	-0.7	-2.5	0.5	18.2	C12 H26 N3 O2 F2
	282.1995	-0.9	-3.2	4.0	4.2	C17 H27 O2 F
	282.1977	0.9	3.2	-1.0	33.6	C12 H30 N2 O3 S

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

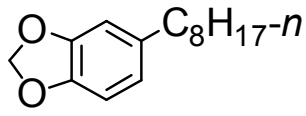
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-2611

Sample Serial Number: MZB-3

Operator: Li

Date: 2011/11/16



$[C_{15}H_{22}O_2]^+$: 234.1620

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
409 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-4 F: 0-2 S: 0-1

Minimum:				-1.5						
Maximum:		2.0	5.0	50.0						
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula				
234.1616	234.1618	-0.2	-0.9	1.5	1.5	C10	H21	N3	O2	F
	234.1620	-0.4	-1.7	5.0	3.1	C15	H22	O2		
	234.1606	1.0	4.3	5.5	1.2	C13	H20	N3	O	

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

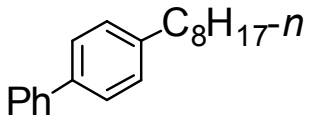
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T*11-12*-2693

Sample Serial Number: MZB-2

Operator: Li

Date: 2011/11/29



$[C_{20}H_{26}]^+$: 266.2035

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
673 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
266.2033	266.2035	-0.2	-0.8	8.0	4.5	C20 H26
	266.2028	0.5	1.9	-1.0	207.9	C12 H30 N2 O2 S

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

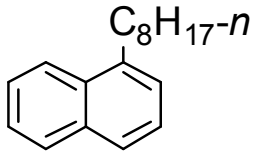
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-2613

Sample Serial Number: MZB-5

Operator: Li

Date: 2011/11/16



$[C_{18}H_{24}]^+$: 240.1878

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
412 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-4 F: 0-2 S: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
240.1882	240.1878	0.4	1.7	7.0	16.4	C18 H24
	240.1887	-0.5	-2.1	-0.5	13.8	C10 H24 N3 O F2
	240.1876	0.6	2.5	3.5	6.1	C13 H23 N3' F
	240.1889	-0.7	-2.9	3.0	9.8	C15 H25 O F

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

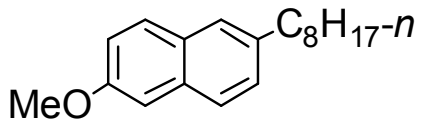
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T*11-12*-2694

Sample Serial Number: MZB-1

Operator: Li

Date: 2011/11/29



$[C_{19}H_{26}O]^+$: 270.1984

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
693 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.1983	270.1984	-0.1	-0.4	7.0	1.3	C19 H26 O
	270.1989	-0.6	-2.2	2.5	1132.3	C16 H29 N Cl
	270.1970	1.3	4.8	7.5	3.7	C17 H24 N3

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

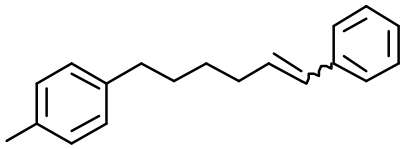
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-05-1141

Sample Serial Number: MZB-01

Operator: Li

Date: 2011/05/26



$C_{19}H_{22}^{+}$: 250.1722

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
469 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-8 F: 0-1 Cl: 0-1

Minimum:				-1.5					
Maximum:		1.5	5.0	50.0					
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula			
250.1724	250.1722	0.2	0.8	9.0	2773915.3	C19	H22		
	250.1720	0.4	1.6	5.5	2773543.5	C14	H21	N3	F
	250.1733	-0.9	-3.6	5.0	2773745.3	C16	H23	O	F

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

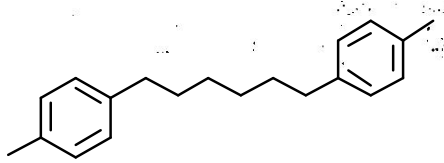
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-2766

Sample Serial Number: MZB-1

Operator: Li

Date: 2011/12/09



$[C_{20}H_{26}]^+$: 266.2035

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
574 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 F: 0-3 I: 0-2

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
266.2032	266.2033	-0.1	-0.4	4.5	22.0	C15 H25 N3 F
	266.2035	-0.3	-1.1	8.0	81.6	C20 H26
	266.2044	-1.2	-4.5	0.5	13.0	C12 H26 N3 O F2

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

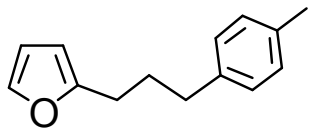
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-11-2610

Sample Serial Number: MZB-2

Operator: Li

Date: 2011/11/16



$[C_{14}H_{16}O]^+$: 200.1201

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
345 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-4 F: 0-2 S: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
200.1204	200.1201	0.3	1.5	7.0	0.9	C14 H16 O
	200.1199	0.5	2.5	3.5	48.4	C9 H15 N3 O F
	200.1211	-0.7	-3.5	-0.5	149.4	C6 H16 N3 O2 F2
	200.1213	-0.9	-4.5	3.0	20.6	C11 H17 O2 F

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

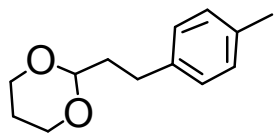
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-2692

Sample Serial Number: MZB-3

Operator: Li

Date: 2011/11/29



$[C_{13}H_{18}O_2]^+$: 206.1307

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions
450 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 S: 0-1 Cl: 0-1 Br: 0-1

Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
206.1309	206.1307	0.2	1.0	5.0	2773012.8	C13 H18 O2
	206.1312	-0.3	-1.5	0.5	2773016.5	C10 H21 N O, Cl

Shanghai Mass Spectrometry Center
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report

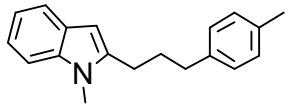
Instrument: Waters Micromass GCT Premier Ionisation Mode: EI+ Electron Energy: 70eV

Card Serial Number: GCT-P-T11-12-2720

Sample Serial Number: MZB-3

Operator: Li

Date: 2011/12/01



$[C_{19}H_{21}N]^+$: 263.1674

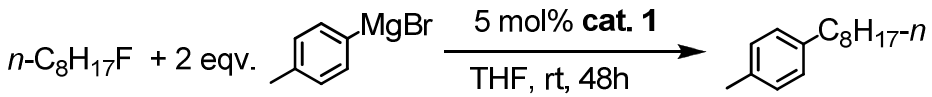
Elemental Composition Report

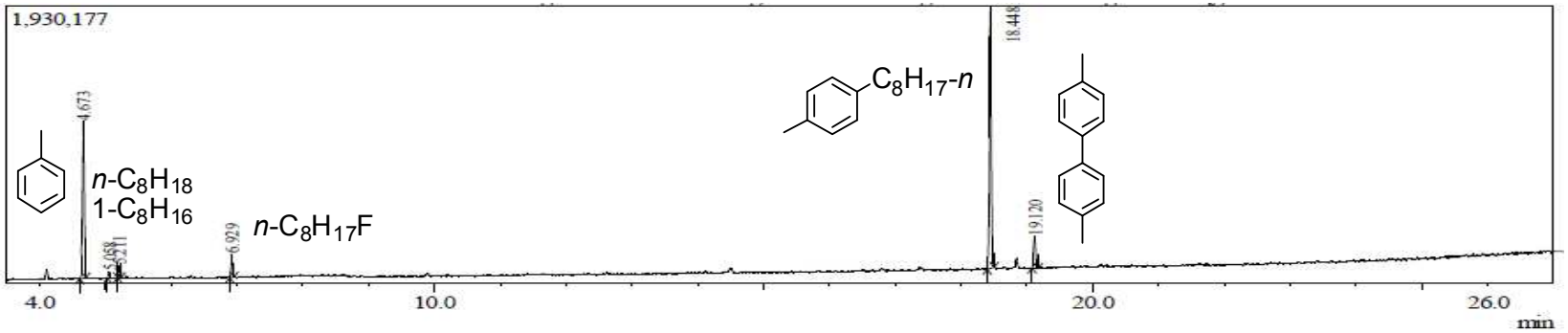
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off

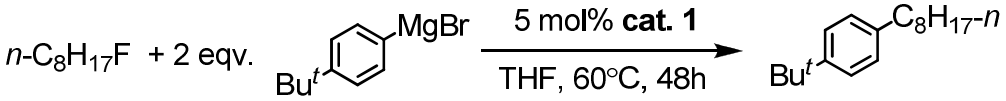
Monoisotopic Mass, Odd and Even Electron Ions
1014 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-80 N: 0-4 O: 0-6 F: 0-3 Cl: 0-2

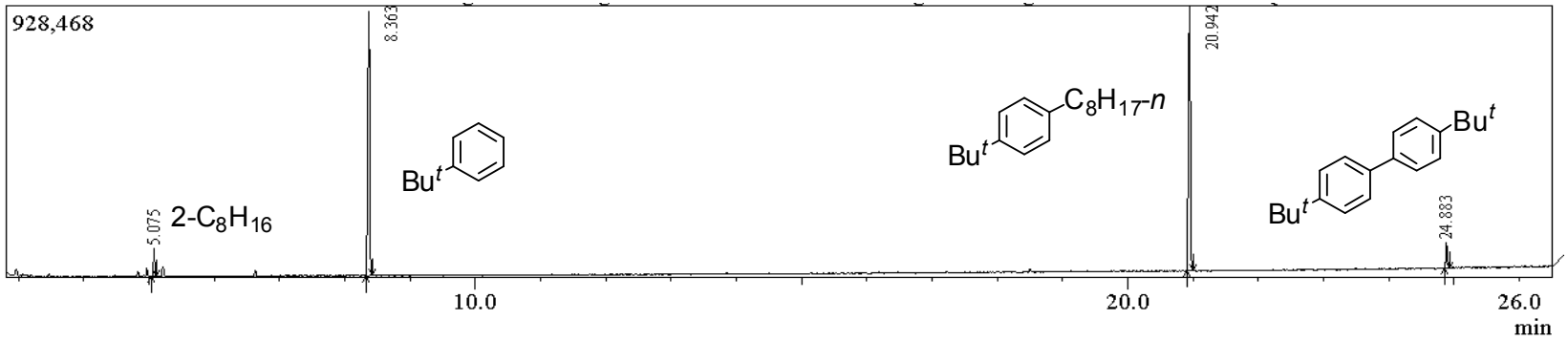
Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
263.1671	263.1672	-0.1	-0.4	6.5	2773045.8	C14 H20 N4 F
	263.1674	-0.3	-1.1	10.0	2773086.8	C19 H21 N
	263.1659	1.2	4.6	1.5	2773072.0	C13 H24 O4 F
	263.1683	-1.2	-4.6	2.5	2773038.0	C11 H21 N4 O F2

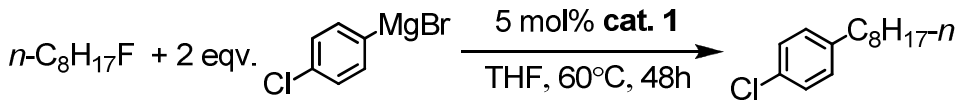
5. Selected GC-MS graphs

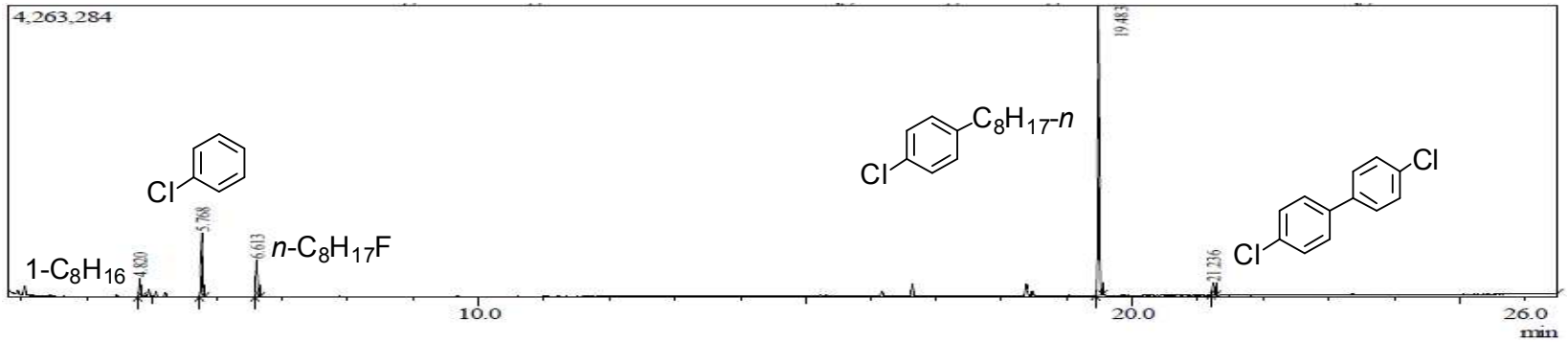


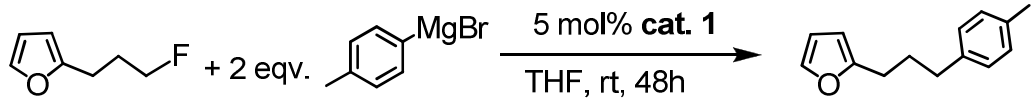


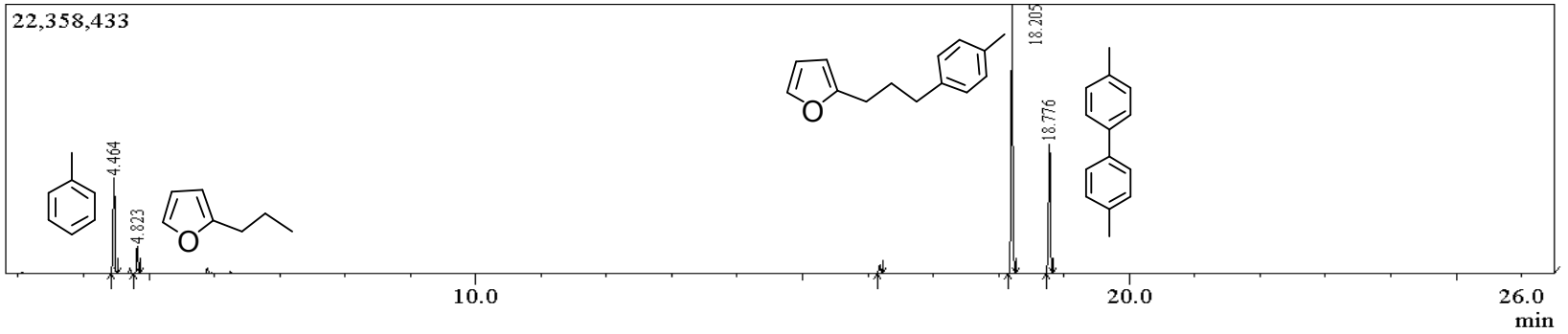


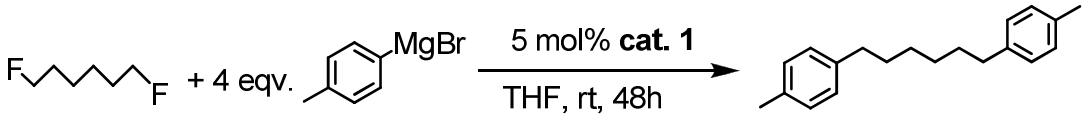


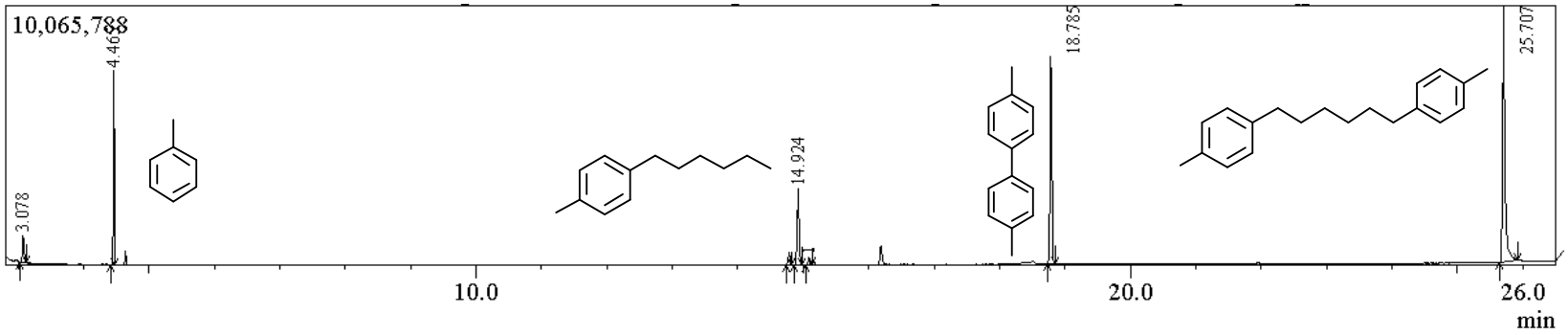

n-C8H17F + 2 eqv.
MgBr
Cl
5 mol% cat. 1
THF, 60°C, 48h
C8H17-n
Cl

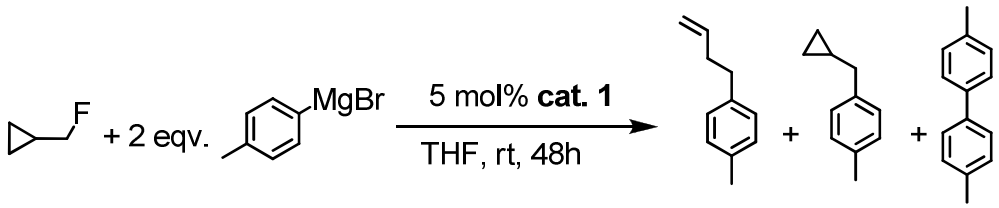

4,263,284
Cl
1-C8H16
4.820
5.768
6.613
n-C8H17F
C8H17-n
Cl
19.483
Cl
21.236
10.0
20.0
26.0
min

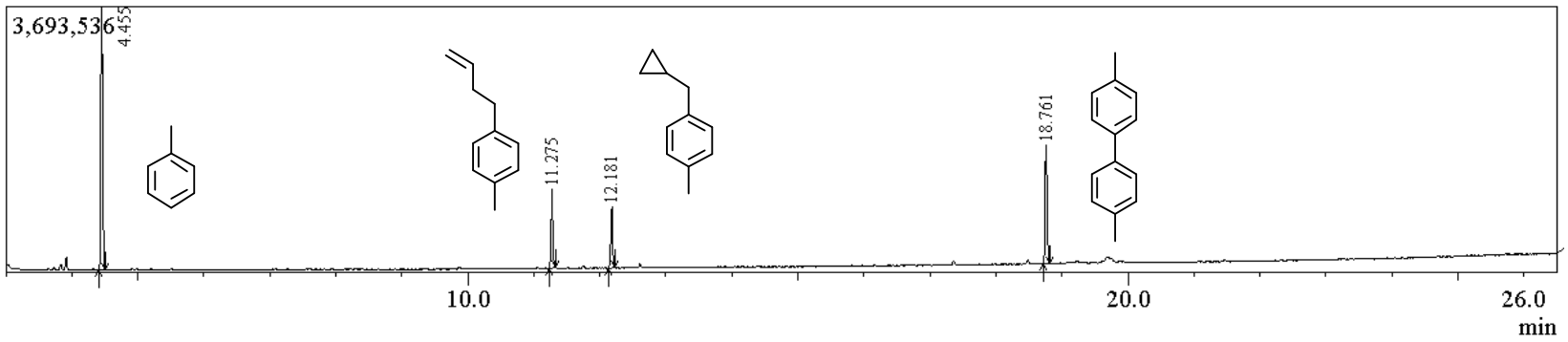

F
+ 2 eqv.
MgBr
5 mol% cat. 1
THF, rt, 48h


22,358,433
4.464
4.823
18.205
18.776
10.0
20.0
26.0
min


F
F
+ 4 eqv.
MgBr
5 mol% cat. 1
THF, rt, 48h


10,065,788
4.465
3.078
14.924
18.785
25.707
10.0
20.0
26.0
min


F
+ 2 eqv.
MgBr
5 mol% cat. 1
THF, rt, 48h
+
+


3,693,536
4.455
11.275
12.181
18.761
10.0
20.0
26.0
min