Electronic Supplementary Information

Room-temperature nickel-catalysed cross-couplings of aryl chlorides with arylzincs

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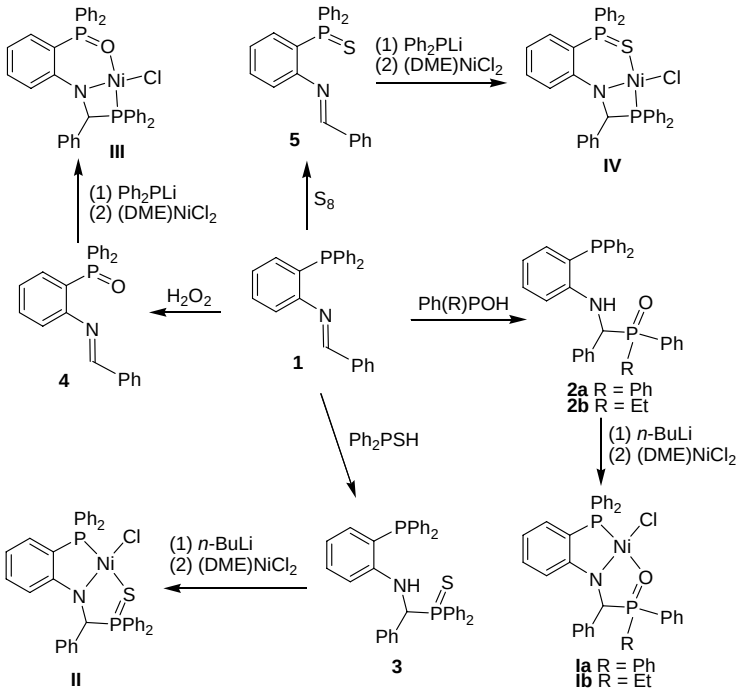


Scheme S1. Synthesis of complexes **Ia-IV**

Experimental Section

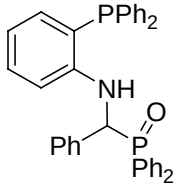
General

All reactions were performed under nitrogen atmosphere using standard Schlenk and vacuum line techniques. Solvents were distilled under nitrogen over sodium (toluene), sodium/benzophenone (THF, Et_2O and n-hexane) and degassed prior to use. NMP and DMA was dried over 4Å molecular sieves, fractionally distilled under reduced pressure and stored

under nitrogen atmosphere. 2-(Ph_2P)C_6H_4N=CHPh,[1] (DME)$NiCl_2$,[2] $Ph_2P(S)H$,[3] Ph_2POH[4] and Ph(Et)POH[4] were prepared according to the reported methods. *n*-BuLi was purchased from Acros Organics and used as received. $CDCl_3$, purchased from Cambridge Isotope Laboratories, Inc., was degassed and stored over 4Å molecular sieves. Zinc dust was purchased from Acros Organics. 2-Furyllithium was prepared from furan by direct lithiation using *n*-BuLi.[5] PhLi, *p*-MeC_6H_4Li, *o*-MeC_6H_4Li and *p*-$Me_2NC_6H_4Li$ were prepared from corresponding aryl bromides and Li according to literature.[6] *p*-$EtO_2CC_6H_4ZnBr$, *p*-$EtO_2CC_6H_4ZnI$ and *p*-MeC_6H_4ZnI was prepared according to the procedure reported in literature.[7,8] NMR spectra were recorded on a Bruker av300 spectrometer at ambient temperature. The chemical shifts of the ^1H and ^{13}C NMR spectra were referenced to TMS or internal solvent resonances. MS data were recorded on an Agilent6890/Micromass GCT-MS spectrometer (EI) or a Thermo Finnigan LCQ Advantage Max ion trap mass spectrometer (ESI). Elemental analysis was performed by the Analytical Center of the University of Science and Technology of China.

1. Synthesis and characterization of compounds 2-5 and nickel complexes I-IV

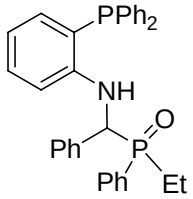
Synthesis of 2-(Ph_2P)C_6H_4NHCH(Ph)P(O)Ph_2 (2a)



A mixture of 2-(Ph_2P)C_6H_4N=CHPh (0.41 g, 1.12 mmol), Ph_2POH (0.24 g, 1.19 mmol) and toluene (15 mL) was stirred overnight at room temperature and then refluxed for 2 hours. The resulting solution was cooled to room temperature, and added hexane (10 mL) to form white precipitate. The precipitate was collected by filtration and dried in vacuo to afford white solid (0.5 g, 78%), mp 184–187 °C. ^1H NMR ($CDCl_3$): δ 5.26 (dd, *J* = 9.3, 16.5 Hz, 1H, CH), 5.64 (q, *J* = 8.7 Hz, 1H, Ar), 6.47 (dd, *J* = 5.4, 8.1 Hz, 1H, Ar), 6.53 (t, *J* = 7.5 Hz, 1H, Ar), 6.64 (t, *J* = 6.3 Hz, 1H, Ar), 6.94–6.97 (m, 2H, Ar), 6.98–7.06 (m, 6H, Ar), 7.08–7.26 (m, 11H, Ar), 7.36–7.42 (m, 4H, Ar), 7.57–7.63 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 57.93 (d, *J* = 75.2 Hz),

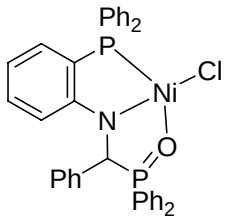
111.66, 118.65, 121.33 (d, J = 9.2 Hz), 127.69, 128.15, 128.31, 128.46, 128.61, 128.91, 130.56, 131.79, 131.90, 132.00, 132.18, 132.30, 132.64, 133.71, 133.89, 133.96, 134.14, 134.40, 134.77, 135.17, 135.26, 148.71 (dd, J = 12.1, 18.7 Hz). ^{31}P NMR ($CDCl_3$): δ –26.41, 26.37. Anal. Calcd for $C_{37}H_{31}NOP_2$: C, 78.29; H, 5.50; N, 2.47. Found: C, 77.95; H, 5.53; N, 2.17.

Synthesis of 2-(Ph_2P)C_6H_4NHCH(Ph)P(O)(Ph)Et (2b)



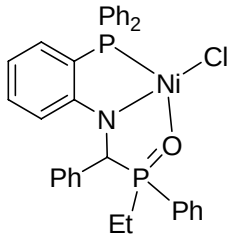
A mixture of 2-(Ph_2P)C_6H_4N=CHPh (0.46 g, 1.26 mmol), Ph(Et)POH (0.20 g, 1.30 mmol) and toluene (15 mL) was stirred overnight at room temperature and then refluxed for 6 hours. Solvent was removed in vacuo, and Et_2O (10 mL) was added into the residue with vigorous stirring until white precipitate generated. The precipitate was collected by filtration and dried in vacuo to give white solid (0.52 g, 80%), mp 124–128 °C. ^{1}H NMR ($CDCl_3$): δ 0.87–1.05 (m, 6H, CH_3), 1.68–1.87 (m, 4H, CH_2), 4.72 (dd, J = 7.5, 13.9 Hz, 1H, CH), 4.83 (dd, J = 9.3, 16.8 Hz, 1H, CH), 5.32 (q, J = 7.6 Hz, 1H, Ar), 5.76 (q, J = 7.5 Hz, 1H, Ar), 6.33 (dd, J = 5.3, 7.5 Hz, 1H, Ar), 6.41 (dd, J = 5.3, 7.8 Hz, 1H, Ar), 6.52 (t, J = 7.3 Hz, 2H, Ar), 6.60 (t, J = 5.8 Hz, 1H, Ar), 6.68 (t, J = 6 Hz, 1H, Ar), 6.86 (d, J = 5.7 Hz, 2H, Ar), 6.91–7.05 (m, 7H, Ar), 7.07–7.72 (m, 31H, Ar). ^{13}C NMR ($CDCl_3$): δ 5.21 (d, J = 4.6 Hz), 5.42 (d, J = 4.5 Hz), 18.37 (d, J = 4.5 Hz), 19.31, 57.66 (d, J = 71 Hz), 59.05 (d, J = 72 Hz), 111.54 (d, J = 18.7 Hz), 118.53 (d, J = 8.5 Hz), 127.54, 127.73, 128.25, 128.37, 128.43, 128.65, 129.00 (d, J = 7.5 Hz), 130.33 (d, J = 14.8 Hz), 131.39 (d, J = 8.1 Hz), 131.80, 132.03, 133.70, 133.96, 134.10, 134.21, 134.26, 134.35, 134.96, 135.26, 135.62, 148.90 (dd, J = 14.9, 29.9 Hz). ^{31}P NMR ($CDCl_3$): δ –24.82, 37.77, 38.26. Anal. Calcd for $C_{33}H_{31}NOP_2$: C, 76.29; H, 6.01; N, 2.70. Found: C, 75.93; H, 6.21; N, 2.77.

Synthesis of [Ni(Cl){2-(Ph_2P)C_6H_4NCH(Ph)P(O)Ph_2}] (Ia)



To a stirred solution of **2a** (0.50 g, 0.88 mmol) in THF (15 mL) was added dropwise *n*-BuLi (0.36 mL, a 2.5 M solution in hexanes, 0.90 mmol) at about −80 °C. The resulting mixture was warmed to room temperature and stirred for 4 h. This solution was added dropwise to a stirred suspension of (DME)$NiCl_2$ (0.20 g, 0.91 mmol) in THF (10 mL) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo and the residue was dissolved in toluene. The resulting solution was filtered and the filtrate was concentrated to afford brown powder (0.38 g, 65%), mp 246–248 °C. ^{1}H NMR ($CDCl_3$): δ 4.62 (d, *J* = 7.5 Hz, 1H, CH), 6.08 (t, *J* = 6.6 Hz, 1H, Ar), 6.15 (t, *J* = 7.2 Hz, 1H, Ar), 6.81 (t, *J* = 8.5 Hz, 2H, Ar), 6.99–7.23 (m, 8H, Ar), 7.26–7.31 (m, 3H, Ar), 7.35–7.44 (m, 3H, Ar), 7.54 –7.69 (m, 5H, Ar), 7.79–7.91 (m, 4H, Ar), 8.19-8.25 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 64.62 (d, *J* = 85.2 Hz), 112.59 (d, *J* = 12.8 Hz), 114.05 (d, *J* = 7.5 Hz), 117.49, 118.22, 125.42, 126.74, 127.82, 127.96, 128.11, 128.40, 128.48, 128.68 (d, *J* = 6.3 Hz), 128.87, 129.25 (d, *J* = 11.7 Hz), 130.84, 132.27 (d, *J* = 9.4 Hz), 132.76, 133.23, 133.35, 133.55 (d, *J* = 10.6 Hz), 135.94, 163.58. ^{31}P NMR ($CDCl_3$): δ 24.91, 58.79. Anal. Calcd for $C_{37}H_{30}NOP_2NiCl$: C, 67.26; H, 4.58; N, 2.12. Found: C, 67.07; H, 4.55, N, 1.92.

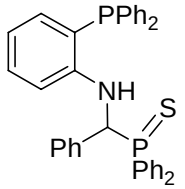
Synthesis of [Ni(Cl){2-(Ph_2P)C_6H_4NCH(Ph)P(O)(Ph)Et}] (IIb)



To a stirred solution of **2b** (0.60 g, 1.15 mmol) in THF (15 mL) was added dropwise *n*-BuLi (0.47 mL, 2.5 M solution in hexanes, 1.17 mmol) at about −80 °C. The resulting mixture was warmed to room temperature and stirred for 4 h. This solution was added dropwise to a stirred suspension of (DME)$NiCl_2$ (0.26 g, 1.18 mmol) in THF (10 mL) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in

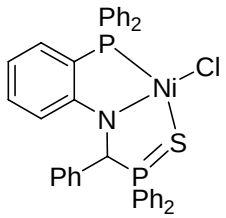
vacuo and the residue was dissolved in toluene. The solution was filtered and the filtrate was concentrated. Et_2O added into the concentrated filtrate to form brown crystals of **2b** (0.36 g, 51%), mp 229–232 °C. ^{1}H NMR ($CDCl_3$): δ 0.69–0.79 (m, 3H, CH_3), 1.42–1.70 (m, 2H, CH_2), 4.30 (dd, *J* = 1.9, 6.5 Hz, 1H, CH), 5.99 (dd, *J* = 5.5, 8.6 Hz, 1H, Ar), 6.14 (t, *J* = 6.1 Hz, 1H, Ar), 6.79 (dd, *J* = 7.3, 14.1 Hz, 2H, Ar), 7.23–7.55 (m, 9H, Ar), 7.64 (s, 3H, Ar), 7.83–7.99 (m, 6H, Ar), 8.29-8.44 (m, 2H, Ar). ^{13}C NMR ($CDCl_3$): δ 4.88, 19.88 (d, *J* = 67 Hz), 65.64 (d, *J* = 80.4 Hz), 112.62 (d, *J* = 12.2 Hz), 113.86, 127.81, 128.49, 128.70, 128.86, 129.13, 129.75, 130.27, 130.84, 131.29, 131.42, 132.70, 132.91, 133.03, 133.24, 133.44, 133.59, 136.95, 163.91. ^{31}P NMR ($CDCl_3$): δ 24.83, 71.33. Anal. Calcd for $C_{33}H_{30}NOP_2NiCl$: C, 64.69; H, 4.94; N, 2.29. Found: C, 64.76; H, 5.15, N, 2.19.

Synthesis of 2-(Ph_2P)C_6H_4NHCH(Ph)P(S)Ph_2 (3)



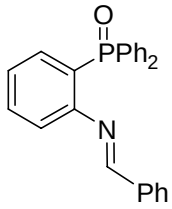
A mixture of 2-(Ph_2P)C_6H_4N=CHPh (0.40 g, 1.09 mmol), Ph_2PSH (0.24 g, 1.10 mmol) and toluene (15 mL) was stirred overnight at room temperature and then refluxed for 2 h. The resulting solution was cooled to room temperature. Hexane (10 mL) was added to the solution to form white precipitate. The precipitate was collected by filtration and dried in vacuo to afford white solid (0.52 g, 81%), mp 174–177 °C. ^{1}H NMR ($CDCl_3$): δ 2.35 (s, PhC*H*$_3$), 5.41 (dd, *J* = 9.4, 12.4 Hz, 1H, CH), 6.39 (q, *J* = 8.9 Hz, 1H, Ar), 6.50–6.61 (m, 2H, Ar), 6.75–6.79 (m, 1H, Ar), 6..84–6.88 (m, 2H, Ar), 6.97 (t, *J* = 7.7 Hz, 2H, Ar), 7.03–7.09 (m, 2H, Ar), 7.14–7.17 (m, 1H, Ar), 7.19–7.39 (m, 12H, Ar), 7.41–7.49 (m, 3H, Ar), 7.68–7.79 (m, 2H, Ar), 8.01–8.13 (m, 1H, Ar). ^{13}C NMR ($CDCl_3$): δ 57.51 (d, *J* = 60 Hz), 111.62, 118.23, 127.61, 127.64, 127.81, 128.01, 128.48, 128.55, 128.68, 128.74, 128.83, 128.97, 130.34, 131,64, 131.70, 131.82, 132.11, 132.24, 132.47, 133.98, 134.13, 134.23, 134.48. ^{31}P NMR: δ –25.69, 47.19. Anal. Calcd for $C_{37}H_{31}NSP_2 \cdot 0.7C_7H_8$: C, 77.64; H, 5.69; N, 2.16. Found: C, 77.72; H, 5.69; N, 2.27.

Synthesis of [Ni(Cl){2-(Ph_2P)C_6H_4NCH(Ph)P(S)Ph_2}] (II)



To a stirred solution of **3**·0.7C_7H_8 (0.37 g, 0.57 mmol) in THF (15 mL) was added dropwise *n*-BuLi (0.24 mL, 2.5 M solution in hexanes, 0.60 mmol) at about −80 °C. The resulting mixture was warmed to room temperature and stirred for 4 h. This solution was added to a stirred suspension of (DME)$NiCl_2$ (0.13 g, 0.59 mmol) in THF (10 mL) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo and the residue was dissolved in toluene. The solution was filtered and the filtrate was concentrated to form red crystals (0.315 g, 69%), mp 205−207 °C. ^{1}H NMR ($CDCl_3$): δ 2.35 (s, PhC*H*$_3$), 5.37 (d, *J* = 9.2 Hz, 1H, CH), 6.23 (s, 2H, Ar), 6.92 (d, *J* = 9.2 Hz, 2H, Ar), 7.00−8.18 (m, 27H, Ar). ^{13}C NMR ($CDCl_3$): δ 70.79 (d, *J* = 74.4 Hz), 112.94 (d, *J* = 13.3 Hz), 113.95 (d, *J* = 6.7 Hz), 127.86 (d, *J* = 2.1 Hz), 128.12 (d, *J* = 3.1 Hz), 128.21, 128.39 (d, *J* = 2.7 Hz), 128.48, 128.63 (d, *J* = 3 Hz), 128.76, 129.23, 129.39, 130.71, 132.17 (d, *J* = 9.1 Hz), 132.65, 132.80, 132.94, 133.15, 133.38, 133.46, 133.52, 133.59, 134.88, 164.89 (d, *J* = 17.8 Hz). ^{31}P NMR ($CDCl_3$): δ 21.72, 55.40. Anal. Calcd for $C_{37}H_{30}NSP_2NiCl$·1.3C_7H_8: C, 69.51; H, 5.11; N, 1.76. Found: C, 69.50; H, 5.23; N, 1.88.

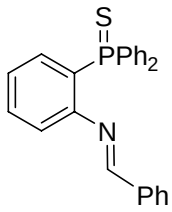
Synthesis of 2-[Ph_2P(O)]C_6H_4N=CHPh (4)



A solution of 2-(Ph_2P)C_6H_4N=CHPh (0.60 g, 1.64 mmol) in THF (15 mL) was cooled to 0 °C. To the solution was added dropwise H_2O_2 (0.23 mL, 30% w/w, 2.03 mmol) and resulting mixture was stirred at 0 °C for 1.5 h. Solvents were removed in vacuo. To the residue was added Et_2O with vigorous stirring until white precipitate generated. The precipitate was collected by filtration and dried in vacuo to yield white solid (0.59 g, 94%), mp 100−101 °C.

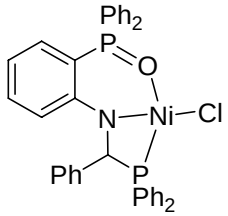
^{1}H NMR ($CDCl_3$): δ 7.02 (dd, *J* = 5.1, 7.7 Hz, 1H, Ar), 7.26–7.42 (m, 12H, Ar), 7.58 (t, *J* = 7.7 Hz, 1H, Ar), 7.79 (dd, *J* = 7.0, 12.3 Hz, 4H, Ar), 7.96–8.03 (m, 1H, Ar), 8.09 (s, 1H, CH). ^{13}C NMR ($CDCl_3$): δ 118.52 (d, *J* = 7.8 Hz), 125.99 (d, *J* = 11.4 Hz), 128.26, 128.42, 128.67, 128.86, 129.38, 131,47, 131.51, 131.84, 132.12, 132.26, 132.41, 133.91, 134.60 (d, *J* = 7.9 Hz), 153.56, 160.71. ^{31}P NMR ($CDCl_3$): δ 23.67. Anal. Calcd for $C_{25}H_{20}NOP$: C, 78.73; H, 5.29; N, 3.67. Found: C, 78.90; H, 5.60; N, 3.61.

Synthesis of 2-[$Ph_2P(S)$]C_6H_4N=CHPh (5)



A mixture of 2-(Ph_2P)C_6H_4N=CHPh (0.50 g, 1.37 mmol), S_8 (0.044 g, 1.37 mmol) and toluene (15 mL) was refluxed for 2 h and then cooled to room temperature. Volatiles were removed in vacuo and the residue was dissolved in Et_2O. The solution was concentrated and added hexane to give pale yellow powder (0.48 g, 88%), mp 119–121 °C. ^{1}H NMR ($CDCl_3$): δ 1.20 (t, *J* = 7.0 Hz, Et_2O), 3.47 (q, *J* = 7.0 Hz, Et_2O), 6.99 (dd, *J* = 5.2, 7.5 Hz, 1H, Ar), 7.25–7.41 (m, 12H, Ar), 7.56 (t, *J* = 7.5 Hz, 1H, Ar), 7.84-7.96 (m, 5H, Ar), 8.08 (s, 1H, CH). ^{13}C NMR ($CDCl_3$): δ 118.67 (d, *J* = 7.4 Hz), 125.81 (d, *J* = 12.9 Hz), 128.14, 128.31, 128.49, 129.33, 130.98 (d, *J* = 2.8 Hz), 131.69, 132.15, 132.30, 133.62 (d, *J* = 2.3 Hz), 134.72, 134.87, 153.87, 160.37. ^{31}P NMR ($CDCl_3$): δ 38.52. Anal. Calcd for $C_{25}H_{20}NSP{\cdot}0.25Et_2O$: C, 75.07; H, 5.45; N, 3.37. Found: C, 74.86; H, 5.21; N, 3.33.

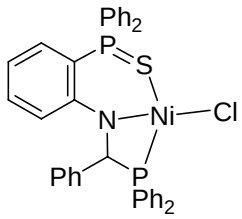
Synthesis of [Ni(Cl){2-($Ph_2P(O)$)C_6H_4NCH(Ph)PPh_2}] (III)



A solution of compoud **4** (0.30 g, 0.78 mmol) in THF (15 mL) was cooled to about −80 °C. To the solution was added dropwise a THF solution of Ph_2PLi [prepared in situ from Ph_2PH

(0.14 g, 0.79 mmol) and Bu^nLi (0.32 mL, 2.5 M solution in hexane, 0.80 mmol) in THF (5 mL)] with stirring. The mixture was warmed to room temperature and stirred for 12 h. The resulting solution was added dropwise into a stirred suspension of $(DME)NiCl_2$ (0.18 g, 0.81 mmol) in THF (10 mL) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in toluene. The resulting solution was filtered. Et_2O was added into the filtrate to form brown powder (0.33 g, 59%), mp 166−170 °C. Anal. Calcd for $C_{37}H_{30}NOP_2NiCl{\cdot}0.5C_7H_8$: C, 68.82; H, 4.85; N, 1.98. Found: C, 68.87; H, 5.19, N, 1.98. ESI-MS: *m*/*z* 665 $[M–Cl+CH_3CN]^+$ (The sample was dissolved in CH_3CN), 624 $[M–Cl]^+$.

Synthesis of [Ni(Cl){2-($Ph_2P(S)$)C_6H_4NCH(Ph)PPh_2}] (IV)



A mixture of compoud **5**·0.25Et_2O (0.33 g, 0.79 mmol) in THF (15 mL) was cooled to about −80 °C. To the solution was added a THF solution of Ph_2PLi [prepared in situ from Ph_2PH (0.15 g, 0.80 mmol) and *n*-BuLi (0.32 mL, 2.5 M solution in hexane, 0.80 mmol) in THF (5 mL)] with stirring. The mixture was warmed to room temperature and stirred for 12 h. The resulting solution was added dropwise into a stirred suspension of $(DME)NiCl_2$ (0.18 g, 0.81 mmol) in THF (10 mL) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in toluene. The resulting solution was filtered and the filtrate was concentrated to give red crystals (0.39 g, 63%), mp 186−188 °C. Anal. Calcd for $C_{37}H_{30}NSP_2NiCl{\cdot}1.1C_7H_8$: C, 68.99; H, 5.03; N, 1.80. Found: C, 69.15; H, 5.10; N, 1.83. ESI-MS: *m*/*z* 676 $[M+1]^+$.

2. X-Ray crystallography

Single crystals of complex **II** were mounted in Lindemann capillaries under nitrogen. Diffraction data were collected at 295(2) K on a Oxford diffraction Gemini S Ultra diffractometer using Cu-K_α radiation (λ = 1.54184 Å). The structure was solved by direct

methods using SHELXS-97 program[9] and refined against F^2 by full-matrix least-squares using SHELXL-97 program.[10] Hydrogen atoms were placed in calculated positions. Crystal data and experimental details of the structure determination are listed in Table S1.

Table S1. Details of the X-ray structure determination of complex **II**

empirical formula	$C_{37}H_{30}ClNNiP_2S$	D_{calcd} (gcm^{-3})	1.386
fw	676.78	$F(000)$	1400
crystal system	monoclinic	μ (mm^{-1})	3.360
space group	P 21/c	no. of reflns collected	25396
a (Å)	9.535(5)	no. of indep reflns (R_{int})	5072 (0.0322)
b (Å)	22.010(5)	restraints/params	12/388
c (Å)	15.523(5)	goodness of fit on F^2	0.999
β (deg)	95.316(5)	final R indices[a] [$I > 2\sigma(I)$]	$R1$ = 0.0492 w$R2$ = 0.1216
V (Å^3)	3244(2)	R indices (all data)	$R1$ = 0.0608 w$R2$ = 0.1276
Z	4	largest diff peak and hole [e.Å^{-3}]	1.823, -0.499

[a] $R1 = \Sigma \left| |Fo| - |Fc| \right| / \Sigma |Fo|$; $wR2 = \left[\Sigma w(Fo^2 - Fc^2)^2 / \Sigma w(Fo^4) \right]^{1/2}$

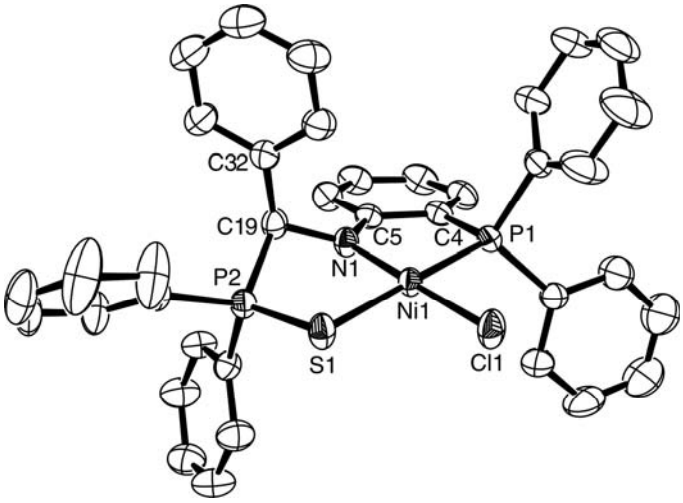


Figure S1. Molecular structure of complex **II** (30% thermal ellipsoids)

The structure of complex **Ia** have been reported by us,[1] but the spectral and analytical data of the complex were not provided then due to minor sample amount. In this study the complex was obtained in gram scale and was characterized by NMR spectroscopy and

elemental analysis.

3. General procedure for the Negishi cross-coupling

(1) Reaction of PhZnCl with *p*-$MeOC_6H_4Cl$ catalyzed by complex **Ia**

A Schlenk tube was charged with *p*-$MeOC_6H_4Cl$ (0.071 g, 0.5 mmol), NMP (1.5 mL) and a solution of complex **Ia** (0.02 mL, 0.05 M solution in THF, 0.001 mmol). To the stirred mixture PhZnCl solution (1.5 mL, 0.5 M solution in THF, 0.75 mmol) was added by syringe. The reaction mixture was stirred at room temperature for 24 h. Water (10 mL) and several drops of hydrochloric acid were successively added. The mixture was extracted with Et_2O (3 × 10 mL). The combined organic phases were dried over anhydrous Na_2SO_4, concentrated by rotary evaporation, and purified by column chromatography (silica gel, eluted using 3% CH_3COOEt-petroleum ether) to afford *p*-$MeOC_6H_4Ph$ (0.09 g, 98 %).

Other reactions of arylzinc chlorides with aryl chlorides followed the same procedure.

(2) Reaction of *p*-$EtOOCC_6H_4ZnBr$ with *p*-$PhC(O)C_6H_4Cl$ catalysed by complex **Ia**

p-$EtOOCC_6H_4ZnBr$ was prepared according to the procedure described in literature.[7] After reaction completed, THF was removed *in vacuo*. The residue was washed with Et_2O to remove $C_{10}H_8$. Then THF was added to prepare a about 0.5 M solution of *p*-$EtOOCC_6H_4ZnBr$ in THF.

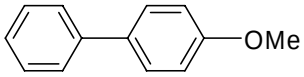
A Schlenk tube was charged *p*-$PhC(O)C_6H_4Cl$ (0.108 g, 0.5 mmol), NMP (1.5 mL), and complex **Ia** (16.5mg, 0.025 mmol). To the stirred mixture *p*-$EtOOCC_6H_4ZnBr$ solution (1.5 mL, 0.5 M solution in THF, 0.75 mmol) was added by syringe. Then the reaction mixture was stirred at room temperature for 12 h. Water (10 mL) and several drops of hydrochloric acid were successively added. The resulting mixture was extracted with Et_2O (3 × 10 mL), and the combined organic layers were dried over anhydrous Na_2SO_4. The Na_2SO_4 was removed by filtration and washed with Et_2O. The resulting Et_2O solution was concentrated by rotary evaporation, and the residue was purified by column chromatography (silica gel, eluted using 5 % CH_3COOEt-petroleum ether) to afford 4-$EtOOCC_6H_4C_6H_4C(O)Ph$-4′ (0.124 g, 75 %).

p-$EtOOCC_6H_4ZnI$ and *p*-MeC_6H_4ZnI were prepared by reaction of corresponding aryl

iodide with activated Zn.[8] Their coupling reactions with aryl chlorides followed the same procedure as above.

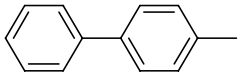
Spectral data of the cross-coupling products

(1) 4-Methoxybiphenyl [11]



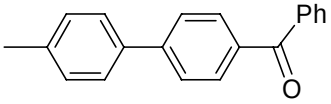
^{1}H NMR ($CDCl_3$): δ 3.87 (s, 3H, CH_3), 7.01 (d, J = 8.8 Hz, 2H, C_6H_4), 7.33 (t, J = 7.5 Hz, 1H, Ph), 7.45 (t, J = 7.8 Hz, 2H, Ph), 7.54–7.61 (m, 4H, Ph+C_6H_4).

(2) 4-Methylbiphenyl [11]



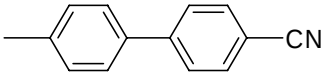
^{1}H NMR ($CDCl_3$): δ 2.35 (s, 3H, CH_3), 7.20 (d, J = 8.1 Hz, 2H, C_6H_4), 7.28 (d, J = 7.3 Hz, 1H, Ph), 7.37 (t, J = 7.5 Hz, 2H, Ph), 7.46 (d, J = 8.1 Hz, 2H, C_6H_4), 7.54 (d, J = 7.7 Hz, 2H, Ph).

(3) (4'-Methylbiphenyl-4-yl)(phenyl)methanone [11]



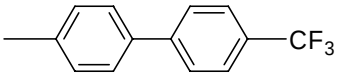
^{1}H NMR ($CDCl_3$): δ 2.28 (s, 3H, CH_3), 7.15 (d, J = 7.8 Hz, 2H, Ar), 7.33–7.48 (m, 5H, Ar), 7.55 (d, J = 8.4 Hz, 2H, Ar), 7.71 (d, J = 7.9 Hz, 2H, Ar), 7.75 (d, J = 8.1 Hz, 2H, Ar).

(4) 4'-Methylbiphenyl-4-carbonitrile [11]



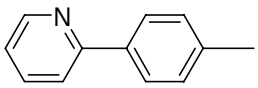
^{1}H NMR ($CDCl_3$): δ 2.29 (s, 3H, CH_3), 7.16 (d, J = 7.9 Hz, 2H, C_6H_4), 7.36 (d, J = 8.2 Hz, 2H, C_6H_4), 7.50–7.57 (m, 4H, C_6H_4).

(5) 4-Methyl-4'-(trifluoromethyl)biphenyl [11]



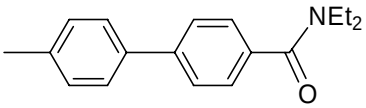
^{1}H NMR ($CDCl_3$): δ 2.40 (s, 3H, CH_3), 7.26 (d, J = 8 Hz, 2H, C_6H_4), 7.48 (d, J = 8.1 Hz, 2H, C_6H_4), 7.65 (s, 4H, C_6H_4).

(6) 2-*p*-Tolylpyridine [11]



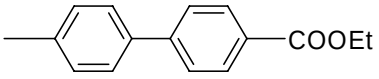
^{1}H NMR ($CDCl_3$): δ 2.39 (s, 3H, CH_3), 7.15–7.19 (m, 1H, pyridyl), 7.27 (d, J = 7.9 Hz, 2H, C_6H_4), 7.66–7.73 (m, 2H, pyridyl), 7.88 (d, J = 8.2 Hz, 2H, C_6H_4), 8.66 (dt, J = 1.4, 4.8 Hz, 1H, pyridyl).

(7) *N*,*N*-Diethyl-4'-methylbiphenyl-4-carboxamide [11]



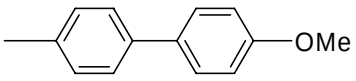
^{1}H NMR ($CDCl_3$): δ 1.20 (b, 6H, CH_3), 2.39 (s, 3H, CH_3), 3.34 (b, 2H, CH_2), 3.54 (b, 2H, CH_2), 7.25 (d, J = 7.9 Hz, 2H, C_6H_4), 7.42 (d, J = 8.3 Hz, 2H, C_6H_4), 7.49 (d, J = 8.1 Hz, 2H, C_6H_4), 7.59 (d, J = 8.3 Hz, 2H, C_6H_4).

(8) Ethyl 4'-methylbiphenyl-4-carboxylate [11]



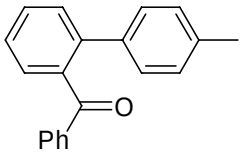
^{1}H NMR ($CDCl_3$): δ 1.26 (t, J = 7.1 Hz, 3H, CH_3), 2.24 (s, 3H, CH_3), 4.25 (q, J = 7.1 Hz, 2H, CH_2), 7.09 (d, J = 8.1 Hz, 2H, C_6H_4), 7.35 (d, J = 8 Hz, 2H, C_6H_4), 7.47 (d, 2H, J = 8.2 Hz, C_6H_4), 7.95 (d, 2H, J = 8.2 Hz, C_6H_4).

(9) 4-Methoxy-4'-methylbiphenyl [11]



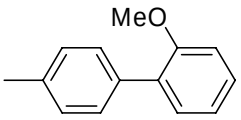
^{1}H NMR ($CDCl_3$): δ 2.28 (s, 3H, CH_3), 3.73 (s, 3H, OCH_3), 6.86 (d, J = 8.8 Hz, 2H, C_6H_4), 7.12 (d, J = 7.9 Hz, 2H, C_6H_4), 7.35 (d, J = 8.1 Hz, 2H, C_6H_4), 7.41 (d, J = 8.8 Hz, 2H, C_6H_4).

(10) (4'-Methylbiphenyl-2-yl)(phenyl)methanone [11]



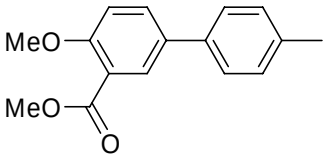
^{1}H NMR ($CDCl_3$): δ 2.24 (s, 3H, CH_3), 7.00 (d, *J* = 7.5 Hz, 2H, Ar), 7.15 (d, *J* = 7.7 Hz, 2H, Ar), 7.27 (t, *J* = 7.8 Hz, 2H, Ar), 7.36–7.59 (m, 5H, Ar), 7.66 (d, *J* = 8.1 Hz, 2H, Ar).

(11) 2-Methoxy-4'-methylbiphenyl [11]



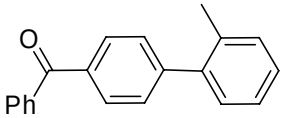
^{1}H NMR ($CDCl_3$): δ 2.29 (s, 3H, CH_3), 3.69 (s, 3H, CH_3), 6.86 (d, *J* = 8.1 Hz, 1H, C_6H_4), 6.93 (d, *J* = 7.4 Hz, 1H, C_6H_4), 7.12 (d, *J* = 7.8 Hz, 2H, C_6H_4), 7.21 (d, *J* = 7.3 Hz, 2H, C_6H_4), 7.33 (d, *J* = 8 Hz, 2H, C_6H_4).

(12) Methyl 2-methoxy-5-(*p*-methylphenyl)benzoate



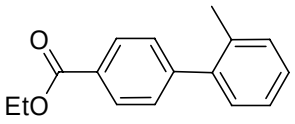
^{1}H NMR ($CDCl_3$): δ 2.40 (s, 3H, CH_3), 3.93 (s, 3H, CH_3), 3.95 (s, 3H, CH_3), 7.05 (d, *J* = 8.7 Hz, 1H, Ar), 7.25 (d, *J* = 8.1 Hz, 2H, Ar), 7.47 (d, *J* = 8.1 Hz, 2H, Ar), 7.69 (dd, *J* = 2.4, 8.6 Hz, 1H, Ar), 8.03 (d, *J* = 2.4 Hz, 1H, Ar). ^{13}C NMR ($CDCl_3$): δ 21.10, 52.11, 56.19, 112.50, 120.27, 126.57, 129.59, 130.04, 131.73, 133.28, 136.87, 136.91, 158.40, 166.76. HR-MS (EI): *m*/*z* 256.1101 $[M]^+$, calcd for $C_{16}H_{16}O_3$ 256.1099.

(13) (2'-Methylbiphenyl-4-yl)(phenyl)methanone [11]



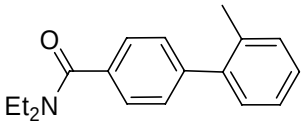
^{1}H NMR ($CDCl_3$): δ 2.19 (s, 3H, CH_3), 7.11–7.18 (m, 4H, Ar), 7.28-7.50 (m, 5H, Ar), 7.73-7.77 (m, 4H, Ar).

(14) Ethyl 2'-methylbiphenyl-4-carboxylate [11]



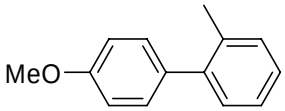
^{1}H NMR ($CDCl_3$): δ 1.30 (t, *J* = 7.1 Hz, 3H, CH_3), 2.14 (s, 3H, CH_3), 4.29 (q, *J* = 7.1 Hz, 2H, CH_2), 7.09–7.16 (m, 4H, C_6H_4), 7.27 (d, *J* = 8.1 Hz, 2H, C_6H_4), 7.99 (d, *J* = 8.1 Hz, 2H, C_6H_4).

(15) *N*,*N*-Diethyl-2'-methylbiphenyl-4-carboxamide [11]



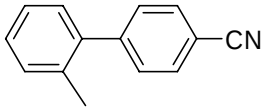
^{1}H NMR ($CDCl_3$): δ 1.20 (b, 6H, CH_3), 2.26 (s, 3H, CH_3), 3.34 (b, 2H, CH_2), 3.56 (b, 2H, CH_2), 7.21–7.26 (m, 4H, C_6H_4), 7.33 (d, *J* = 8.1 Hz, 2H, C_6H_4), 7.43 (d, *J* = 8.1 Hz, 2H, C_6H_4).

(16) 4'-Methoxy-2-methylbiphenyl [11]



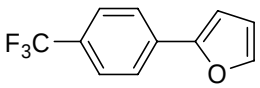
^{1}H NMR ($CDCl_3$): δ 2.27 (s, 3H, CH_3), 3.83 (s, 3H, OCH_3), 6.94 (d, *J* = 8.7 Hz, 2H, C_6H_4), 7.21–7.26 (m, 6H, C_6H_4).

(17) 2'-Methylbiphenyl-4-carbonitrile [12]



^{1}H NMR ($CDCl_3$): δ 2.13 (s, 3H, CH_3), 7.17 (d, *J* = 7.5 Hz, 1H, C_6H_4), 7.25 (d, *J* = 7.5 Hz, 2H, C_6H_4), 7.31-7.37 (m, 3H, C_6H_4), 7.61 (d, *J* = 8.5 Hz, 2H, C_6H_4).

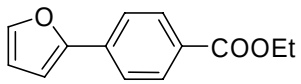
(18) 2-(4-(Trifluoromethyl)phenyl)furan [11]



^{1}H NMR ($CDCl_3$): δ 6.49 (dd, *J* = 1.8, 3.3 Hz, 1H, furyl), 6.74 (d, *J* = 3.3 Hz, 1H, furyl),

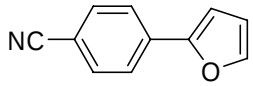
7.49 (s, 1H, furyl), 7.61 (d, J = 8.6 Hz, 2H, C_6H_4), 7.73 (d, J = 8.5 Hz, 2H, C_6H_4).

(19) Ethyl 4-(furan-2-yl)benzoate [11]



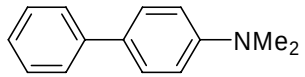
^{1}H NMR ($CDCl_3$): δ 1.29 (t, J = 7.1 Hz, 3H, CH_3), 4.27 (q, J = 7.1 Hz, 2H, CH_2), 6.38 (dd, J = 1.8, 3.4 Hz, 1H, furyl), 6.65 (d, J = 3.4 Hz, 1H, furyl), 7.39 (d, J = 1.8 Hz, 1H, furyl), 7.60 (d, J = 8.3 Hz, 2H, C_6H_4), 7.94 (d, J = 8.3 Hz, 2H, C_6H_4).

(20) 4-(Furan-2-yl)benzonitrile [11]



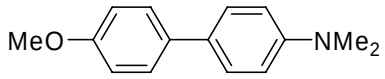
^{1}H NMR ($CDCl_3$): δ 6.43 (dd, J = 1.7, 3.3 Hz, 1H, furyl), 6.71 (d, J = 3.3 Hz, 1H, furyl), 7.43 (s, 1H, furyl), 7.54 (d, J = 8.6 Hz, 2H, C_6H_4), 7.63 (d, J = 8.1 Hz, 2H, C_6H_4).

(21) *N*,*N*-Dimethylbiphenyl-4-amine [11]



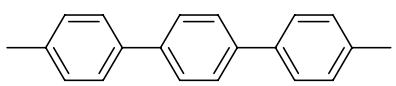
^{1}H NMR ($CDCl_3$): δ 2.86 (s, 6H, CH_3), 6.69 (d, J = 8.8 Hz, 2H, Ar), 7.11-7.17 (m, 1H, Ar), 7.26-7.31 (m, 2H, Ar), 7.39–7.47 (m, 4H, Ar).

(22) 4'-Methoxy-*N*,*N*-dimethylbiphenyl-4-amine [11]



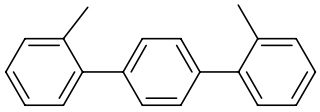
^{1}H NMR ($CDCl_3$): δ 2.97 (s, 6H, NCH_3), 3.82 (s, 3H, OCH_3), 6.79 (d, J = 8.8 Hz, 2H, C_6H_4), 6.94 (d, J = 8.8 Hz, 2H, C_6H_4), 7.46 (t, J = 8.5 Hz, 4H, C_6H_4).

(23) 1,4-Di(*p*-methylphenyl)benzene [12]



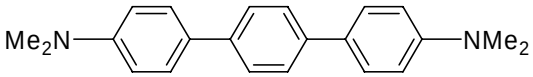
^{1}H NMR ($CDCl_3$): δ 2.40 (s, 6H, CH_3), 7.26 (d, J = 7.2 Hz, 4H, C_6H_4), 7.53 (d, J = 8 Hz, 4H, C_6H_4), 7.64 (s, 4H, C_6H_4).

(24) 1,4-Di(o-methylphenyl)benzene [11]



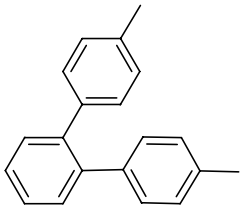
^{1}H NMR ($CDCl_3$): δ 2.35 (s, 6H, CH_3), 7.25–7.32 (m, 8H, C_6H_4), 7.37 (s, 4H, C_6H_4).

(25) 4-[4-(4-dimethylaminophenyl)phenyl]-*N*,*N*-dimethylaniline [13]



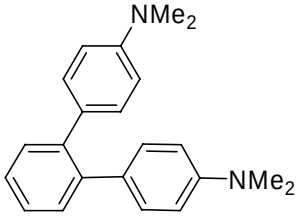
^{1}H NMR ($CDCl_3$): δ 3.00 (s, 12H, NMe), 6.82 (d, J = 8.8 Hz, 4H, C_6H_4), 7.55 (d, J = 8.8 Hz, 4H, C_6H_4), 7.59 (s, 4H, C_6H_4).

(26) 1,2-Di(*p*-methylphenyl)benzene [11]



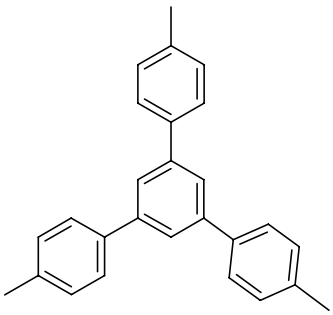
^{1}H NMR ($CDCl_3$): δ 2.32 (s, 6H, CH_3), 7.04 (s, 8H, C_6H_4), 7.40 (s, 4H, C_6H_4).

(27) 4-[2-(4-dimethylaminophenyl)phenyl]-*N*,*N*-dimethylaniline [14]



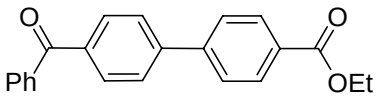
^{1}H NMR ($CDCl_3$): δ2.99 (s, 12H, NMe), 6.69 (d, J = 8 Hz, 4H, C_6H_4), 7.15 (d, J = 6.9 Hz, 4H, C_6H_4), 7.37-7.48 (m, 4H, C_6H_4).

(28) 1,3,5-tris(*p*-tolyl)benzene[15]



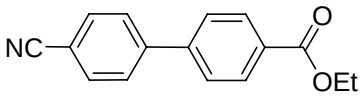
^{1}H NMR ($CDCl_3$): δ 2.29 (s, 9H, CH_3), 7.16 (d, *J* = 7.8 Hz, 6H, C_6H_4), 7.48 (d, *J* = 7.9 Hz, 6H, C_6H_4), 7.63 (s, 3H, C_6H_3).

(29) Ethyl 4-(4-benzoylphenyl)benzoate[16]



^{1}H NMR ($CDCl_3$): δ 1.42 (t, *J* = 7.1 Hz, 3H, Me), 4.40 (q, *J* = 7.1 Hz, 2H, CH_2), 7.50 (t, *J* = 7.5 Hz, 2H, Ph), 7.58-7.62 (m, 1H, Ph), 7.71 (t, *J* = 7.9 Hz, 4H, Ph+C_6H_4), 7.82-7.84 (m, 2H, C_6H_4), 7.90 (d, *J* = 8.5 Hz, 2H, C_6H_4), 8.23 (d, *J* = 8.5 Hz, 2H, C_6H_4).

(30) Ethyl 4-(4-cyanophenyl)benzoate[17]



^{1}H NMR ($CDCl_3$): δ 1.42 (t, *J* = 7.1 Hz, 3H, Me), 4.41 (q, *J* = 7.1 Hz, 2H, CH_2), 7.65 (d, *J* = 8.6 Hz, 2H, C_6H_4), 7.73 (q, *J* = 7.7 Hz, 4H, C_6H_4), 8.15 (d, *J* = 8.6 Hz, 2H, C_6H_4).

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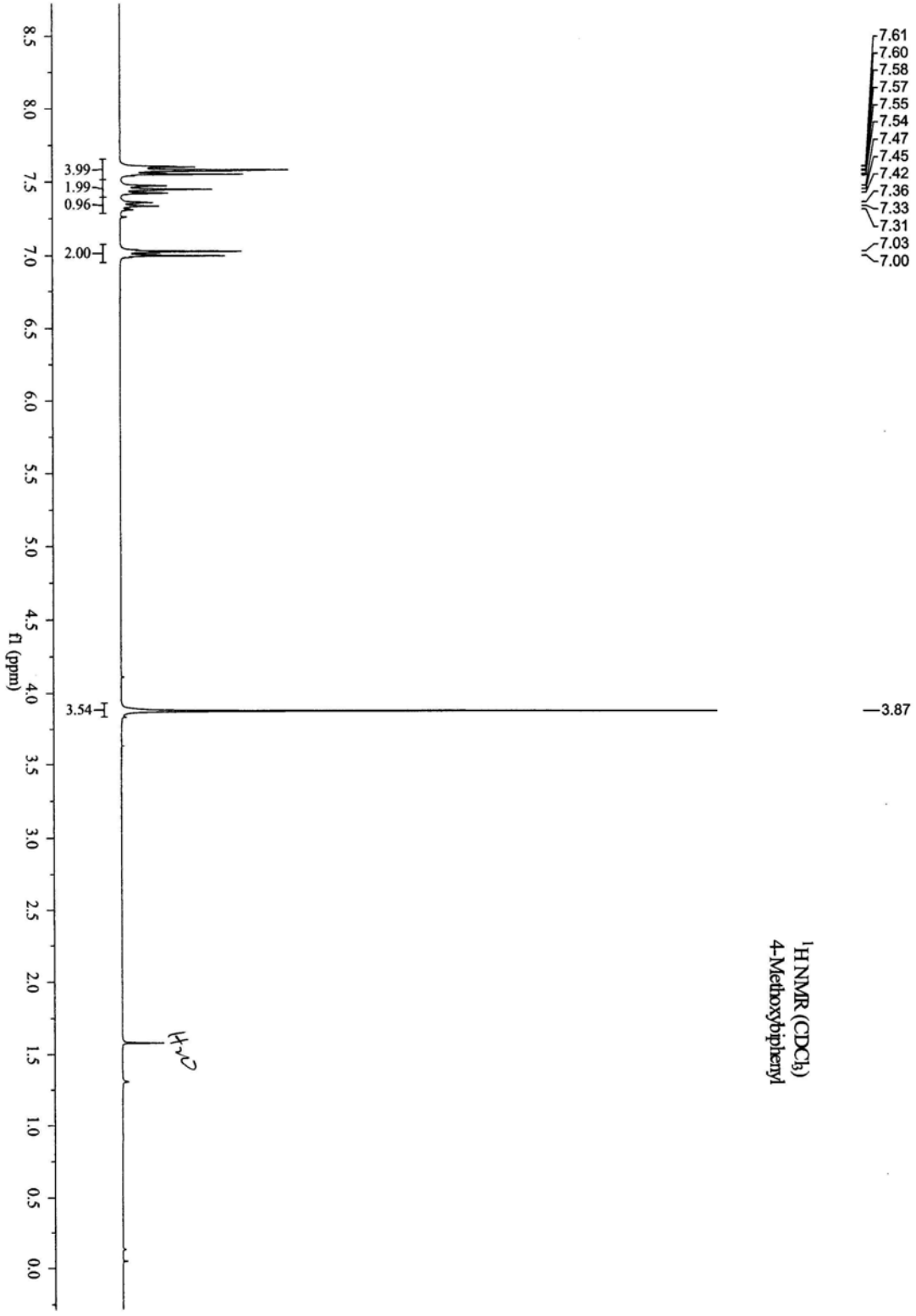
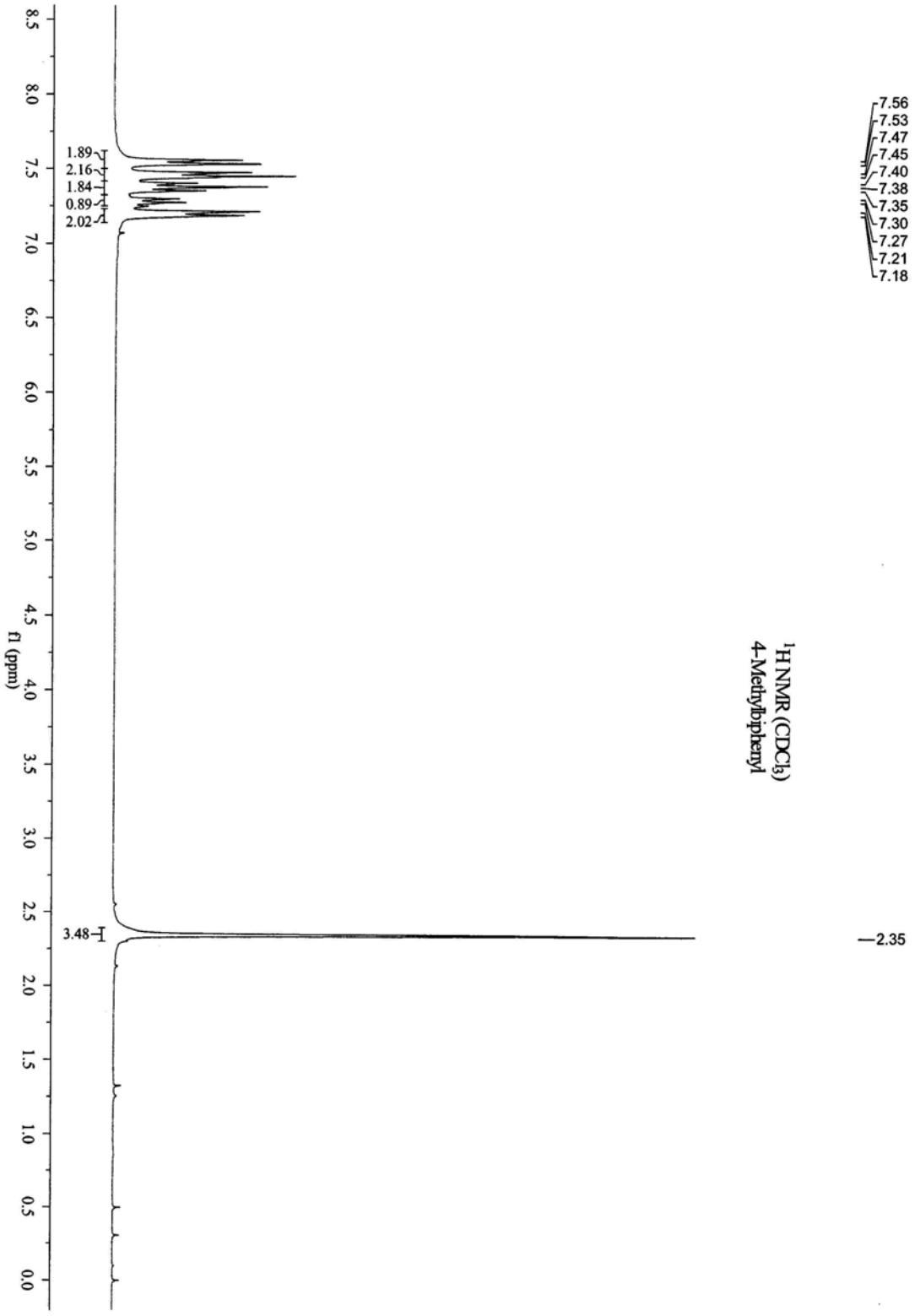
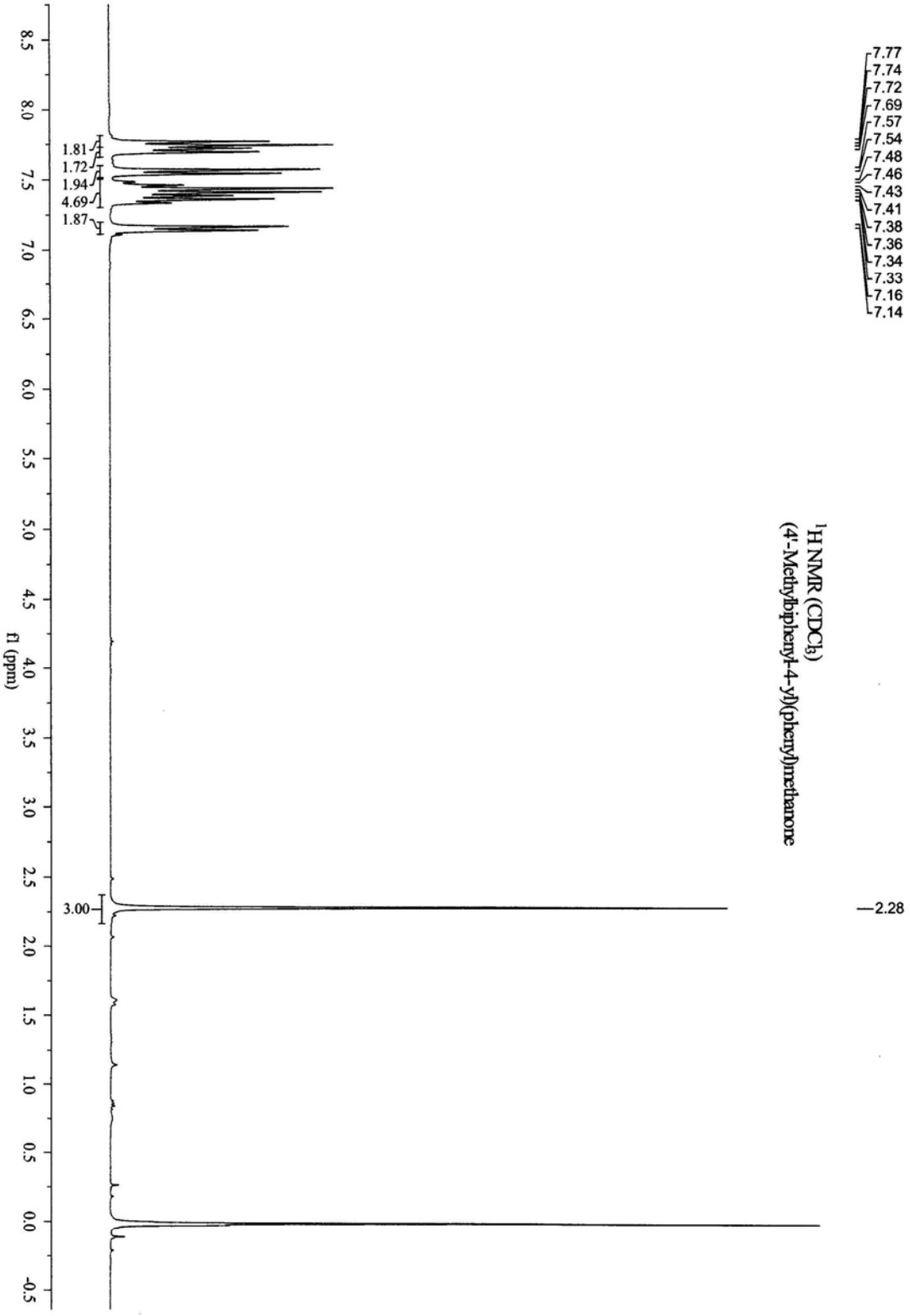
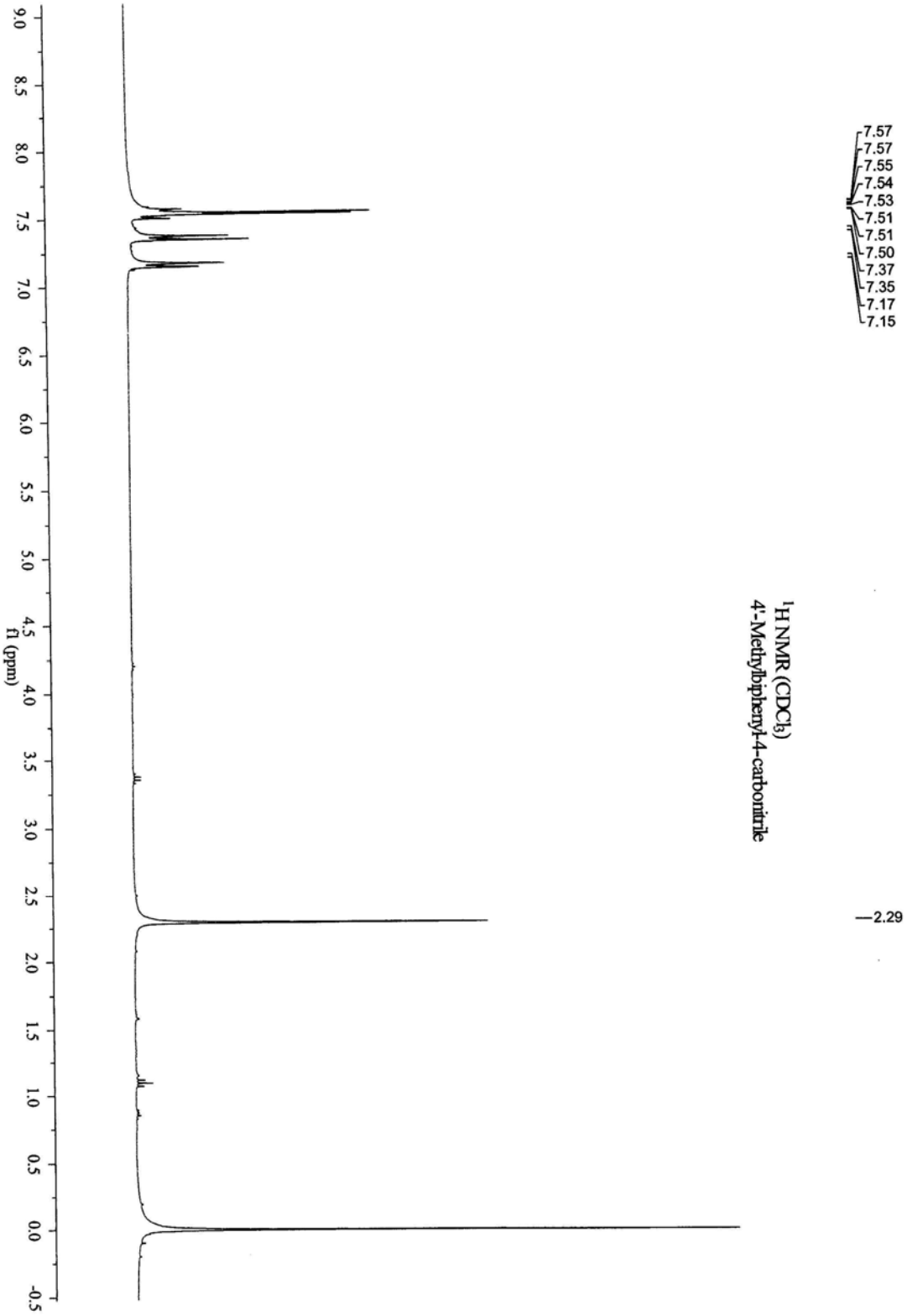
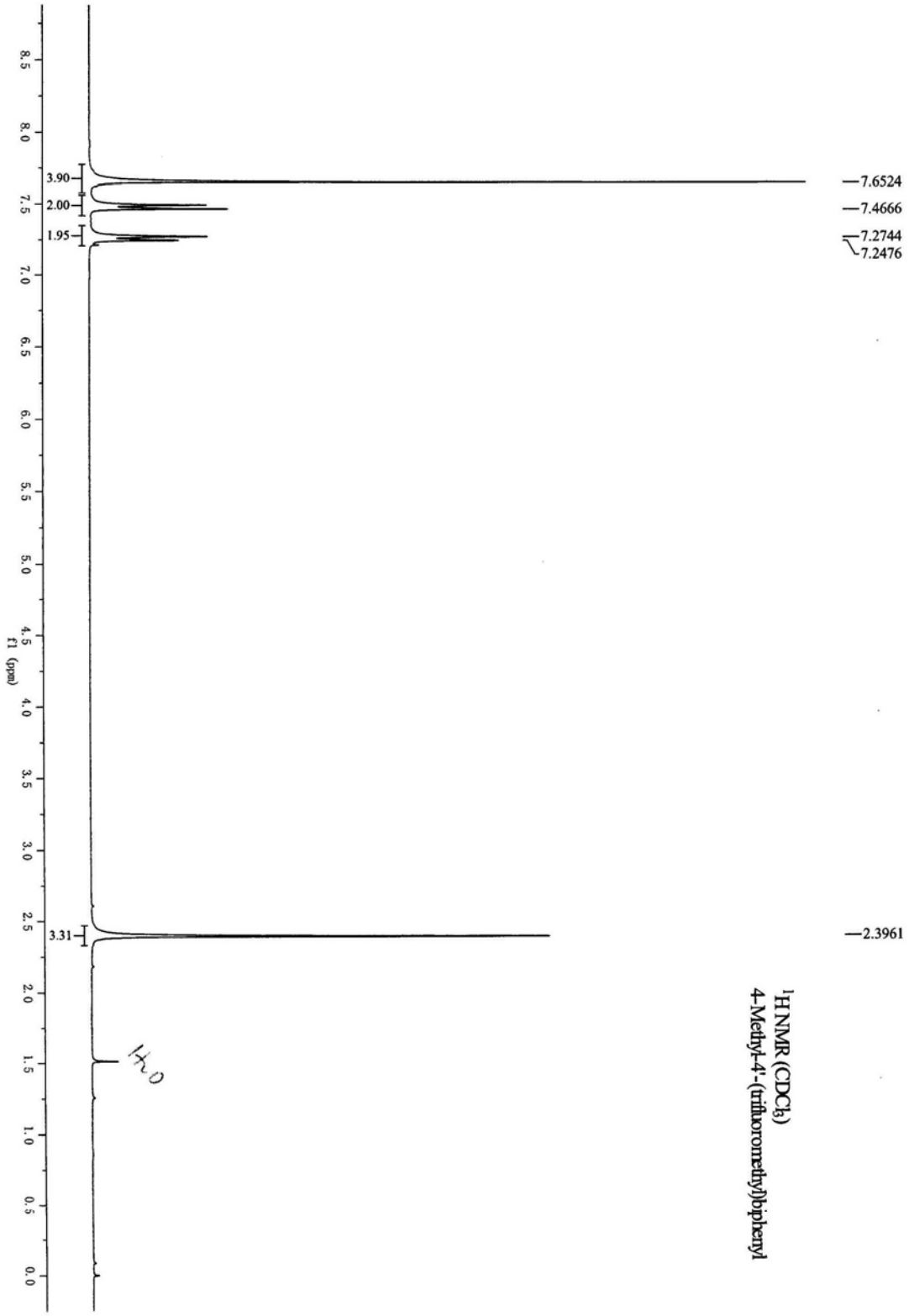
Scanned NMR spectra

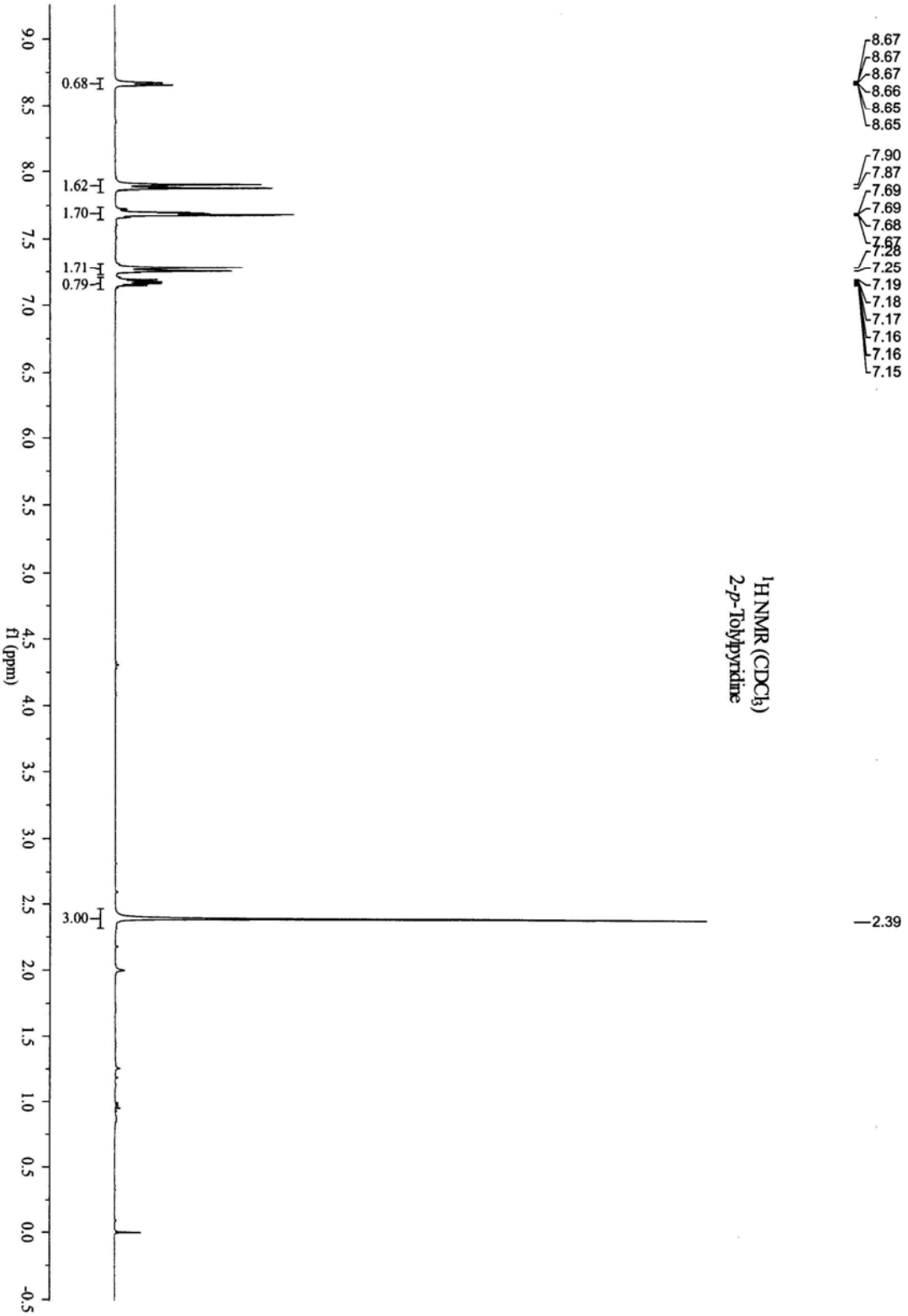


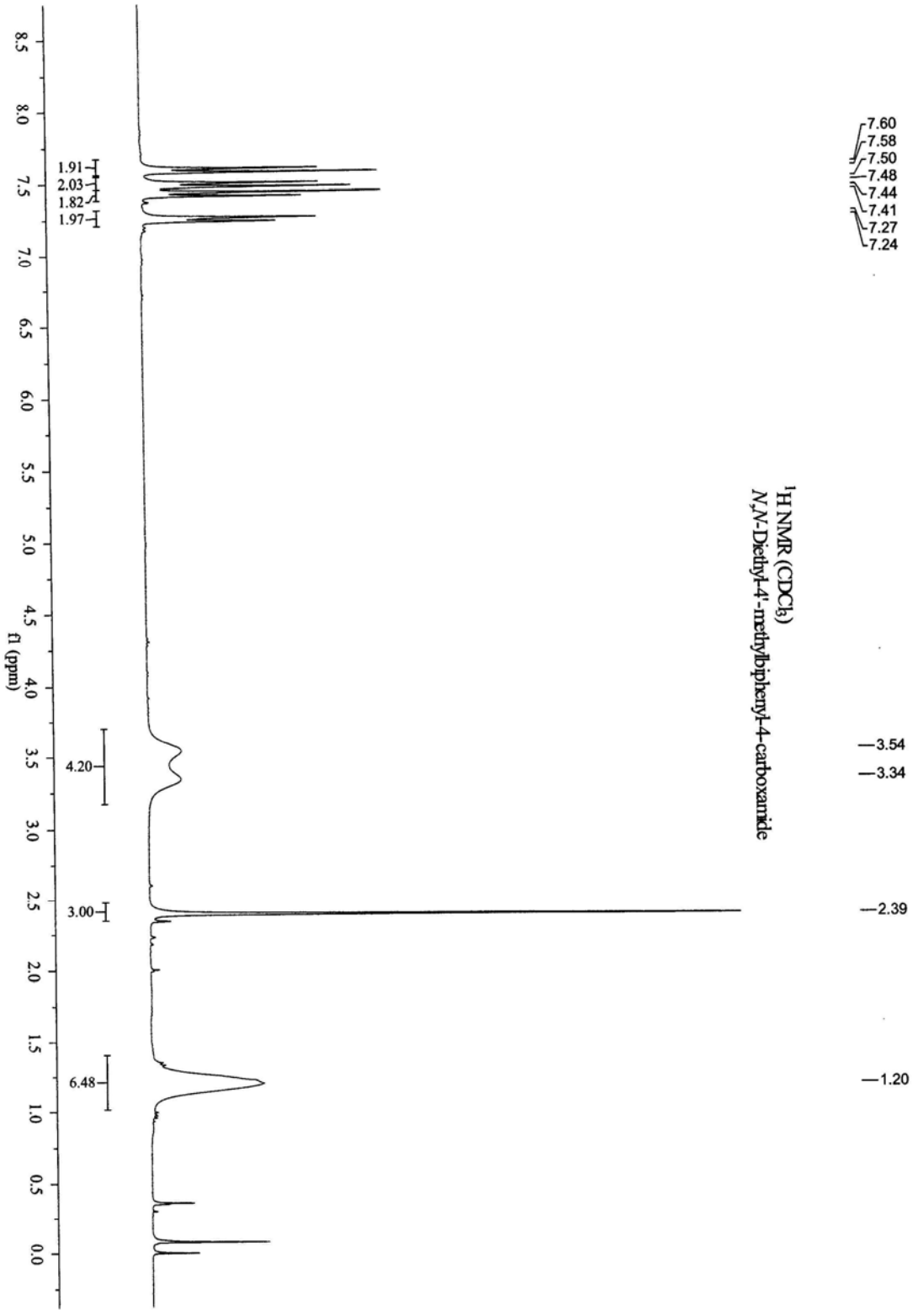

^{1}H NMR (CDCl$_3$)
4-Methylbiphenyl
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.89
2.16
1.84
0.89
2.02
3.48
7.56
7.53
7.47
7.45
7.40
7.38
7.35
7.30
7.27
7.21
7.18
2.35

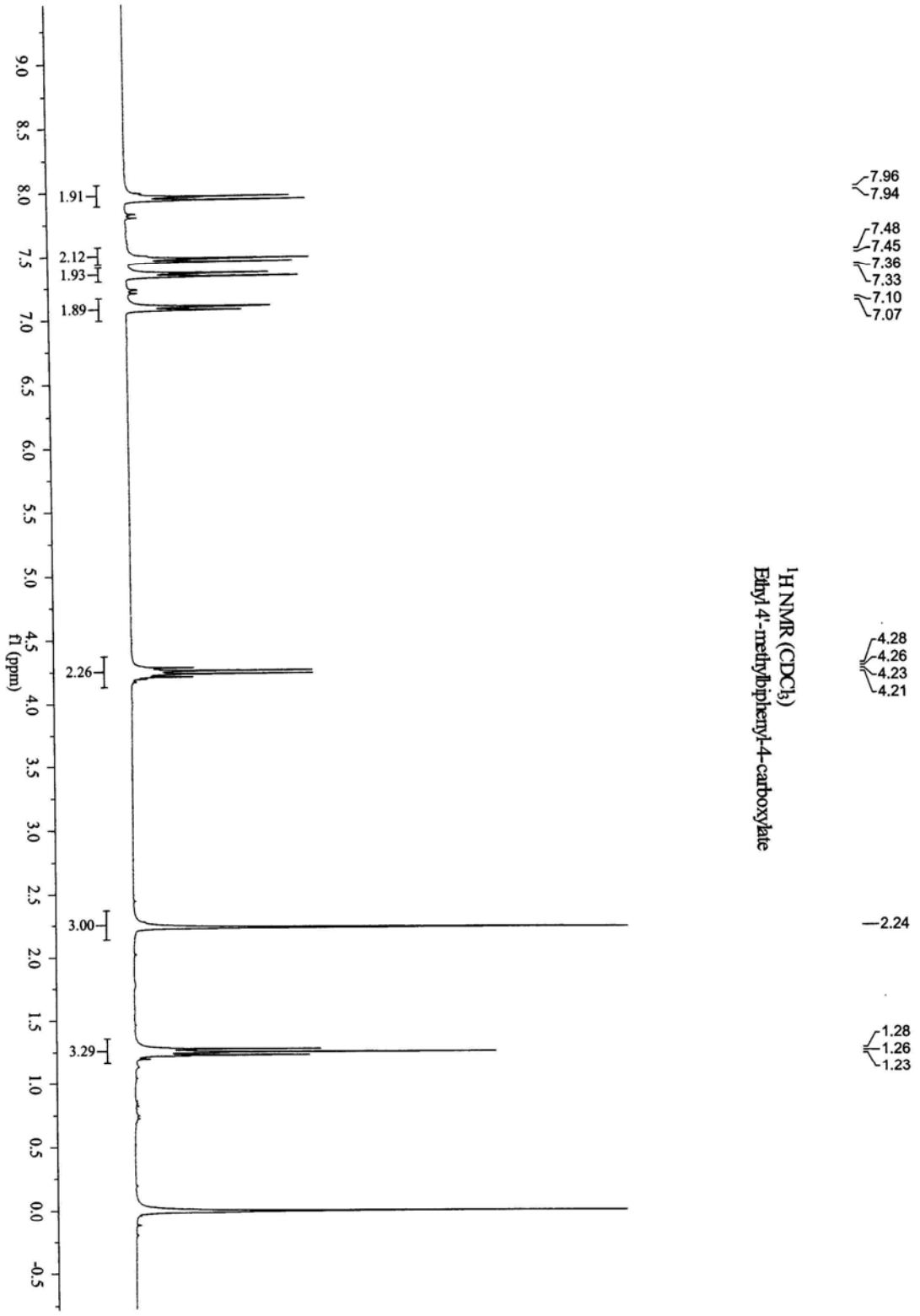

^{1}H NMR (CDCl$_3$)
(4'-Methylbiphenyl-4-yl)(phenyl)methanone
7.77
7.74
7.72
7.69
7.57
7.54
7.48
7.46
7.43
7.41
7.38
7.36
7.34
7.33
7.16
7.14
1.81
1.72
1.94
4.69
1.87
3.00
2.28
f1 (ppm)
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

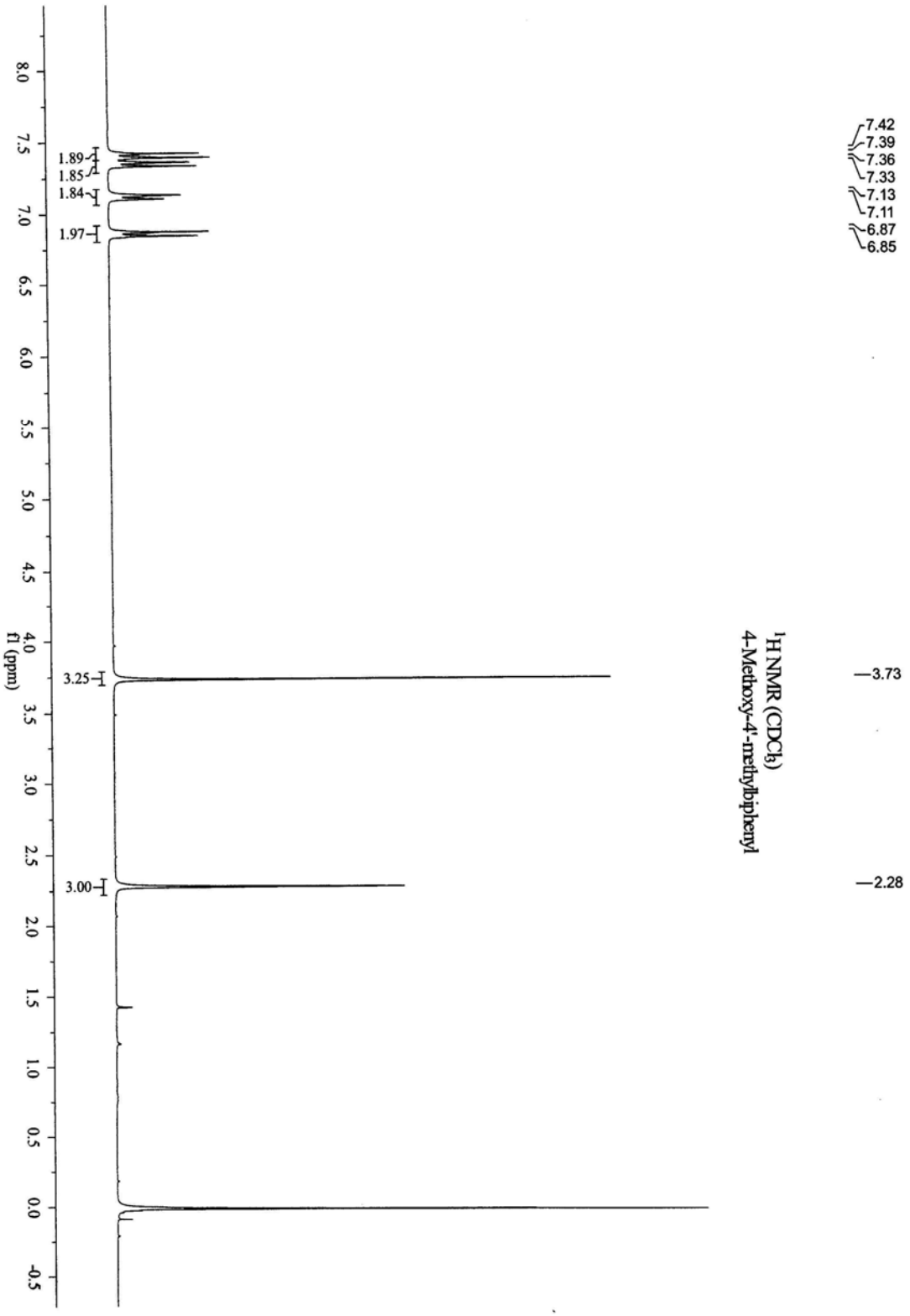

7.57
7.57
7.55
7.54
7.53
7.51
7.51
7.50
7.37
7.35
7.17
7.15
2.29
^{1}H NMR (CDCl$_3$)
4'-Methylbiphenyl-4-carbonitrile
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

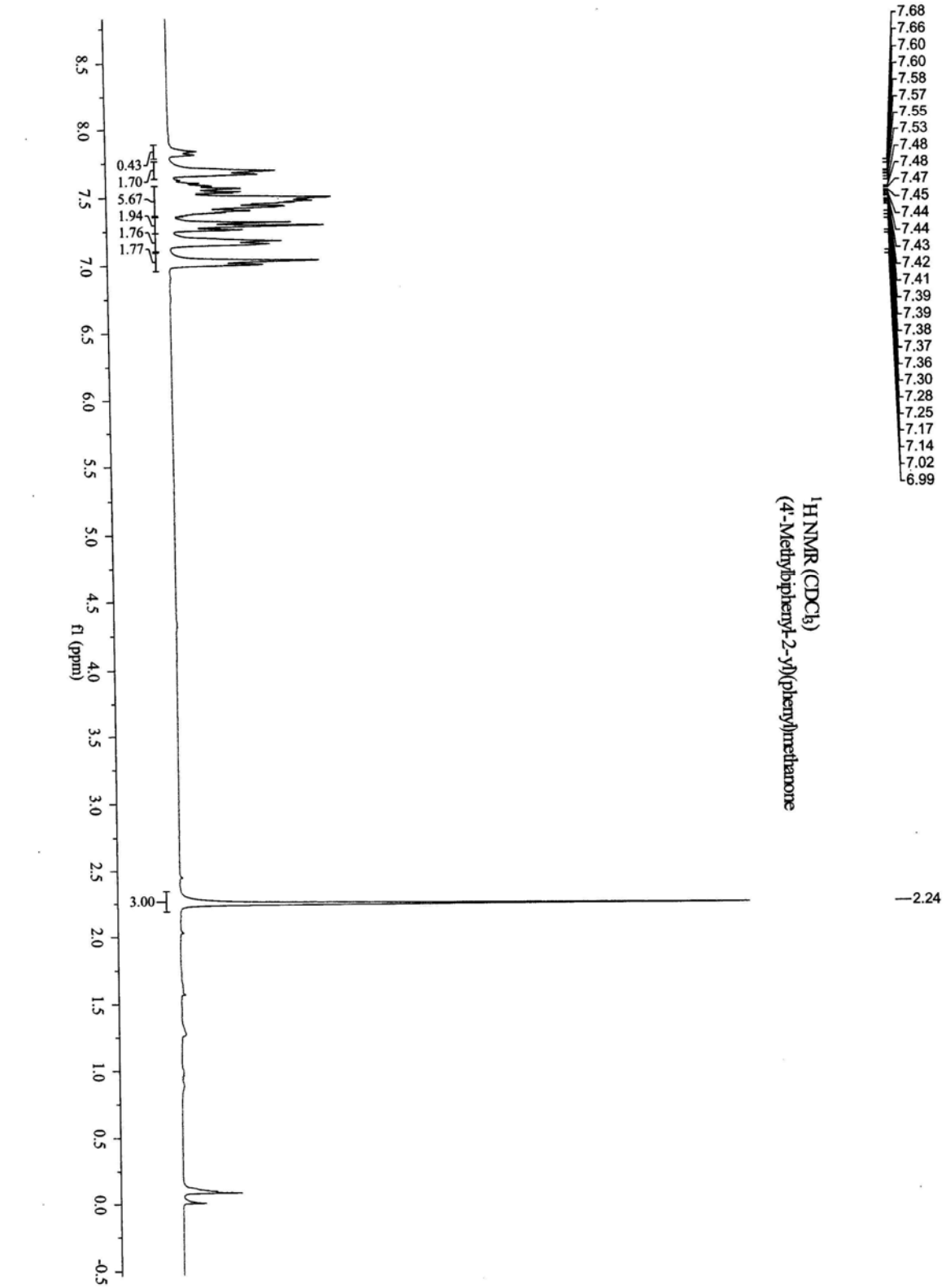

3.90
2.00
1.95
3.31
7.6524
7.4666
7.2744
7.2476
2.3961
f1 (ppm)
^{1}H NMR (CDCl$_3$)
4-Methyl-4'-(trifluoromethyl)biphenyl

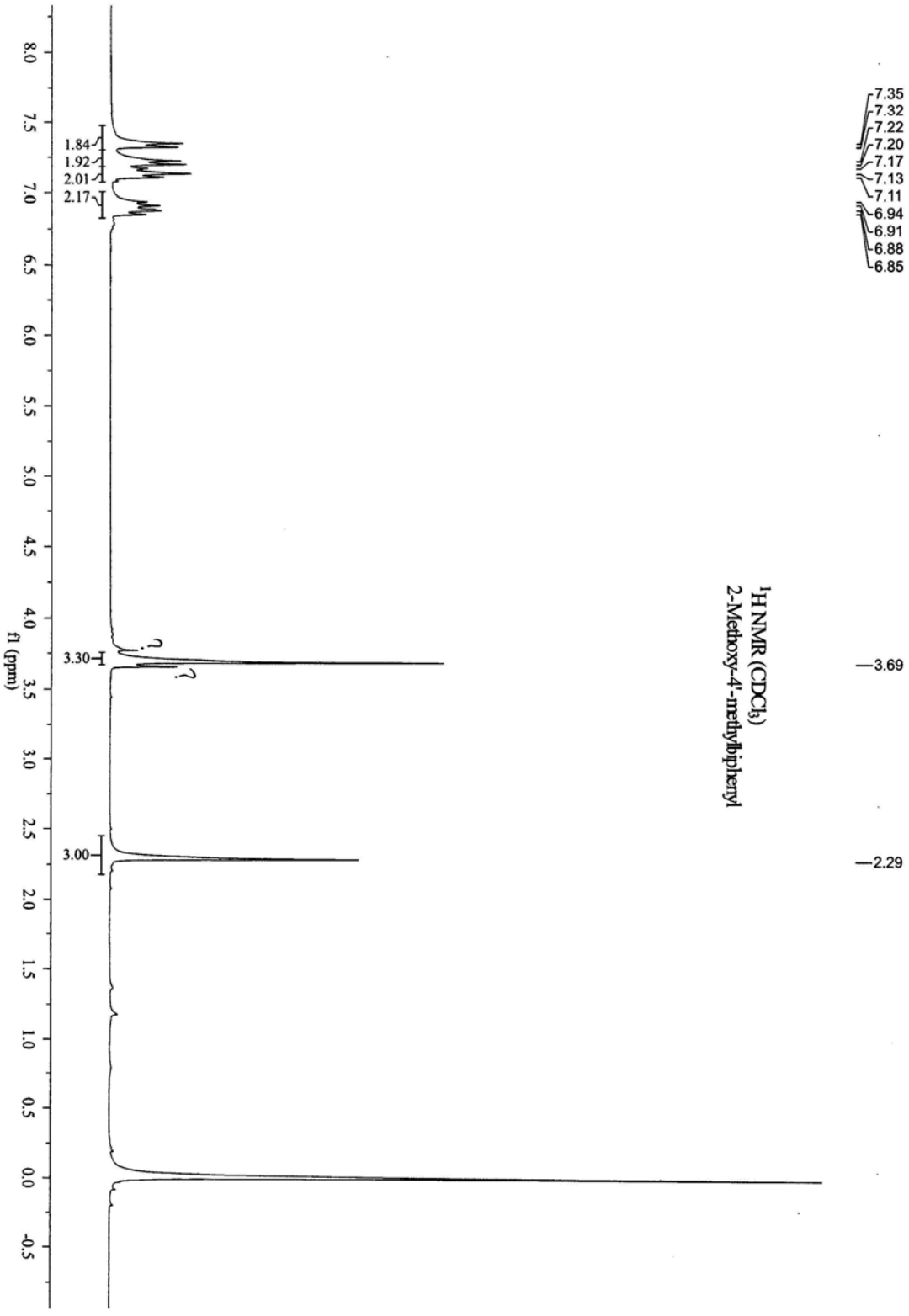

^{1}H NMR (CDCl$_3$)
2-*p*-Tolylpyridine
8.67
8.67
8.67
8.66
8.65
8.65
7.90
7.87
7.69
7.69
7.68
7.67
7.28
7.25
7.19
7.18
7.17
7.16
7.16
7.15
2.39
0.68
1.62
1.70
1.71
0.79
3.00
f1 (ppm)

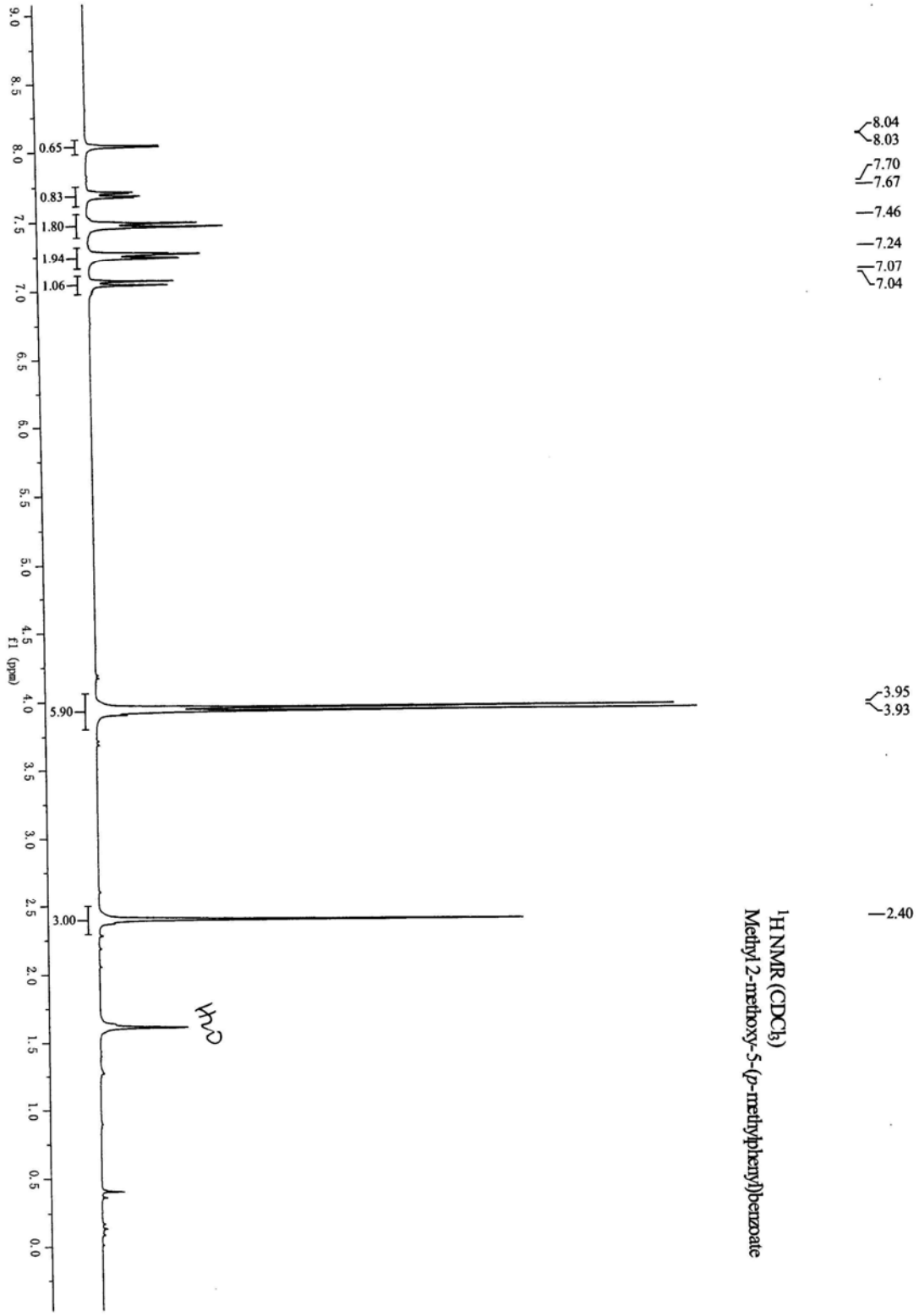

^{1}H NMR (CDCl$_3$)
N,N-Diethyl-4'-methylbiphenyl-4-carboxamide
f1 (ppm)
1.91
2.03
1.82
1.97
4.20
3.00
6.48
7.60
7.58
7.50
7.48
7.44
7.41
7.27
7.24
3.54
3.34
2.39
1.20


^{1}H NMR (CDCl$_3$)
Ethyl 4'-methylbiphenyl-4-carboxylate
7.96
7.94
7.48
7.45
7.36
7.33
7.10
7.07
4.28
4.26
4.23
4.21
2.24
1.28
1.26
1.23
1.91
2.12
1.93
1.89
2.26
3.00
3.29
f1 (ppm)

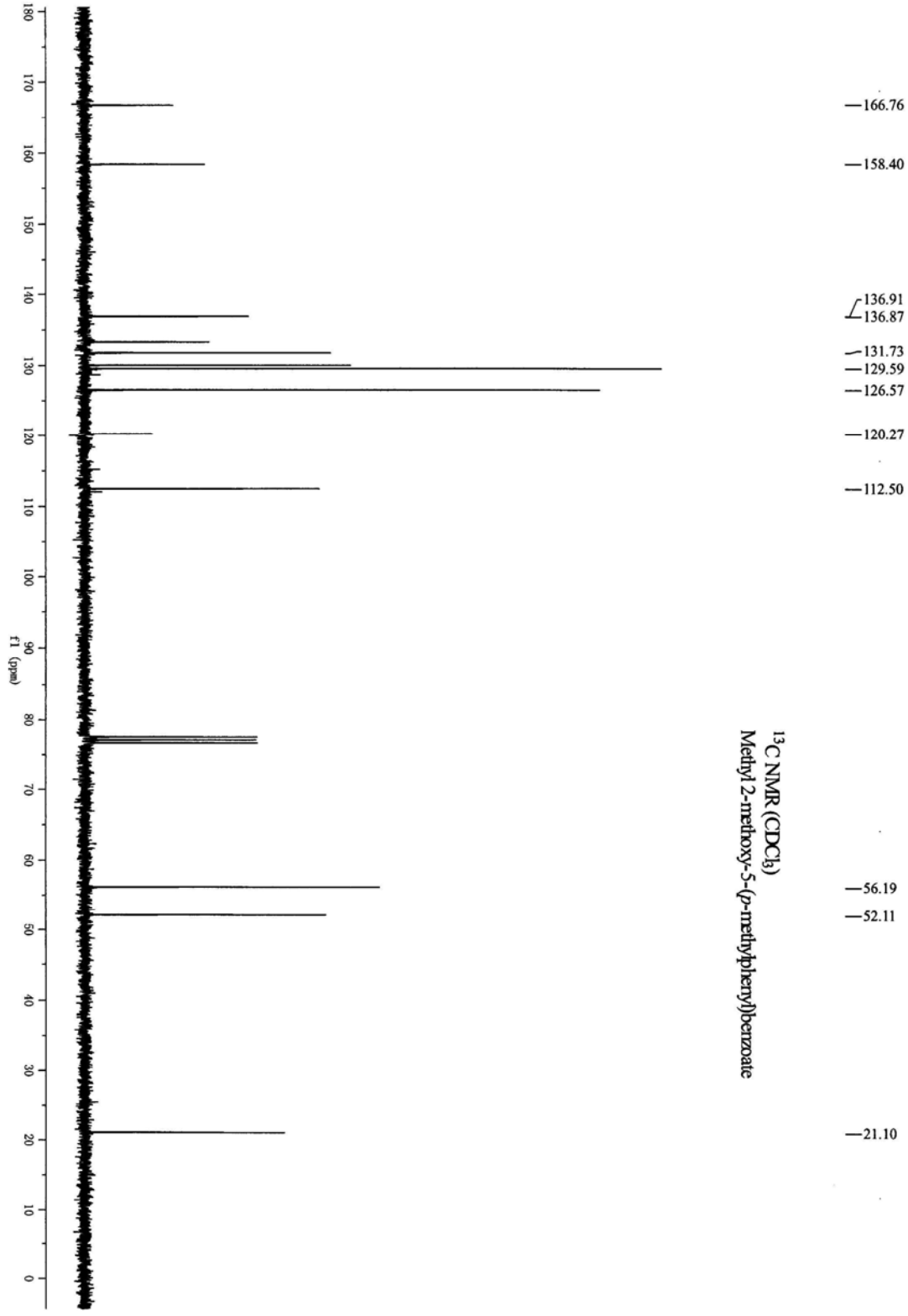

^{1}H NMR (CDCl$_3$)
4-Methoxy-4'-methylbiphenyl
f1 (ppm)
1.89
1.85
1.84
1.97
3.25
3.00
7.42
7.39
7.36
7.33
7.13
7.11
6.87
6.85
3.73
2.28


^{1}H NMR (CDCl$_3$)
(4'-Methylbiphenyl-2-yl)(phenyl)methanone
7.68
7.66
7.60
7.60
7.58
7.57
7.55
7.53
7.48
7.48
7.47
7.45
7.44
7.44
7.43
7.42
7.41
7.39
7.39
7.38
7.37
7.36
7.30
7.28
7.25
7.17
7.14
7.02
6.99
2.24
0.43
1.70
5.67
1.94
1.76
1.77
3.00
f1 (ppm)

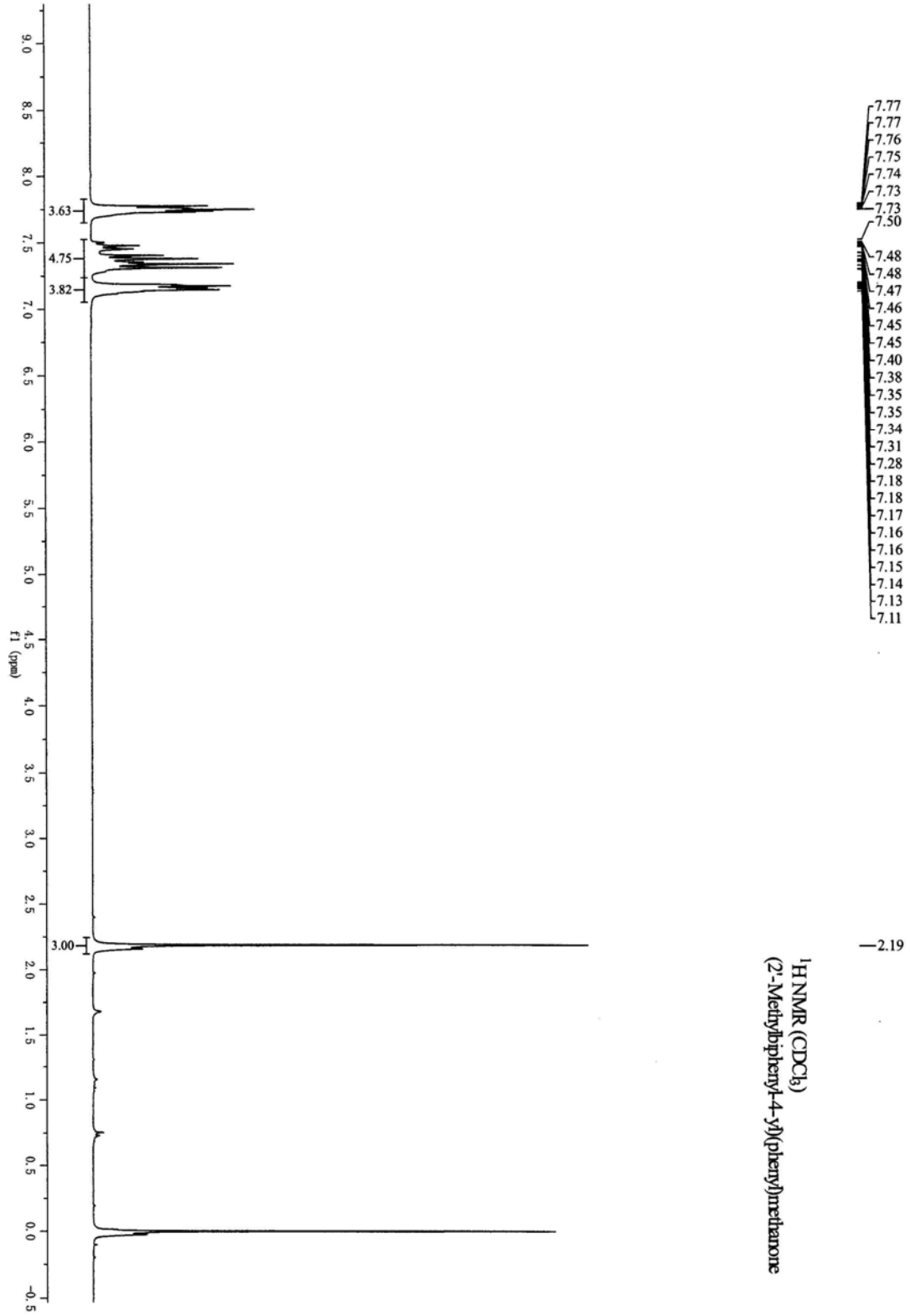

^{1}H NMR (CDCl$_3$)
2-Methoxy-4'-methylbiphenyl
7.35
7.32
7.22
7.20
7.17
7.13
7.11
6.94
6.91
6.88
6.85
3.69
2.29
1.84
1.92
2.01
2.17
3.30
3.00
f1 (ppm)



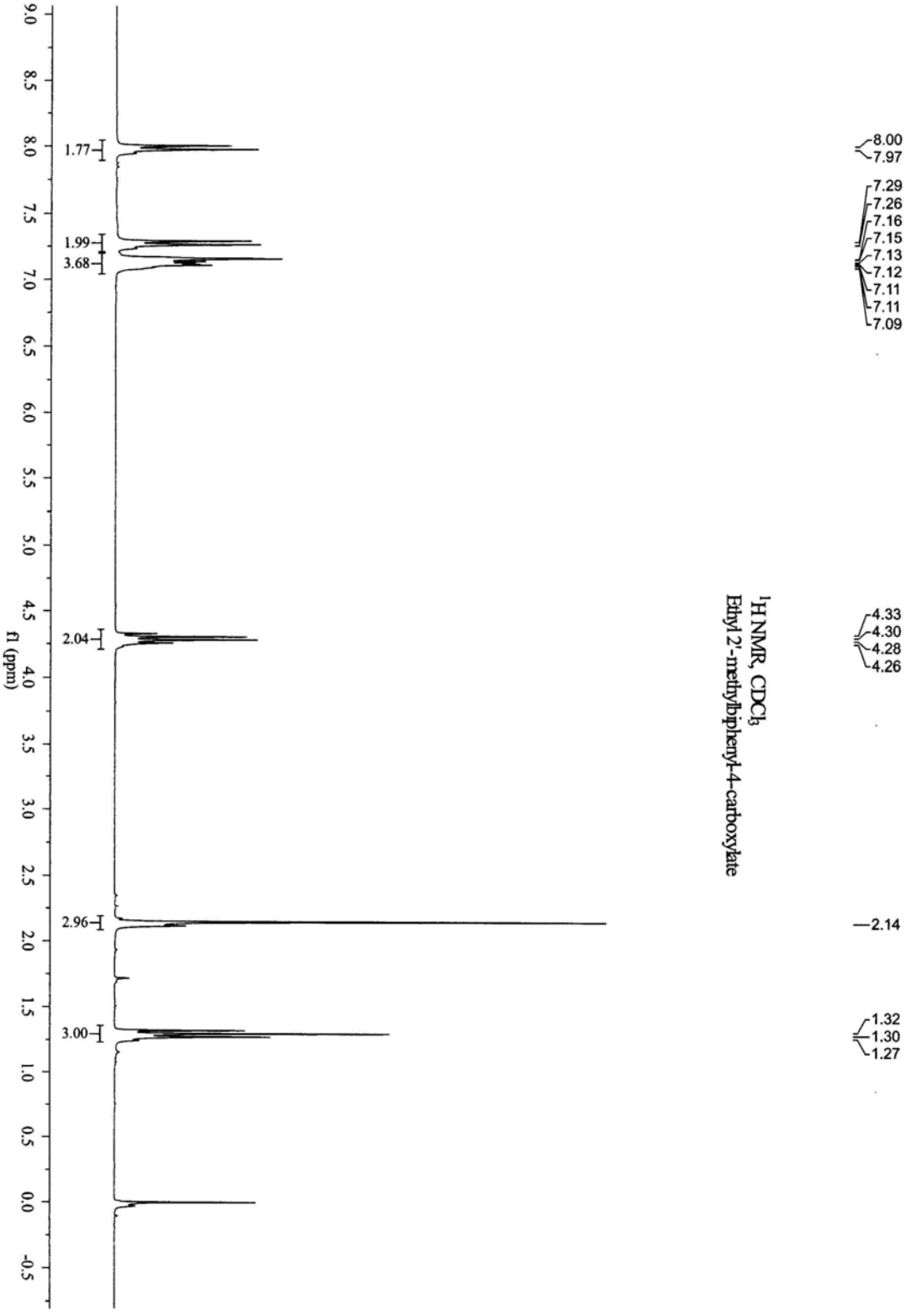
^{1}H NMR ($CDCl_3$)
Methyl 2-methoxy-5-(*p*-methylphenyl)benzoate

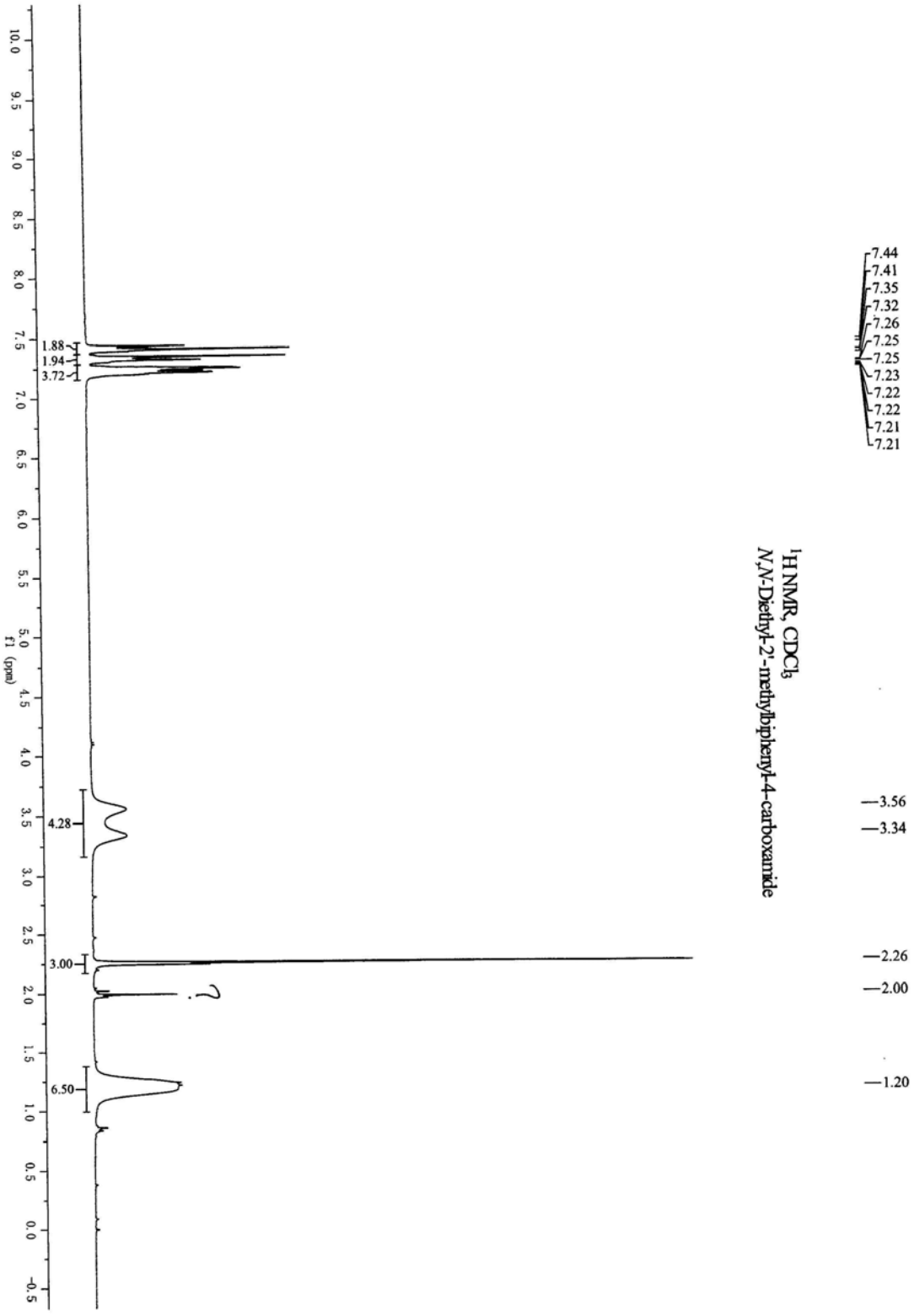


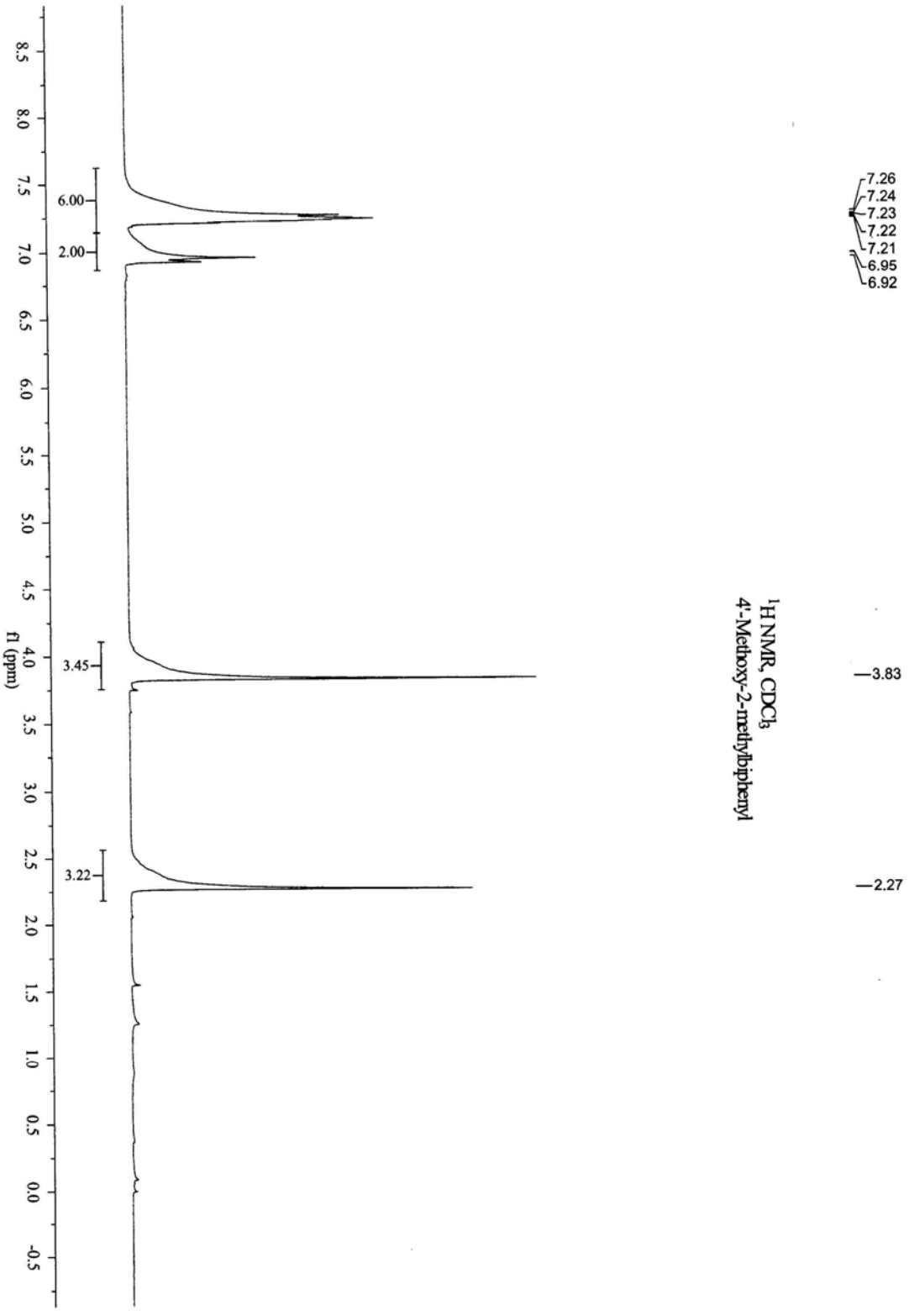
^{13}C NMR ($CDCl_3$)
Methyl 2-methoxy-5-(*p*-methylphenyl)benzoate

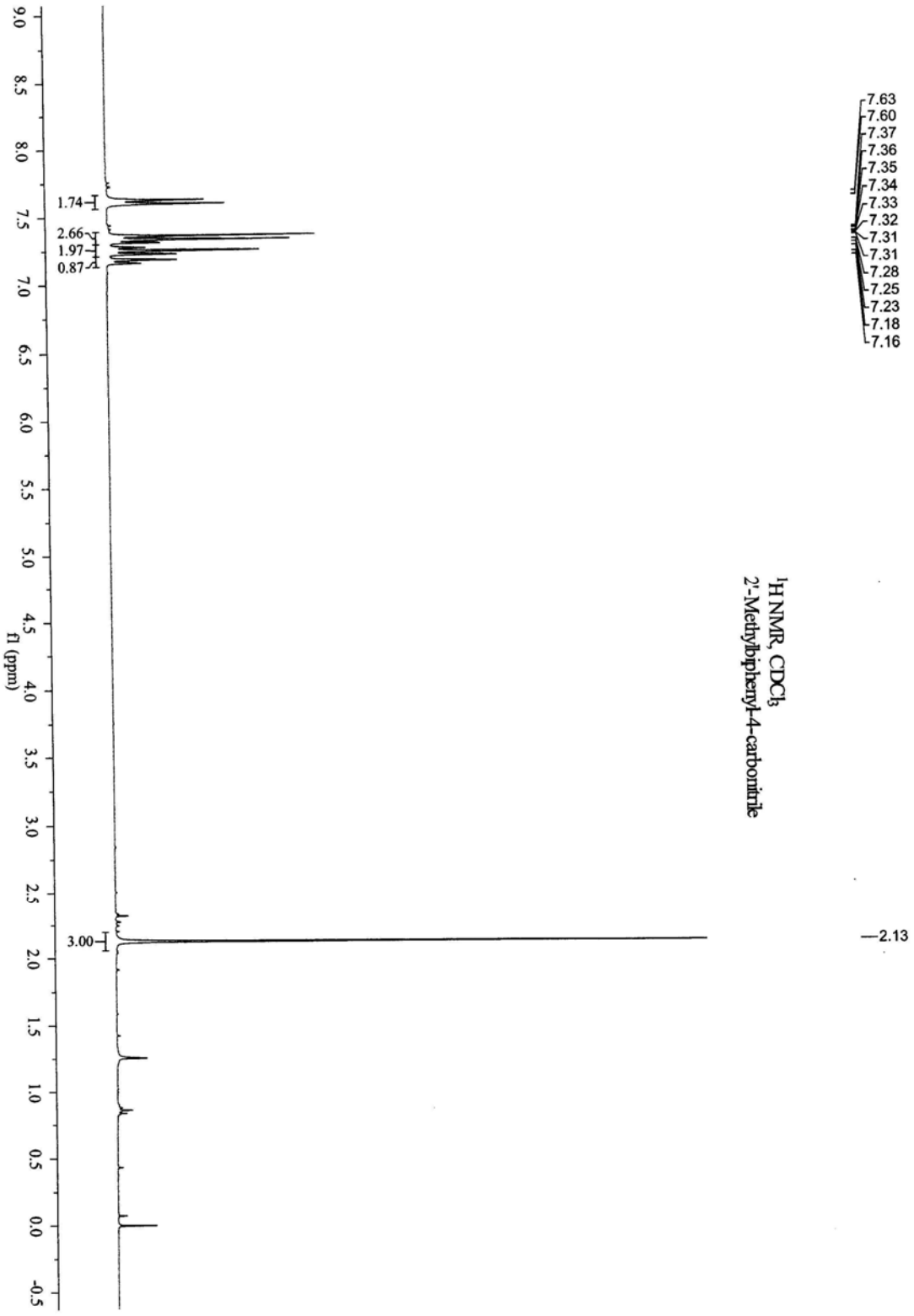


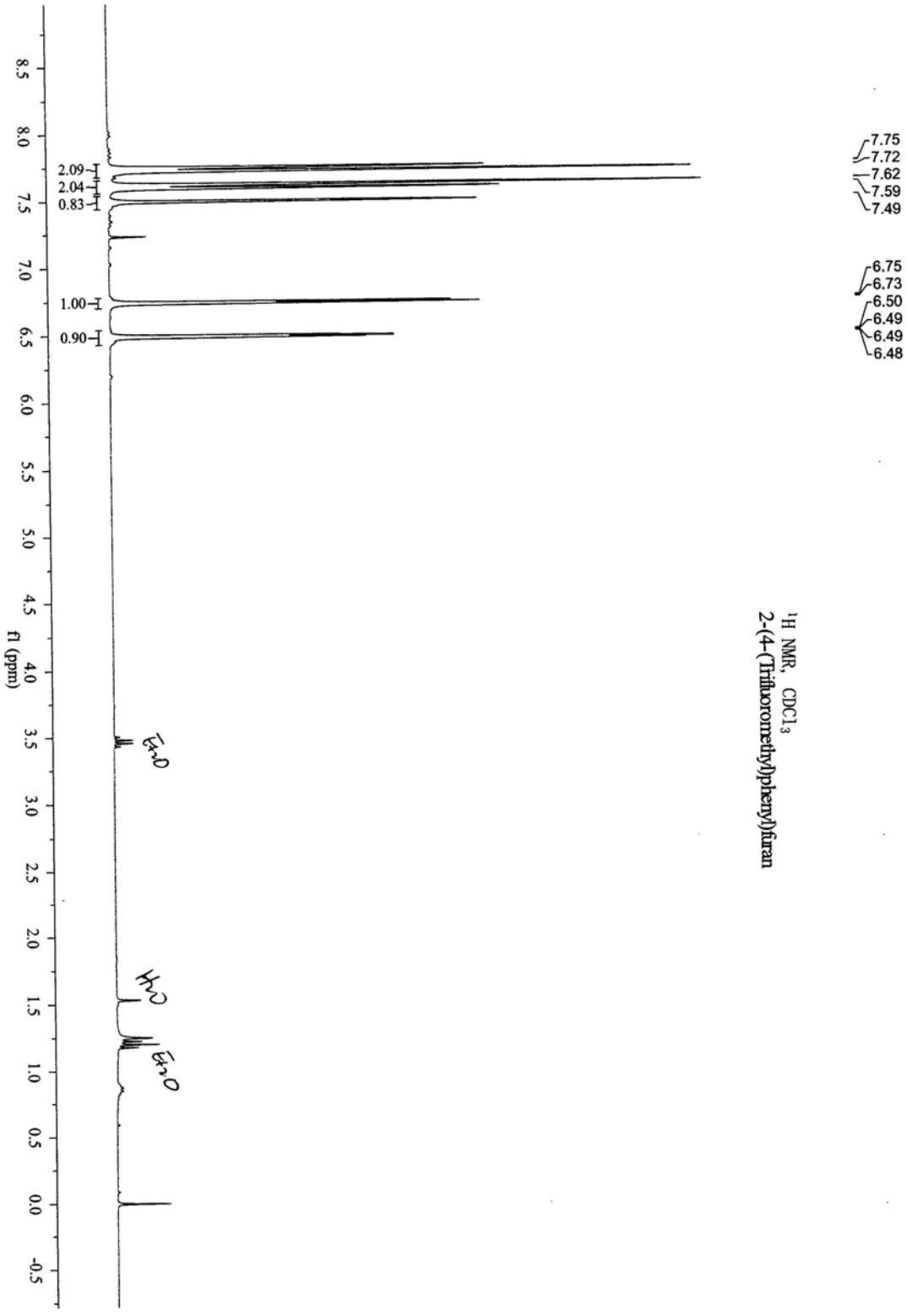
^{1}H NMR ($CDCl_3$)
(2'-Methylbiphenyl-4-yl)(phenyl)methanone

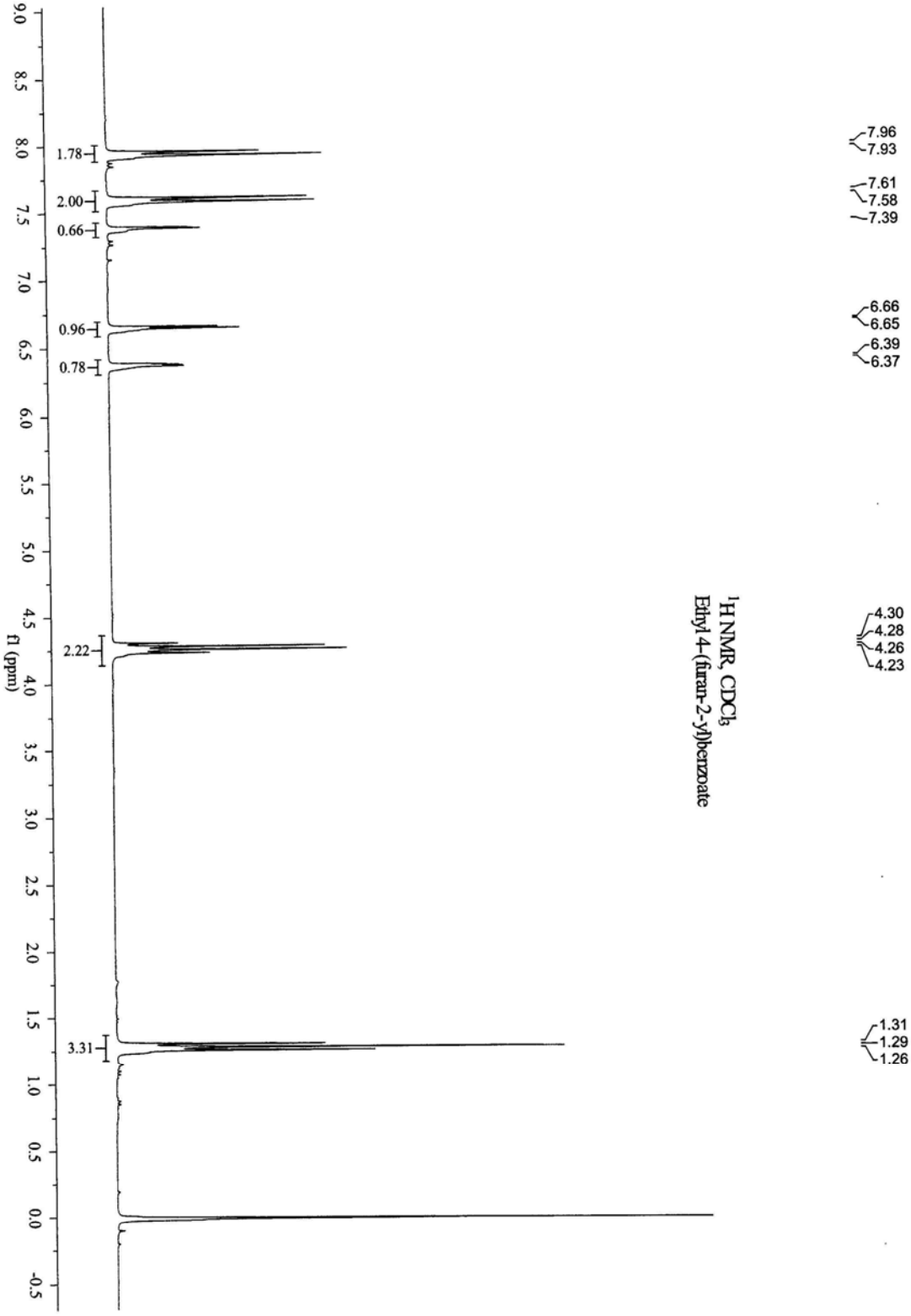

^{1}H NMR, CDCl$_3$
Ethyl 2'-methylbiphenyl-4-carboxylate
f1 (ppm)
1.77
1.99
3.68
2.04
2.96
3.00
8.00
7.97
7.29
7.26
7.16
7.15
7.13
7.12
7.11
7.11
7.09
4.33
4.30
4.28
4.26
2.14
1.32
1.30
1.27


^{1}H NMR, CDCl$_3$
N,N-Diethyl-2'-methylbiphenyl-4-carboxamide
7.44
7.41
7.35
7.32
7.26
7.25
7.25
7.23
7.22
7.22
7.21
7.21
3.56
3.34
2.26
2.00
1.20
1.88
1.94
3.72
4.28
3.00
6.50
f1 (ppm)


^{1}H NMR, CDCl$_3$
4'-Methoxy-2-methylbiphenyl
7.26
7.24
7.23
7.22
7.21
6.95
6.92
3.83
2.27
6.00
2.00
3.45
3.22
f1 (ppm)


^{1}H NMR, CDCl$_3$
2'-Methylbiphenyl-4-carbonitrile
7.63
7.60
7.37
7.36
7.35
7.34
7.33
7.32
7.31
7.31
7.28
7.25
7.23
7.18
7.16
2.13
1.74
2.66
1.97
0.87
3.00
f1 (ppm)


7.75
7.72
7.62
7.59
7.49
6.75
6.73
6.50
6.49
6.49
6.48
2.09
2.04
0.83
1.00
0.90
f1 (ppm)
^{1}H NMR, CDCl$_3$
2-(4-(Trifluoromethyl)phenyl)furan


^{1}H NMR, CDCl$_3$
Ethyl 4-(furan-2-yl)benzoate
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
1.78
2.00
0.66
0.96
0.78
2.22
3.31
7.96
7.93
7.61
7.58
7.39
6.66
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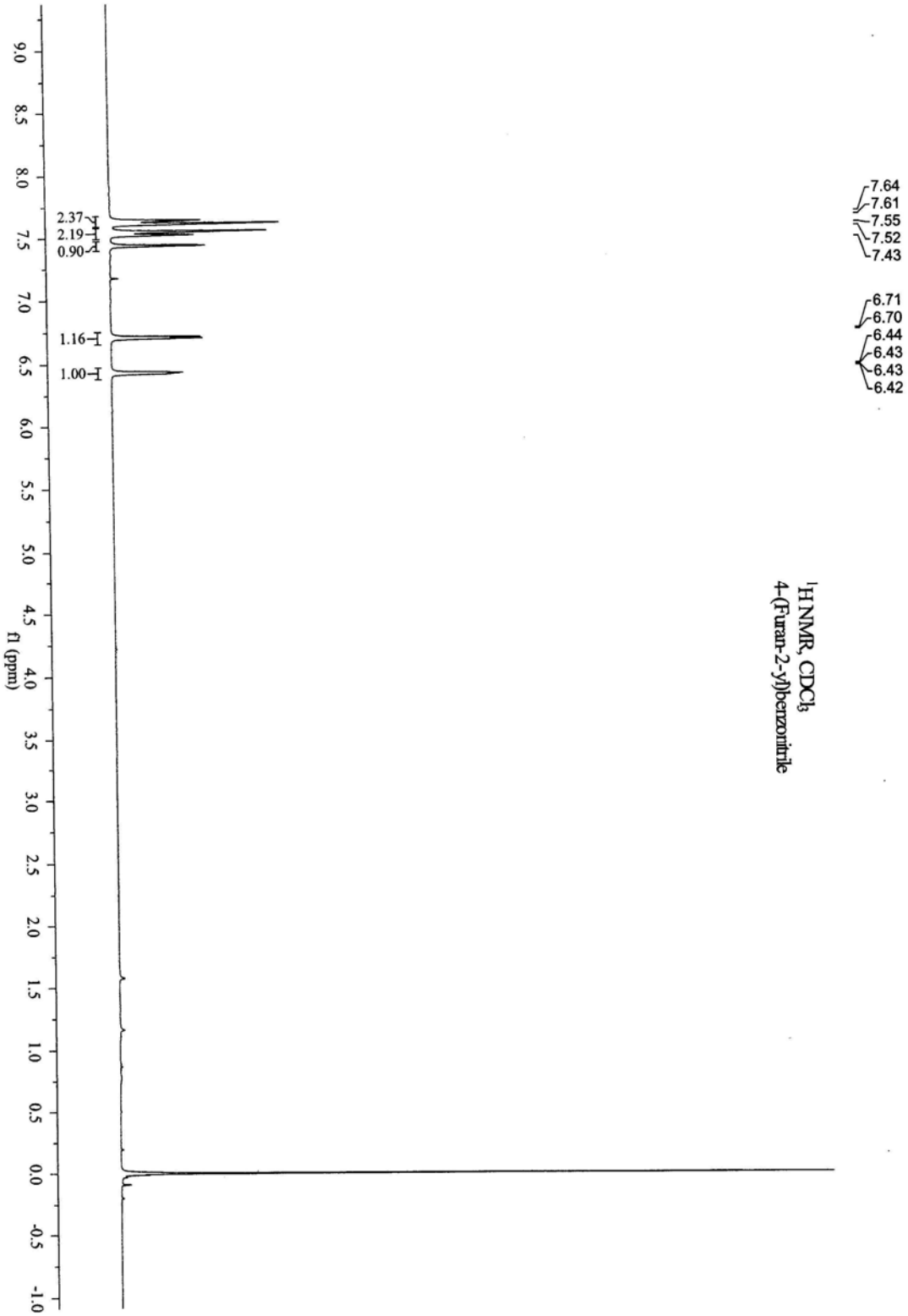
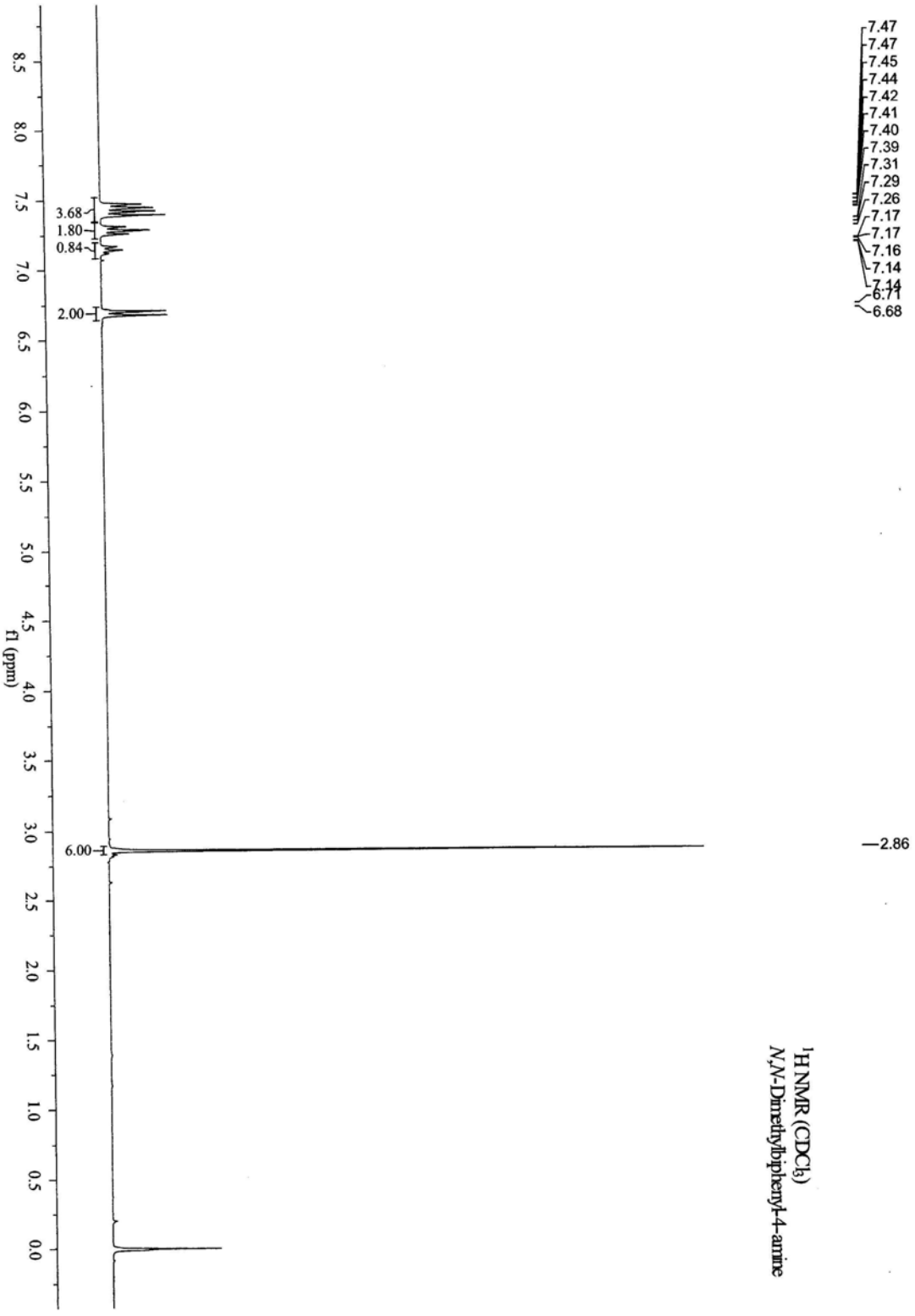
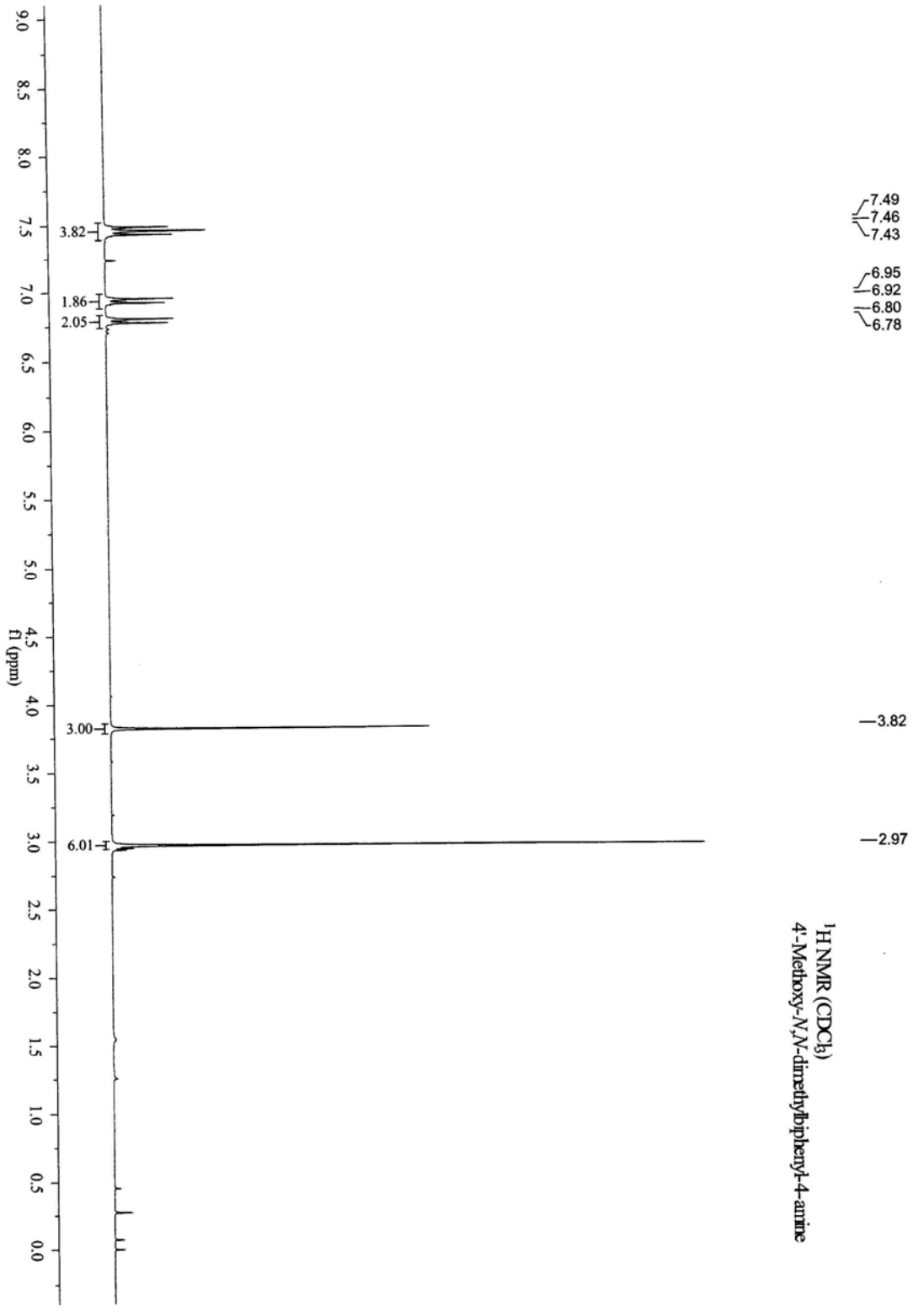
4.28
4.26
4.23
1.31
1.29
1.26

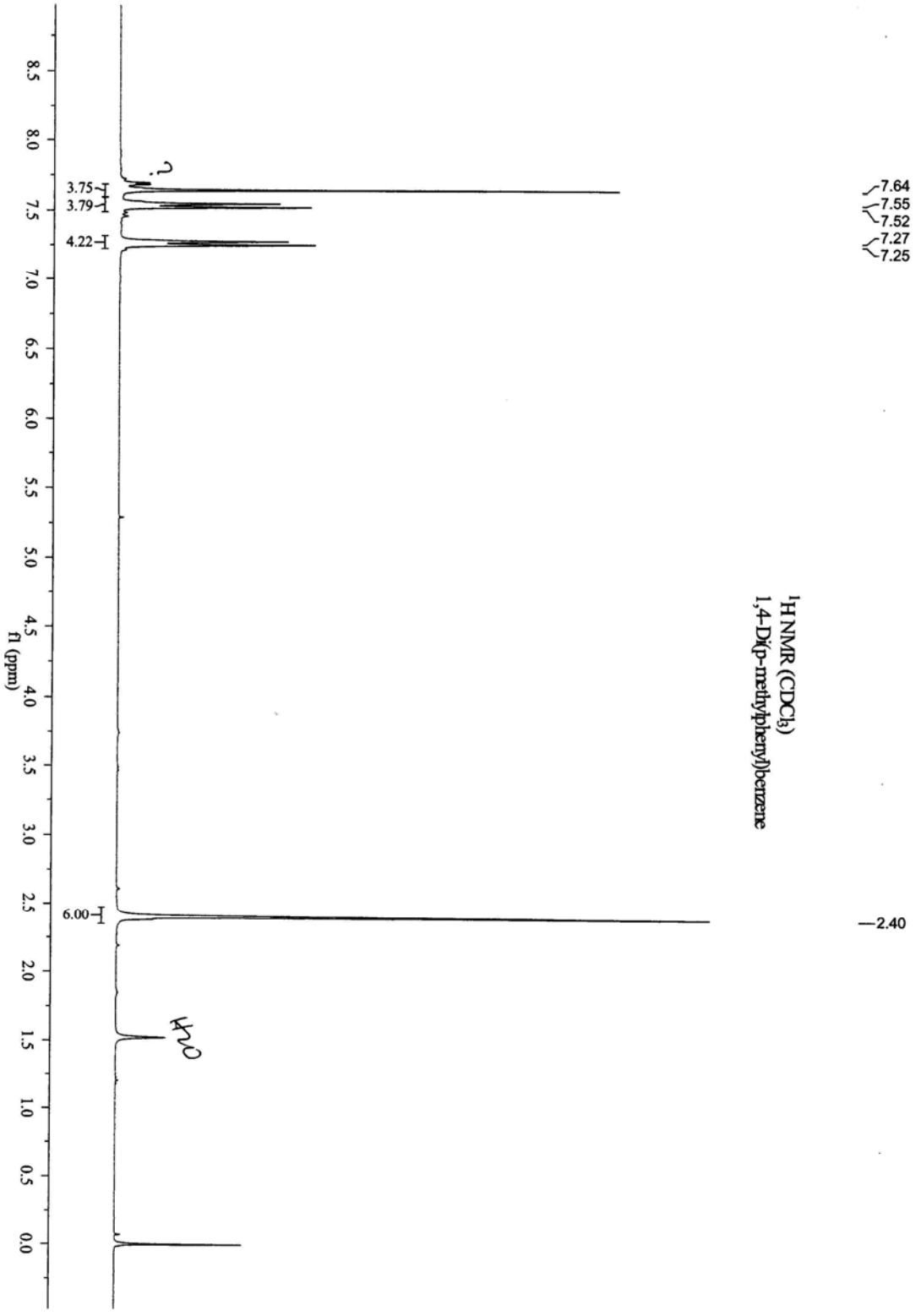

^{1}H NMR, $CDCl_3$
4-(Furan-2-yl)benzonitrile
7.64
7.61
7.55
7.52
7.43
6.71
6.70
6.44
6.43
6.43
6.42
2.37
2.19
0.90
1.16
1.00
f1 (ppm)

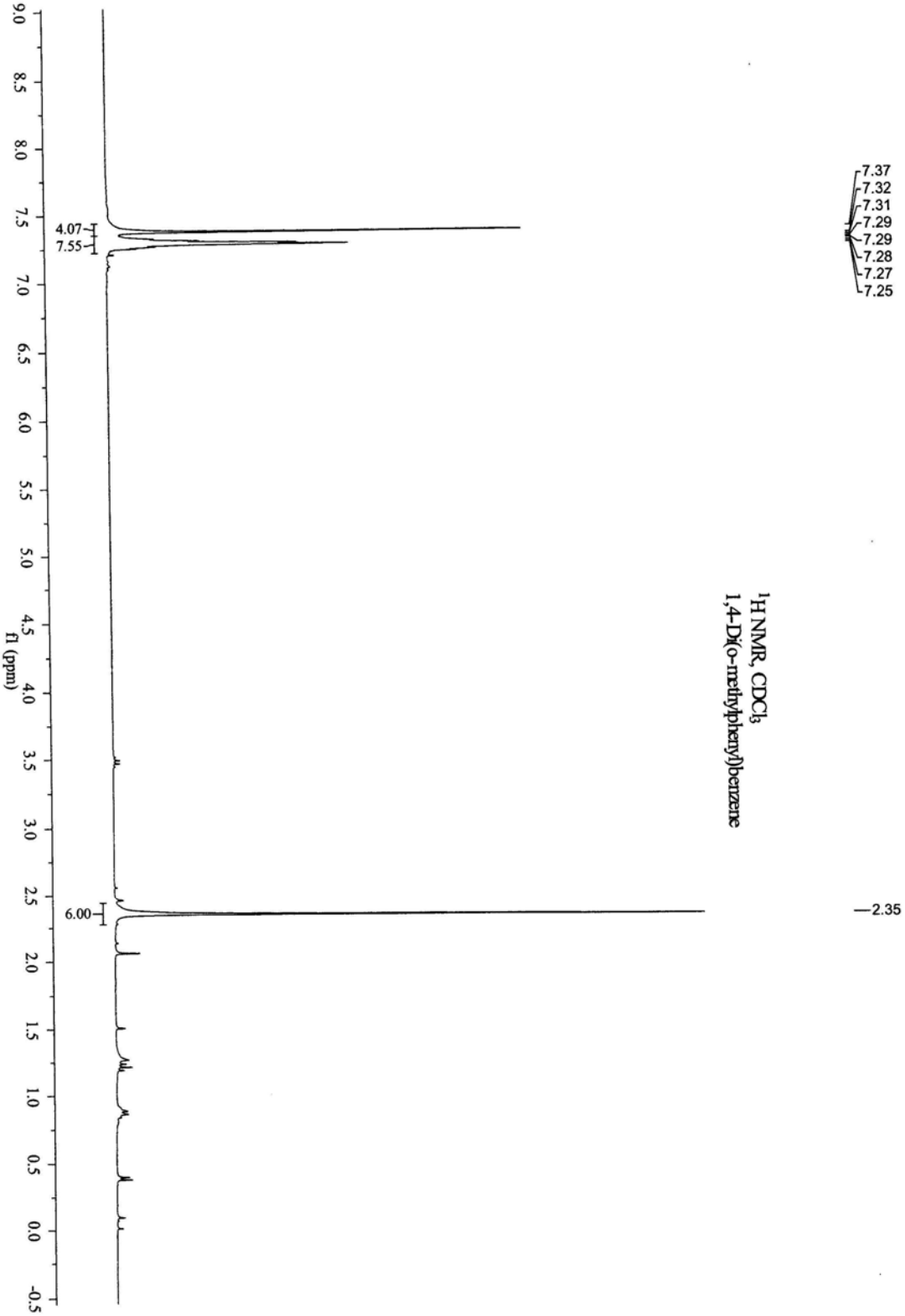


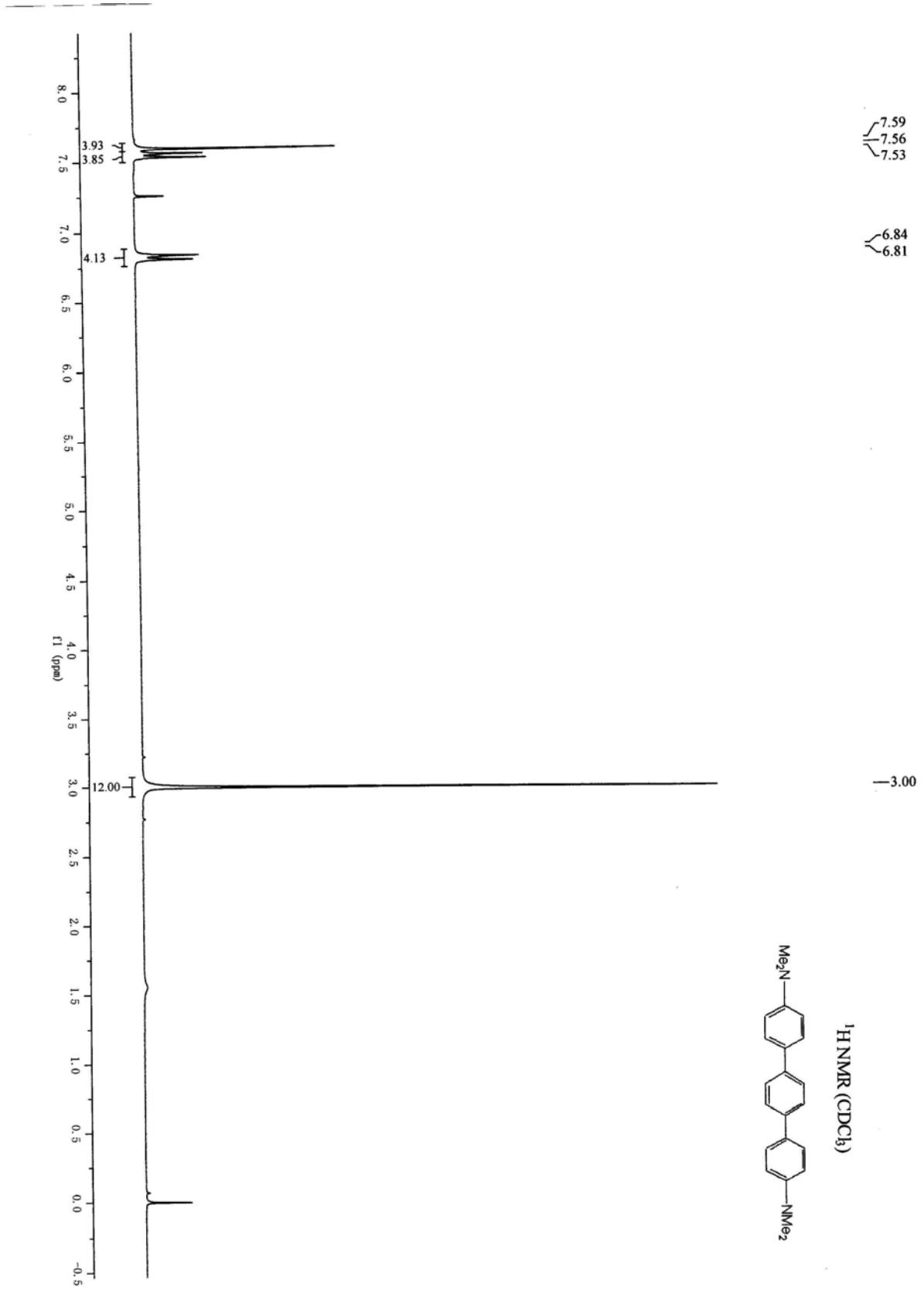
^{1}H NMR ($CDCl_3$)
N,N-Dimethylbiphenyl-4-amine

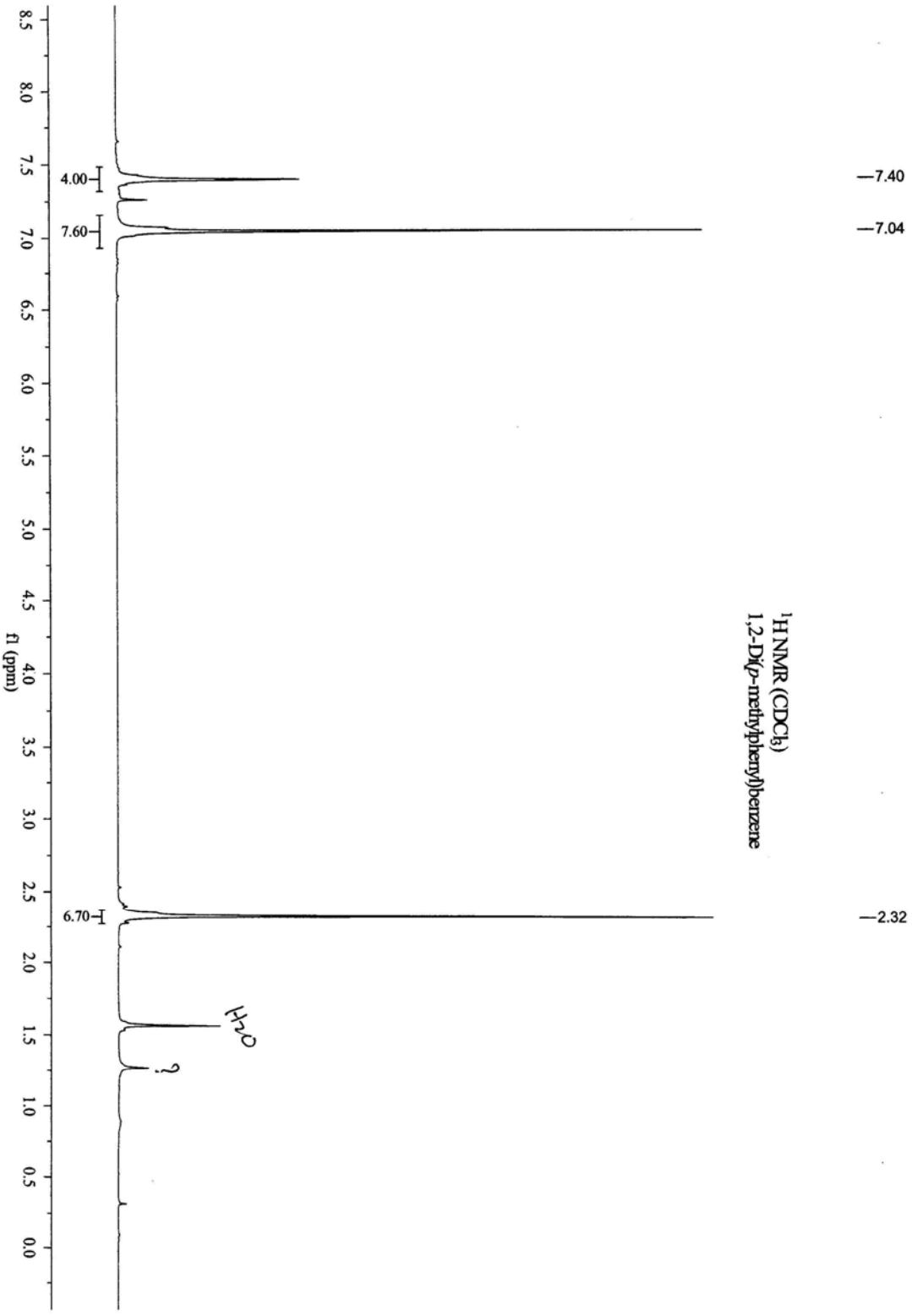


^{1}HNMR ($CDCl_3$)
4'-Methoxy-*N*,*N*-dimethylbiphenyl-4-amine

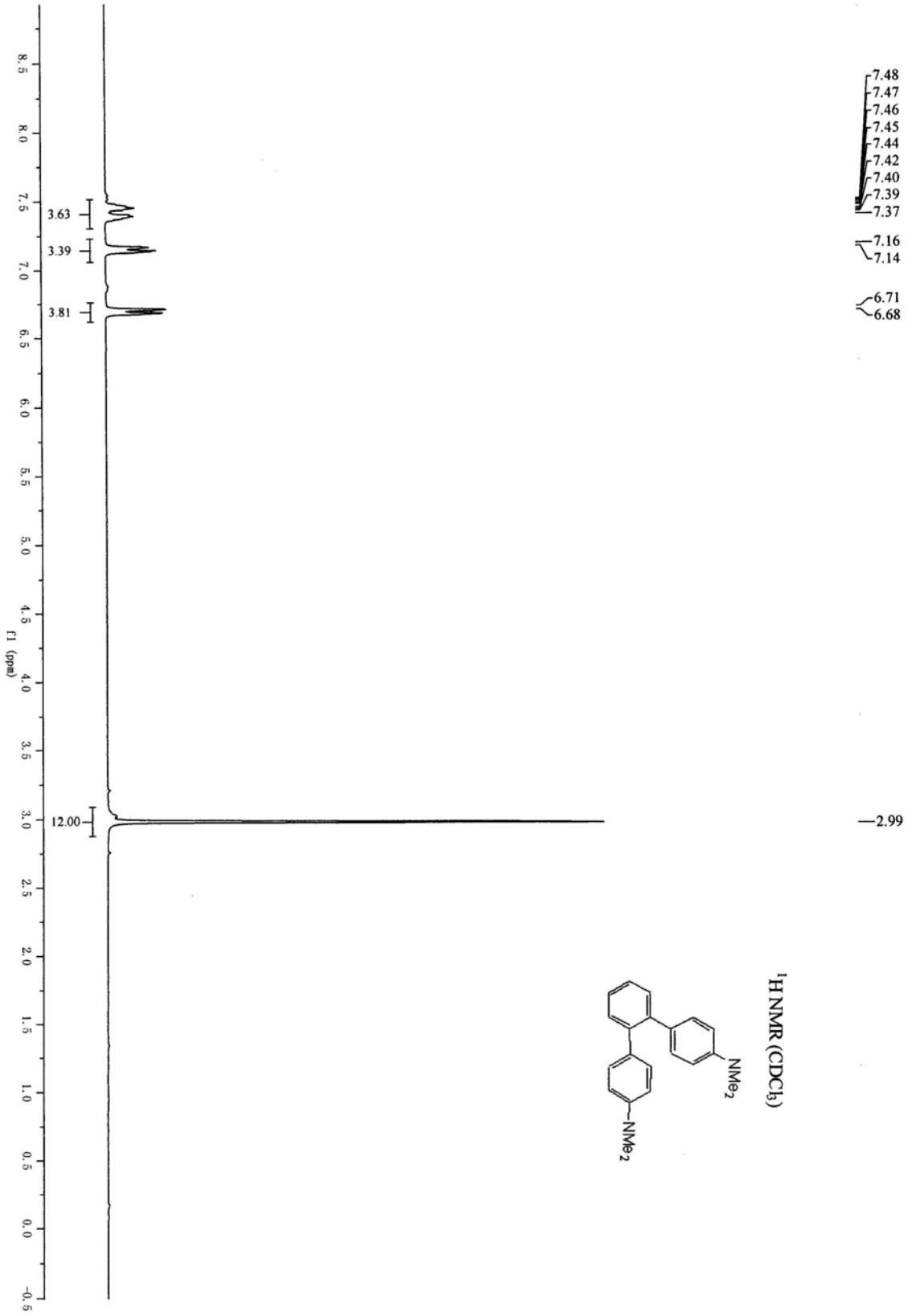

^{1}H NMR (CDCl$_3$)
1,4-Di(p-methylphenyl)benzene
7.64
7.55
7.52
7.27
7.25
2.40
3.75
3.79
4.22
6.00
H2O
f1 (ppm)


^{1}H NMR, CDCl$_3$
1,4-Di(o-methylphenyl)benzene
7.37
7.32
7.31
7.29
7.29
7.28
7.27
7.25
2.35
4.07
7.55
6.00
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5

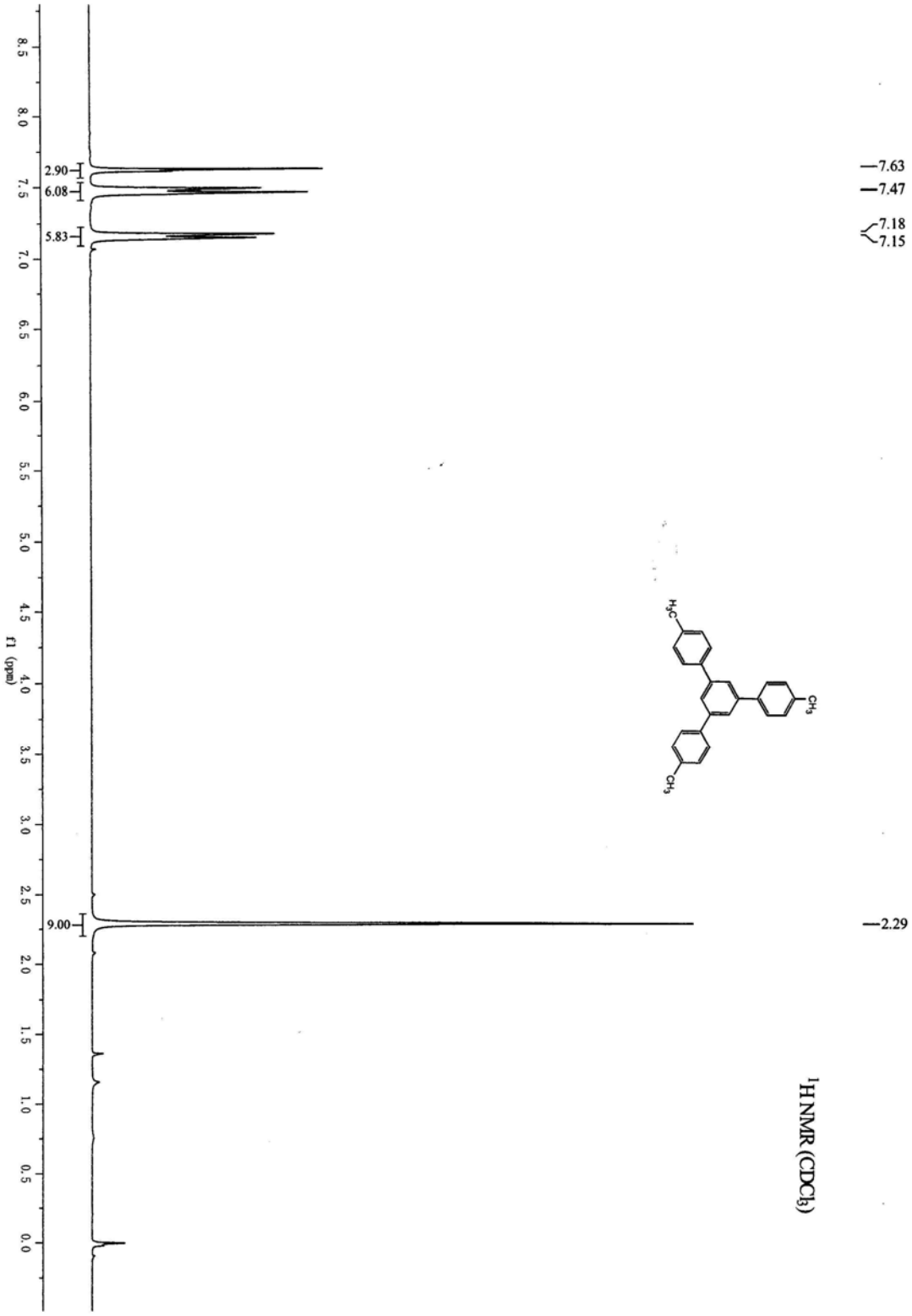

7.59
7.56
7.53
6.84
6.81
3.93
3.85
4.13
12.00
3.00
f1 (ppm)
Me2N
NMe2
1H NMR (CDCl3)

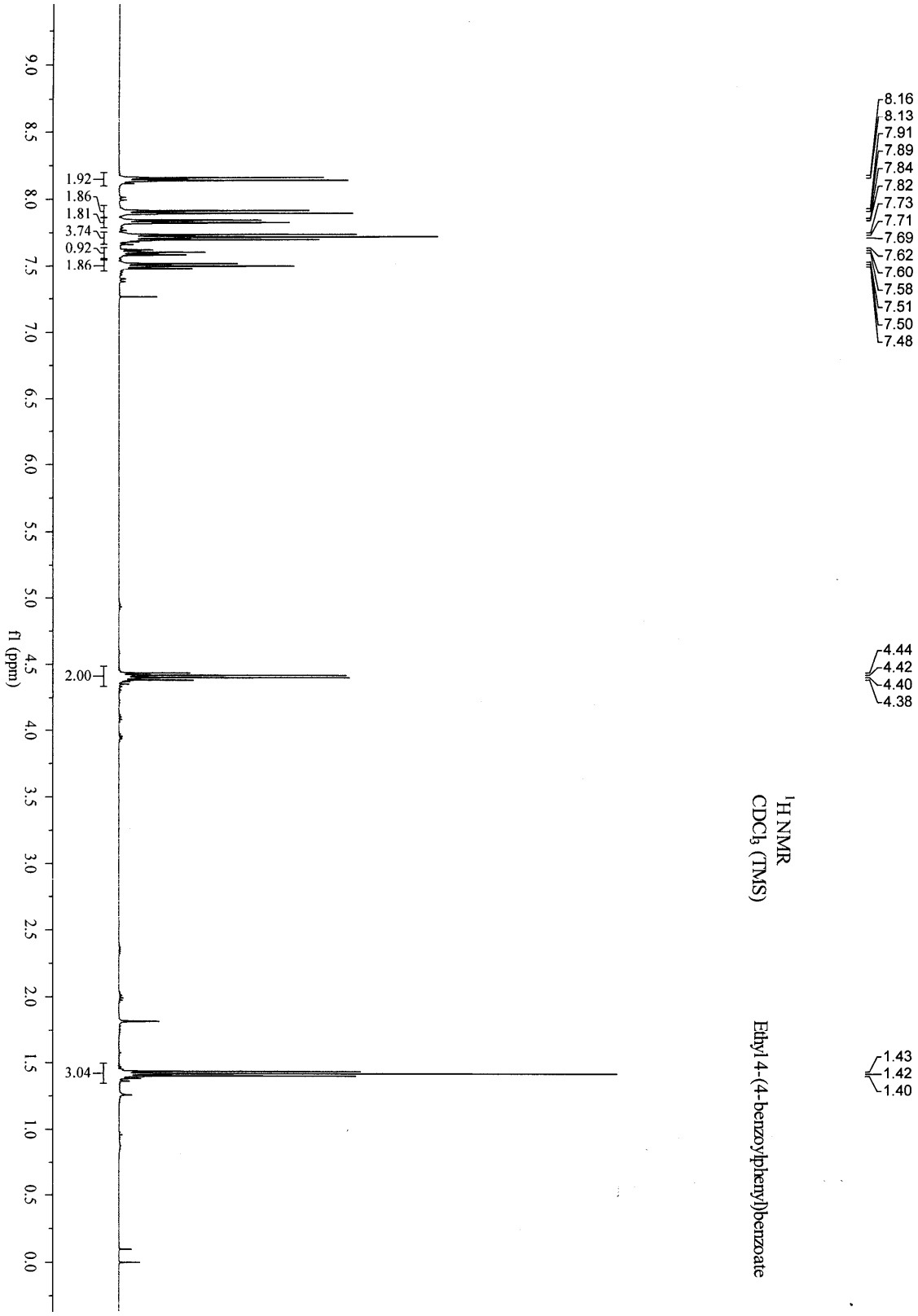


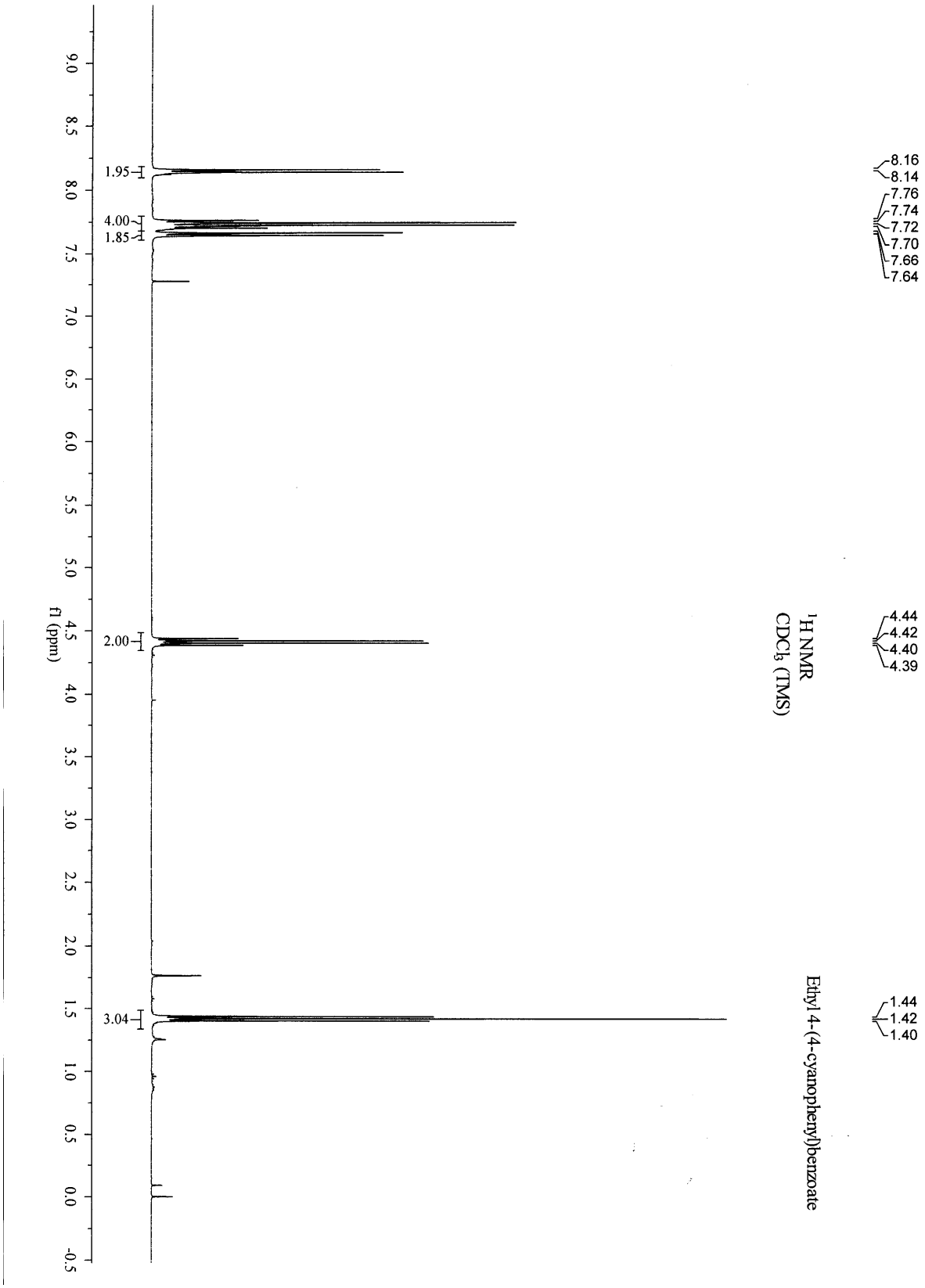
^{1}HNMR ($CDCl_3$)
1,2-Di(*p*-methylphenyl)benzene


7.48
7.47
7.46
7.45
7.44
7.42
7.40
7.39
7.37
7.16
7.14
6.71
6.68
2.99
3.63
3.39
3.81
12.00
f1 (ppm)
NMe2
NMe2

^{1}H NMR ($CDCl_3$)


2.90
6.08
5.83
9.00
7.63
7.47
7.18
7.15
2.29
f1 (ppm)
^{1}H NMR (CDCl$_3$)


8.16
8.13
7.91
7.89
7.84
7.82
7.73
7.71
7.69
7.62
7.60
7.58
7.51
7.50
7.48
4.44
4.42
4.40
4.38
1.43
1.42
1.40
1.92
1.86
1.81
3.74
0.92
1.86
2.00
3.04
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
^{1}H NMR
$CDCl_3$ (TMS)
Ethyl 4-(4-benzoylphenyl)benzoate


Ethyl 4-(4-cyanophenyl)benzoate
^{1}H NMR
$CDCl_3$ (TMS)
8.16
8.14
7.76
7.74
7.72
7.70
7.66
7.64
4.44
4.42
4.40
4.39
1.44
1.42
1.40
1.95
4.00
1.85
2.00
3.04
f1 (ppm)
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5