

Palladium-Catalyzed Selective Heck-type Diarylation of Allylic Esters with Aryl Halides Involving a β -OAc Elimination Process

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Supporting Information

List of Contents

| | |
|--------------------------------------------|---------|
| (A) Typical experimental procedure | S2 |
| (B) Analytical data of 3-13, 15, and 17-28 | S2-S8 |
| (C) References | S8-S9 |
| (D) Spectra of 3-13, 15, and 17-28 | S10-S57 |

(A) Typical Experimental Procedure

(a) Typical Experimental Procedure for the Palladium-Catalyzed Diarylation Reactions of Allylic Esters (1) with Aryl Iodides (2).

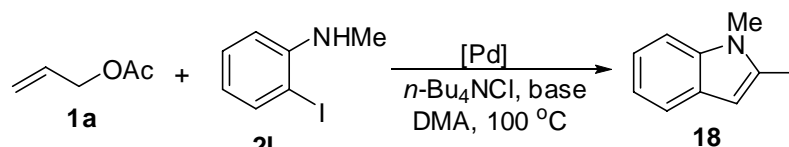
To a Schlenk tube were added allylic esters **1** (0.2 mmol), aryl iodides **2** (0.5 mmol), Pd(OAc)₂ (4.5 mg, 10 mol %), *n*-Bu₄NCl (83.4mg, 1.5 equiv), Et₃N (161.9 mg, 8.0 equiv) and anhydrous MeCN (2 mL). Then the tube was stirred at 120 °C (oil bath temperature) under the air atmosphere for the indicated time until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was cooled to room temperature, diluted in diethyl ether, and washed with brine. The aqueous phase was re-extracted with diethyl ether. The combined organic extracts were dried over Na₂SO₄ and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the corresponding product.

(b) Typical Experimental Procedure for the Synthesis of Indoles and Benzofurans.

To a Schlenk tube were added allylic esters **1** (0.2 mmol), aryl halides **2** (0.3 mmol), PdCl₂ (7.1 mg, 10 mol %), *n*-Bu₄NCl (83.4 mg, 1.5 equiv), K₂CO₃ (55.2 mg, 2.0 equiv) and anhydrous DMA (2 mL). Then the tube was stirred at 100 °C (oil bath temperature) under the air atmosphere for the indicated time until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was cooled to room temperature, diluted in diethyl ether, and washed with brine. The aqueous phase was re-extracted with diethyl ether. The combined organic extracts were dried over Na₂SO₄ and concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the Indoles or Benzofurans.

(c) Table S1

Table S1. Screening Optimal Conditions Applications in the Synthesis of Indole^a



| entry | [Pd] (mol %) | Base | Solvent | T (°C) | yield (%) ^b |
|----------------|---------------------------|------------------------------------------|---------|--------|------------------------|
| 1 ^c | Pd(OAc) ₂ (10) | Et ₃ N (8 equiv) | MeCN | 120 | 38 |
| 2 ^d | Pd(OAc) ₂ (10) | Et ₃ N (2 equiv) | MeCN | 100 | 42 |
| 3 ^e | Pd(OAc) ₂ (10) | Et ₃ N (2 equiv) | MeCN | 80 | 20 |
| 4 ^f | Pd(OAc) ₂ (10) | Et ₃ N (2 equiv) | DMA | 100 | 65 |
| 5 ^g | Pd(OAc) ₂ (10) | K ₂ CO ₃ (2 equiv) | DMA | 100 | 84 |
| 6 | PdCl ₂ (10) | K ₂ CO ₃ (2 equiv) | DMA | 100 | 88 |

^a Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol), PdCl₂ (10 mol %), *n*-Bu₄NCl (1.5 equiv), base and solvent (2 mL) under air atmosphere. DMA = *N,N*-dimethylacetamide. ^b Isolated yield.

(B) Analytical data for 3-13, 15, and 17-28

(*E*)-4,4'-(Prop-1-ene-1,3-diyl)bis(methoxybenzene) (3)¹

White solid; mp: 47-49 °C; ¹H NMR (300 MHz, CDCl₃) δ: 7.27 (t, *J* = 7.5 Hz, 2H), 7.15 (d, *J* = 8.5 Hz, 2H), 6.86-6.81 (m, 4H), 6.37 (d, *J* = 15.8 Hz, 1H), 6.24-6.16 (m, 1H), 3.78 (s, 6H); 3.46 (d, *J* = 6.6 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 158.8, 158.0, 132.5, 130.4, 130.1, 129.6, 127.5, 127.1, 113.9, 113.9, 55.3 (2C), 38.4; LRMS (EI 70 ev): *m/z* (%): 254 (M⁺, 100), 223 (49), 145 (38), 115 (32), 121 (23).

(*E*)-2,2'-(prop-1-ene-1,3-diyl)bis(methoxybenzene) (4)

Yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.42 (d, *J* = 6.3 Hz, 1H), 7.22-7.14 (m, 3H), 6.92-6.83 (m, 5H), 6.41-6.32 (m, 1H), 3.84 (s, 3H), 3.83 (s, 3H), 3.56 (d, *J* = 6.0 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 157.3, 156.4, 139.5, 129.8, 129.5, 129.1, 127.9, 127.3, 126.6, 125.5, 120.6, 120.5, 110.9, 110.4, 55.5, 55.4, 33.8; LRMS (EI 70 ev): *m/z* (%): 254 (M⁺, 100), 223 (62), 91 (52), 115 (35), 145 (29); HRMS *m/z* (ESI) calcd for C₁₇H₁₁O₂ (M+H)⁺ 255.1372, found 255.1380.

(*E*)-prop-1-ene-1,3-diyl dibenzene (5)¹

Colourless liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.38-7.20 (m, 10H), 6.46 (d, *J* = 15.9 Hz, 1H), 6.40-6.56 (m, 1H), 3.55 (d, *J* = 6.3 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 140.2, 137.5, 131.1, 129.3, 128.7, 128.5, 128.3, 127.1, 126.2, 126.1, 39.4; LRMS (EI 70 ev): *m/z* (%): 194 (M⁺, 100), 115 (93), 93 (54), 179 (44), 116 (57).

(E)-4,4'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (6)¹

Pale yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.24 (d, *J* = 7.2 Hz, 2H), 7.12-7.08 (m, 5H), 6.41 (d, *J* = 15.8 Hz, 1H), 6.33-6.23 (m, 1H), 3.49 (d, *J* = 6.6 Hz, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ: 137.3, 136.8, 135.6, 134.8, 130.7, 129.2, 129.1, 128.5, 128.5, 126.0, 38.9, 21.1, 21.0; LRMS (EI 70 ev): *m/z* (%): 222 (M⁺, 97), 207 (100), 115 (82), 129 (64).

(E)-2,2'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (7)¹

Colourless liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.43-7.39 (m, 1H), 7.16-7.11 (m, 7H), 6.63 (d, *J* = 15.0 Hz, 1H), 6.24-6.14 (m, 1H), 3.55 (dd, *J* = 6.6 Hz, 2H), 2.35 (s, 3H), 2.30 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ: 168.4, 136.7, 136.3, 135.0, 130.2, 130.1, 129.9, 129.1, 128.9, 127.0, 126.4, 126.1, 126.0, 125.6, 37.2, 19.8, 19.4; LRMS (EI 70 ev): *m/z* (%): 222 (M⁺, 83), 104 (100), 115 (84), 130 (72).

(E)-3,3'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (8)

Colourless liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.21-7.16 (m, 4H), 7.05-7.01 (m, 4H), 6.42 (d, *J* = 15.8 Hz, 1H), 6.36-6.30 (m, 1H), 3.50 (dd, *J* = 3.9 Hz, 2H), 2.33 (s, 3H), 2.32 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ: 140.2, 138.1, 138.0, 137.5, 131.0, 129.5, 129.2, 128.4, 128.4, 127.9, 126.9, 126.9, 125.7, 123.3, 39.3, 21.4 (2C); LRMS (EI 70 ev): *m/z* (%): 222 (M⁺), 115 (100), 207 (94), 129 (76), 130 (48); HRMS *m/z* (ESI) calcd for C₁₇H₁₈ (M+H)⁺ 223.1482, found 223.1485.

(E)-4,4'-(prop-1-ene-1,3-diyl)dianiline (9)

Yellow solid; ¹H NMR (300 MHz, CDCl₃) δ: 7.17 (d, *J* = 9.0 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.66-6.20 (m, 4H), 6.32 (d, *J* = 15.0 Hz, 1H), 6.15-6.09 (m, 1H), 3.59 (s, 4H), 3.40 (d, *J* = 6.9 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 145.4, 144.5, 130.7, 130.2, 129.5, 128.5, 127.2, 126.4, 115.3, 115.2, 38.5; LRMS (EI 70 ev): *m/z* (%): 224 (M⁺, 100), 130 (84), 106 (57), 223 (43), 118 (30); HRMS *m/z* (ESI) calcd for C₁₅H₁₆N₂ (M+H)⁺ 225.1389, found 225.1386.

(E)-4-chloro-1-(3-(5-chloro-2-methoxyphenyl)allyl)-2-methoxybenzene (10)

Yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.37 (d, *J* = 2.4 Hz, 1H), 7.16-7.10 (m, 3H), 6.79-6.74 (m, 2H), 6.71 (d, *J* = 16.9 Hz, 1H), 6.35-6.26 (m, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.50 (d, *J* = 6.0 Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 155.9, 155.0, 130.5, 129.8, 129.6, 128.2, 127.5, 127.0,

126.3, 125.7, 125.4, 124.9, 112.0, 111.5, 55.8, 55.7, 33.7; LRMS (EI 70 ev): m/z (%): 324 ($M^+ + 2$, 30), 322 (M^+ , 45), 145 (100), 186 (67), 178 (47), 125 (35), 89 (30); HRMS m/z (ESI) calcd for 323.0594, found 323.0600

(E)-4,4'-(prop-1-ene-1,3-diyl)bis(acetophenone) (11)²

White solid; mp: 94-96 °C; ¹H NMR (300 MHz, CDCl₃) δ: 7.91 (d, $J = 8.4$ Hz, 2H), 7.43 (d, $J = 8.4$ Hz, 2H), 7.34 (d, $J = 8.4$ Hz, 2H), 6.49 (d, $J = 4.0$ Hz, 2H), 3.64 (d, $J = 2.4$ Hz, 2H), 2.60 (s, 3H), 2.59 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ: 197.8, 197.5, 145.2, 144.4, 141.8, 136.6, 135.9, 135.6, 131.2, 130.9, 129.0, 128.9, 128.8, 128.8, 127.5, 126.2, 39.3, 26.6, 26.5; LRMS (EI 70 ev): m/z (%): 278 (M^+ , 100), 263 (97), 235 (41), 124 (32), 207 (26).

(E)-3,3'-(prop-1-ene-1,3-diyl)bis((trifluoromethyl)benzene) (12)

Yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.60 (s, 1H), 7.54-7.41 (m, 7H), 6.53-6.36 (m, 2H), 3.60 (d, $J = 6.0$ Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 140.5, 137.9, 132.1, 130.6, 130.1, 129.3, 129.0, 125.4, 125.4, 123.9, 123.3, 123.3, 122.9, 122.8, 39.0; LRMS (EI 70 ev): m/z (%): 330 (M^+ , 92), 261 (100), 115 (50), 183 (34), 311 (18); HRMS m/z (ESI) calcd for C₁₇H₁₂F₆ ($M+H$)⁺ 331.0910, found 331.0916.

(E)-2,2'-(prop-1-ene-1,3-diyl)dithiophene (13)

Yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.25-7.11 (m, 2H), 6.96-6.91 (m, 3H), 6.86-6.85 (m, 1H), 6.61 (d, $J = 15.9$ Hz, 1H), 6.25-6.16 (m, 1H), 3.70 (d, $J = 6.9$ Hz, 2H); ¹³C NMR (75 MHz, CDCl₃) δ: 142.7, 142.3, 128.0, 127.3, 127.0, 125.1, 124.9, 124.6, 123.9, 123.8, 33.1; LRMS (EI 70 ev): m/z (%): 206 (M^+ , 100), 97 (34), 205 (32), 173 (26); HRMS m/z (ESI) calcd for ($M+H$)⁺ 207.0292, found 207.0297.

(E)-4-(4-methoxyphenyl)-2-methylbut-3-en-2-ol (15)⁴

Yellow liquid; ¹H NMR (300 MHz, CDCl₃) δ: 7.31 (d, $J = 8.7$ Hz, 2H), 6.85 (d, $J = 8.7$ Hz, 2H), 6.52 (d, $J = 16.1$ Hz, 1H), 6.22 (d, $J = 16.1$ Hz, 1H), 3.80 (s, 3H), 1.77 (s, 1H), 1.41 (s, 6H); ¹³C NMR (75 MHz, CDCl₃) δ: 159.1, 135.4, 129.7, 127.6, 125.8, 114.0, 71.0, 55.3, 31.6, 29.9 (2C); LRMS (EI 70 ev): m/z (%): 192 (M^+), 121 (100), 159 (76), 177 (60), 144 (56).

(Z)-4,4'-(3-phenylprop-1-ene-1,3-diyl)bis(methoxybenzene) (17)

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.33-7.21 (m, 7H), 7.15 (d, $J = 8.6$ Hz, 2H), 6.86-6.82 (m, 4H), 6.55-6.47 (m, 1H), 6.26 (d, $J = 15.6$ Hz, 1H), 4.82 (d, $J = 7.2$ Hz, 1H), 3.80 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ : 159.0, 158.1, 144.1, 135.9, 130.8, 130.6, 130.2, 129.6, 128.6, 128.4, 127.4, 126.6, 126.3, 113.9, 113.8, 55.3, 55.3, 53.4; LRMS (EI 70 ev): m/z (%): 330 (M^+ , 100), 222 (90), 299 (56), 121 (41), 221 (33); HRMS m/z (ESI) calcd for $\text{C}_{23}\text{H}_{22}\text{O}_2$ ($\text{M}+\text{H}$) $^+$ 331.1692, found 331.1693.

1,2-Dimethyl-1H-indole (18)⁵

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.51 (d, $J = 7.5$ Hz, 1H), 7.24 (d, $J = 8.6$ Hz, 1H), 7.17-7.03 (m, 2H), 6.24 (s, 1H), 3.64 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 136.0, 135.0, 129.0, 120.9, 119.6, 110.1, 100.4, 13.7; LRMS (EI 70 ev): m/z (%): 145 (M^+ , 20), 144 (100), 115 (11), 143 (10).

1-(2-Methyl-1H-indol-1-yl)ethanone (19)⁶

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.99 (d, $J = 8.1$ Hz, 1H), 7.47-7.44 (m, 1H), 7.26-7.22 (m, 2H), 6.38 (s, 1H), 2.73 (s, 3H), 2.64 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 170.3, 137.3, 136.5, 129.8, 123.5, 123.1, 119.8, 115.2, 109.7, 27.4, 17.6; LRMS (EI 70 ev): m/z (%): 173 (M^+ , 29), 131 (94), 130 (100), 77 (14).

2-Methyl-1H-indole (20)⁷

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.87 (brs, 1H), 7.51 (d, $J = 7.2$ Hz, 1H), 7.39-7.26 (m, 1H), 7.11-7.04 (m, 2H), 6.22 (s, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 136.0, 135.0, 129.0, 120.9, 119.6 (2C), 110.1, 100.4, 13.7; LRMS (EI 70 ev): m/z (%): 131 (M^+ , 72), 130 (100), 77 (12), 65 (12).

1,2,5-Trimethyl-1H-indole (21)

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.29 (s, 1H), 7.12 (d, $J = 8.3$ Hz, 1H), 6.96-6.94 (m, 1H), 6.14 (s, 1H), 3.61 (s, 3H), 2.42 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 136.8, 135.7, 128.3, 128.1, 121.9, 119.4, 108.3, 99.0, 29.4, 21.4, 12.7; LRMS (EI 70 ev): m/z (%): 159 (M^+ , 100), 158 (98), 144 (29), 115 (15); HRMS m/z (ESI) calcd for $\text{C}_{11}\text{H}_{13}\text{N}$ ($\text{M}+\text{H}$) $^+$ 160.1118, found 160.1121.

1,2-Dimethyl-5-(trifluoromethyl)-1H-indole (22)

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.79 (s, 1H), 7.37-7.34 (m, 1H), 7.28-7.24 (m, 1H), 6.31 (s, 1H), 3.66 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 138.8, 138.6, 127.3, 126.7, 124.5, 121.7, 121.4, 117.3, 117.2 (2C), 108.8, 100.6, 29.6, 12.8; LRMS (EI 70 ev): m/z (%): 213 (M^+ , 92), 122 (100), 143 (10), 106 (9). HRMS m/z (ESI) calcd for $\text{C}_{11}\text{H}_{10}\text{F}_3\text{N}$ ($\text{M}+\text{H}$) $^+$ 214.0833, found 214.0838.

1,2,2-Trimethyl-1,2-dihydroquinoline (23)⁸

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.24-7.18 (m, 2H), 6.74-6.60 (m, 3H), 6.20 (d, J = 15.9 Hz, 1H), 2.85 (s, 3H), 1.45 (s, 6H); ^{13}C NMR (75 MHz, CDCl_3) δ : 146.4, 140.0, 128.7, 127.3, 123.3, 121.8, 117.2, 110.1, 71.3, 30.8, 30.1; LRMS (EI 70 ev): m/z (%): 173 (M^+ , 98), 158 (100), 143 (88), 130 (47).

1,2,3-trimethyl-1H-indole (24)⁹

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.48 (d, J = 7.5 Hz, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.17-7.05 (m, 2H), 3.65 (s, 3H), 2.35 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 140.2, 136.4, 132.6, 128.3, 120.4, 118.5, 117.9, 108.6, 29.5, 10.1, 8.8; LRMS (EI 70 ev): m/z (%): 159 (M^+ , 87), 158 (100), 144 (63), 143 (21).

2-Ethyl-1-methyl-1H-indole (25)¹⁰

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.54 (d, J = 7.7 Hz, 1H), 7.27 (d, J = 10.1 Hz, 1H), 7.18-7.04 (m, 3H), 6.26 (s, 1H), 3.71 (s, 3H), 2.78-2.73 (m, 2H), 1.36 (t, J = 10.1 Hz, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 15142.9, 137.4, 127.5, 120.5, 119.7, 118.0, 108.6, 97.8, 29.3, 20.1, 12.7; LRMS (EI 70 ev): m/z (%): 159 (M^+ , 47), 144 (100), 143 (13).

2-Methylbenzofuran (26)¹¹

Colourless liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.48-7.45 (m, 1H), 7.41-7.38 (m, 1H), 7.20-7.14 (m, 2H), 6.36 (s, 1H), 2.45 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ : 155.4, 154.8, 129.2, 123.0, 122.4, 120.1, 110.6, 102.6, 14.1; LRMS (EI 70 ev): m/z (%): 132 (M^+ , 5), 131 (100), 77 (16), 103 (14).

(E)-N-Methyl-N-(2-(prop-1-enyl)phenyl)acetamide (27)

Yellow liquid; ^1H NMR (500 MHz, CDCl_3) δ : 7.49 (d, $J = 9.0$ Hz, 1H), 7.22 (t, $J = 8.5$ Hz, 1H), 7.17 (t, $J = 7.5$ Hz, 1H), 7.04 (t, $J = 9.0$ Hz, 1H), 3.12 (s, 3H), 1.83 (t, $J = 5.5$ Hz, 3H), 1.70 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 171.0, 141.2, 135.4, 129.4, 128.4, 128.1, 128.0, 126.4, 125.3, 36.4, 22.2, 18.9; LRMS (EI 70 eV): m/z (%): 189 (M^+ , 25), 146 (100). HRMS (ESI) for $\text{C}_{12}\text{H}_{16}\text{O}_3$ ($\text{M}+\text{H}$) $^+$: calcd. 190.1232, found 190.1235.

(E)-3-(2-(Hydroxymethyl)phenyl)allyl acetate (28)

Yellow liquid; ^1H NMR (300 MHz, CDCl_3) δ : 7.45-7.42 (m, 1H), 7.30-7.28 (m, 1H), 7.23-7.19 (m, 2H), 6.93 (d, $J = 9.3$ Hz, 1H), 6.17, 6.14 (tt, $J = 3.6$ Hz, 3.9 Hz, 1H), 4.69-4.67 (m, 4H), 2.04 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ : 170.9, 137.7, 135.3, 130.1, 128.5, 128.3, 128.2, 126.4, 125.8, 65.2, 63.4, 21.0; MS (EI, 70 eV) m/z (%): 206 (M^+ , 1), 117 (100), 115 (82), 131 (68), 128 (63), 146 (62); HRMS (ESI) for $\text{C}_{12}\text{H}_{14}\text{O}_3$ ($\text{M}+\text{H}$) $^+$: calcd.207.1018, found 207.1015.

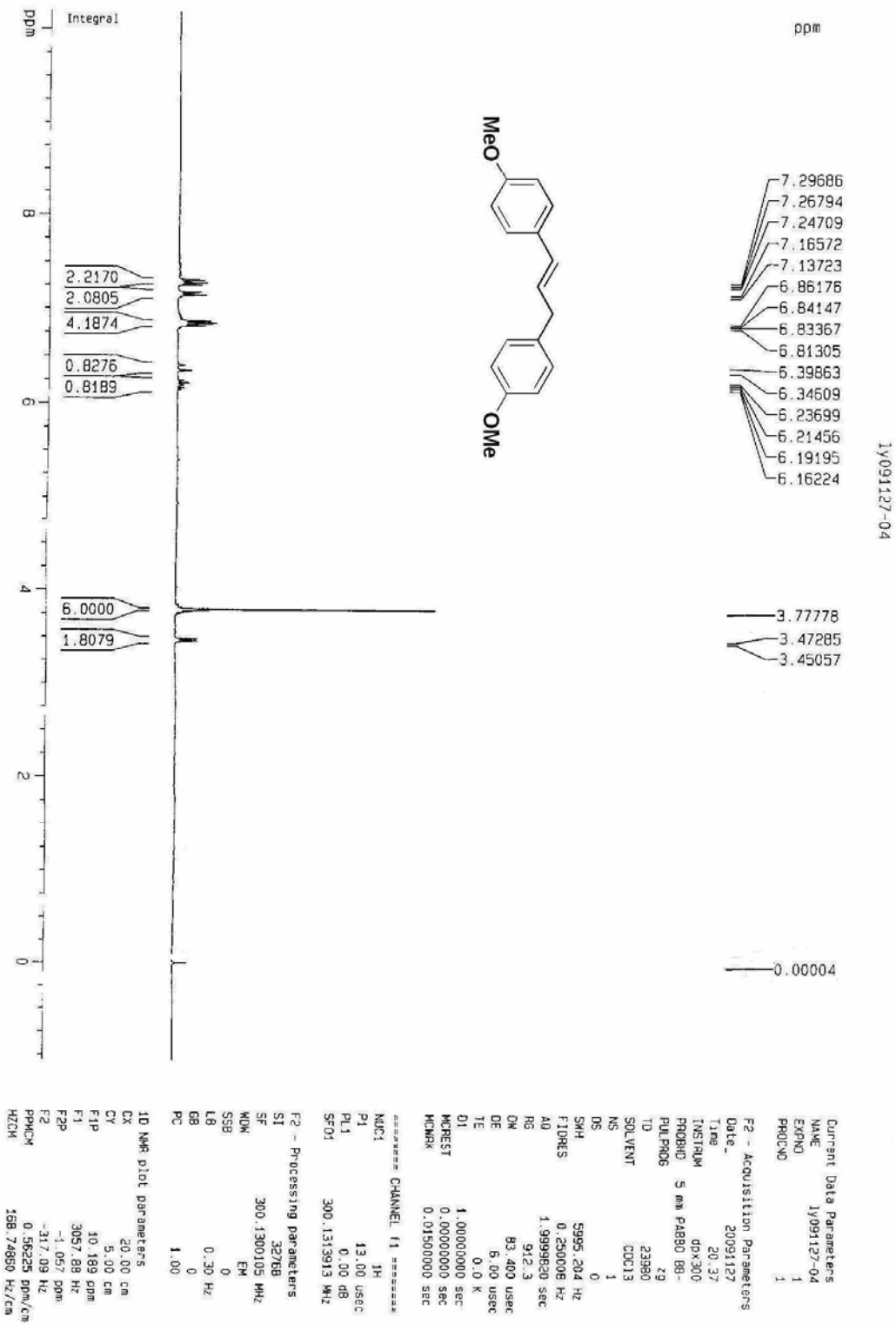
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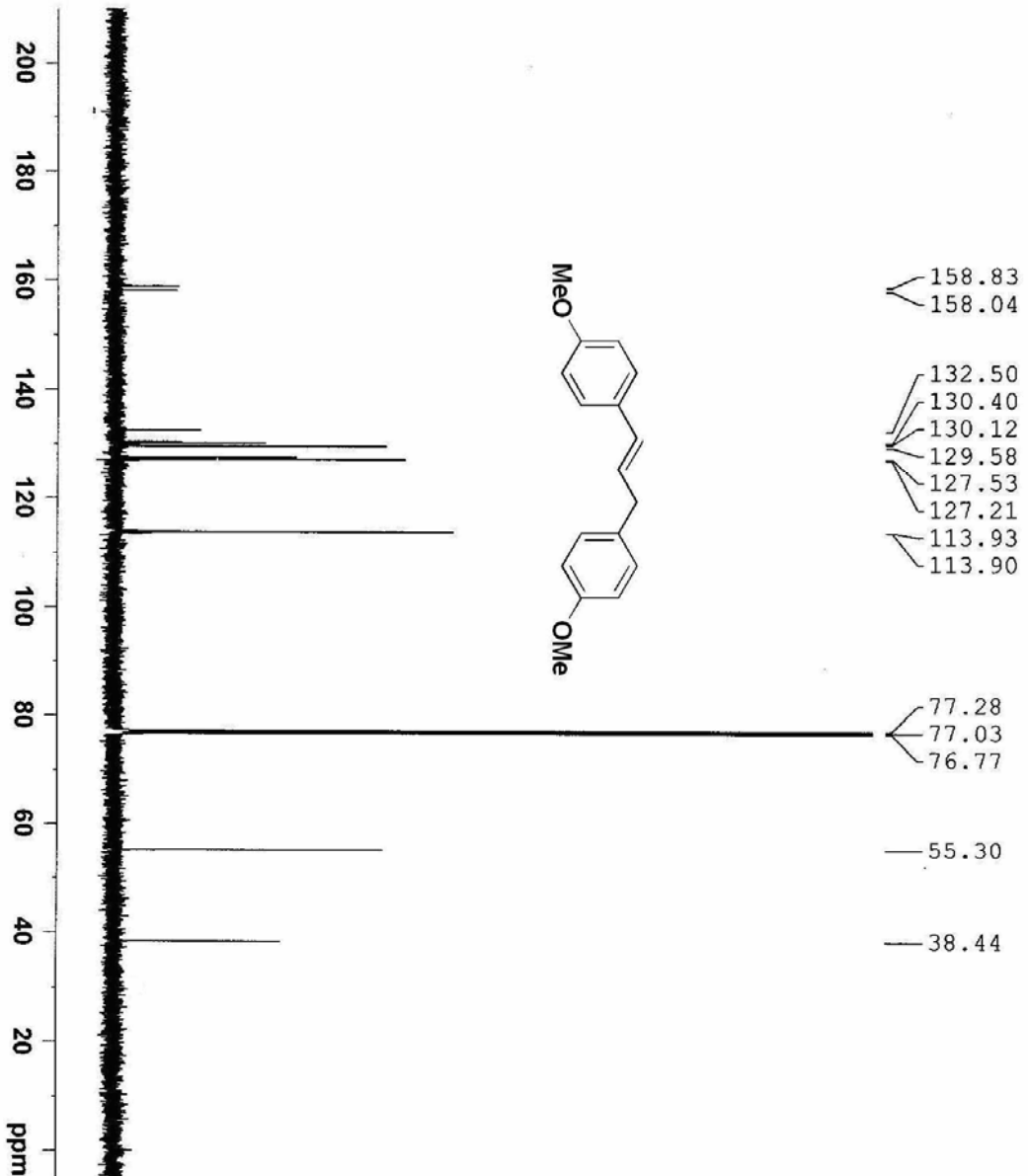
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(C) Spectra

(E)-4,4'-(Prop-1-ene-1,3-diyl)bis(methoxybenzene) (3)



(E)-4,4'-(Prop-1-ene-1,3-diyl)bis(methoxybenzene) (3)



1y091105-01

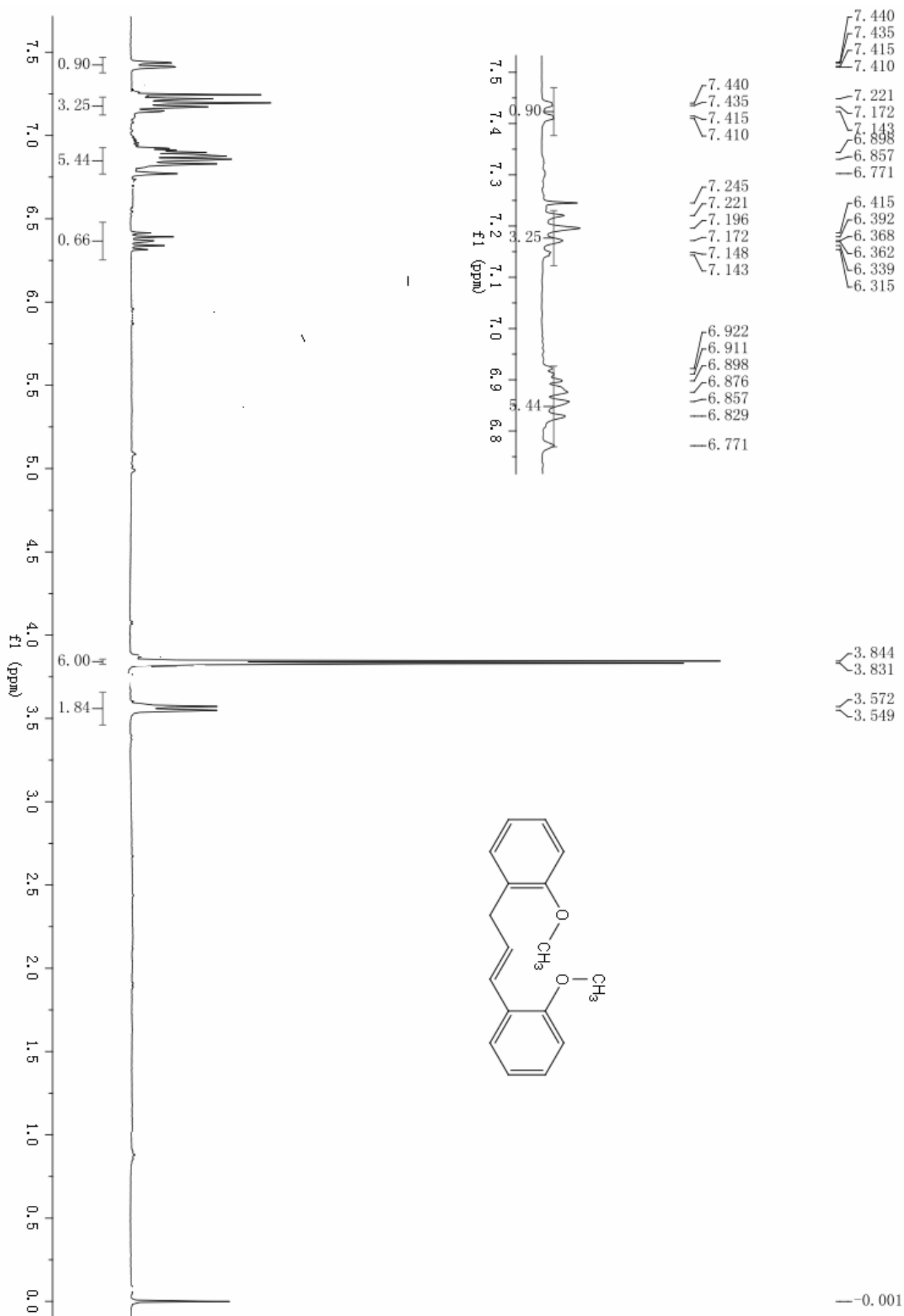
```

NAME 1y091105-01
EXPNO 2
PROCNO 1
Date_ 20091105
Time 16.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 233
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DE 16.800 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

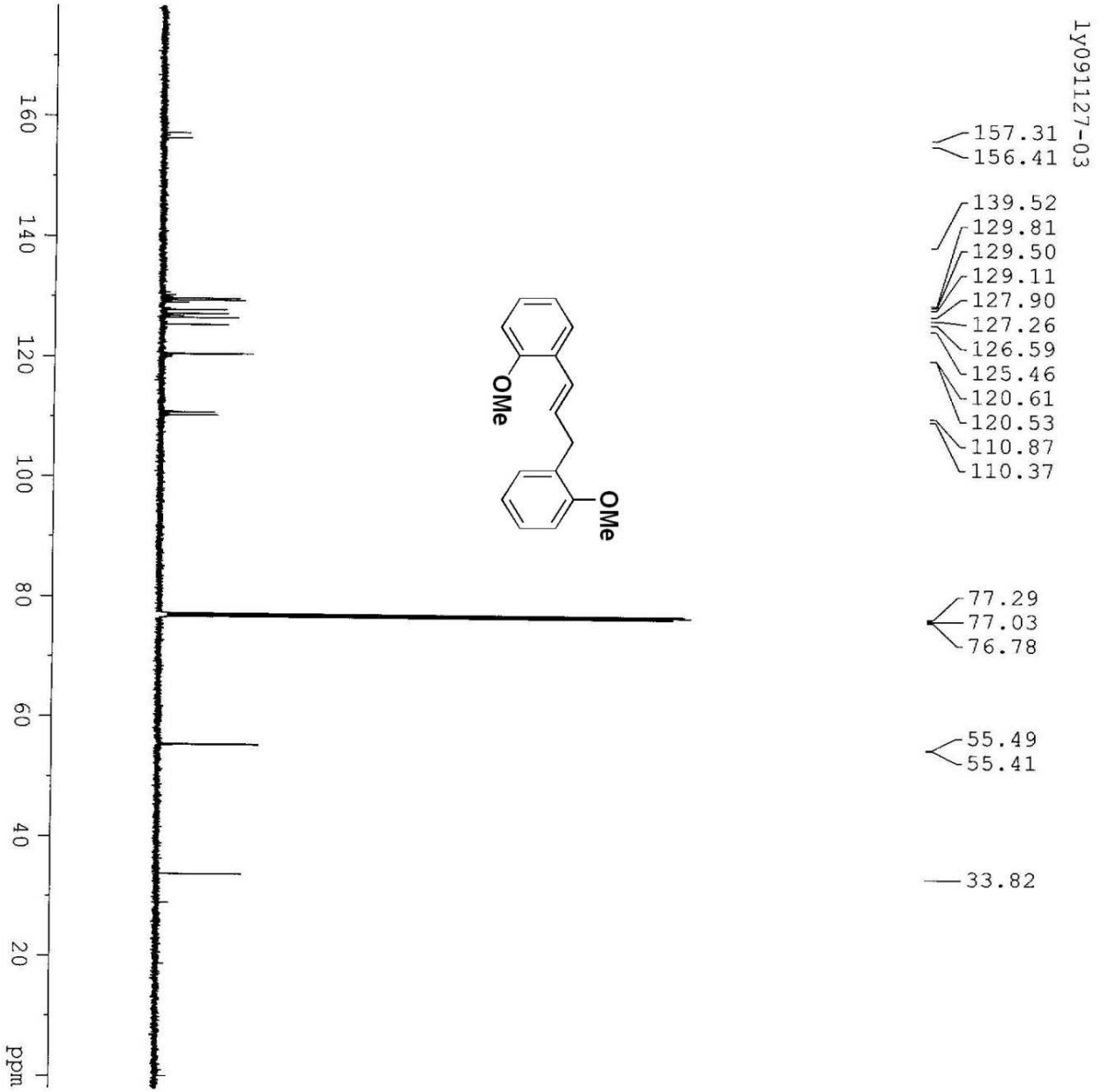
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL1W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SF02 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
GB 0
PC 1.40
    
```

(E)-2,2'-(prop-1-ene-1,3-diyl)bis(methoxybenzene) (4)



(E)-2,2'-(prop-1-ene-1,3-diyl)bis(methoxybenzene) (4)



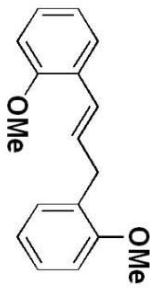
1y091127-03

157.31
156.41
139.52
129.81
129.50
129.11
127.90
127.26
126.59
125.46
120.61
120.53
110.87
110.37

77.29
77.03
76.78

55.49
55.41

33.82



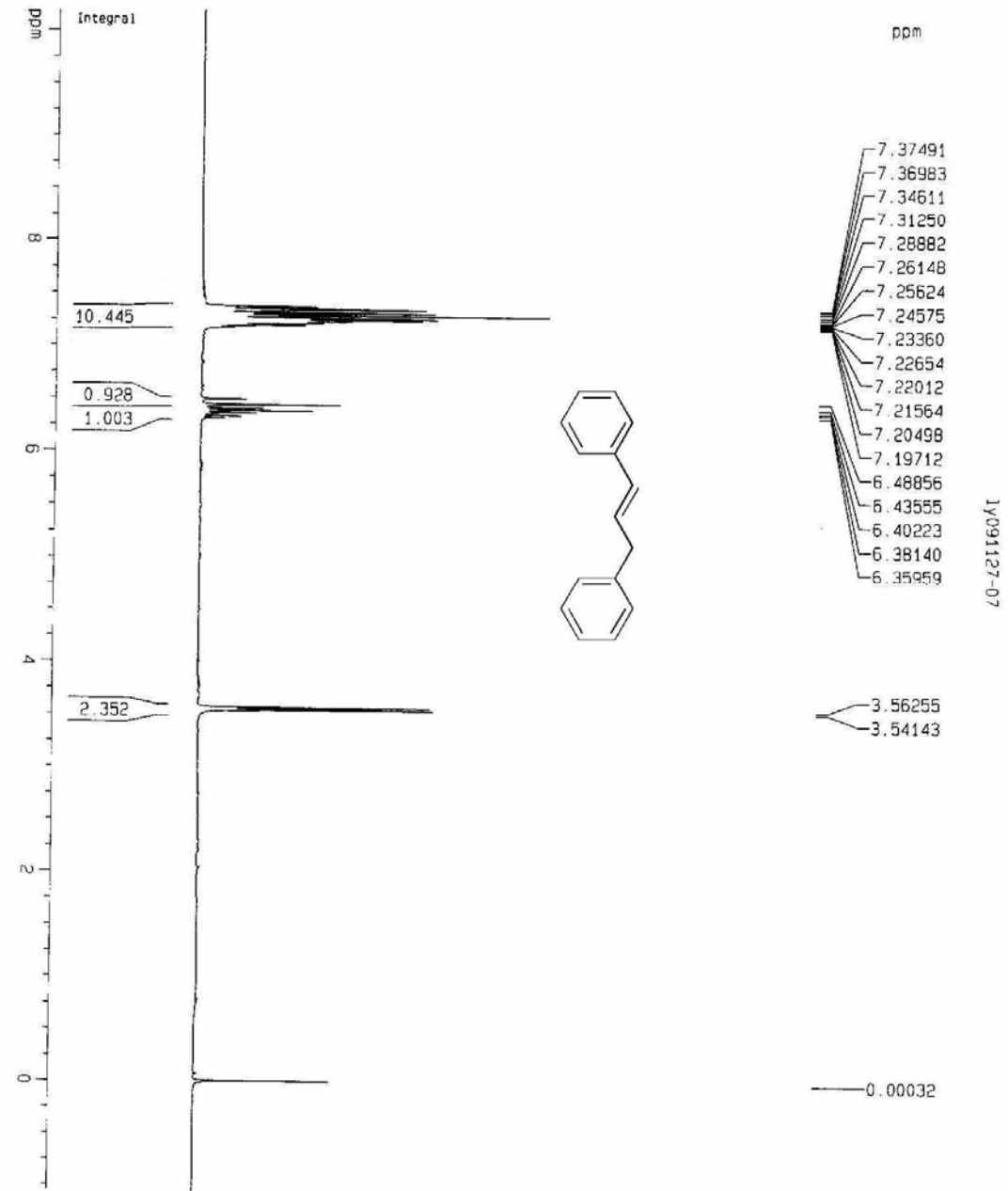
```

NAME          1y091127-03
EXPNO         2
PROCNO        1
Date_         20091130
Time_         10.16
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            256
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            203
DE            16.800 usec
DW            6.50 usec
TE            300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
PL1           0.00 dB
PL1W          90.67910004 W
SFO1          125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           1.90 dB
PL12         16.86 dB
PL13         16.86 dB
PL2W         14.92065334 W
PL12W        0.47619823 W
PL13W        0.47619823 W
SFO2         500.1320005 MHz
SI           32768
SE           125.7577890 MHz
MDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

(E)-prop-1-ene-1,3-diylidibenzene (5)



Current Data Parameters
 NAME 1Y091127-07
 EXPNO 1
 PROCNO 1

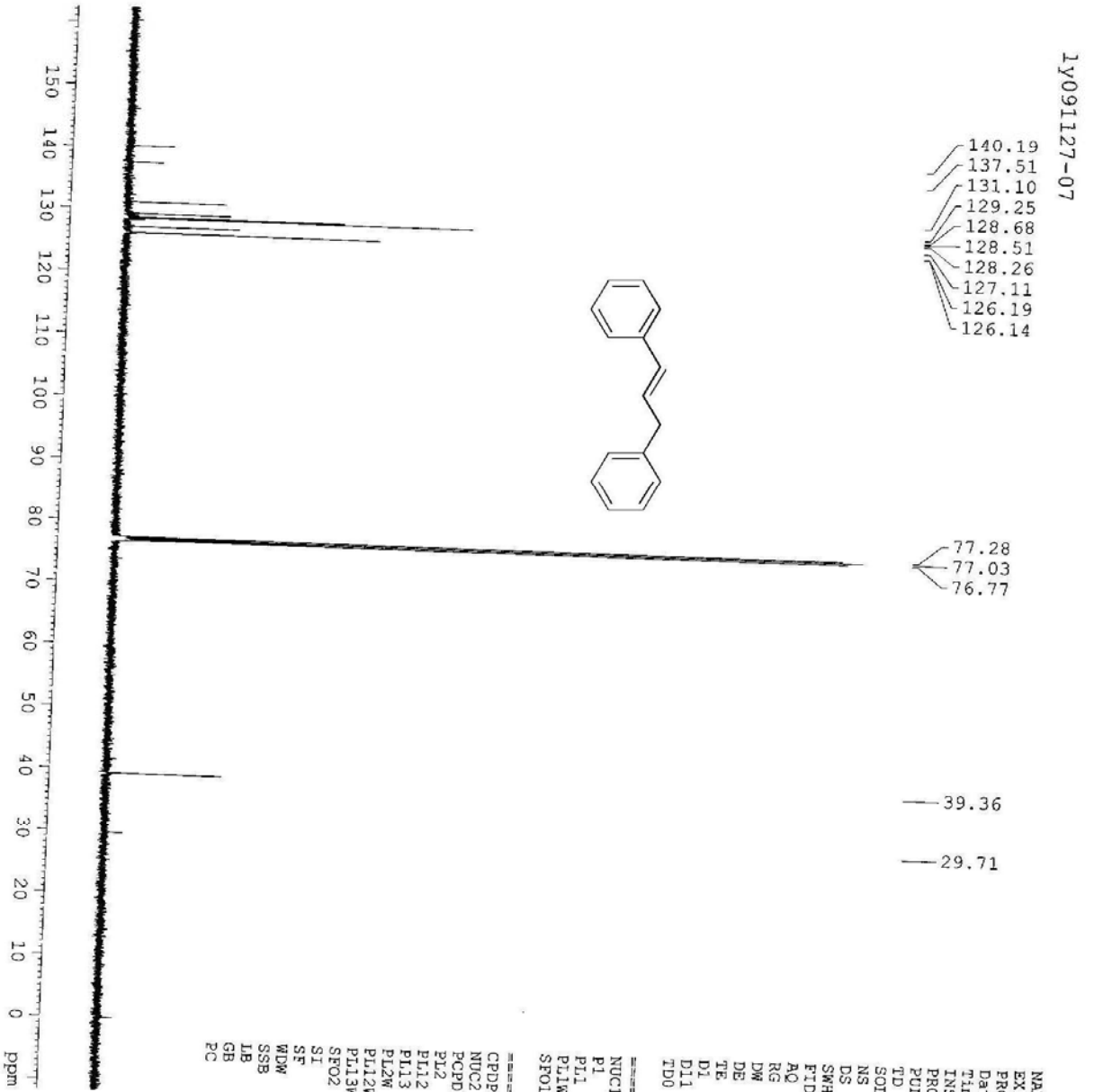
F2 - Acquisition Parameters
 Date_ 20091127
 Time 21.12
 INSTRUM gp-300
 PROBNM 5 mm PABBO BB-
 PULPROG zg
 TD 23980
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5985.204 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 RG 912.3
 DM 83.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCOREST 0.00000000 sec
 MCORR 0.01500000 sec

***** CHANNEL f1 *****
 NUCl 1H
 P1 13.00 usec
 PL1 0.00 dB
 SF01 300.1313913 MHz

F2 - Processing parameters
 S1 32759
 SF 300.1300109 MHz
 KHZW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

10 NMR plot parameters
 CX 20.00 cm
 CY 4.00 cm
 F1P 10.189 ppm
 F1 3057.88 Hz
 F2P -1.057 ppm
 F2 -317.09 Hz
 PPM1M 0.56229 ppm/cm
 HZCM 168.74850 Hz/cm

(E)-prop-1-ene-1,3-diylidibenzene (5)



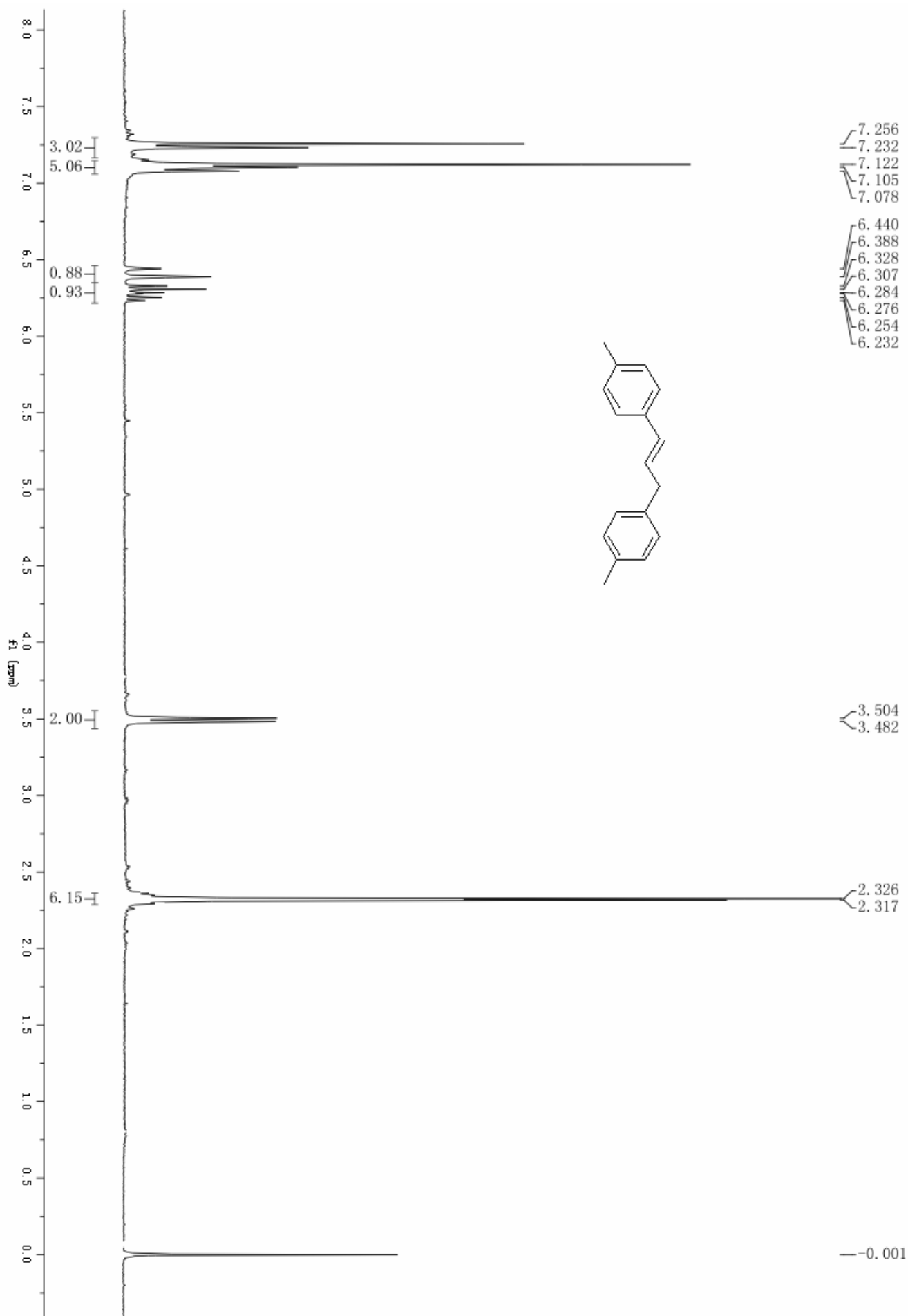
```

NAME 1y091127-07
EXPNO 2
PROCNO 1
Date_ 20091130
Time_ 11.09
INSTRUM 5 mm PABBO BB-
PROBHD spect
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

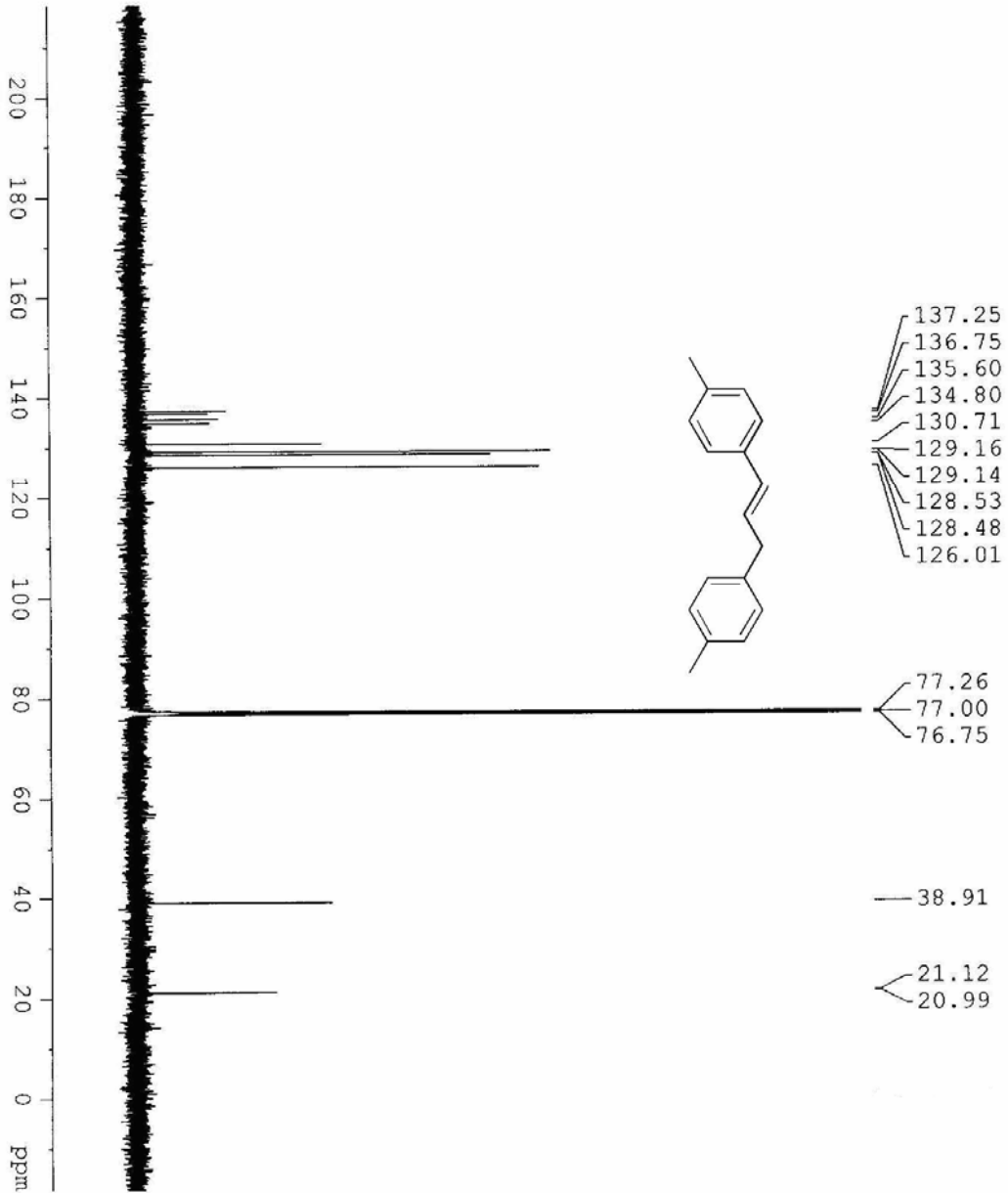
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL1W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

(E)-4,4'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (6)



(E)-4,4'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (6)

1Y09112702



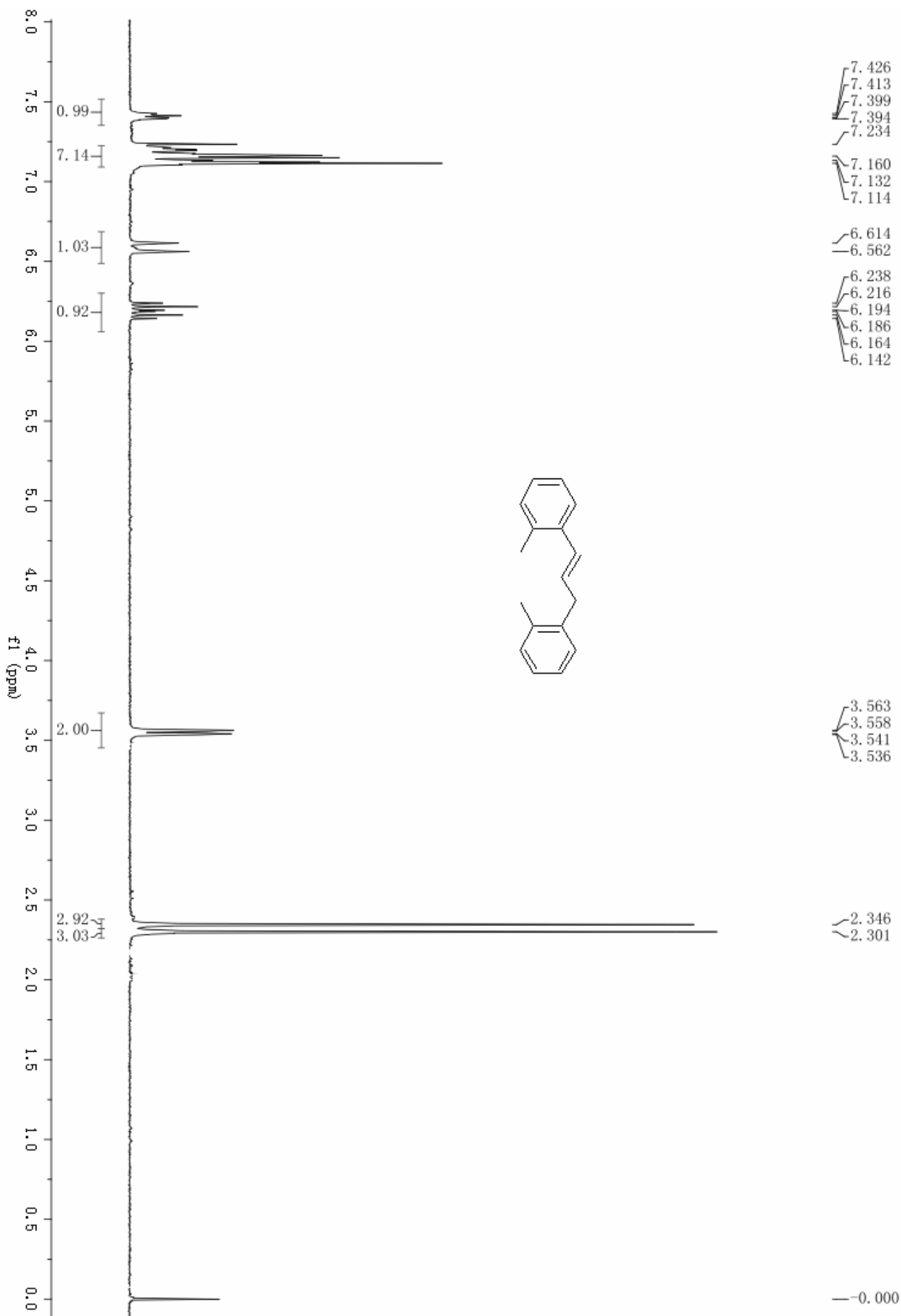
```

NAME 1Y09112702
EXPNO 2
PROCNO 1
Date_ 20091208
Time 1.58
INSTRUM spect
PROBHD 5 mm PABBO Bb-
PULPROG zgpg30
TD 65536
F2 1024
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DM 16.800 usec
DE 5.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.6791004 W
SFO1 125.7703643 KHz

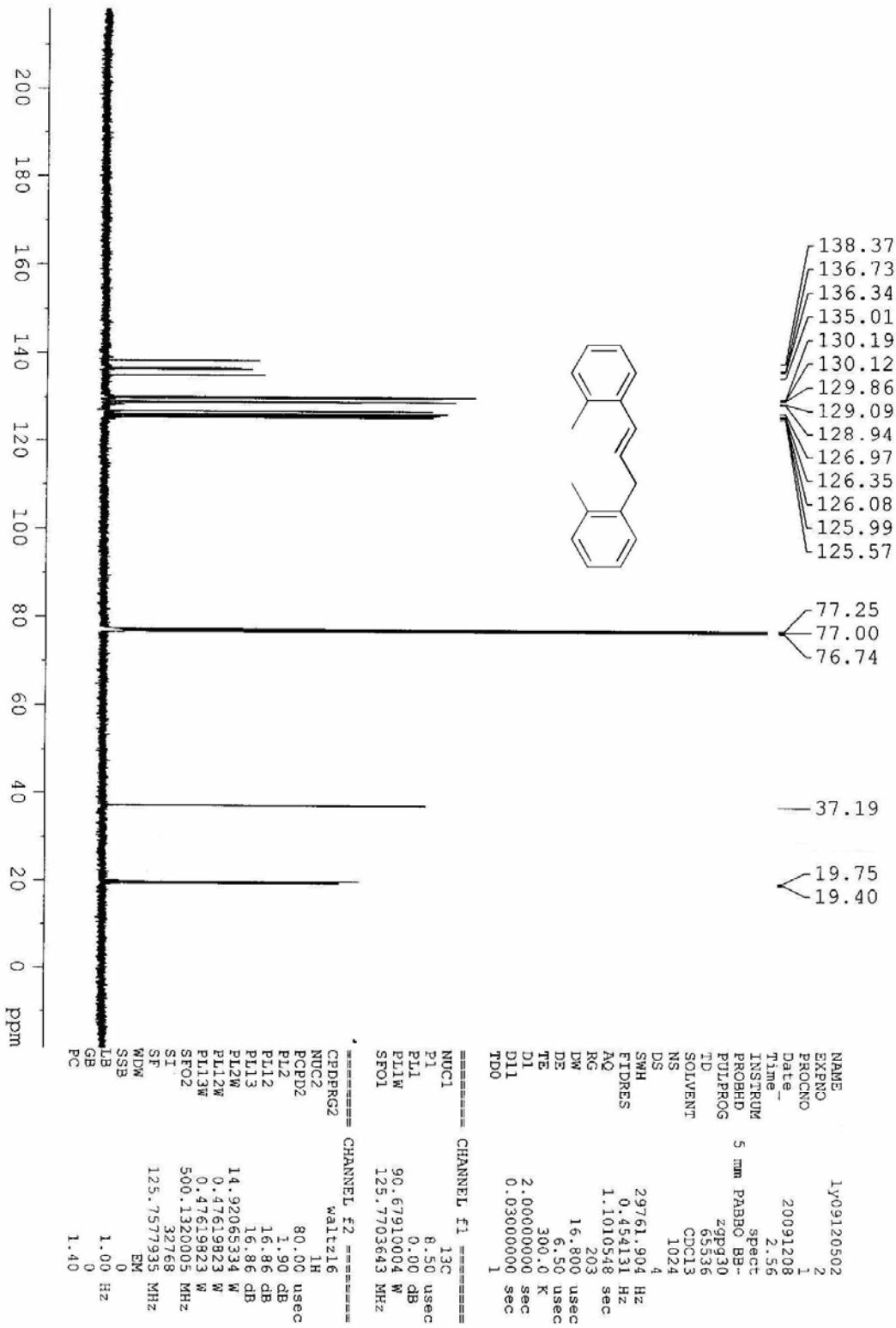
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL12W 14.92065334 W
PL13W 0.47619823 W
SFO2 500.1320005 KHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

(E)-2,2'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (7)



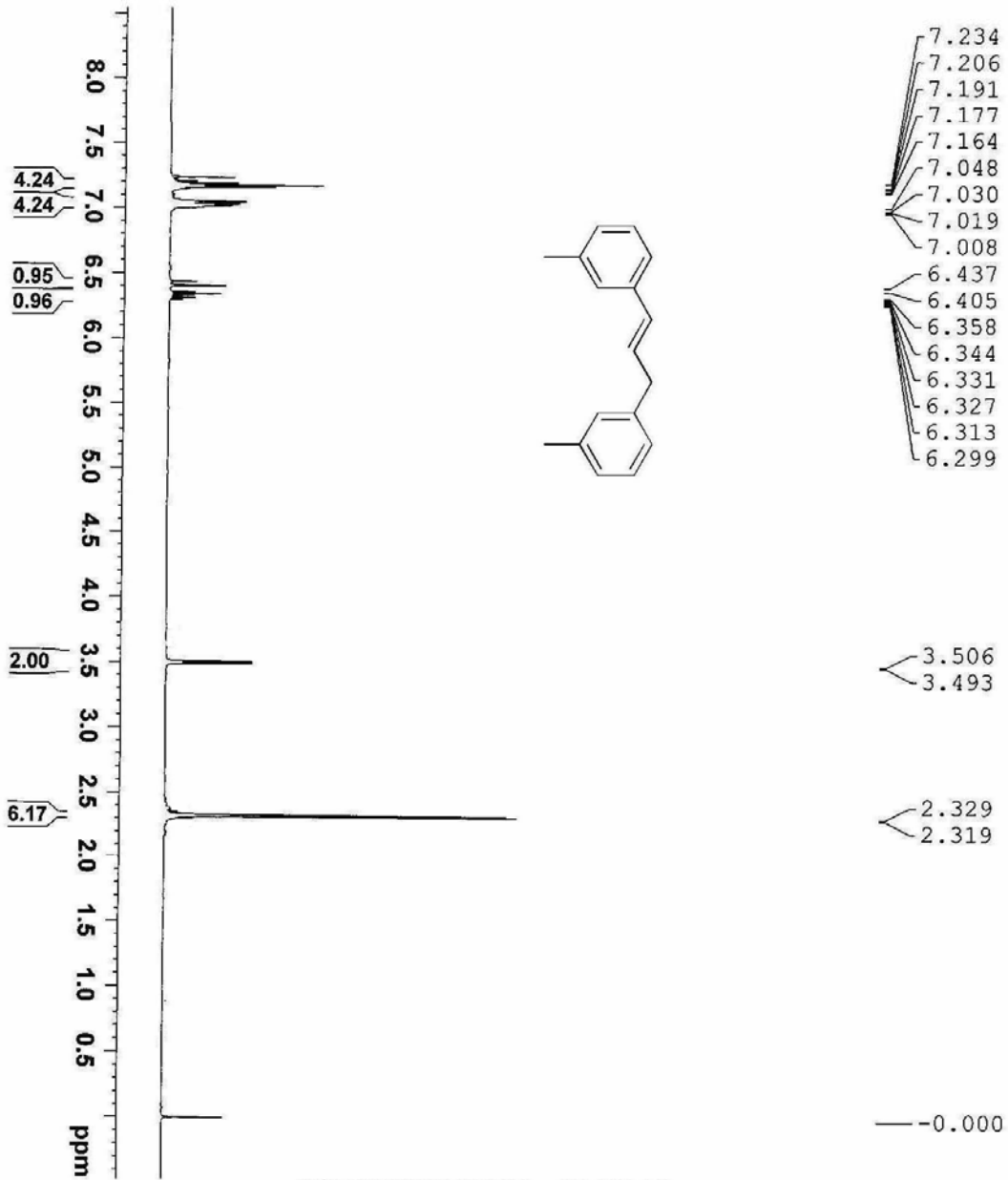
(E)-2,2'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (7)

1y09120502



(E)-3,3'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (8)

1y10060402

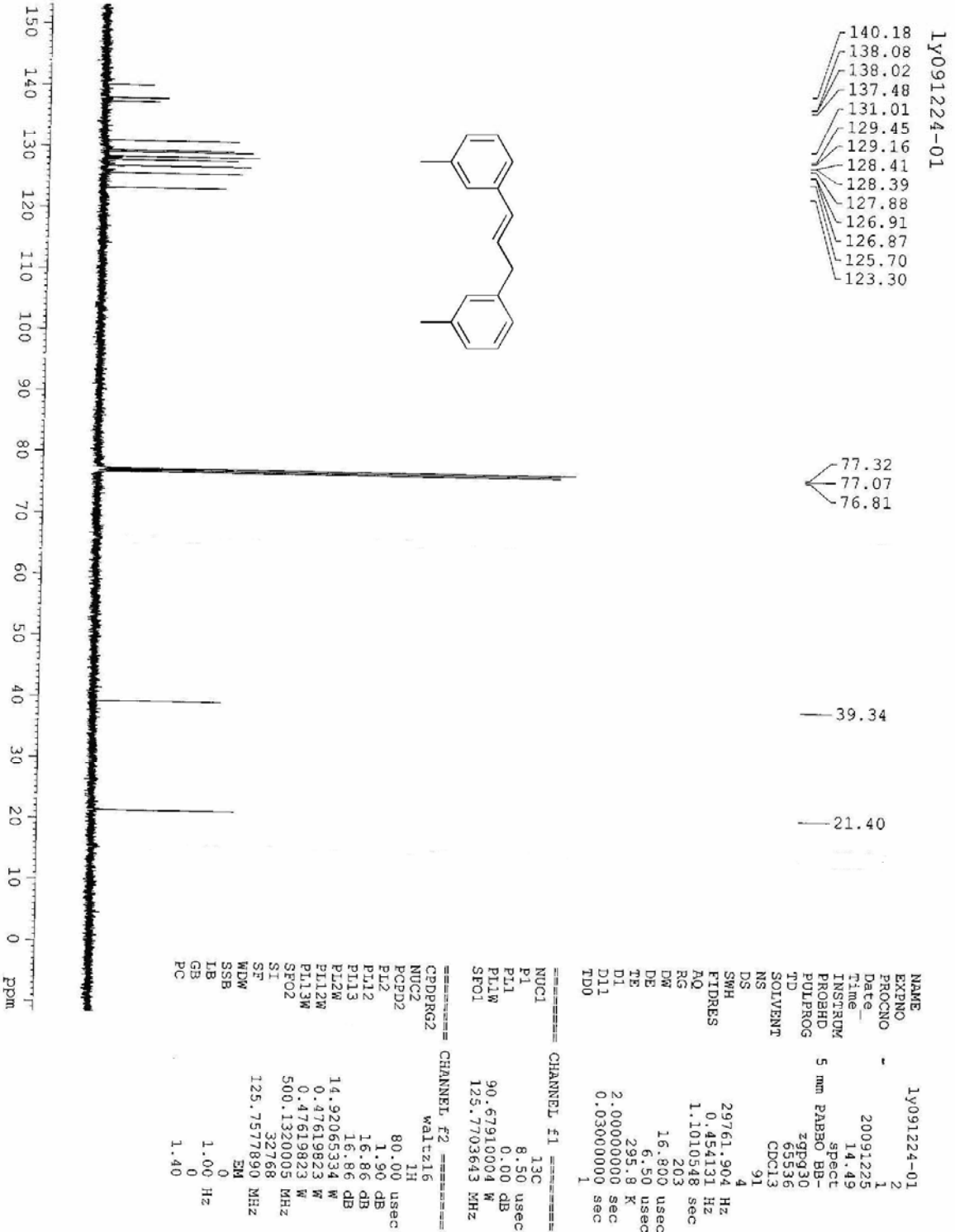


```

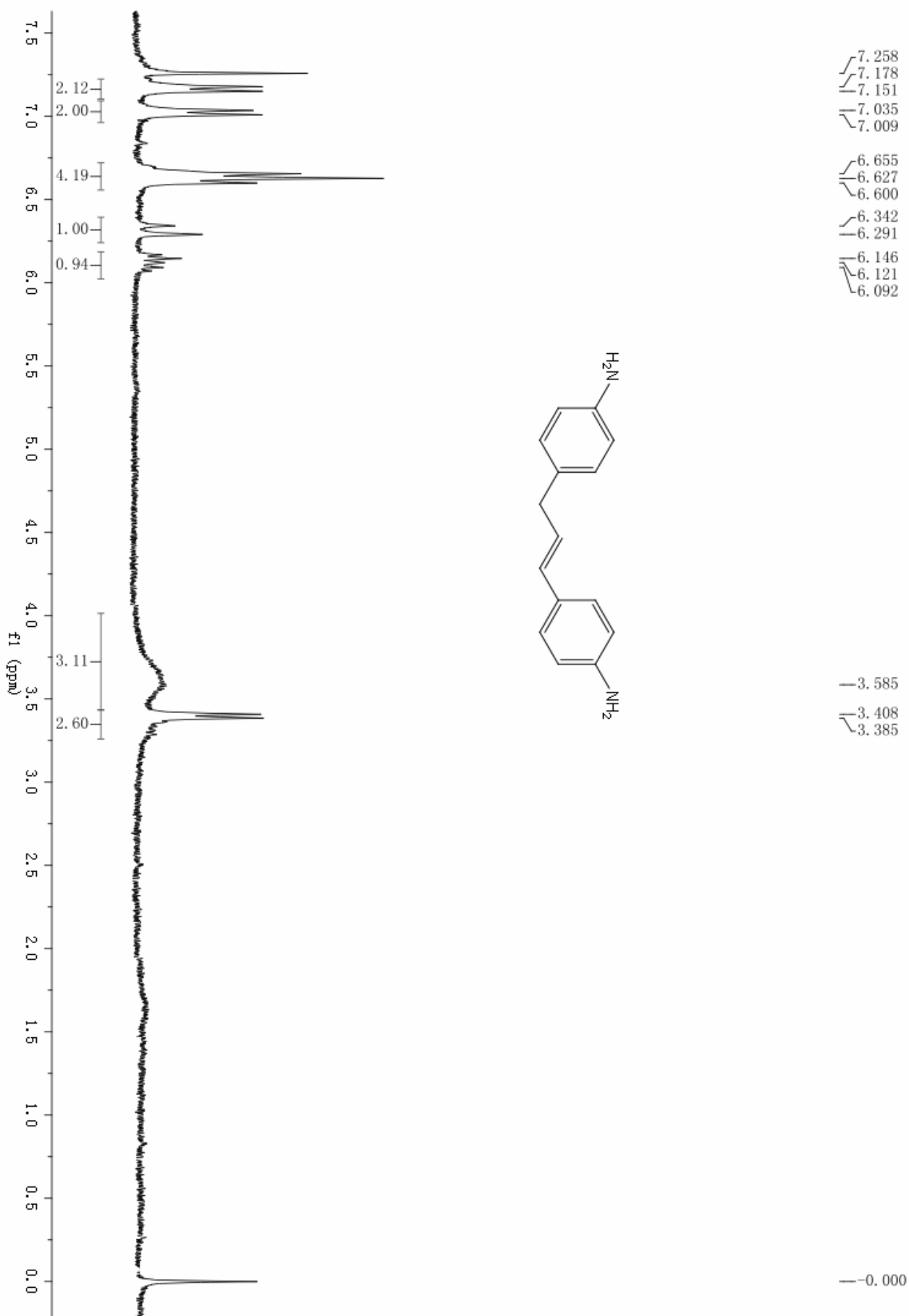
NAME          1y10060402
EXPNO         1
PROCNO        1
Date_         20100605
Time         6.38
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      CDCl3
NS           16
DS           2
SWH          10330.578 Hz
FIDRES       0.157632 Hz
AQ           3.1719923 sec
RG           161
DE           48.400 usec
TE           298.7 K
D1           1.00000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          1H
P1           14.00 usec
PL1          1.90 dB
PL1W         14.92065334 W
SFO1         500.1330885 MHz
SI           32768
SF           500.1300260 MHz
WDW          EM
SSB          0
IB           0.30 Hz
GB           0
PC           1.00
    
```

(E)-3,3'-(prop-1-ene-1,3-diyl)bis(methylbenzene) (8)

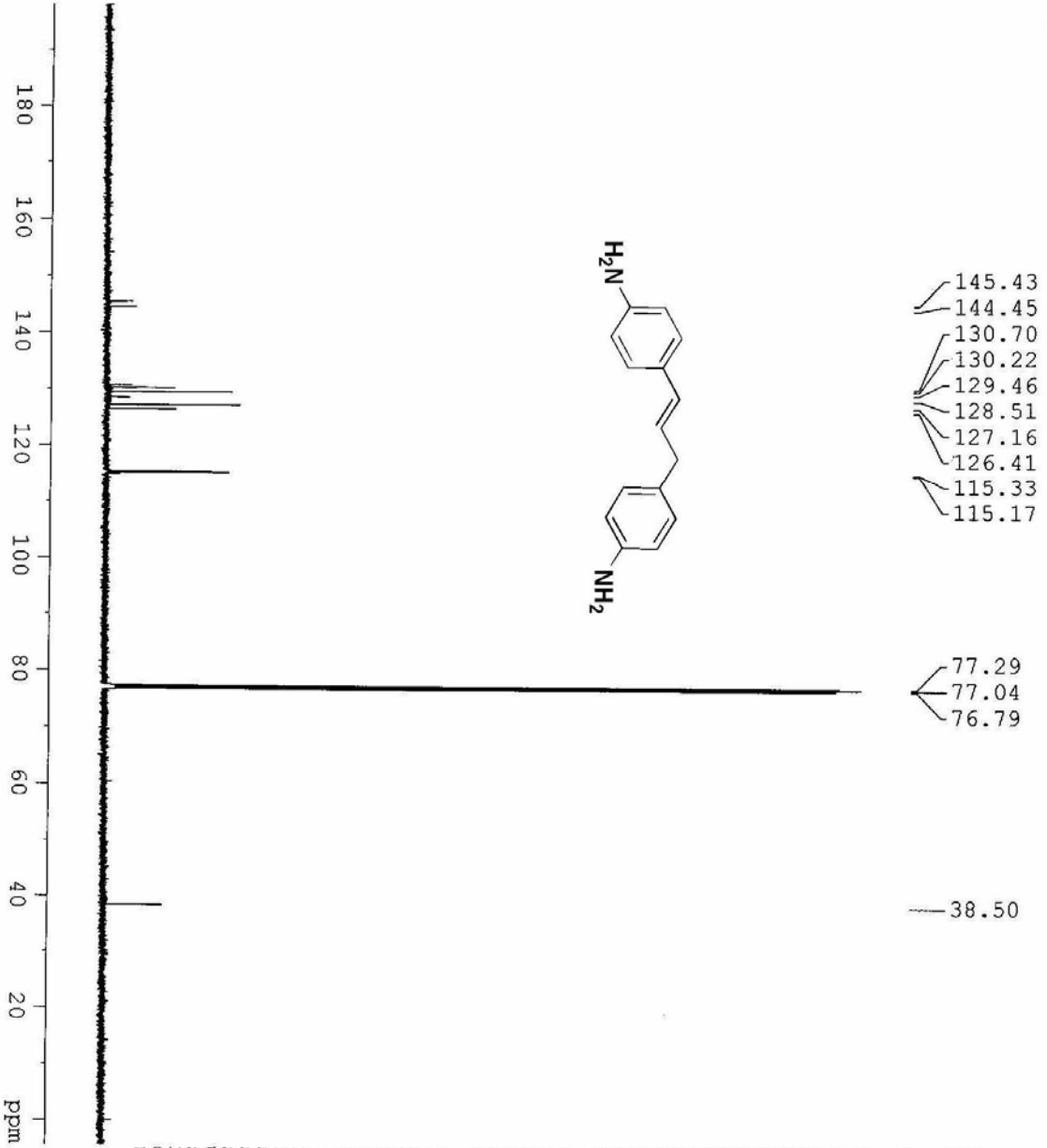


(E)-4,4'-(prop-1-ene-1,3-diyl)dianiline (9)



(E)-4,4'-(prop-1-ene-1,3-diyl)dianiline (9)

1y100409-02

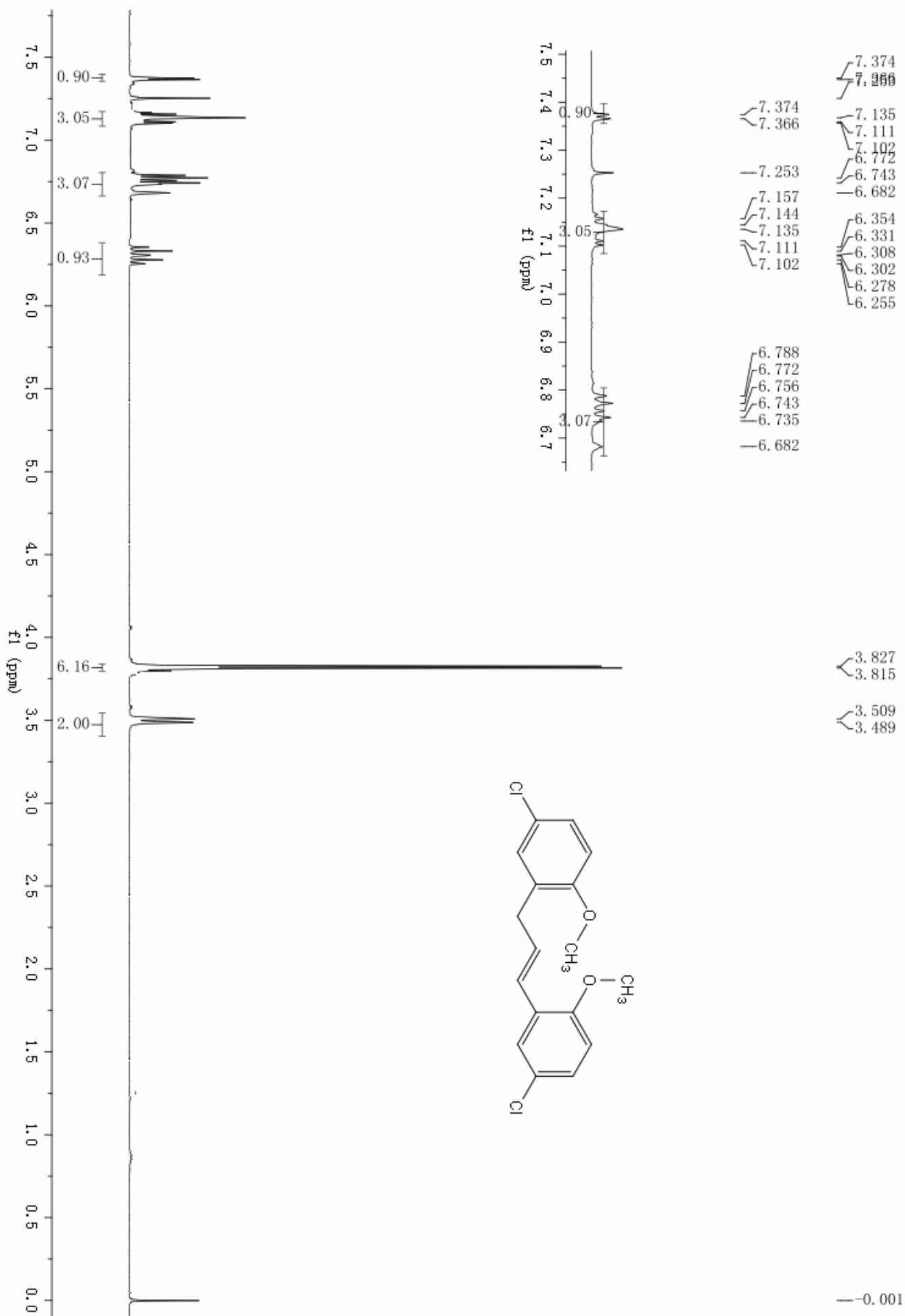


| | |
|---------|----------------|
| NAME | 1y100409-02 |
| EXPNO | 2 |
| PROCNO | 1 |
| Date_ | 20100413 |
| Time | 11.10 |
| INSTRUM | 5 mm PABBO BB- |
| PROBHD | spect |
| PULPROG | zgpg30 |
| TD | 65536 |
| SOLVENT | CDCl3 |
| NS | 512 |
| DS | 4 |
| SWH | 29761.904 Hz |
| FIDRES | 0.454131 Hz |
| AQ | 1.1010548 sec |
| RG | 203 |
| DW | 16.800 usec |
| DE | 6.50 usec |
| TE | 295.8 K |
| D1 | 2.00000000 sec |
| D11 | 0.03000000 sec |
| TD0 | 1 |

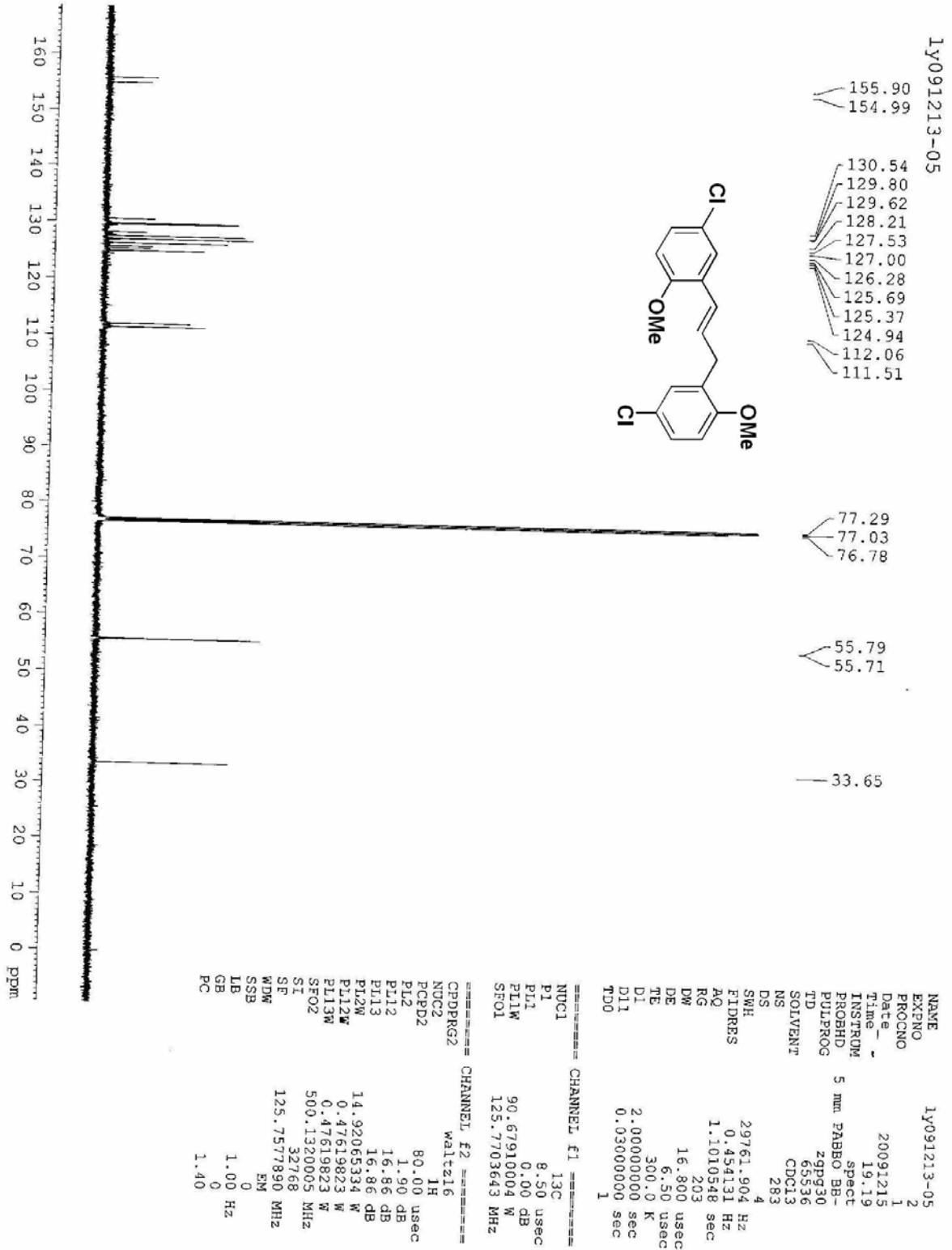
| | |
|------------------------|-----------------|
| ===== CHANNEL F1 ===== | |
| NUC1 | 13C |
| P1 | 8.50 usec |
| PL1 | 0.00 dB |
| PL1W | 90.57910004 W |
| SFO1 | 125.7703643 MHz |

| | |
|------------------------|-----------------|
| ===== CHANNEL F2 ===== | |
| CPDPRG2 | waltz16 |
| NUC2 | 1H |
| PCPD2 | 80.00 usec |
| PL2 | 1.90 dB |
| PL12 | 16.86 dB |
| PL13 | 16.86 dB |
| PL2W | 14.92065334 W |
| PL12W | 0.47619823 W |
| PL13W | 0.47619823 W |
| SFO2 | 500.1320005 MHz |
| SI | 32768 |
| SF | 125.7577890 MHz |
| WDM | EM |
| SSB | 0 |
| LB | 1.00 Hz |
| GB | 0 |
| PC | 1.40 |

(E)-4-chloro-1-(3-(5-chloro-2-methoxyphenyl)allyl)-2-methoxybenzene (10)



(E)-4-chloro-1-(3-(5-chloro-2-methoxyphenyl)allyl)-2-methoxybenzene (10)



(E)-4,4'-(prop-1-ene-1,3-diyl)bis(acetophenone) (11)



1y091127-01

Current Data Parameters
NAME 1y091127-01
EXPNO 1
PROCNO 1

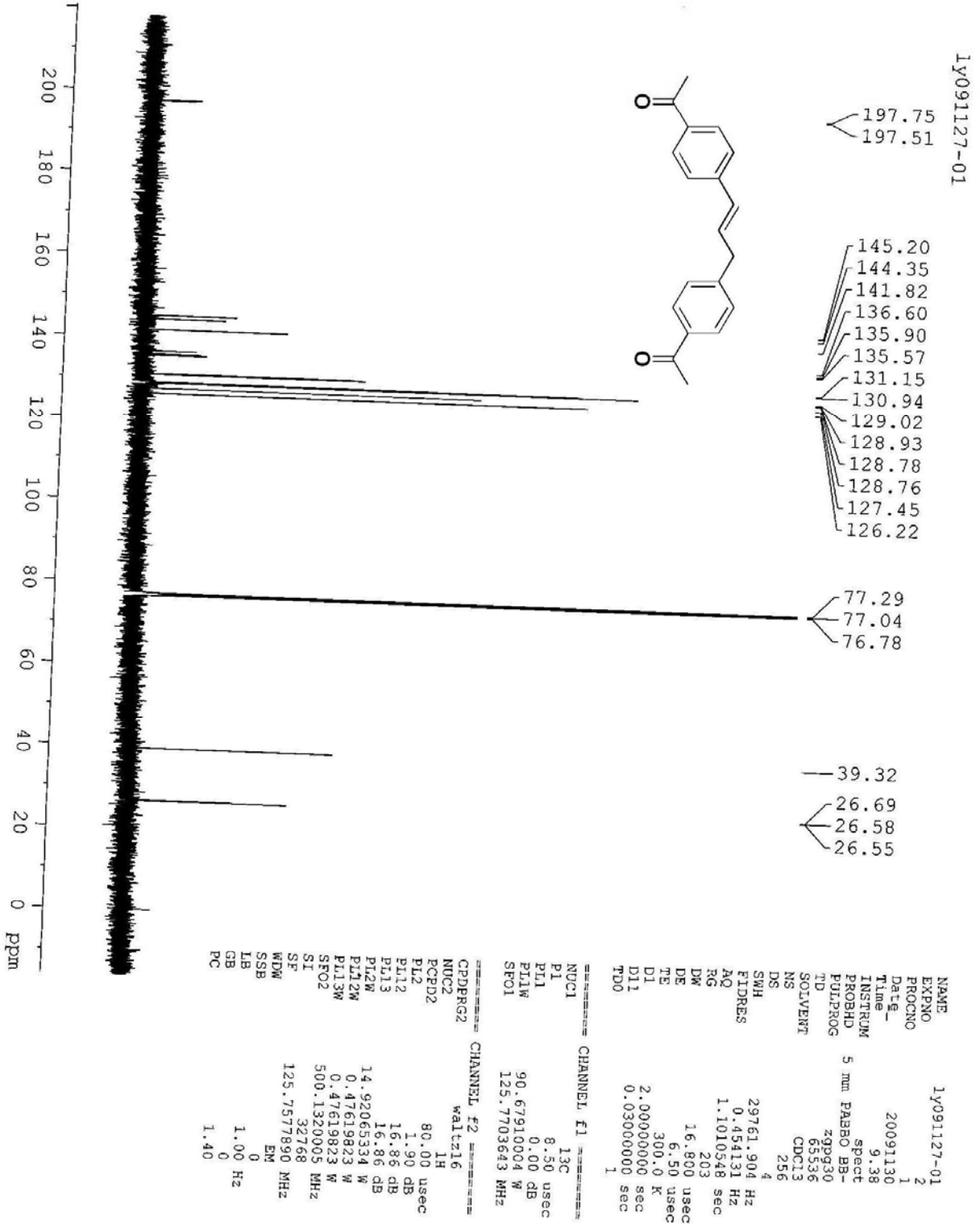
F2 - Acquisition Parameters
Date_ 20091127
Time 20.00
INSTRUM dpX300
PROBHD 5 mm PA880 B8-
PULPROG zg
TD 23880
SOLVENT CDCl3
NS 2
DS 0
SWH 5996.204 Hz
FIDRES 0.250008 Hz
AQ 1.9998820 sec
RG 912.3
DM 83.400 usec
DE 6.00 usec
TE 0.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCMRK 0.01500000 sec

***** CHANNEL f1 *****
NUC1 1H
P1 13.00 usec
PL1 0.00 dB
SFO1 300.1313913 MHz

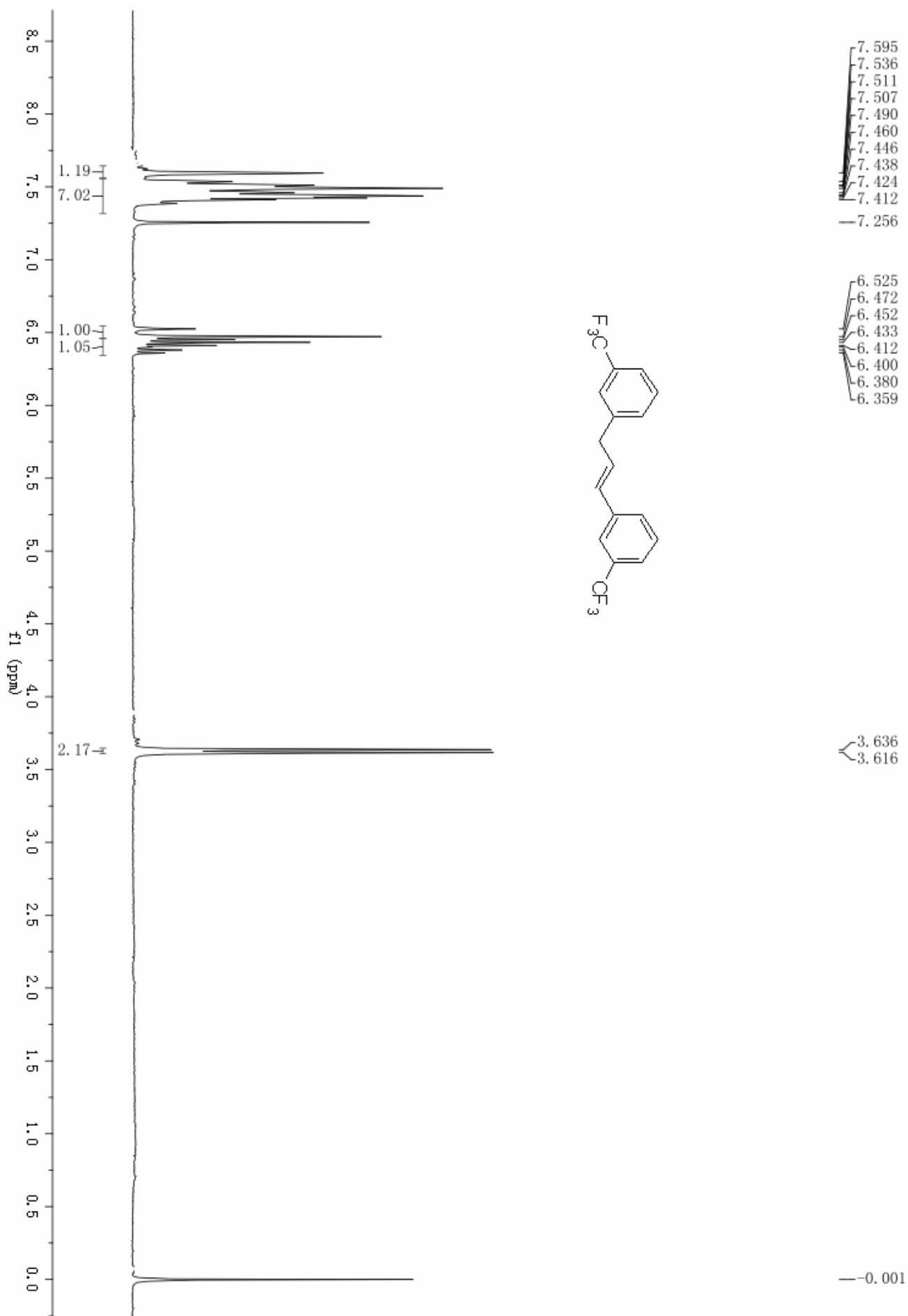
F2 - Processing parameters
SI 32768
SF 300.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.189 DDM
F1 3057.98 Hz
F2P -1.057 ppm
F2 -317.09 Hz
PPMCK 0.56225 ppm/cm
HZCM 188.74660 Hz/cm

(E)-4,4'-(prop-1-ene-1,3-diyl)bis(acetophenone) (11)

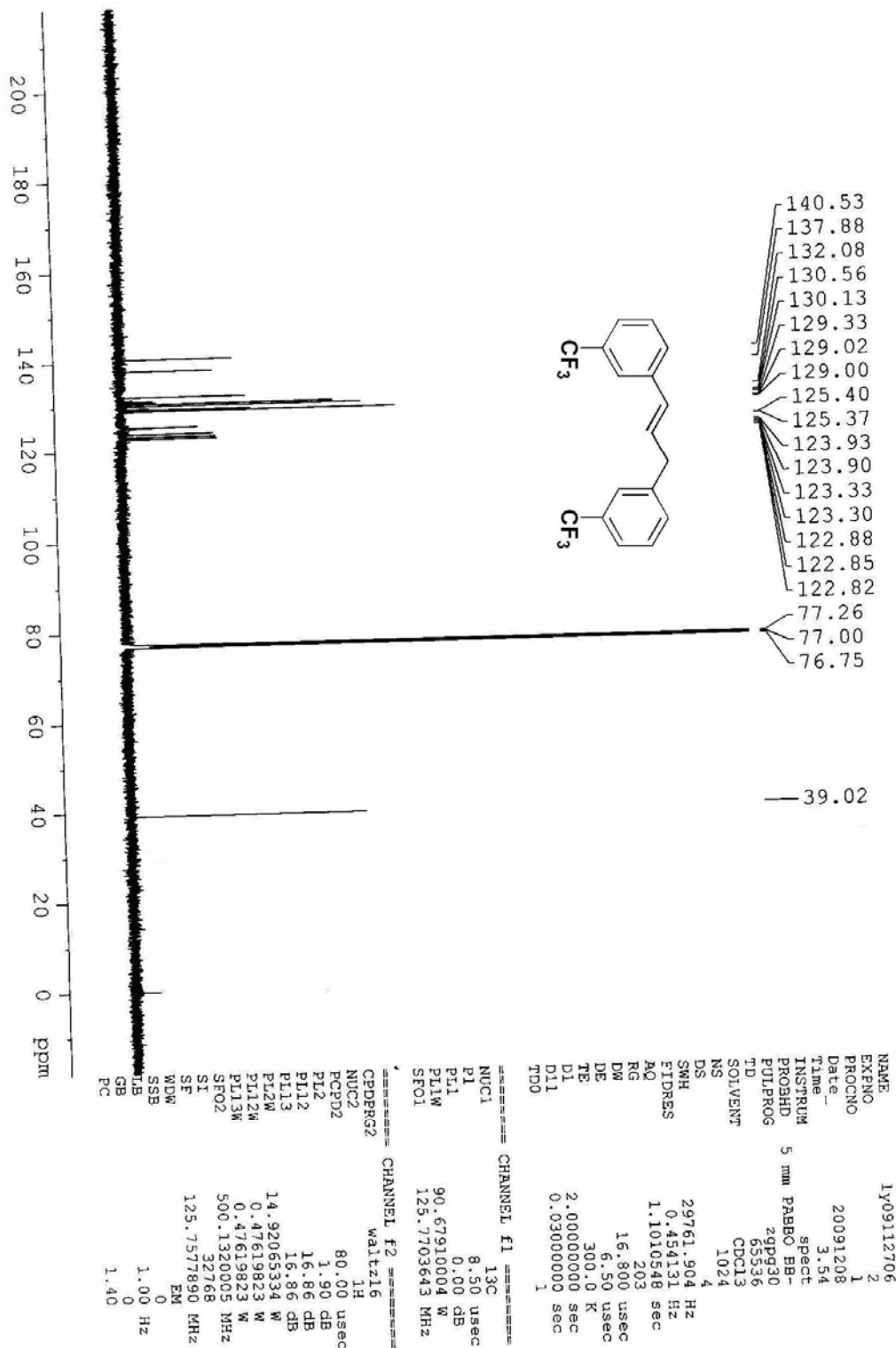


(E)-3,3'-(prop-1-ene-1,3-diyl)bis((trifluoromethyl)benzene) (12)

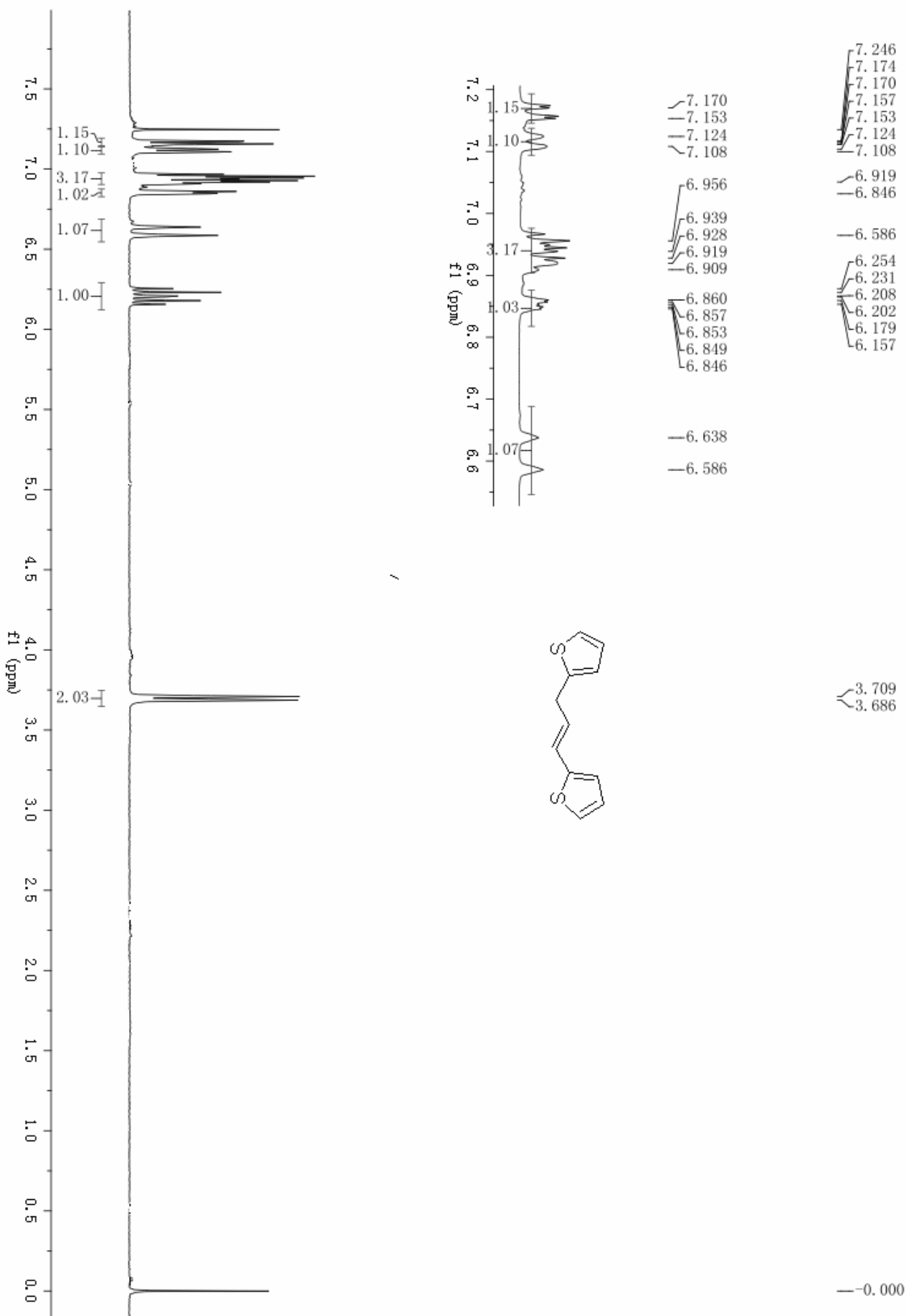


(E)-3,3'-(prop-1-ene-1,3-diyl)bis((trifluoromethyl)benzene) (12)

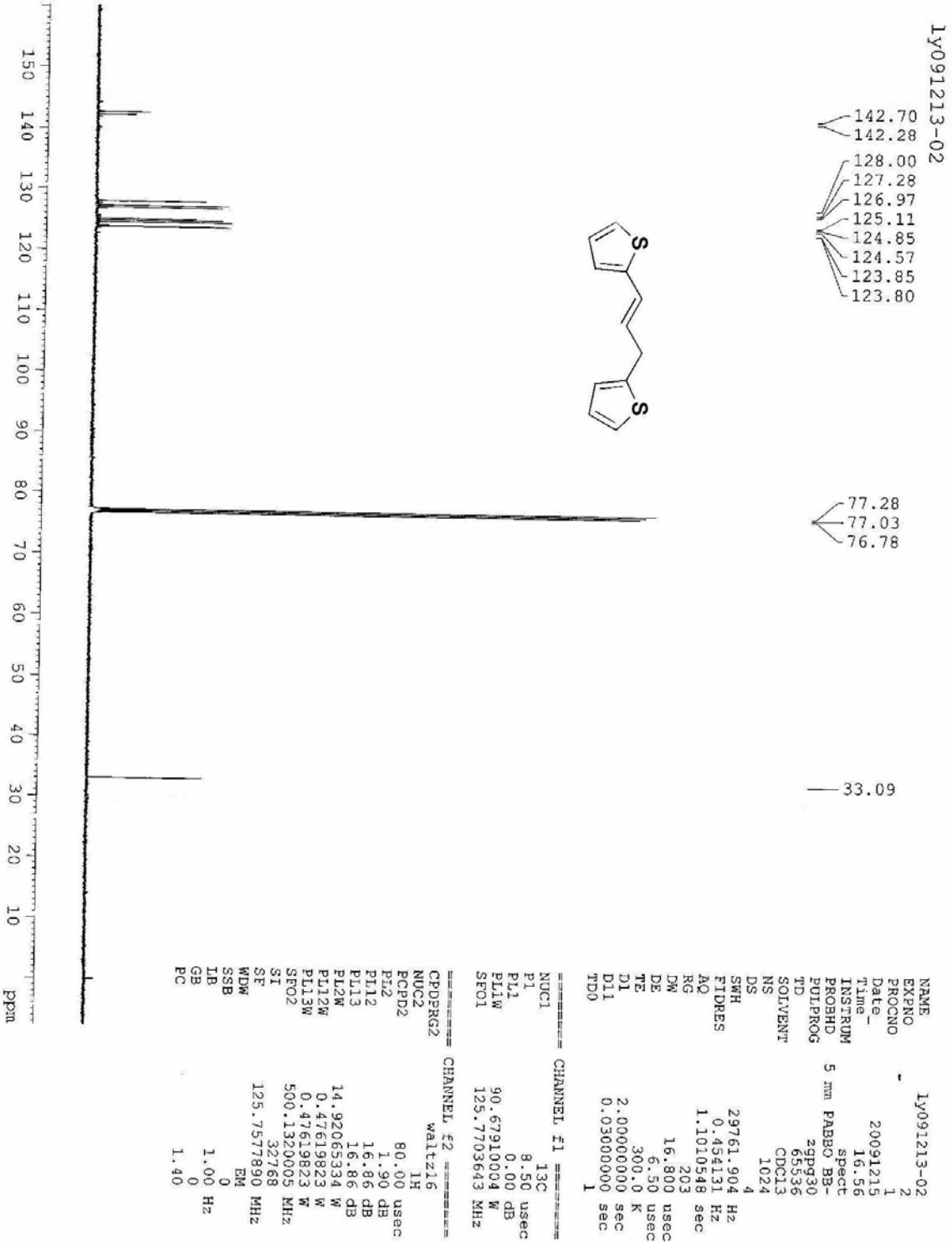
1Y09112706



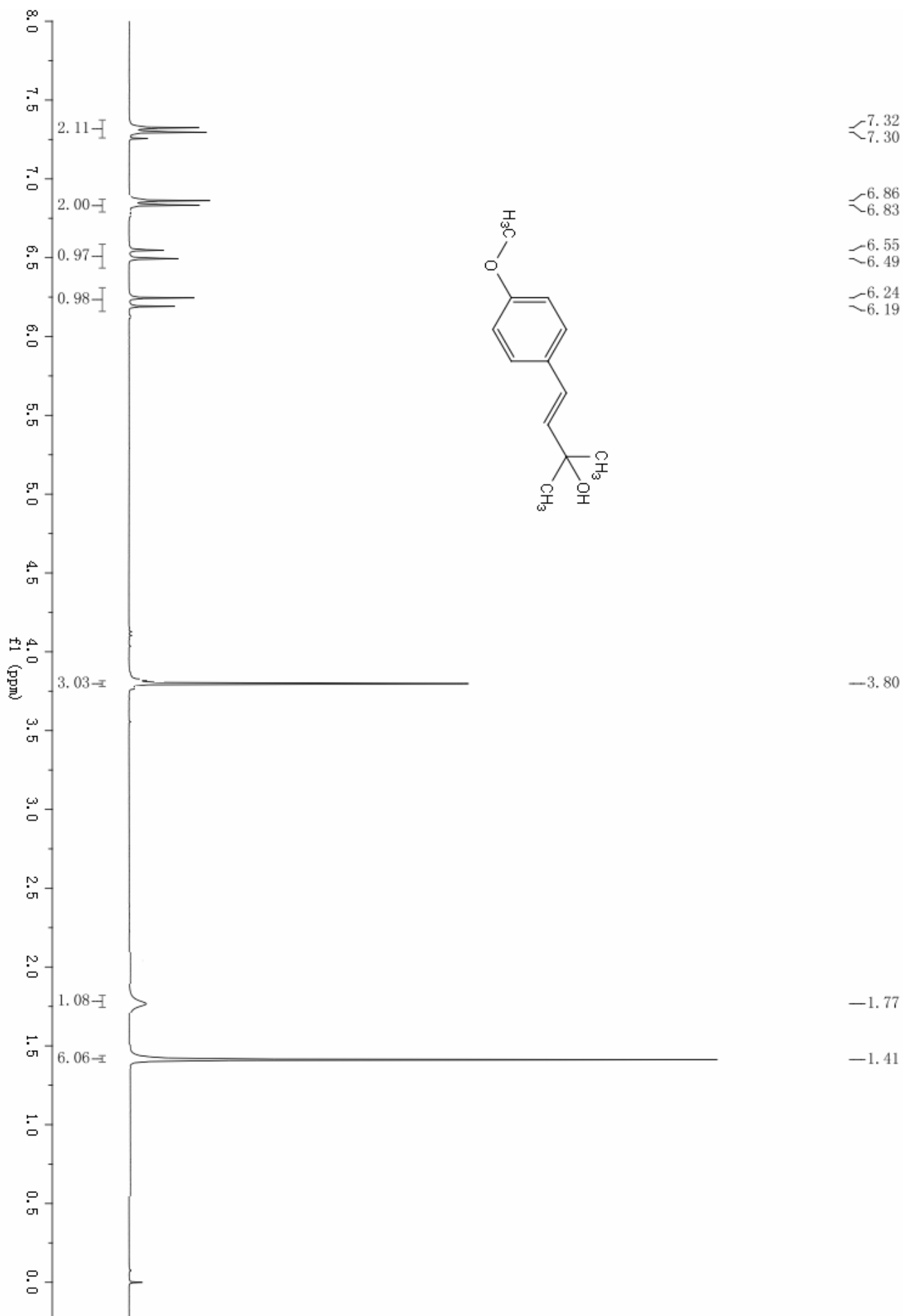
(E)-2,2'-(prop-1-ene-1,3-diyl)dithiophene (13)



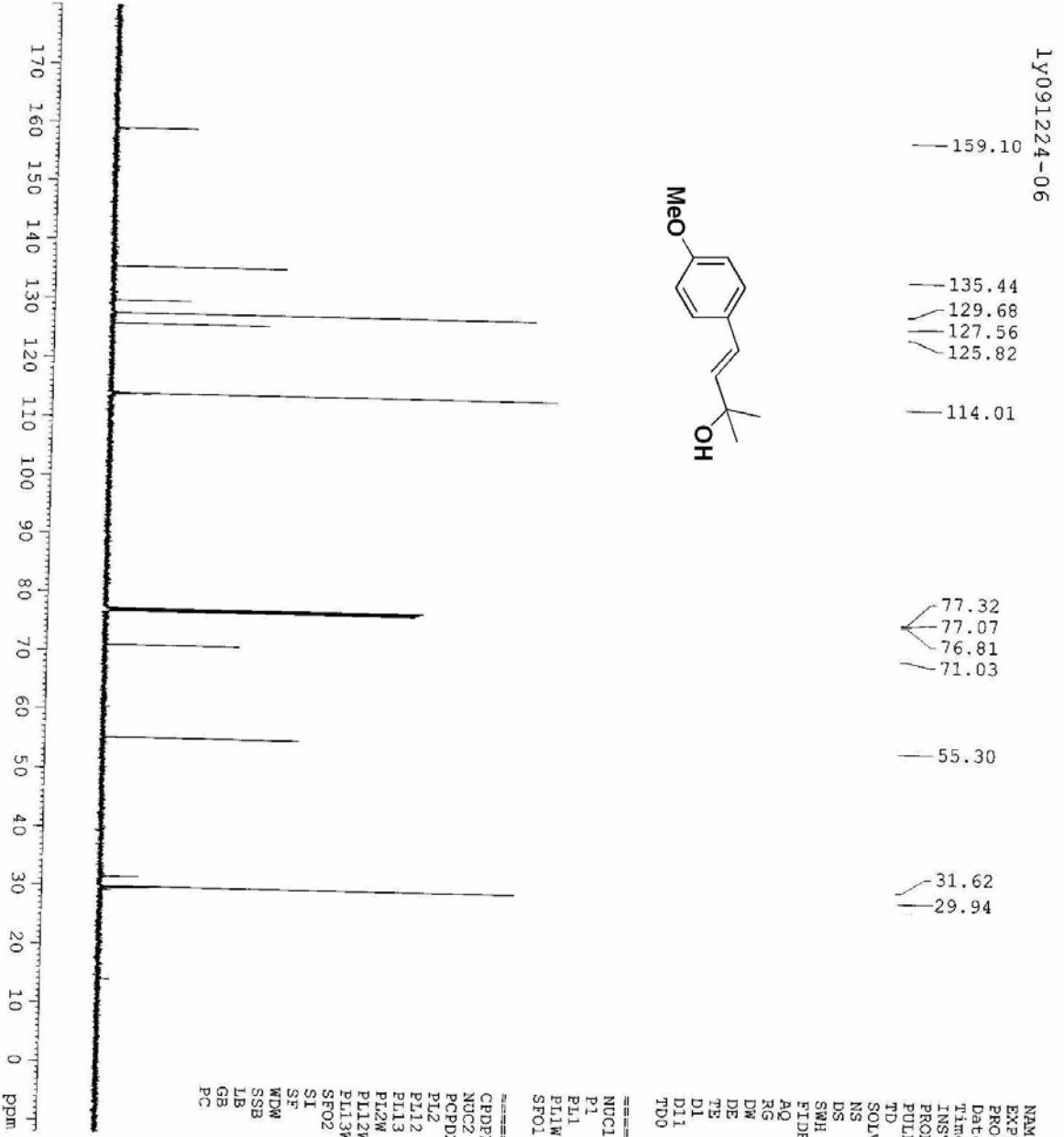
(E)-2,2'-(prop-1-ene-1,3-diyl)dithiophene (13)



(E)-4-(4-methoxyphenyl)-2-methylbut-3-en-2-ol (15)



(E)-4-(4-methoxyphenyl)-2-methylbut-3-en-2-ol (15)



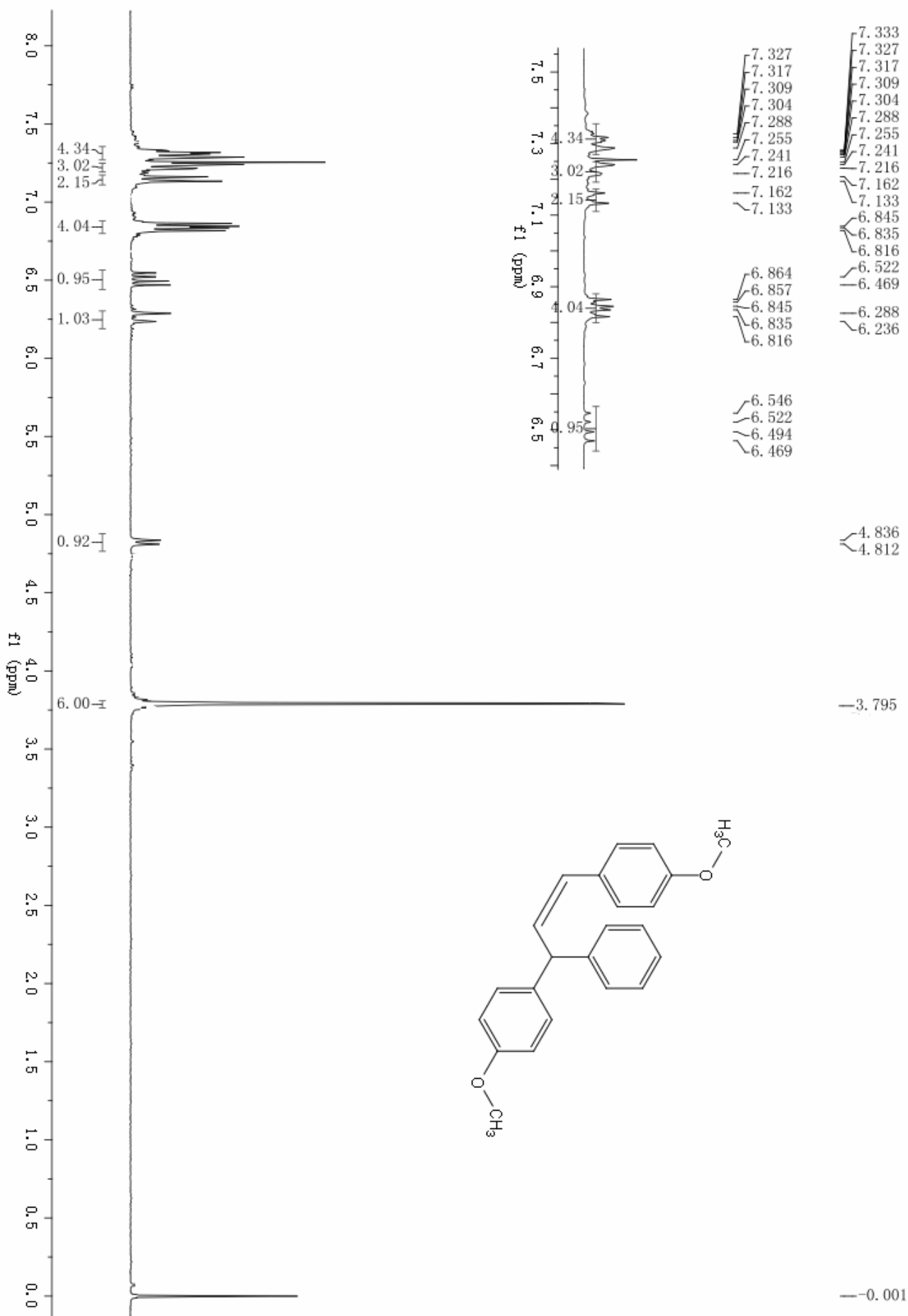
```

NAME 1y091224-06
EXPNO 2
PROCNO 1
Date_ 20091225
Time 16:57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 138
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DM 16.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL13 *
PL12W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

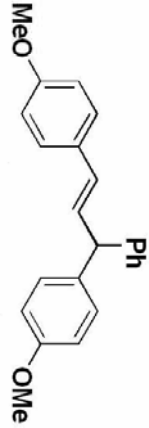
(Z)-4,4'-(3-phenylprop-1-ene-1,3-diyl)bis(methoxybenzene) (17)



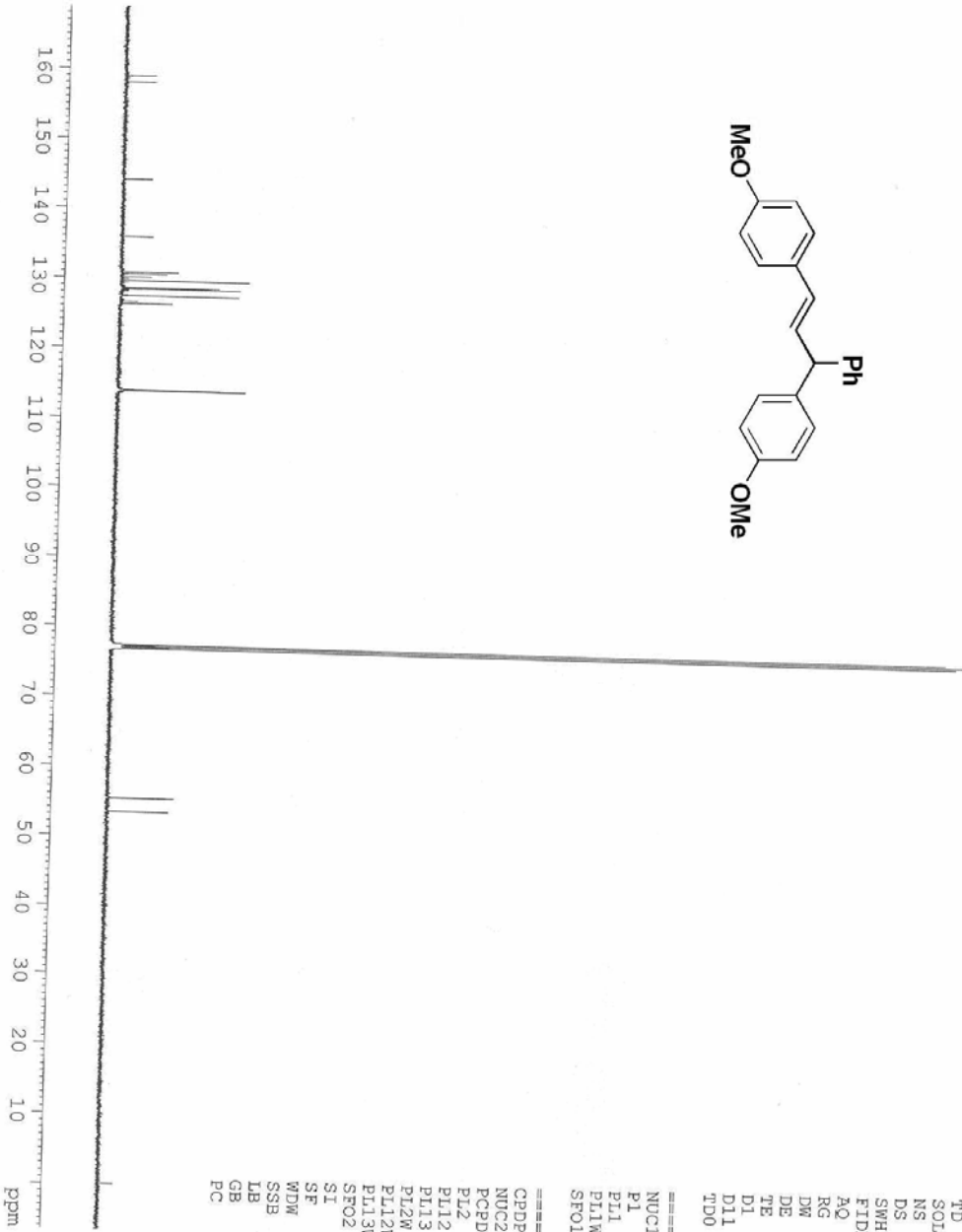
(Z)-4,4'-(3-phenylprop-1-ene-1,3-diyl)bis(methoxybenzene) (17)

1y09122901

- 158.98
- 158.11
- 144.08
- 135.90
- 130.80
- 130.55
- 130.16
- 129.61
- 128.61
- 128.44
- 127.42
- 126.63
- 126.31
- 113.93
- 113.83



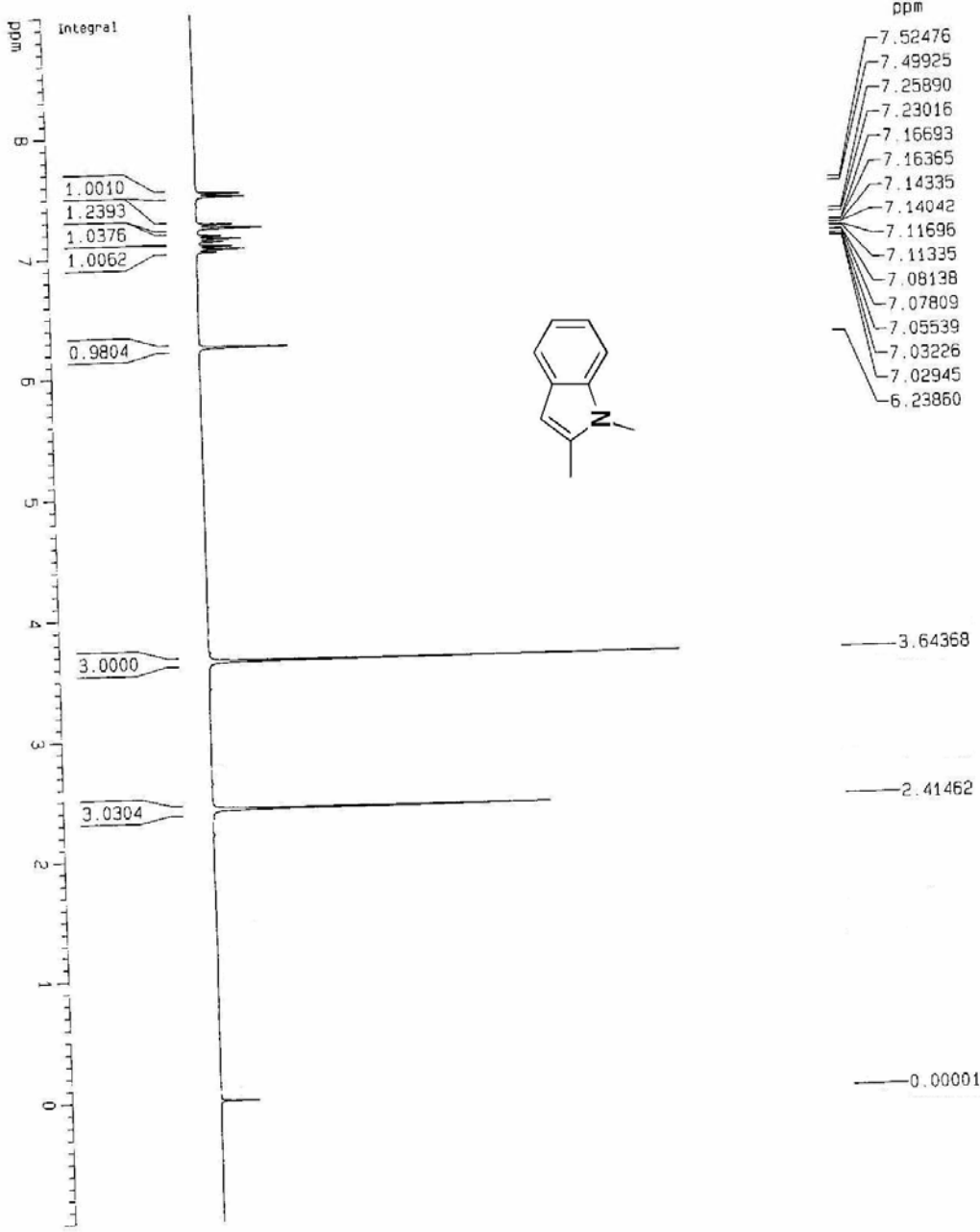
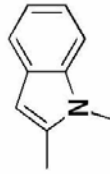
- 55.31
- 55.27
- 53.35



```

NAME 1y09122901
EXPNO 2
PROCNO 1
Date_ 20091230
Time 14.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DE 16.800 usec
TE 295.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL12W 14.92065334 W
PL12M 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

1,2-Dimethyl-1H-indole (18)



1y100107-01

Current Data Parameters
 NAME 1y100107-01
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20100107
 Time 20.01
 INSTRUM gpcx300
 PROBHD 5 mm PAB90 BB-
 PULPROG zgpg30
 TD 23980
 FIDRES 0.15000000
 SOLVENT cdc13
 NS 4
 DS 0
 SWH 7485.030 Hz
 FIDRES 0.312136 Hz
 AQ 1.6019140 sec
 RG 206
 DE 56.800 usec
 TE 300.2 K
 D1 1.00000000 sec
 MCOREST 0.00000000 sec
 MCORRK 0.01500000 sec

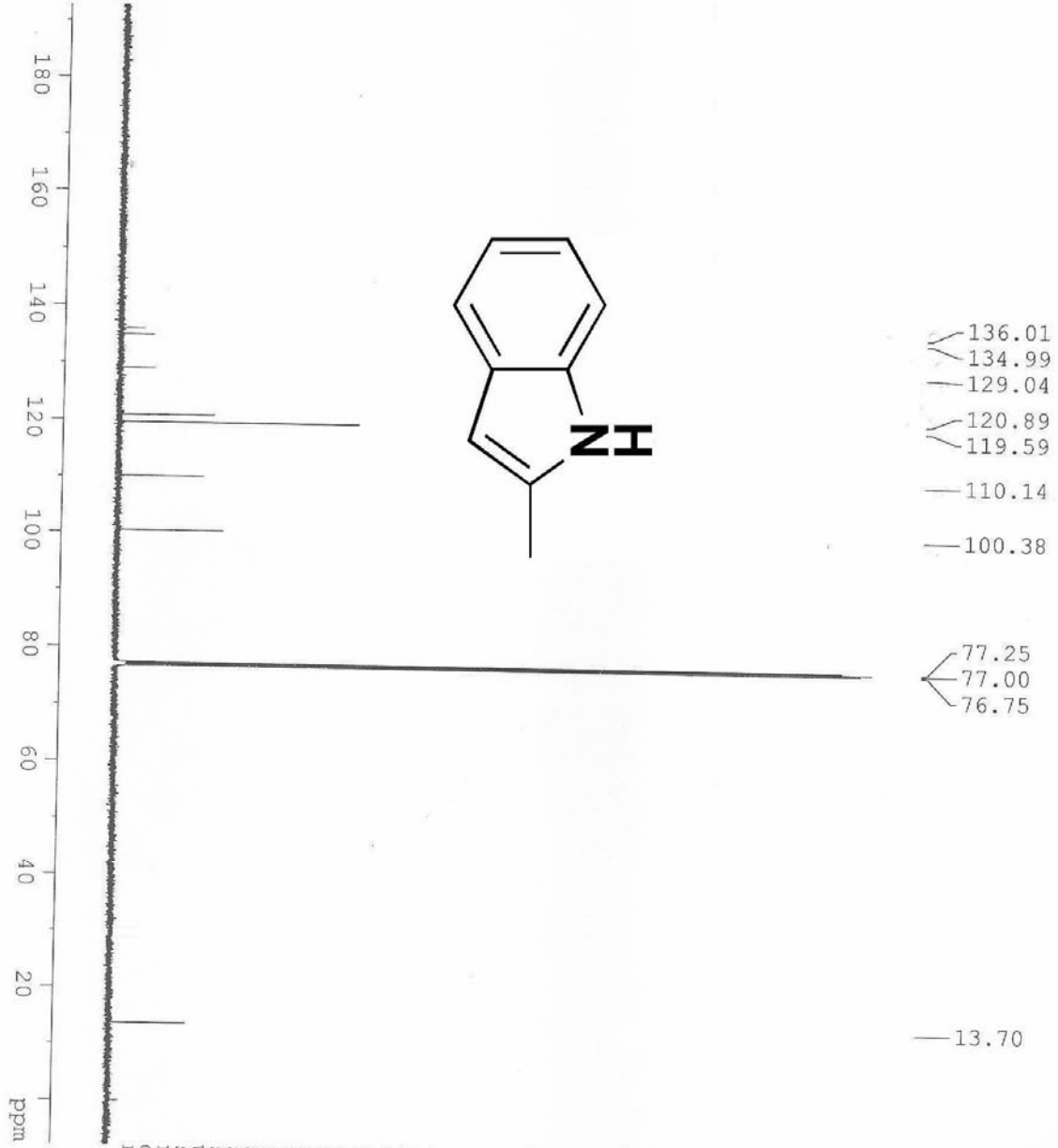
===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 300.1313913 MHz

F2 - Processing parameters
 S1 32768
 SF 300.1300152 MHz
 K0N EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ID NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 F1P 9.000 ppm
 F1 2701.17 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCK 0.50000 ppm/cm
 HZCM 150.06500 Hz/cm

1,2-Dimethyl-1H-indole (18)

1y100409-01



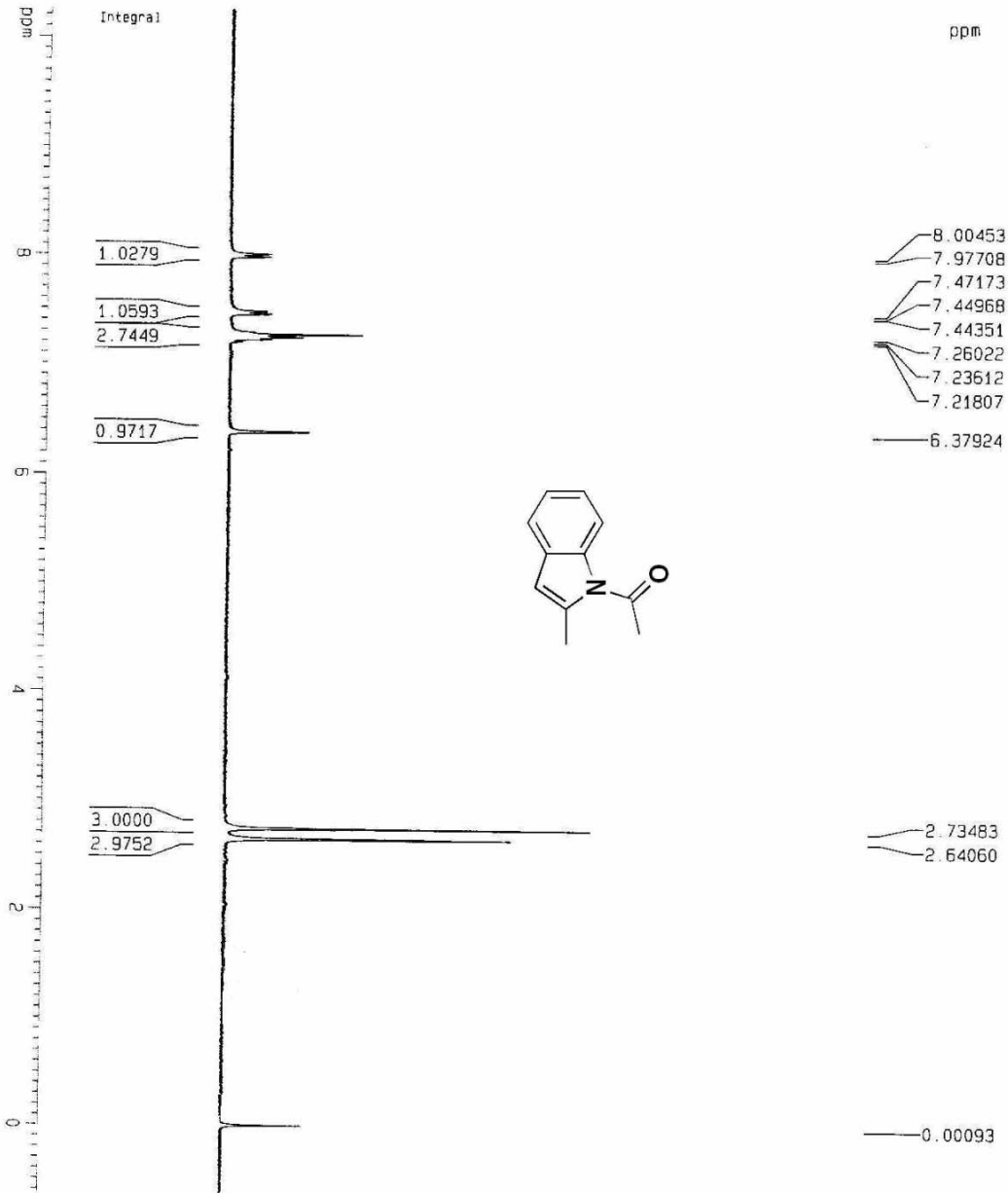
```

NAME 1y100409-01
EXPNO 2
PROCNO 1
Date_ 20100413
Time_ 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.30 dB
PL12 16.86 dB
PL13 16.86 dB
PL2W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577931 MHz
WDW EM
SSB 0
GB 0
PC 1.40
    
```

1-(2-Methyl-1H-indol-1-yl)ethanone (19)



1Y100409-04

Current Data Parameters
 NAME 1Y100409-04
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100409
 Time 16.37
 INSTRUM dx300
 PROCNO 5 mm PABBO 89-
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 4
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.182959 Hz
 AQ 2.7329011 sec
 RG 32
 DW 83.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 3.00000000 sec
 MCRCST 0.00000000 sec
 MCNKR 0.01500000 sec

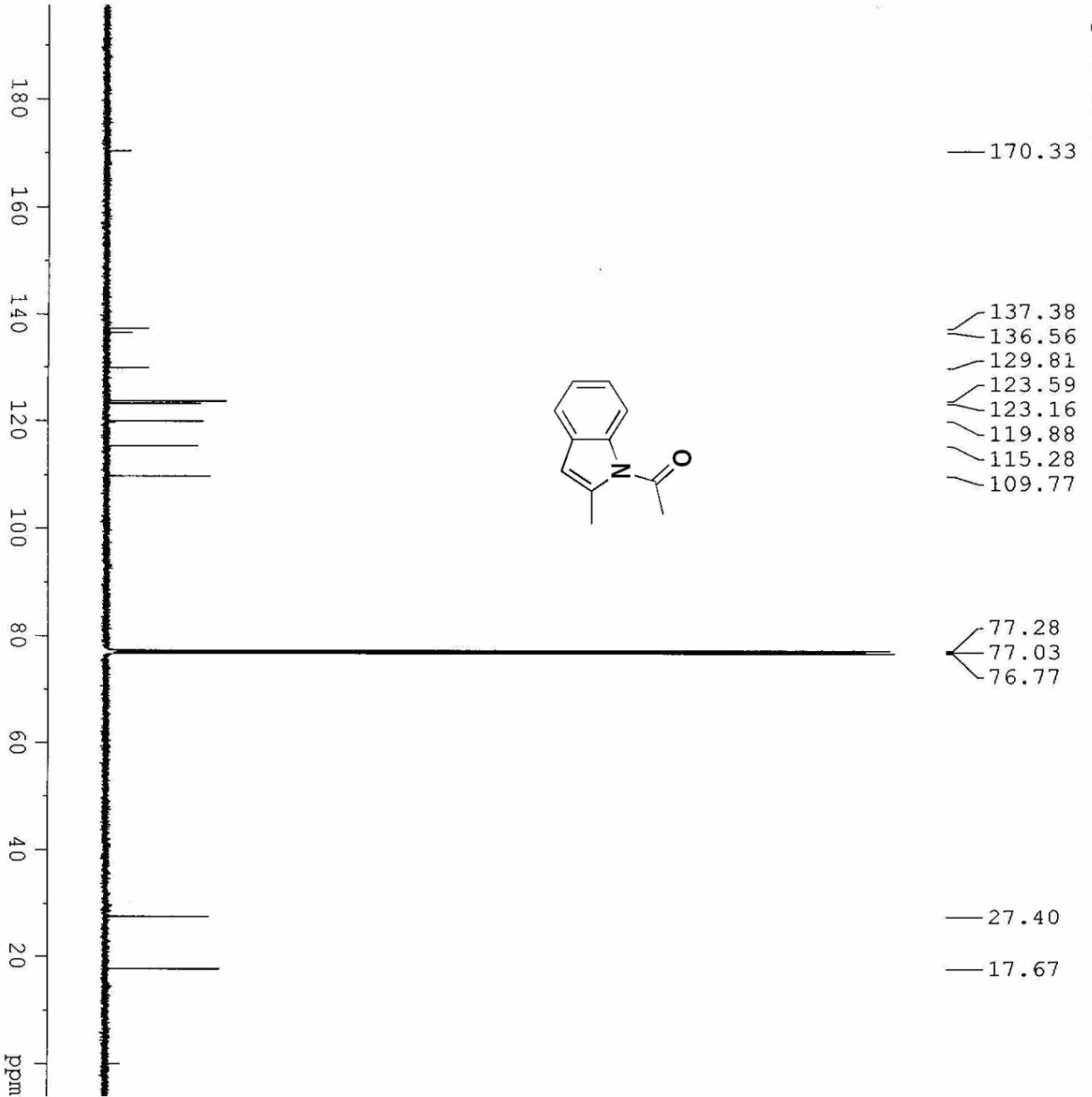
===== CHANNEL f1 =====
 NU1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 300.1381009 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300054 MHz
 MDX EM
 SSB 0
 LB 0.03 Hz
 GB 0
 PC 1.00

1D NMR plot parameters
 CX 20.00 cm
 CY 6.00 cm
 FXP 10.249 ppm
 F1 3076.17 Hz
 FSP -0.628 ppm
 F2 -188.39 Hz
 PPM0M 0.54386 ppm/cm
 HZCM 153.28803 Hz/cm

1-(2-Methyl-1H-indol-1-yl)ethanone (19)

LY100409-04



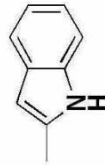
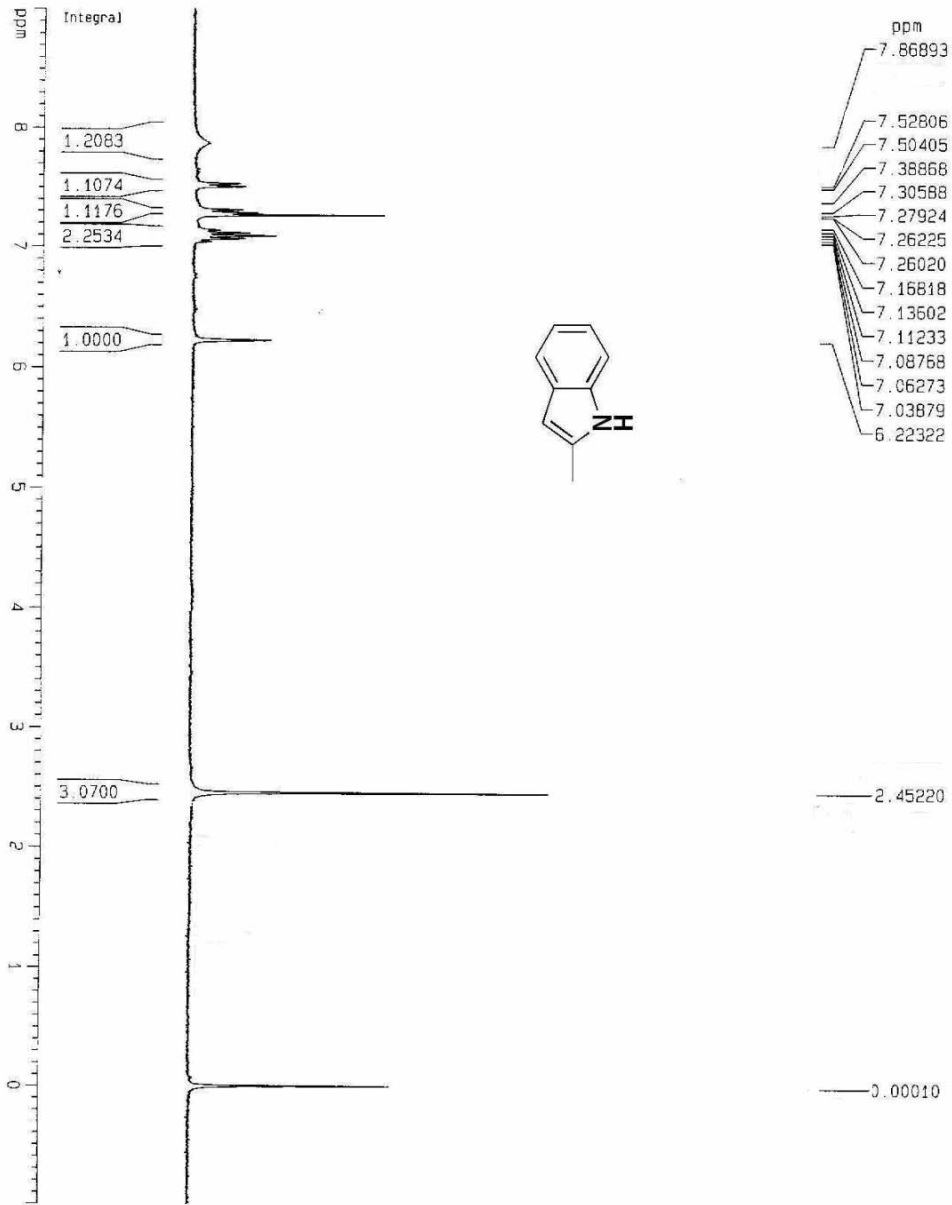
```

=====
NAME          LY100409-04
EXPNO         2
PROCNO        1
Date_         20100413
Time_         1.18
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            512
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010548 sec
RG            203
DW            16.800 usec
DE            6.50 usec
TE            296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1          13C
P1            8.50 usec
PL1           0.00 dB
PL1W          90.67910004 W
SFO1         125.7703643 MHz

===== CHANNEL f2 =====
CDDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
P12          1.90 dB
PL12         16.86 dB
PL13         16.86 dB
PL2W         14.92065334 W
PL12W        0.47619823 W
PL13W        0.47619823 W
SFO2         500.1320005 MHz
SI           32768
SF           125.7577890 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
    
```

2-Methyl-1H-indole (20)



1Y10011301

Current Data Parameters
 NAME 1Y10011301
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20100113
 Time 16.24
 INSTRUM dpX300
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 23960
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 7485.030 Hz
 FIDRES 0.312136 Hz
 AQ 1.6019140 sec
 RG 206
 DM 66.800 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

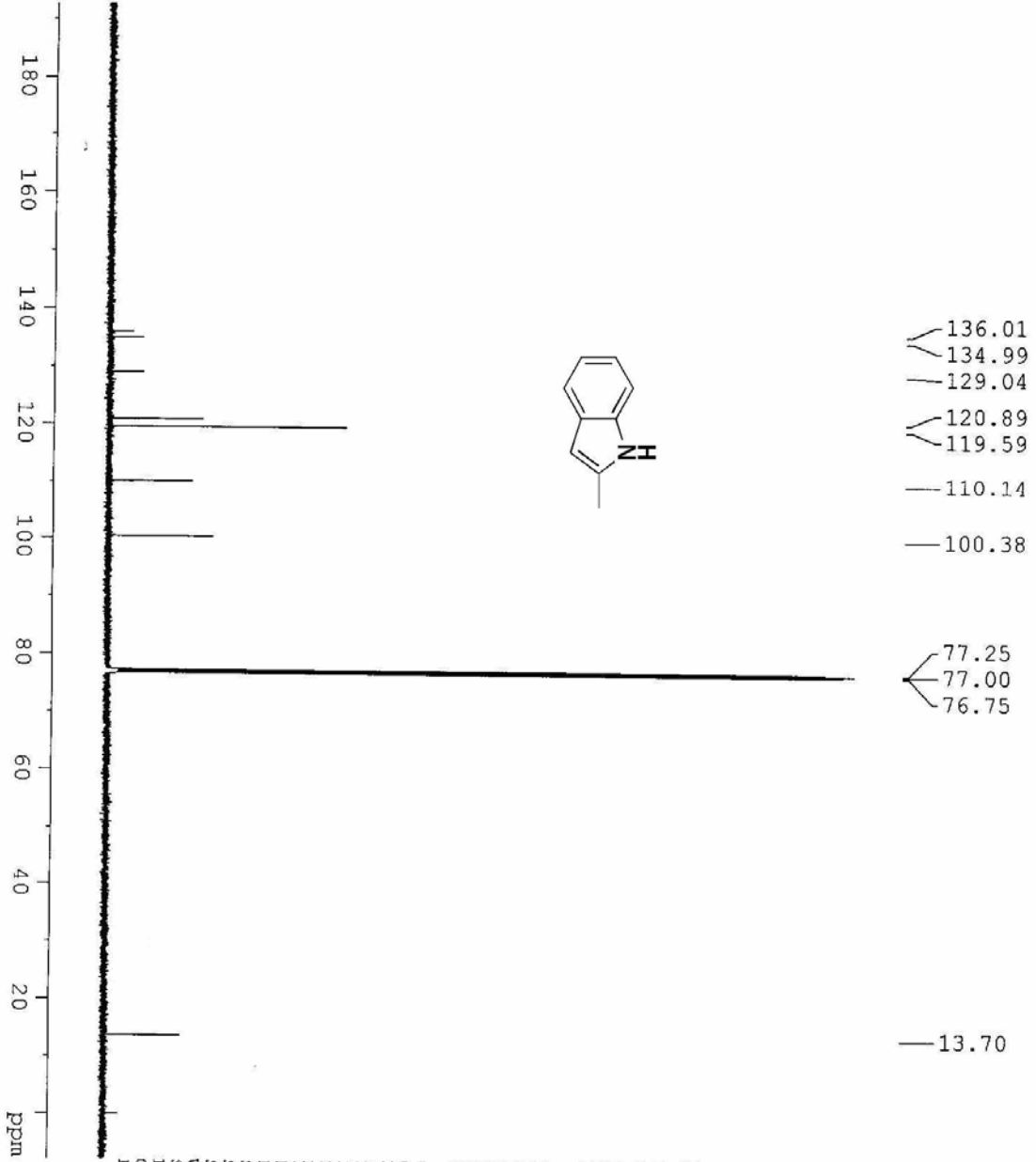
***** CHANNEL f1 *****
 NUCL1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 300.1313913 MHz

F2 - Processing parameters:
 SI 32768
 SF 300.1300054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

1D NMR plot parameters:
 CX 20.00 cm
 CY 5.00 cm
 F1P 9.000 ppm
 F1 2701.17 Hz
 F2P -1.000 ppm
 F2 -300.13 Hz
 PPMCM 0.50000 ppm/cm
 HZCM 150.06500 Hz/cm

2-Methyl-1H-indole (20)

Ly100409-01



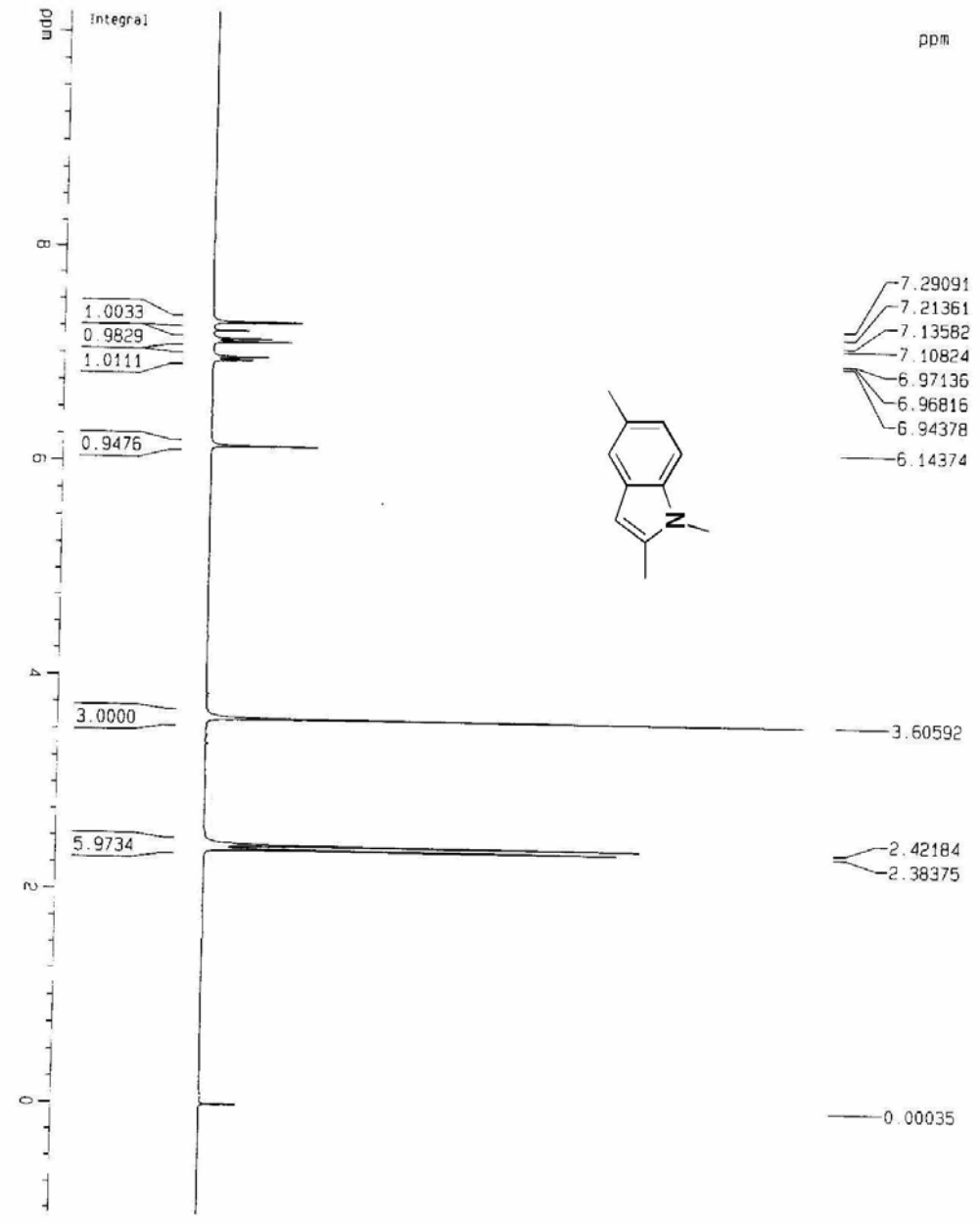
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NAME Ly100409-01
EXPNO 2
PROCNO 1
Date_ 20100413
Time_ 0.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL2W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SE 125.7577931 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

1,2,5-Trimethyl-1H-indole (21)



1Y100304-01

Current Data Parameters
 NAME 1Y100304-01
 EXPNO 1
 PROCNO 1

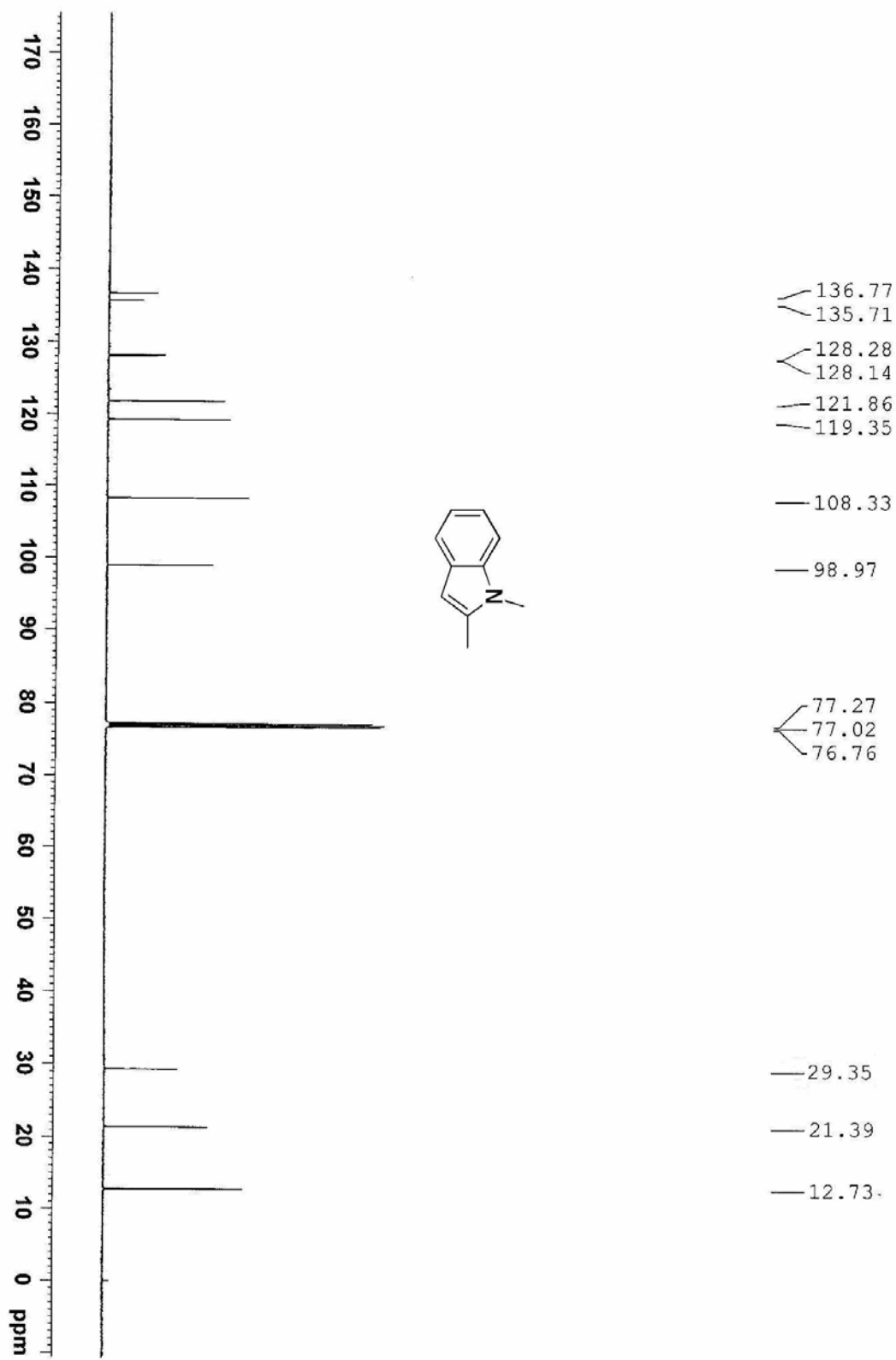
F2 - Acquisition Parameters
 Date_ 20100304
 Time 19 21
 INSTRUM dpx300
 PROBRD 5 nm PAB90 BR-
 PULPROG zg
 TD 23980
 SOLVENT CDCl3
 NS 4
 DS 0
 SMH 5995.204 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 RG 912.3
 DW 83.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCHREST 0.00000000 sec
 MCNMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 300.1313913 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300202 MHz
 WDM EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

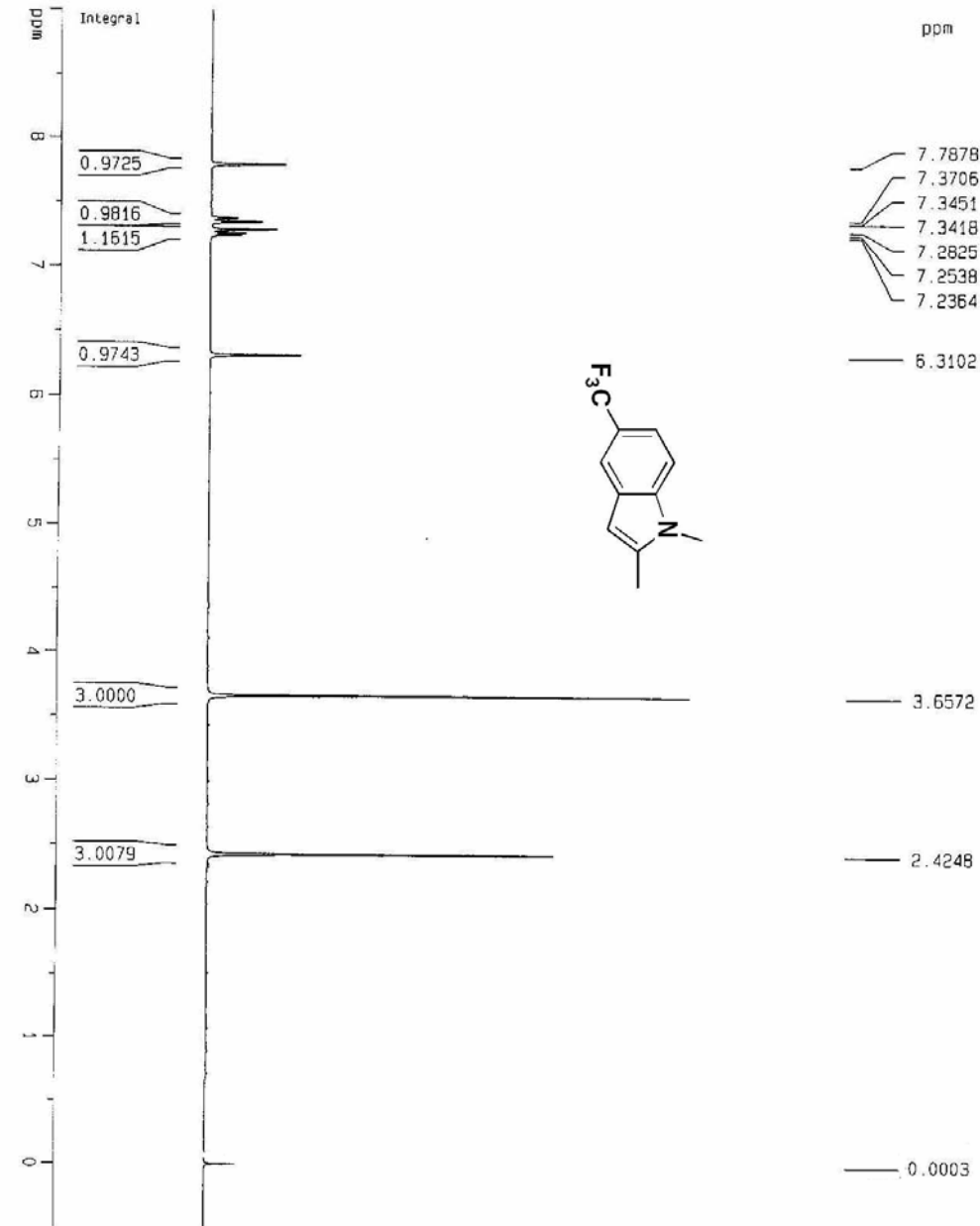
10 NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 FXP 10.189 ppm
 F1 3057.88 Hz
 F2P -1.057 ppm
 F2 -317.09 Hz
 PPMCM 0.56225 ppm/cm
 HZCM 168.74863 Hz/cm

1,2,5-Trimethyl-1*H*-indole (21)



LY100304-01

1,2-Dimethyl-5-(trifluoromethyl)-1H-indole (22)



1Y100309-04

Current Data Parameters
 NAME 1Y100309-04
 EXPNO 1
 PROCNO 1

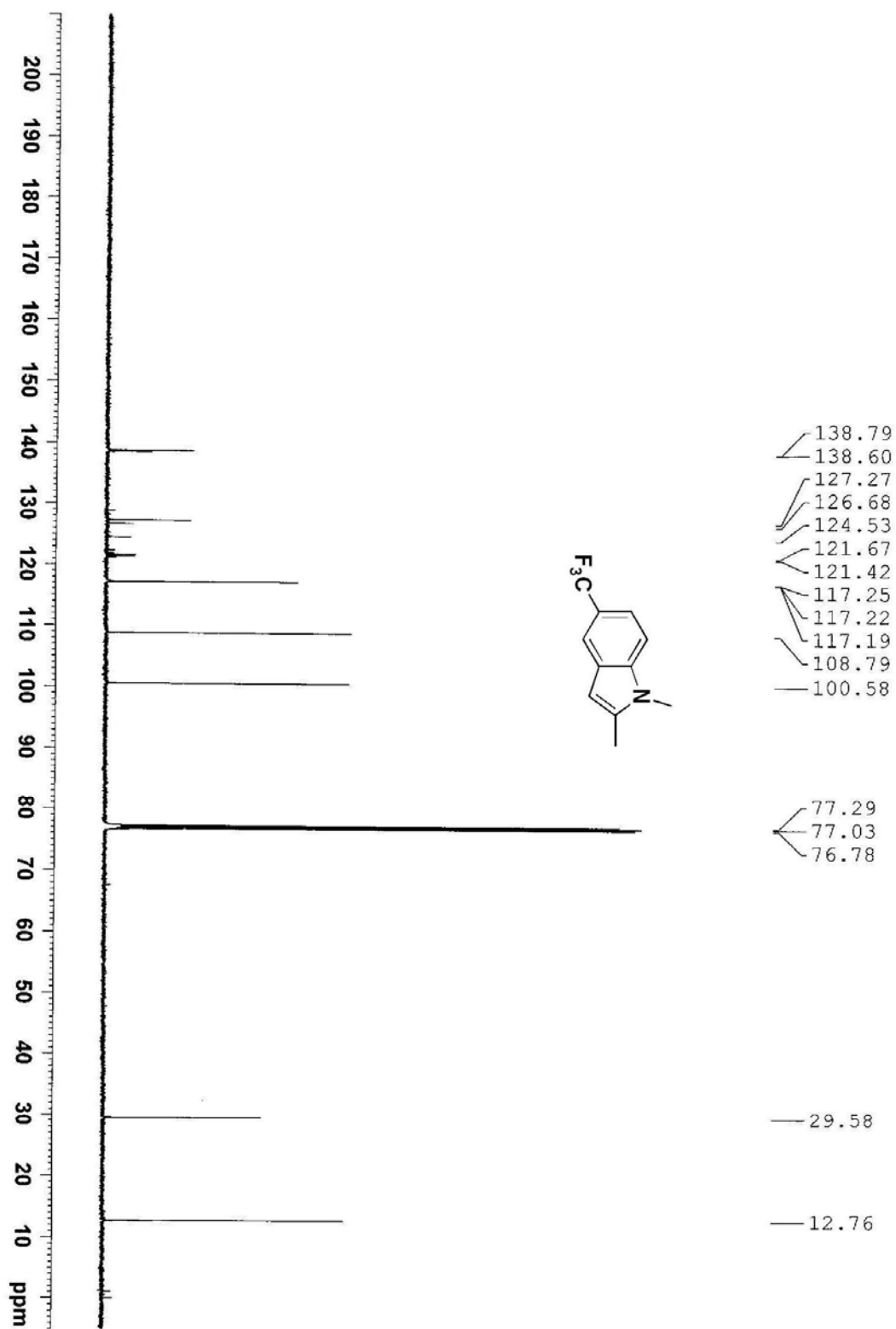
F2 - Acquisition Parameters
 Date_ 20100309
 Time 17:31
 INSTRUM dpx300
 PROBRD 5 mm PABBO BB-
 PULPROG zg
 TO 23960
 SOLVENT CDCl3
 NS 6
 DS 0
 SMH 5995.204 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 R6 256
 CW 63.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCNKR 0.01500000 sec

***** CHANNEL f1 *****
 NUCl1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 300.1313913 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300132 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

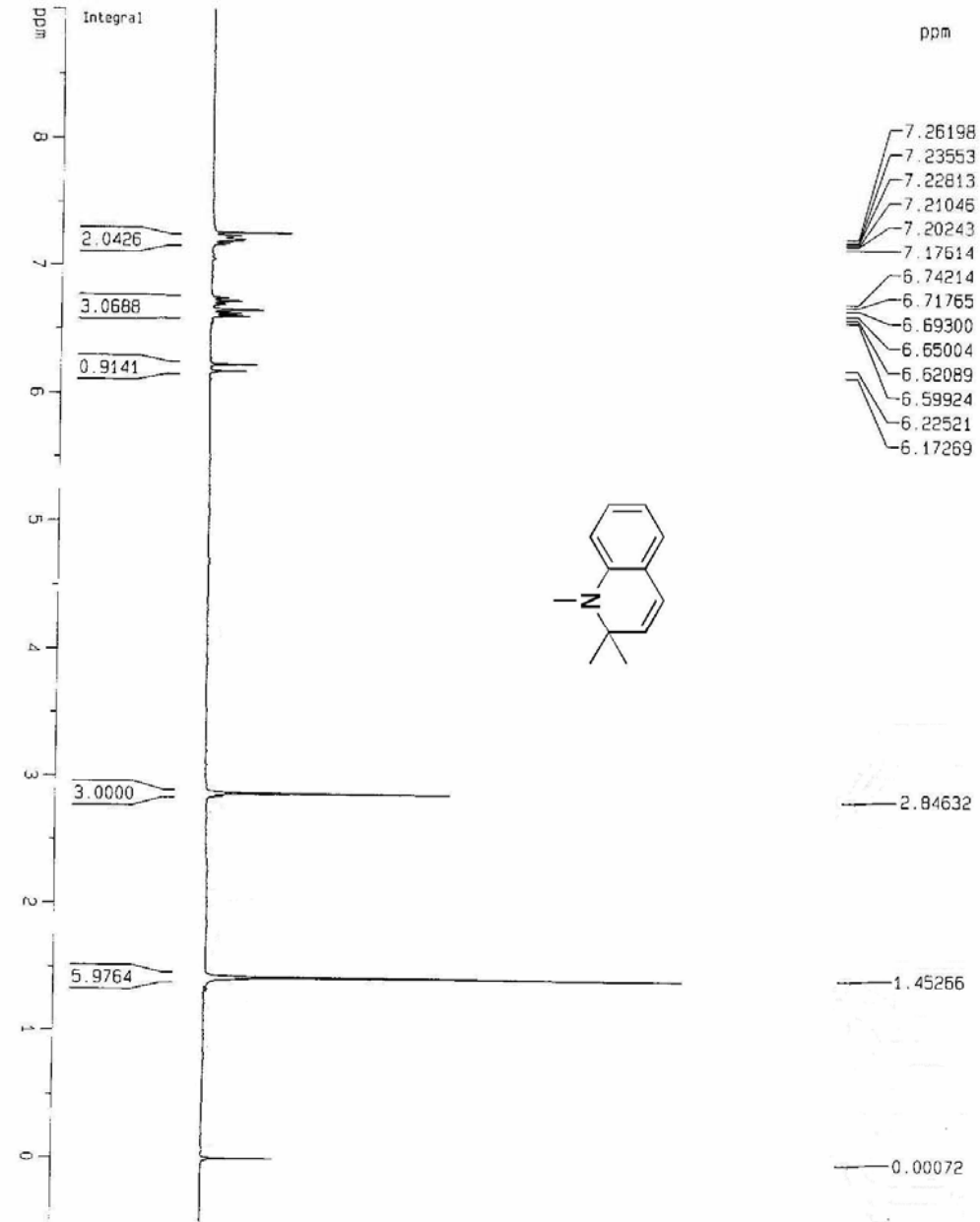
10 NMR plot parameters.
 CX 20.00 cm
 CY 8.00 cm
 FXP 9.000 ppm
 F1 2701.17 Hz
 F2 -0.500 ppm
 PPKCM 150.06 Hz
 PPKCM 0.47500 ppm/cm
 HZCM 142.56175 Hz/cm

1,2-Dimethyl-5-(trifluoromethyl)-1*H*-indole (22)

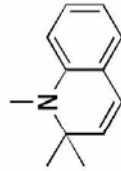


LY100309-04

1,2,2-Trimethyl-1,2-dihydroquinoline (23)



1Y100309-03



Current Data Parameters
 NAME 1Y100309-03
 EXPNO 1
 PROCNO 1

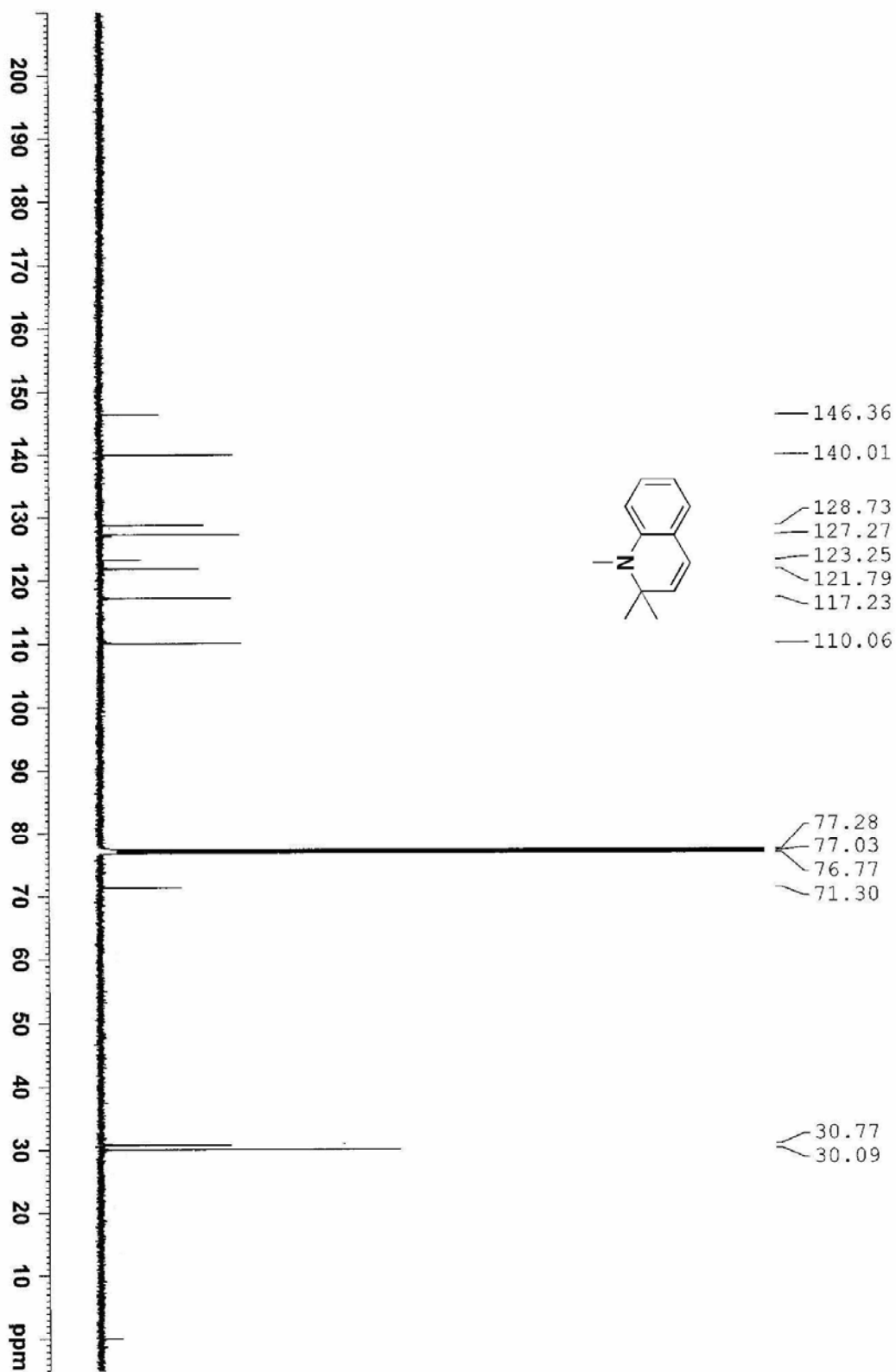
F2 - Acquisition Parameters
 Date_ 20100309
 Time 17.20
 INSTRUM dxp300
 PROBDW 5 mm PAB90 BB-
 PULPROG zg
 TD 23980
 SOLVENT CDCl3
 NS 6
 DS 0
 SMH 5995.204 Hz
 FIDRES 0.250008 Hz
 AQ 1.9999820 sec
 RG 255
 DM 83.400 usec
 DE 6.00 usec
 TE 0.0 K
 D1 1.00000000 sec
 MCRES1 0.00000000 sec
 MCNRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SFO1 300.1313913 MHz

F2 - Processing parameters
 SI 32758
 SF 300.1300056 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

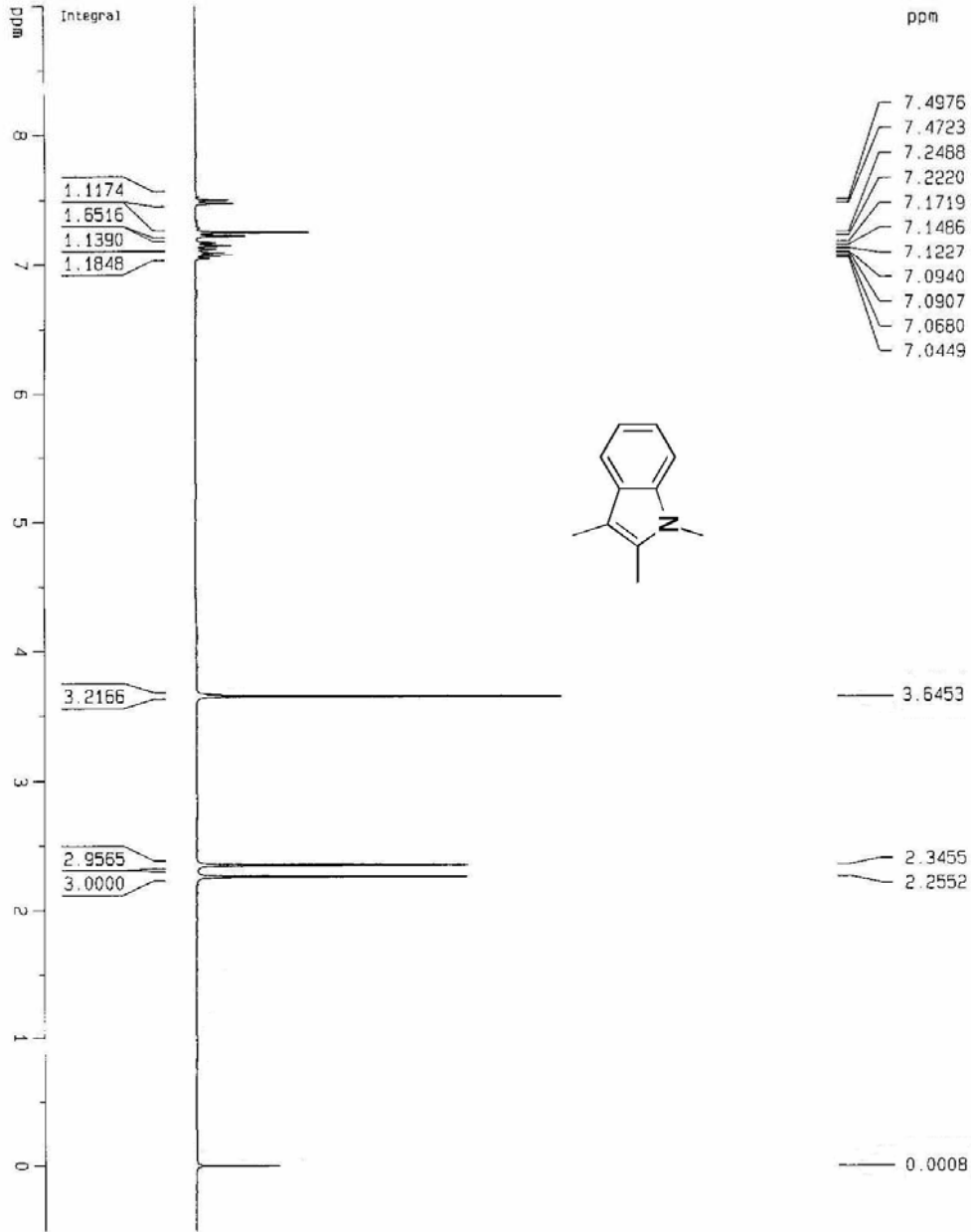
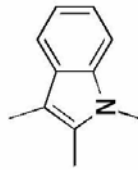
10 NMR plot parameters
 CX 20.00 cm
 CY 8.00 cm
 FIP 9.000 ppm
 F1 2701.17 Hz
 F2 -0.500 ppm
 PPM0H -150.06 Hz
 0.47500 ppm/cm
 HZCM 142.56175 Hz/cm

1,2,2-Trimethyl-1,2-dihydroquinoline (23)



LY100309-03

1,2,3-trimethyl-1H-indole (24)



1Y100309-06

Current Data Parameters
 NAME 1Y100309-05
 EXPNO 1
 PROCNO 1

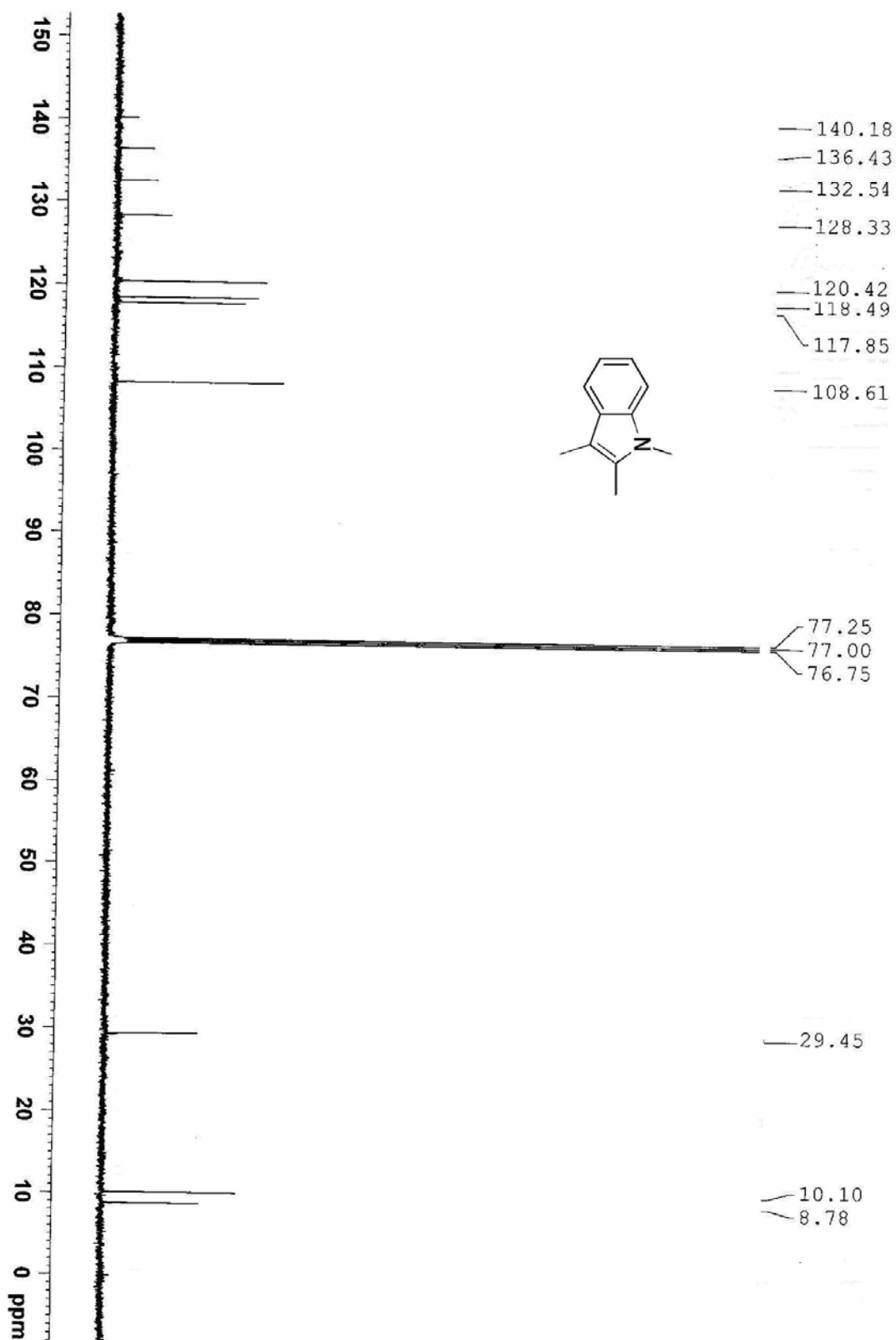
F2 - Acquisition Parameters
 Date_ 20100309
 Time 17.36
 INSTRUM dpx300
 PROBHD 5 mm PAB90 B8-
 PULPROG zg
 TD 23980
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 5995.204 Hz
 FIDRES 0.250008 Hz
 AQ 1.9998820 sec
 RG 256
 DM 83.400 usec
 DE 6.00 usec
 TE 0.0 K
 O1 1.00000000 sec
 MCRES1 0.00000000 sec
 MCRRK 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 12.00 usec
 PL1 -2.00 dB
 SF01 300.1313913 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1300094 MHz
 MDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

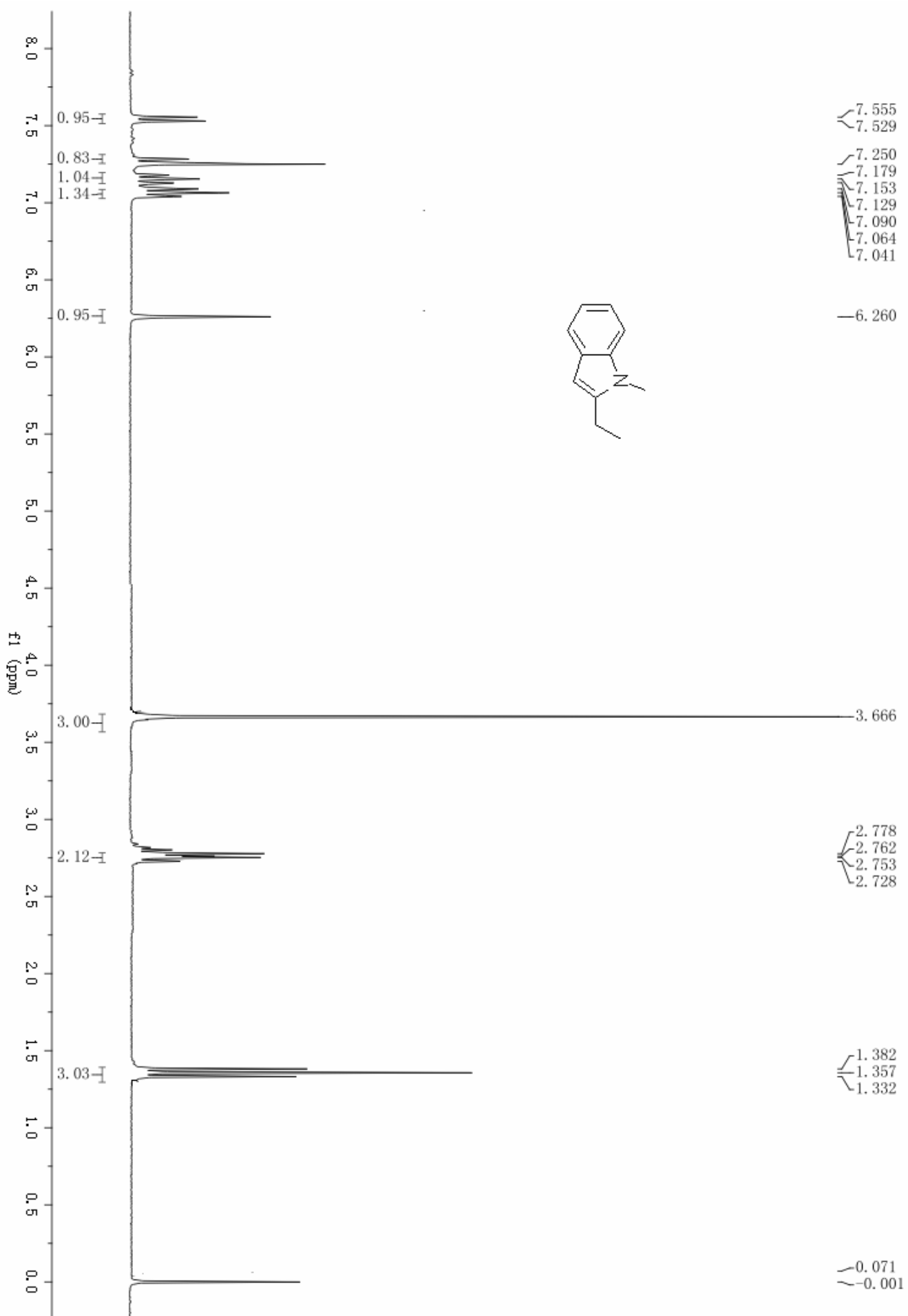
1D NMR Plot Parameters
 CX 20.00 cm
 CY 6.00 cm
 FAP 9.000 dpm
 F1 2701.17 Hz
 F2P -0.500 dpm
 F2 0.47500 dpm/cm
 FPNCH 142.56175 Hz/cm
 HZCM

1,2,3-trimethyl-1*H*-indole (24)

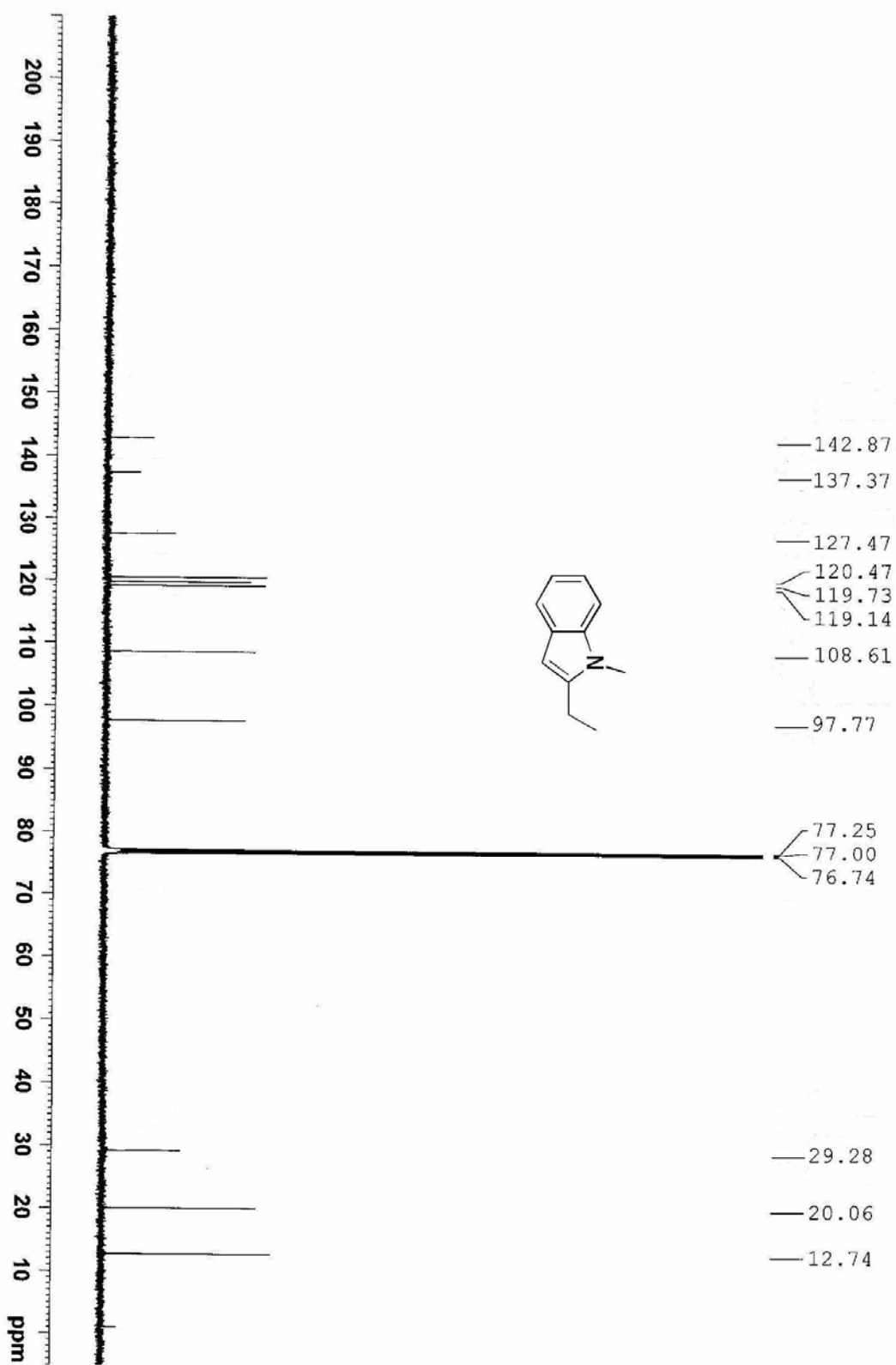


LY100309-06

2-Ethyl-1-methyl-1H-indole (25)

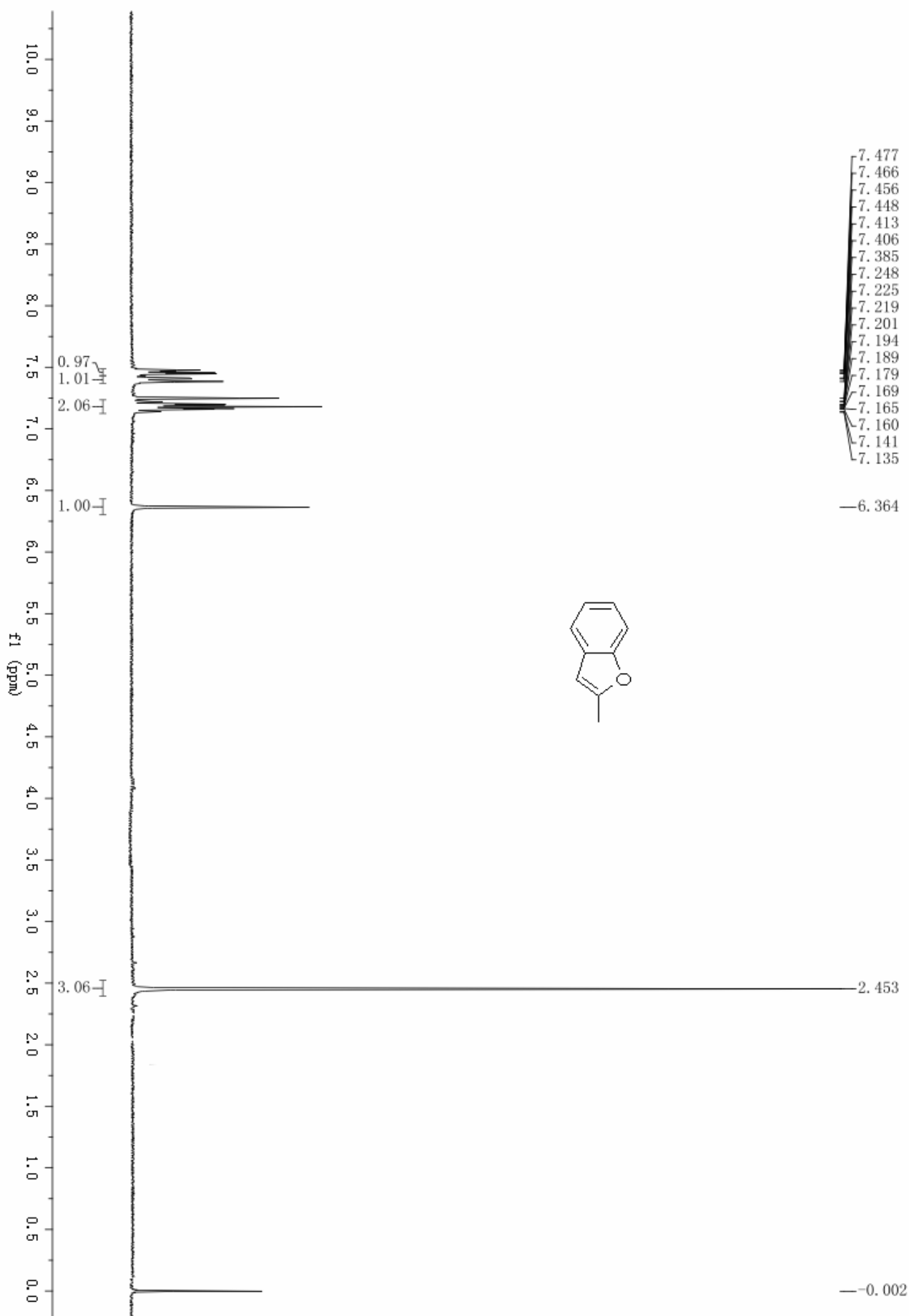


2-Ethyl-1-methyl-1H-indole (25)

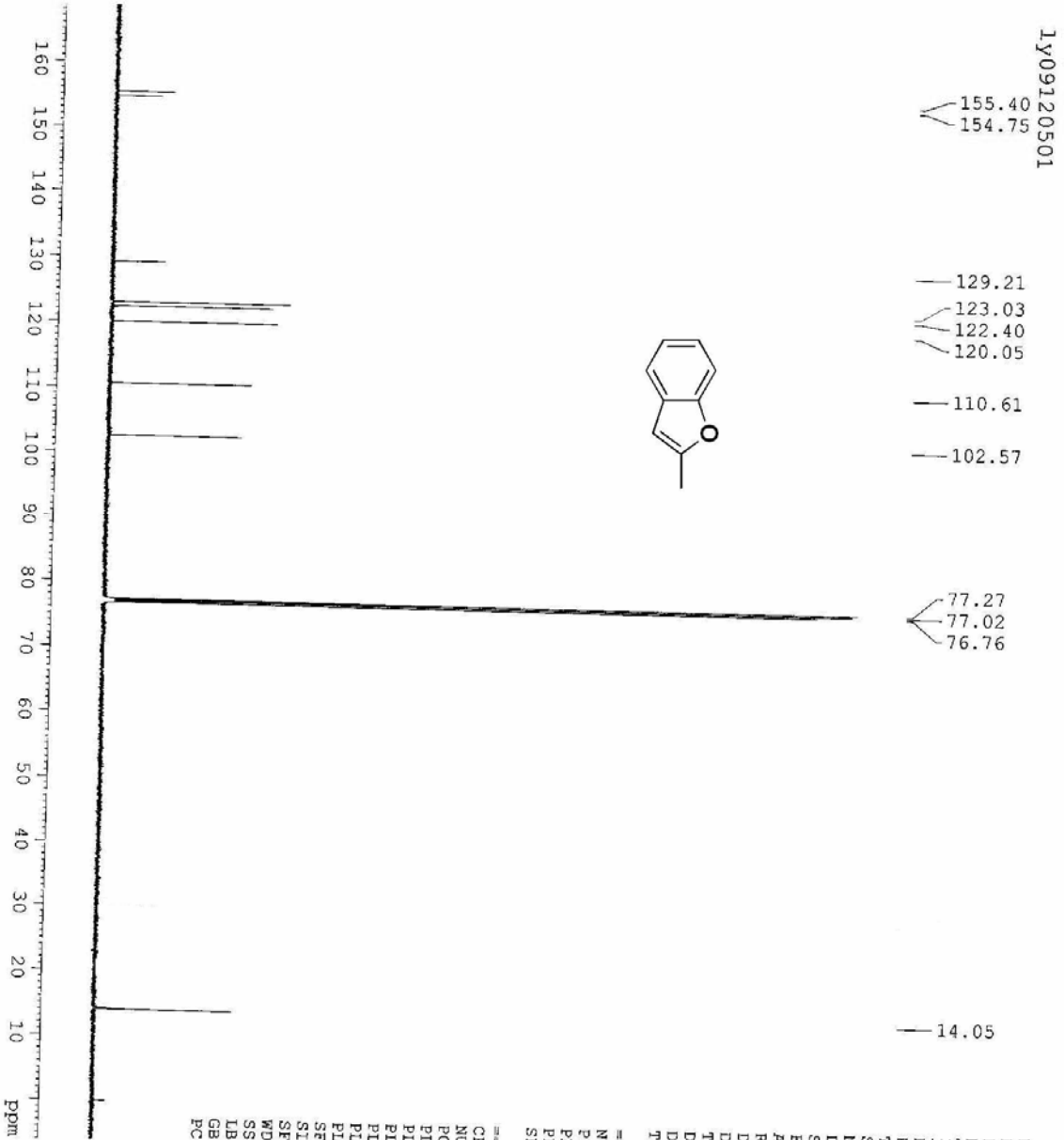
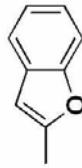


LY100309-01

2-Methylbenzofuran (26)



2-Methylbenzofuran (26)



1Y09120501

155.40
154.75

129.21
123.03
122.40
120.05

110.61
102.57

77.27
77.02
76.76

14.05

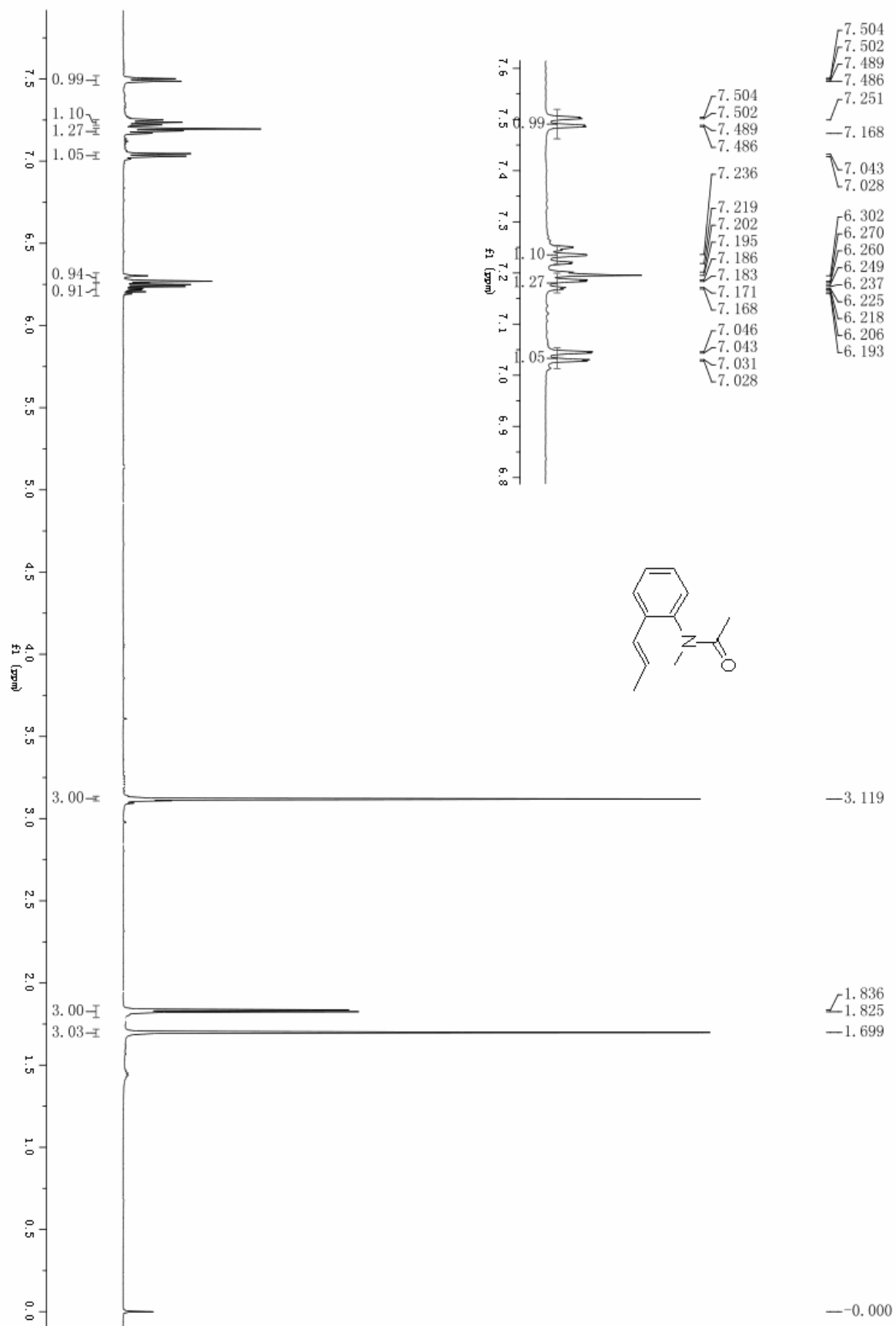
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NAME 1Y09120501
EXPNO 2
PROCNO 1
Date_ 20091208
Time_ 5.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65336
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

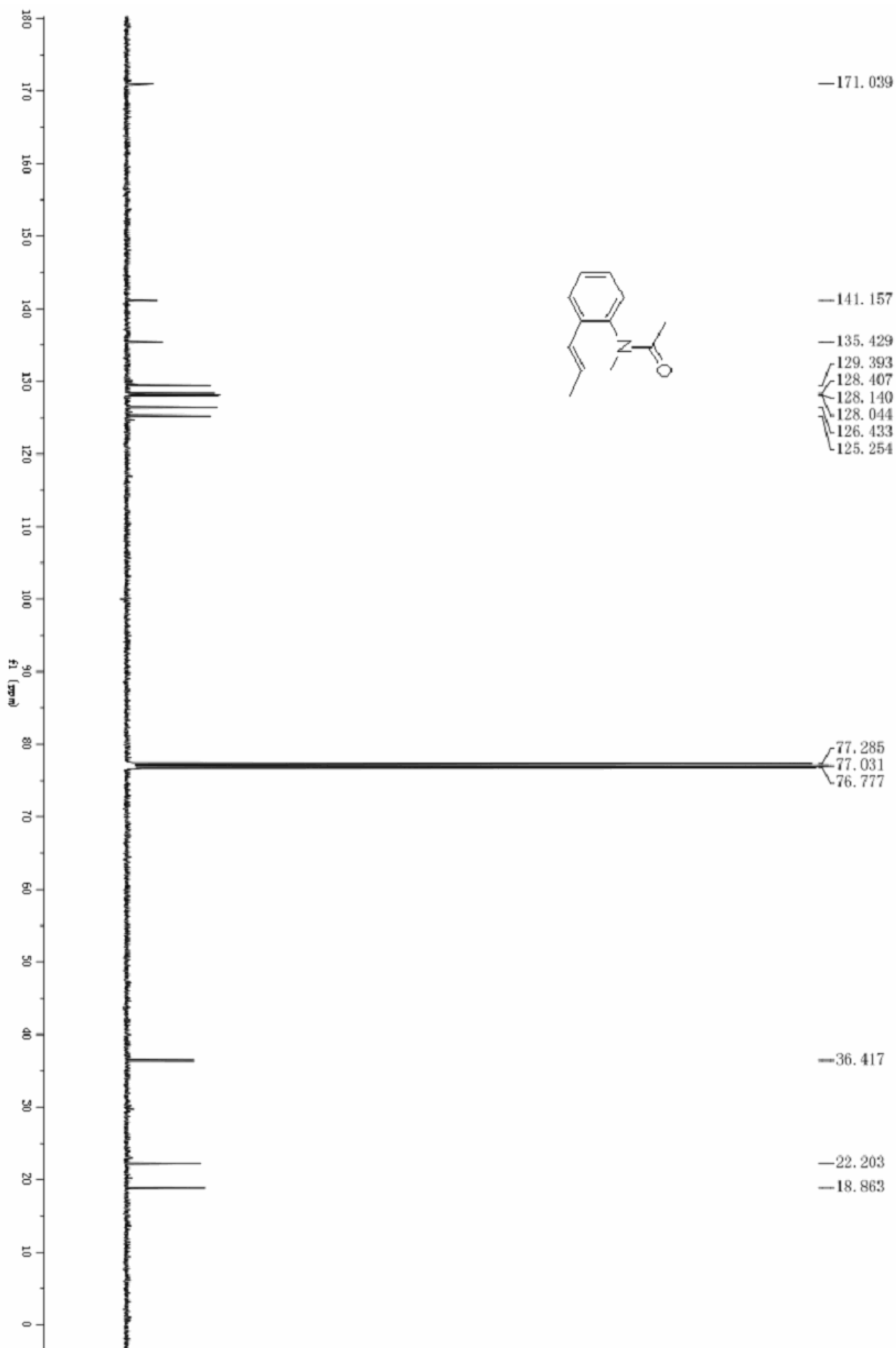
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 usec
PL1 0.00 dB
PL1W 90.67910004 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
P12 1.90 dB
PL12 16.86 dB
PL13 16.86 dB
PL2W 14.92065334 W
PL12W 0.47619823 W
PL13W 0.47619823 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
    
```

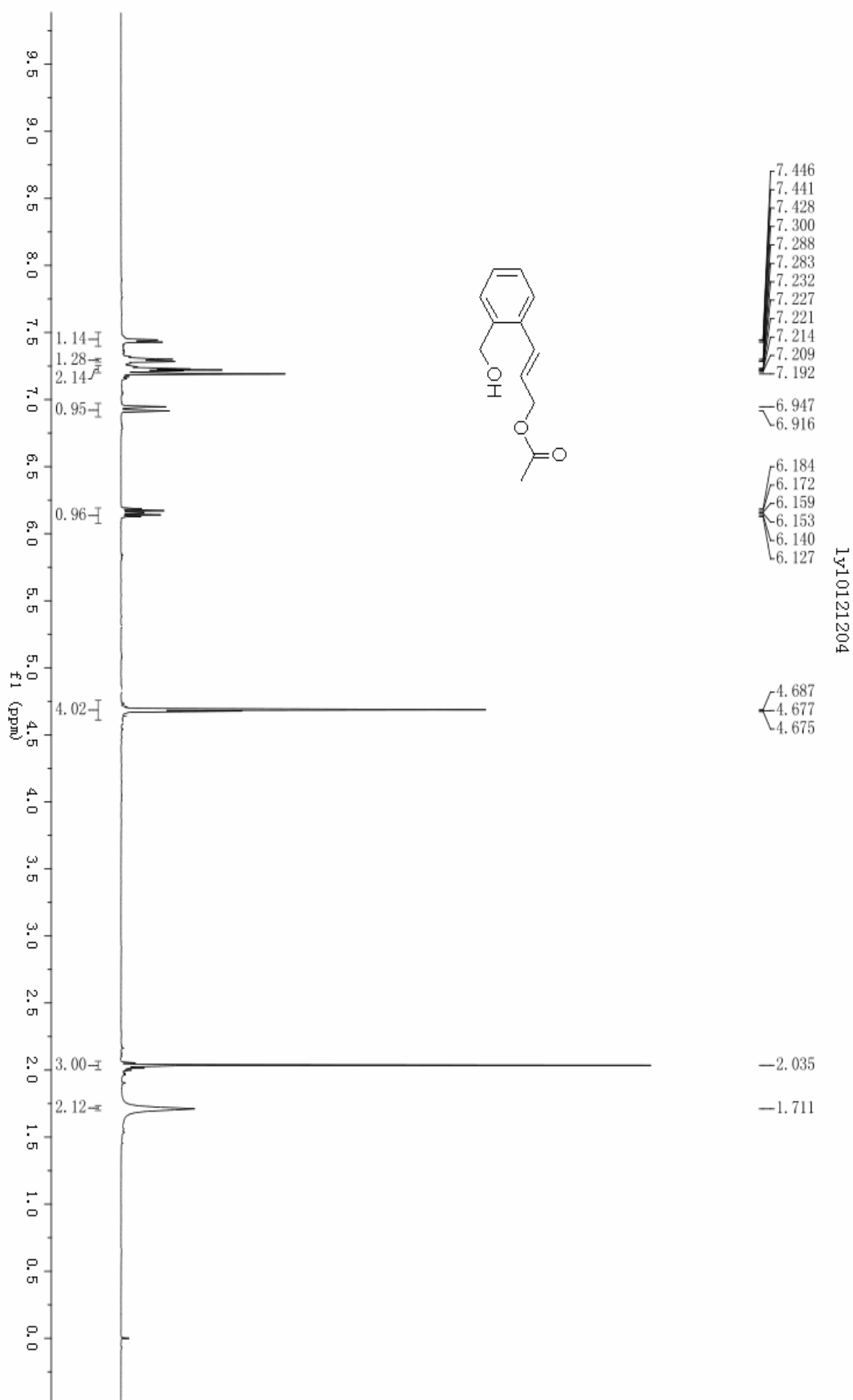
(E)-N-Methyl-N-(2-(prop-1-enyl)phenyl)acetamide (27)



(E)-N-Methyl-N-(2-(prop-1-enyl)phenyl)acetamide (27)



(E)-3-(2-(Hydroxymethyl)phenyl)allyl acetate (28)



(E)-3-(2-(Hydroxymethyl)phenyl)allyl acetate (28)

