Electronic Supplementary Information

Orthogonal Aerobic Conversion of *N*-Benzyl Amidoximes to 1,2,4-Oxadiazoles or Quinazolinones

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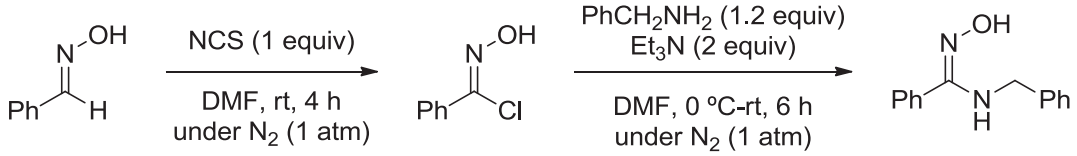
1. General

^{1}H NMR (400 MHz) spectra were recorded on a Bruker Avance 400 spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{1}H, δ = 7.26) or DMSO-d_6 (for ^{1}H, δ = 2.50) as the internal standard]. ^{13}C NMR (100 MHz) spectra on a Bruker Avance 400 spectrometer in $CDCl_3$ [using $CDCl_3$ (for ^{13}C, δ = 77.0) or DMSO-d_6 (for ^{13}C, δ = 39.5) as internal standard]. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, ddd = doublet of doublet of doublet, dt = doublet of triplet, sep = septet, m = multiplet, s br = single broad. IR spectra were recorded on a Shimazu IR Prestige-21 FT-IR Spectrometer. High-resolution mass spectra were obtained with a Q-Tof Premier LC HR mass spectrometer. X-ray crystallography analysis was performed on Bruker X8 APEX X-ray diffractionmeter. Melting points were uncorrected and were recorded on a Buchi B-54 melting point apparatus. IR spectra were recorded on a Shimadzu IR Prestige-21 FT-IR Spectrometer. Flash column chromatography was performed using Merck silica gel 60 with distilled solvents. DMSO (anhydrous), DMF (anhydrous), K_3PO_4, K_2CO_3 and Cs_2CO_3 were purchased from Sigma-Aldrich Co., Inc.

2. Preparation of amidoximes 1

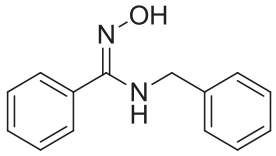
A typical procedure for synthesis of amidoxime **1a**:[1]



To the solution of oxime (2.043 g, 16.88 mmol) in *N*,*N*-dimethylformamide (55.0 mL) at room temperature was added *N*-chlorosuccinimide (2.254 g, 16.88 mmol) in five portions. During each addition, the reaction mixture became yellow and then gradually returned to near colorless. After the addition was complete, the reaction mixture was stirred at room temperature for 4 h. The chlorooxime generated was used in situ. Benzylamine (2.21 mL, 20.26 mmol) and triethylamine (4.71 mL, 33.76 mmol) was added dropwise at 0 °C to the reaction mixture. The reaction mixture was stirred at 0 °C for 2 h and room temperature for 4 h. After that, the reaction

mixture was diluted with H_2O, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude material was purified by flash column chromatography (silica gel; hexane: ethyl acetate = 75 : 25) to afford benzylamidoxime (3.015 g, 13.32 mmol, 79% yield) as a white solid.

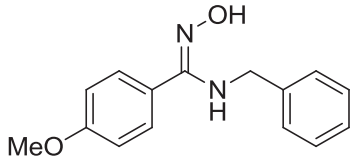
***(Z)*-*N*-benzyl-*N'*-hydroxybenzimidamide (1a):**



79% yield as a white solid from benzaldehyde oxime[2] and benzylamine.

mp: 117-118 °C; IR (NaCl) 3392, 3053, 2986, 1628, 1576, 1497, 1477, 1146 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.24 (2H, s), 5.70 (1H, s), 7.19-7.25 (3H, m), 7.30 (2H, dd, J = 7.2, 7.6 Hz), 7.33-7.42 (3H, m), 7.46-7.48 (2H, m), 8.68 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.4, 126.8, 127.2, 128.4, 128.5, 128.6, 129.6, 131.2, 139.5, 156.5; ESIHRMS: Found: *m/z* 227.1183. Calcd for $C_{14}H_{15}N_2O$: $(M+H)^+$ 227.1184.

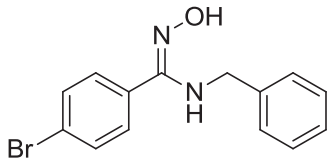
***(Z)*-*N*-benzyl-*N'*-hydroxy-4-methoxybenzimidamide (1c):**



98% yield as a white solid from 4-methoxybenzaldehyde oxime[3] and benzylamine.

mp: 139-140 °C; IR (NaCl) 3395, 3053, 2986, 1624, 1609, 1521, 1421, 1175 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.79 (3H, s), 4.24 (2H, s), 5.71 (1H, s), 6.86-6.88 (2H, m), 7.19-7.24 (3H, m), 7.27-7.31 (2H, m), 7.39 (2H, d, J = 8.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.4, 55.2, 113.8, 123.5, 126.7, 127.1, 128.5, 129.8, 139.7, 156.3, 160.6; ESIHRMS: Found: *m/z* 257.1285. Calcd for $C_{15}H_{17}N_2O_2$: $(M+H)^+$ 257.1290.

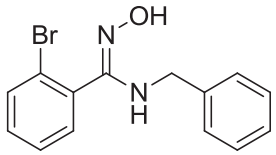
***(Z)*-*N*-benzyl-4-bromo-*N'*-hydroxybenzimidamide (1d):**



85% yield as a white solid from 4-bromobenzaldehyde oxime[4] and benzylamine.

mp: 138-140 °C; IR (NaCl) 3394, 3053, 2986, 1631, 1494, 1421, 1150, 1070 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.21 (2H, d, *J* = 5.2 Hz), 5.70 (1H, s), 7.18 (2H, d, *J* = 6.8 Hz), 7.23-7.26 (1H, m), 7.29-7.34 (4H, m), 7.49 (2H, d, *J* = 8.4 Hz), 8.75 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.4, 124.0, 126.7, 127.3, 128.7, 130.1 (overlapped), 131.7, 139.2, 155.7; ESIHRMS: Found: *m/z* 305.0293. Calcd for $C_{14}H_{14}N_2O^{79}Br$: $(M+H)^+$ 305.0289.

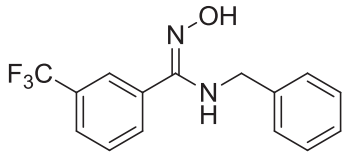
***(Z)*-*N*-benzyl-2-bromo-*N′*-hydroxybenzimidamide (1e):**



82% yield as a white solid from 2-bromobenzaldehyde oxime, which was prepared by condensation of 2-bromobenzaldehyde and hydroxylamine hydrochloride in the presence of sodium acetate in ethanol.[5] The crude oxime was used directly without further purification.

mp: 124-126 °C; IR (NaCl) 3404, 3053, 2985, 1636, 1483, 1451, 1208, 1153 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.06 (2H, s), 5.72 (1H, s), 7.16-7.33 (8H, m), 7.59 (1H, dd, *J* = 2.0, 7.2 Hz), 8.66 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 46.9, 123.5, 127.2 (overlapped), 127.3, 128.5, 130.9, 131.7, 132.4, 132.9, 138.9, 154.3; ESIHRMS: Found: *m/z* 305.0286. Calcd for $C_{14}H_{14}N_2O^{79}Br$: $(M+H)^+$ 305.0289.

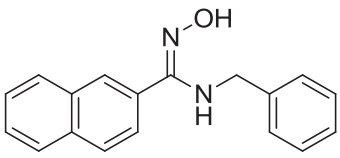
***(Z)*-*N*-benzyl-*N′*-hydroxy-3-(trifluoromethyl)benzimidamide (1f):**



48% yield as a pale yellow solid from 3-(trifluoromethyl)benzaldehyde oxime, which was prepared by condensation of 3-(trifluoromethyl)benzaldehyde and hydroxylamine hydrochloride in the presence of sodium acetate in ethanol.[5] The crude oxime was used directly without further purification.

mp: 107-109 °C; IR (NaCl) 3394, 3053, 2985, 1634, 1591, 1494, 1452, 1130 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.19 (2H, d, *J* = 5.6 Hz), 5.76 (1H, s), 7.15 (2H, d, *J* = 7.2 Hz), 7.22-7.31 (3H, m), 7.47 (1H, dd, *J* = 7.6, 8.0 Hz), 7.64 (2H, t, *J* = 9.2 Hz), 7.72 (1H, s), 9.23 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.5, 123.7 (q, *J* = 270.7), 125.6 (q, *J* = 3.6 Hz), 126.3 (q, *J* = 3.4 Hz), 126.7, 127.4, 128.7, 128.9, 130.9 (q, *J* = 32.5 Hz), 131.82, 132.0, 139.1, 155.4; ESIHRMS: Found: *m/z* 295.1059. Calcd for $C_{15}H_{14}N_2OF_3$: $(M+H)^+$ 295.1058.

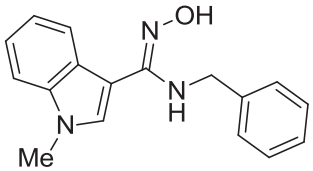
***(Z)*-*N*-benzyl-*N'*-hydroxy-2-naphthimidamide (1g):**



64% yield as a pale yellow solid from 2-naphthaldehyde oxime[6] and benzylamine.

mp: 105-107 °C; IR (NaCl) 3394, 3053, 2986, 1635, 1475, 1420, 1146 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.27 (2H, d, *J* = 3.2 Hz), 5.77 (1H, s), 7.19-7.31 (5H, m), 7.47-7.56 (3H, m), 7.81-7.85 (3H, m), 7.98 (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.6, 125.6, 126.4, 126.77, 126.84, 127.2, 127.7, 128.1, 128.4, 128.59, 128.61, 132.9, 133.8, 139.5,156.7; ESIHRMS: Found: *m/z* 277.1338. Calcd for $C_{18}H_{17}N_2O$: $(M+H)^+$ 277.1341.

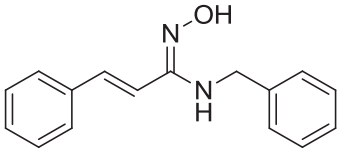
***(Z)*-*N*-benzyl-*N'*-hydroxy-1-methyl-1H-indole-3-carboximidamide (1h):**



42% yield as a pale yellow solid from 1-methyl-1H-indole-3-carbaldehyde oxime[7] and benzylamine.

mp: decompose temperature: 195-198 °C; IR (NaCl) 3402, 3053, 2986, 1630, 1560, 1479, 1422, 1157 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 3.78 (3H, s), 4.27 (2H, d, *J* = 6.8 Hz), 6.11 (1H, t, *J* = 6.8 Hz), 7.08 (1H, dd, *J* = 7.2, 8.0 Hz), 7.16-7.20 (4H, m), 7.26 (2H, dd, *J* = 7.2, 8.0 Hz), 7.44-7.45 (2H, m), 7.68 (1H, d, *J* = 8.0 Hz), 9.58 (1H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 32.5, 46.7, 106.1, 109.9, 119.7, 120.1, 121.5, 126.2, 126.5 (overlapped), 128.1, 129.7, 136.4, 141.2, 150.5; ESIHRMS: Found: *m/z* 280.1452. Calcd for $C_{17}H_{18}N_3O$: $(M+H)^+$ 280.1450.

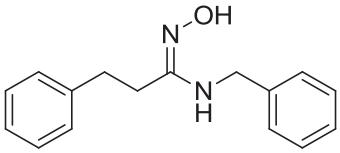
***(Z)-N*-benzyl-*N'*-hydroxycinnamimidamide (1j):**



81% yield as a pale yellow solid from cinnamaldehyde oxime[8] and benzylamine.

IR (NaCl) 3385, 3053, 2986, 1653, 1494, 1450, 1419 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.43 (2H, s), 5.63 (1H, s), 6.49 (1H, d, *J* = 16.0 Hz), 7.18 (1H, d, *J* = 16.0 Hz), 7.24-7.38 (10H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 46.7, 116.7, 126.7, 127.0, 127.2, 128.5 (overlapped), 128.6, 135.7, 135.9, 139.4, 153.8; ESIHRMS: Found: *m/z* 253.1345. Calcd for $C_{16}H_{17}N_2O$: $(M+H)^+$ 253.1341.

***(Z)-N*-benzyl-*N'*-hydroxy-3-phenylpropanimidamide (1k):**

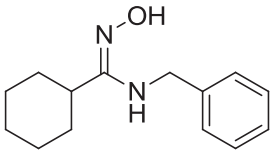


67% yield as a yellow solid from 3-phenylpropanal oxime[9] and benzylamine.

mp: 81-83 °C; IR (NaCl) 3211, 3053, 2986, 2868, 2831, 1643, 1497, 1452, 1421, 1153 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 2.49-2.53 (2H, m), 2.86-2.90 (2H, m), 4.34 (2H, d, *J* = 6.0 Hz), 5.59 (1H, s), 7.15-7.21 (3H, m), 7.25-7.29 (5H, m), 7.33-7.36 (2H,

m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.6, 32.8, 46.0, 126.2, 126.8, 127.4, 128.3, 128.5, 128.7, 139.1, 141.0, 154.8; ESIHRMS: Found: *m/z* 255.1496. Calcd for $C_{16}H_{19}N_2O$: $(M+H)^+$ 255.1497.

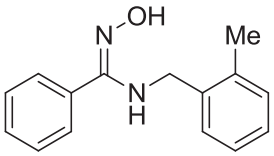
***(Z)*-*N*-benzyl-*N'*-hydroxycyclohexanecarboximidamide (1l):**



67% yield as a white solid from cyclohexanecarbaldehyde oxime[10] and benzylamine.

mp: 124-126 °C; IR (NaCl) 3315, 3053, 2983, 1636, 1494, 1450, 1420, 1340, 1140 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16-1.26 (3H, m), 1.39 (2H, q, *J* = 12.0 Hz), 1.65-1.66 (1H, m), 1.75-1.76 (2H, m), 1.87 (2H, d, *J* = 13.2 Hz), 2.22-2.30 (1H, m), 4.34 (2H, d, *J* = 5.6 Hz), 5.50 (1H, s), 7.25-7.36 (5H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 26.0, 26.3, 30.6, 37.4, 45.8, 126.9, 127.3, 128.6, 139.4, 158.2; ESIHRMS: Found: *m/z* 233.1653. Calcd for $C_{14}H_{21}N_2O$: $(M+H)^+$ 233.1654.

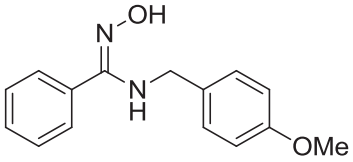
***(Z)*-*N'*-hydroxy-*N*-(2-methylbenzyl)benzimidamide (1m):**



81% yield as a white solid from benzaldehyde oxime and *o*-tolylmethanamine.

mp: 145-148 °C; IR (NaCl) 3053, 2985, 1629, 1575, 1419, 1344, 1153 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.16 (3H, s), 4.18 (2H, s), 5.58 (1H, s), 7.09-7.11 (1H, m), 7.13-7.18 (2H, m), 7.24-7.27 (1H, m), 7.34-7.41 (3H, m), 7.46-7.48 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.8, 45.6, 126.2, 127.2, 127.3, 128.38, 128.44, 129.6, 130.2, 131.3, 135.5, 137.2, 156.5; ESIHRMS: Found: *m/z* 241.1337. Calcd for $C_{15}H_{17}N_2O$: $(M+H)^+$ 241.1341.

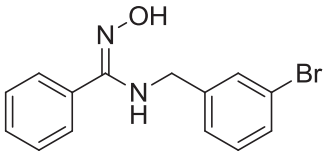
***(Z)*-*N'*-hydroxy-*N*-(4-methoxybenzyl)benzimidamide (1n):**



88% yield as a pale yellow solid from benzaldehyde oxime and (4-methoxyphenyl)methanamine.

mp: 75-77 °C; IR (NaCl) 3393, 3053, 2956, 1628, 1576, 1512, 1463, 1445, 1175 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.78 (3H, s), 4.15 (2H, s), 5.63 (1H, s), 6.81-6.84 (2H, m), 7.10 (2H, d, *J* = 8.4 Hz), 7.34-7.40 (3H, m), 7.45-7.48 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 46.9, 55.2, 113.9, 128.1, 128.4, 128.5, 129.5, 131.3, 131.6, 156.4, 158.7; ESIHRMS: Found: *m/z* 257.1283. Calcd for $C_{15}H_{17}N_2O_2$: $(M+H)^+$ 257.1290.

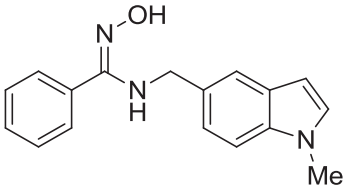
***(Z)*-*N*-(3-bromobenzyl)-*N'*-hydroxybenzimidamide (1o):**



84% yield as a pale yellow solid from benzaldehyde oxime and (3-bromophenyl)methanamine.

mp: 106-108 °C; IR (NaCl) 3396, 3053, 2985, 1631, 1572, 1473, 1445, 1422, 1150 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20 (2H, s), 5.72 (1H, s), 7.10-7.18 (2H, m), 7.32-7.44 (7H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 46.7, 122.7, 125.3, 128.4, 128.5, 129.7, 129.8, 130.1, 130.3, 130.8, 141.9, 156.2; ESIHRMS: Found: *m/z* 305.0289. Calcd for $C_{14}H_{14}N_2O^{79}Br$: $(M+H)^+$ 305.0289.

***(Z)*-*N'*-hydroxy-*N*-((1-methyl-1*H*-indol-5-yl)methyl)benzimidamide (1p):**

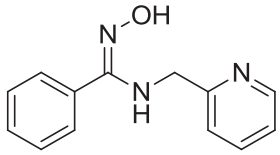


72% yield as a yellow solid from benzaldehyde oxime and (1-methyl-1H-indol-5-yl)methanamine, which was prepared by reduction of

1-methylindole-5-carbonitrile[11] with lithium aluminum hydride in tetrahydrofuran.[12] The crude amine was used directly without further purification.

mp: 172-175 °C; IR (NaCl) 3383, 3053, 2986, 1636, 1422, 1153 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 3.74 (3H, s), 4.22 (2H, d, *J* = 6.8 Hz), 6.12 (1H, t, *J* = 6.8 Hz), 6.34 (1H, d, *J* = 2.8 Hz), 6.92 (1H, dd, *J* = 1.2, 8.4 Hz), 7.26-7.32 (3H, m), 7.37-7.41 (5H, m), 9.82 (1H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 32.4, 40.1, 47.0, 100.1, 109.4, 118.3, 120.4, 127.9, 128.10, 128.13, 128.9, 129.7, 131.2, 132.6, 135.5, 155.0; ESIHRMS: Found: *m/z* 280.1449. Calcd for $C_{17}H_{18}N_3O$: $(M+H)^+$ 280.1450.

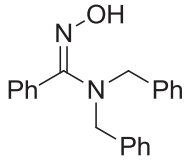
***(Z)-N′*-hydroxy-*N*-(pyridin-4-ylmethyl)benzimidamide (1q):**



74% as a white solid from benzaldehyde oxime and pyridin-2-ylmethanamine.

mp: 166-168 °C; IR (NaCl) 3420, 3053, 2986, 1628, 1568, 1512, 1437, 1422, 1130 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6) δ 4.24 (2H, d, *J* = 6.4 Hz), 6.53 (1H, t, *J* = 6.4 Hz), 7.22 (1H, dd, *J* = 5.6, 7.2 Hz), 7.29 (1H, d, *J* = 8.0 Hz), 7.34-7.41 (5H, m), 7.75 (1H, dt, *J* = 2.0, 7.6 Hz), 8.44 (1H, d, *J* = 4.8 Hz), 9.88 (1H, s); ^{13}C NMR (100 MHz, DMSO-d_6) δ 48.1, 120.7, 121.9, 128.0, 128.2, 128.9, 132.4, 136.6, 148.7, 154.6, 159.3; ESIHRMS: Found: *m/z* 228.1137. Calcd for $C_{13}H_{14}N_3O$: $(M+H)^+$ 228.1137.

***(Z)-N,N*-dibenzyl-*N′*-hydroxybenzimidamide (1r):**

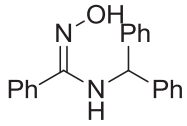


The preparation of **1r** was slightly modified from the general procedure. In this reaction, 2 equiv of oxime and 2 equiv of *N*-chlorosuccinimide were used in the first step while 1 equiv of dibenzylamine and 2.5 equiv of triethylamine were employed in the second step.

80% yield as a white solid from benzaldehyde oxime and dibenzylamine.

mp: 144-146 °C; IR (NaCl) 3394, 3053, 2986, 2864, 1630, 1495, 1452, 1420, 1141 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.20 (4H, s), 6.29 (1H, s br), 7.19 (4H, d, *J* = 7.2 Hz), 7.23-7.27 (2H, m), 7.31 (4H, dd, *J* = 7.2, 7.6 Hz), 7.39-7.47 (3H, m), 7.51 (2H, d, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 50.6, 127.1, 127.9, 128.4, 128.5, 128.9, 129.4, 131.1, 137.8, 160.9; ESIHRMS: Found: *m/z* 317.1655. Calcd for $C_{21}H_{21}N_2O$: $(M+H)^+$ 317.1654.

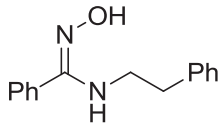
(*Z*)-*N*-benzhydryl-*N'*-hydroxybenzimidamide (1s):



58% yield as a white solid from benzaldehyde oxime and diphenylmethanamine.

mp: 161-163 °C; IR (NaCl) 3392, 3055, 2986, 1632, 1492, 1452, 1379, 1134 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.49 (1H, d, *J* = 9.6 Hz), 5.97 (1H, d, *J* = 9.6 Hz), 7.15 (4H, d, *J* = 7.6 Hz), 7.22-7.38 (11H, m), 7.84 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 60.9, 127.2, 127.3, 128.3, 128.4, 128.5, 129.6, 131.4, 142.5, 156.1; ESIHRMS: Found: *m/z* 303.1498. Calcd for $C_{20}H_{19}N_2O$: $(M+H)^+$ 303.1497.

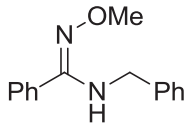
(*Z*)-*N*'-hydroxy-*N*-phenethylbenzimidamide (1t):



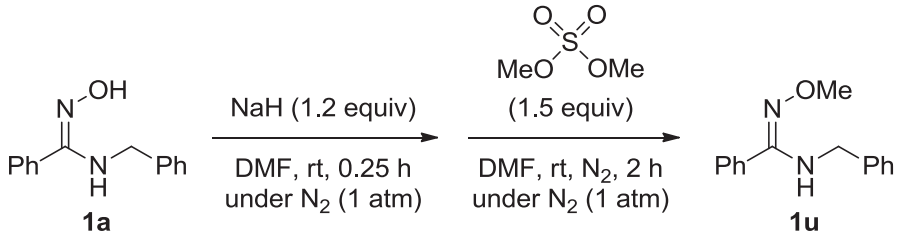
72% yield as a colourless oil from benzaldehyde oxime and 2-phenethylamine.

IR (NaCl) 3385, 3061, 2941, 1627, 1494, 1454, 1392, 1145 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.69 (2H, d, *J* = 7.2 Hz), 3.25 (2H, d, *J* = 6.8 Hz), 5.39 (1H, s br), 7.05-7.07 (2H, m), 7.17-7.26 (3H, m), 7.34-7.42 (5H, m), 8.74 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 37.9, 45.1, 126.4, 128.3, 128.5, 128.8, 129.4, 131.5, 138.5, 156.3; ESIHRMS: Found: *m/z* 241.1336. Calcd for $C_{20}H_{19}N_2O$: $(M+H)^+$ 241.1341.

(*Z*)-*N*-benzyl-*N*'-methoxybenzimidamide (1u):



Procedure for synthesis of **1u**:

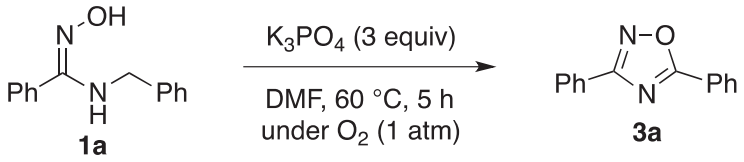


To a suspension of NaH 60 % dispersion in mineral oil (148.7 mg, 3.719 mmol) in DMF (5.0 mL) was added the solution of *(Z)*-*N*-benzyl-*N*'-hydroxybenzimidamide (701.1 mg, 3.099 mmol) in DMF (6 mL) dropwise at room temperature. After the addition was complete, the reaction mixture was stirred at room temperature for 15 min. Then dimethyl sulfate (381 μL, 4.028 mmol) was added dropwise to the reaction mixture. The reaction mixture was stirred at room temperature for 4 h. After that, the reaction mixture was diluted with H_2O, and the aqueous layer was extracted three times with EtOAc. The combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated. The crude material was purified by flash column chromatography (silica gel; hexane: ethyl acetate = 7 : 3) to afford (*Z*)-*N*-benzyl-*N*'-methoxybenzimidamide (1u) (564.6 mg, 2.350 mmol, 76% yield) as a colourless oil.

IR (NaCl) 3398, 1614, 1573, 1497, 1464, 1402, 1354, 1265, 1145 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.88 (3H, s), 4.21 (2H, d, J = 6.4 Hz), 5.59 (1H, s br), 7.20-7.27 (3H, m), 7.30-7.40 (5H, m), 7.46-7.48 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 47.4, 61.2, 126.7, 127.1, 128.3, 128.48, 128.49, 129.5, 131.0, 139.4, 156.0; ESIHRMS: Found: *m/z* 241.1340. Calcd for $C_{15}H_{16}N_2O$: $(M+H)^+$ 241.1341.

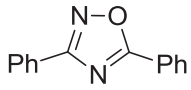
3. Synthesis of 1,2,4-oxadiazoles 3

A typical procedure for synthesis of **3a**:



To a solution of (*Z*)-*N*-benzyl-*N*′-hydroxybenzimidamide (113.8 mg, 0.503 mmol) in DMF (5 mL) was added K_3PO_4 (320.3 mg, 1.509 mmol). The reaction mixture was then stirred for 5 h at 60 ºC under an O_2 atmosphere. The resulting mixture was diluted with water and extracted three times with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$ and concentrated. Purification of the crude product by flash column chromatography (silica gel; hexane: ethyl acetate = 75 : 25) afforded **3a** (87.5 mg, 0.394 mmol, 78% yield) as a white solid.

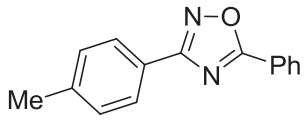
3,5-diphenyl-1,2,4-oxadiazole (3a):[13]



Reaction time: 5 h.

Yield: 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50-7.63 (6H, m), 8.17-8.20 (2H, m), 8.21-8.24 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.3, 126.9, 127.5, 128.1, 128.8, 129.1, 131.2, 132.7, 168.9, 175.7.

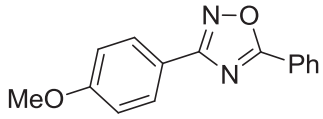
5-phenyl-3-(p-tolyl)-1,2,4-oxadiazole (3b):[14]



Reaction time: 5 h.

Yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.40 (3H, s), 7.29 (2H, d, J = 8.0 Hz), 7.49-7.57 (3H, m), 8.04-8.07 (2H, m), 8.18-8.20 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 124.3, 124.7, 127.4, 128.1, 129.0, 129.5, 132.6, 141.4, 168.9, 175.4.

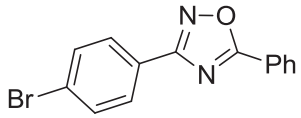
3-(4-methoxyphenyl)-5-phenyl-1,2,4-oxadiazole (3c):[15]



Reaction time: 10 h.

Yield: 83%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.85 (3H, s), 7.00 (2H, d, *J* = 8.8 Hz), 7.50-7.57 (3H, m), 8.10 (2H, d, *J* = 8.8 Hz), 8.19 (2H, d, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.3, 114.2, 119.4, 124.3, 128.0, 128.96, 129.04, 132.5, 161.8, 168.6, 175.3.

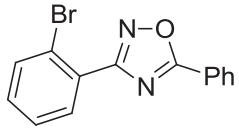
3-(4-bromophenyl)-5-phenyl-1,2,4-oxadiazole (3d):[16]



Reaction time: 5 h.

Yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.67 (5H, m), 8.06 (2H, dd, *J* = 1.6, 6.8 Hz), 8.21 (2H, dd, *J* = 1.6, 8.0 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.0, 125.7, 125.8, 128.1, 128.9, 129., 132.0, 132.8, 168.1, 175.8.

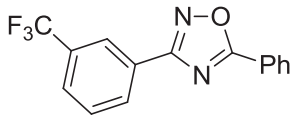
3-(2-bromophenyl)-5-phenyl-1,2,4-oxadiazole (3e):



Reaction time: 10 h.

Yield: 48%; Pale yellow solid, mp: 76-78 °C; IR (NaCl) 2985, 2829, 1610, 1558, 1489, 1464, 1421, 1361, 1141 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (1H, ddd, *J* = 1.6, 7.6, 8.0 Hz), 7.46 (1H, ddd, *J* = 1.2, 7.6, 8.0 Hz), 7.54-7.58 (2H, m), 7.61-7.64 (1H, m), 7.76 (1H, dd, *J* = 0.8, 8.0 Hz), 7.92 (1H, dd, *J* = 0.8, 7.6 Hz), 8.22-8.24 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 122.2, 124.0, 127.4, 128.2, 128.3, 129.1, 131.8, 131.9, 132.8, 134.1, 168.5, 175.3; ESIHRMS: Found: *m/z* 300.9969. Calcd for $C_{14}H_{10}{}^{79}BrN_2O$: $(M+H)^+$ 300.9976.

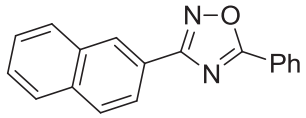
5-phenyl-3-(3-(trifluoromethyl)phenyl)-1,2,4-oxadiazole (3f):



Reaction time: 2 h.

Yield: 70%; White solid, mp: 90-92 °C; IR (NaCl) 3053, 2985, 1610, 1562, 1421, 1377, 1321, 1170 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (1H, s), 8.34 (1H, d, *J* = 8.0 Hz), 8.19-8.21 (2H, m), 7.76 (1H, d, *J* = 8.0 Hz), 7.59-7.64 (2H, m), 7.52-7.56 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 123.8 (q, *J* = 270.8 Hz), 124.0, 124.5 (q, *J* = 3.8 Hz), 127.7 (q, *J* = 3.6 Hz), 127.9, 128.2, 129.1, 129.4, 130.6, 131.4 (q, *J* = 32.7 Hz), 132.9, 167.9, 176.1; ESIHRMS: Found: *m/z* 291.0746. Calcd for $C_{15}H_{10}N_2OF_3$: $(M+H)^+$ 291.0745.

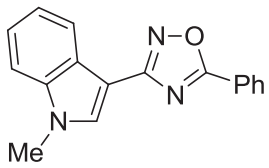
3-(naphthalen-2-yl)-5-phenyl-1,2,4-oxadiazole (3g):



Reaction time: 3 h.

Yield: 94%; White solid, mp: 121-123 °C; IR (NaCl) 3053, 2985, 1635, 1562, 1421, 1377, 1157 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.59 (5H, m), 7.85 (1H, dd, *J* = 4.0, 5.2 Hz), 7.91 (1H, d, *J* = 8.4 Hz), 7.94 (1H, dd, *J* = 4.0, 5.2 Hz), 8.19-8.22 (3H, m), 8.69 (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 123.9, 124.21, 124.23, 126.6, 127.4, 127.8, 128.0, 128.1, 128.6, 128.8, 129.0, 132.6, 133.0, 134.6, 168.9, 175.6; ESIHRMS: Found: *m/z* 273.1028. Calcd for $C_{18}H_{13}N_2O$: $(M+H)^+$ 273.1028.

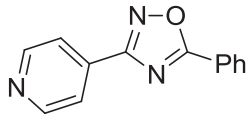
3-(1-methyl-1H-indol-3-yl)-5-phenyl-1,2,4-oxadiazole (3h):



Reaction time: 9 h.

Yield: 62%; Pale yellow solid, mp: 133-135 °C; IR (NaCl) 3053, 2985, 1610, 1587, 1562, 1494, 1479, 1421, 1303, 1118 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.78 (3H, s), 7.29-7.33 (3H, m), 7.48-7.57 (3H, m), 7.83 (1H, s), 8.18-8.21 (2H, m), 8.30-8.34 (1H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.1, 102.9, 109.6, 121.2, 121.9, 122.8, 124.5, 125.4, 128.0, 128.9, 131.4, 132.3, 137.3, 165.7, 174.2; ESIHRMS: Found: *m/z* 276.1135. Calcd for $C_{17}H_{14}N_3O$: $(M+H)^+$ 276.1137.

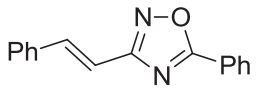
5-phenyl-3-(pyridin-4-yl)-1,2,4-oxadiazole (3i):



Reaction time: 2 h.

Yield: 72%; White solid, mp: 149-151 °C; IR (NaCl) 3053, 2985, 1635, 1421, 1370, 1155 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.56 (2H, dd, *J* = 7.2, 7.6 Hz), 7.61-7.65 (1H, m), 8.03 (2H, dd, *J* = 1.6, 4.4 Hz), 8.20-8.22 (2H, m), 8.80 (2H, dd, *J* = 1.6, 4.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 121.3, 123.8, 128.2, 129.1, 133.1, 134.3, 150.6, 167.4, 176.4; ESIHRMS: Found: *m/z* 224.0822. Calcd for $C_{13}H_{10}N_3O$: $(M+H)^+$ 224.0824.

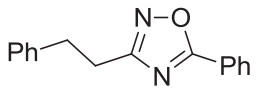
(*E*)-5-phenyl-3-styryl-1,2,4-oxadiazole (3j):



Reaction temperature: 80 ºC; reaction time: 4 h.

Yield: 65%; Pale yellow solid, mp: 101-103°C; IR (NaCl) 3053, 2985, 1645, 1610, 1564, 1504, 1447, 1421, 1378, 1157 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 7.11 (1H, d, *J* = 16.0 Hz), 7.33-7.42 (3H, m), 7.51-7.60 (5H, m), 7.81 (1H, d, *J* = 16.0 Hz), 8.18 (2H, dd, *J* = 1.6, 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 112.9, 124.2, 127.4, 128.1, 128.8, 129.0, 129.4, 132.7, 135.3, 139.1, 168.4, 174.9; ESIHRMS: Found: *m/z* 249.1023. Calcd for $C_{16}H_{13}N_2O$: $(M+H)^+$ 249.1028.

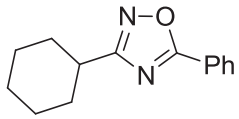
3-phenethyl-5-phenyl-1,2,4-oxadiazole (3k):



Reaction temperature: 80 ºC; reaction time: 7 h.

Yield: 76%; White solid, mp: 36-38°C; IR (NaCl) 3053, 2985, 1636, 1610, 1562, 1481, 1450, 1421, 1373, 1159 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.10-3.16 (4H, m), 7.19-7.32 (5H, m), 7.51 (2H, dd, *J* = 7.2, 7.6 Hz), 7.56-7.59 (1H, m), 8.11-8.14 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 28.0, 33.1, 124.2, 126.3, 128.0, 128.3, 128.5, 129.0, 132.6, 140.3, 170.5, 175.4; ESIHRMS: Found: *m/z* 251.1184. Calcd for $C_{16}H_{15}N_2O$: $(M+H)^+$ 251.1184.

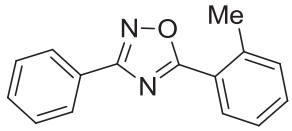
3-cyclohexyl-5-phenyl-1,2,4-oxadiazole (3l):[16]



Reaction time: 32 h.

Yield: 53%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.27-1.48 (3H, m), 1.60-1.78 (3H, m), 1.84-1.88 (2H, m), 2.07-2.11 (2H, m), 2.83-2.91 (1H, m), 7.50 (2H, dd, *J* = 7.2, 7.6 Hz), 7.57 (1H, t, *J* = 7.2 Hz), 8.12 (2H, d, *J* = 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 25.7, 25.8, 30.7, 36.0, 124.5, 128.0, 128.9, 132.4, 174.7, 175.1.

3-phenyl-5-(*o*-tolyl)-1,2,4-oxadiazole (3m):

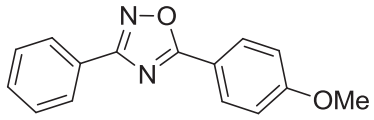


Reaction time: 10 h.

Yield: 65%; White solid, mp: 101-103°C; IR (NaCl) 3053, 2985, 1637, 1608, 1444, 1421, 1362, 1117 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.79 (3H, s), 7.35-7.39 (2H, m), 7.45-7.53 (4H, m), 8.16-8.20 (3H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.9, 123.4,

126.2, 127.1, 127.5, 128.8, 130.1, 131.1, 131.8, 132.1, 139.1, 168.5, 176.3; ESIHRMS: Found: *m/z* 237.1023. Calcd for $C_{15}H_{13}N_2O$: $(M+H)^+$ 237.1028.

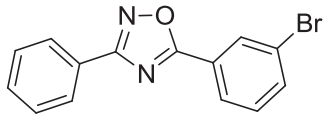
5-(4-methoxyphenyl)-3-phenyl-1,2,4-oxadiazole (3n):[17]



Reaction time: 9 h.

Yield: 59%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.86 (3H, s), 7.01 (2H, dd, *J* = 2.0, 7.2 Hz), 7.49-7.50 (3H, m), 8.13-8.17 (4H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.4, 114.4, 116.8, 127.1, 127.4, 128.8, 130.0, 131.0, 163.1, 168.7, 175.5.

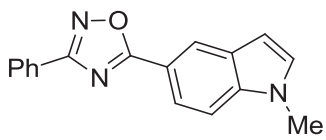
5-(3-bromophenyl)-3-phenyl-1,2,4-oxadiazole (3o):



Reaction time: 3 h.

Yield: 86%; White solid, mp: 110-112°C; IR (NaCl) 3053, 2985, 1638, 1556, 1444, 1421, 1361, 1072 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (1H, t, *J* = 8.0 Hz), 7.47-7.52 (3H, m), 7.69-7.71 (1H, m), 8.10-8.16 (3H, m), 8.34 (1H, dd, *J* = 1.6, 1.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 123.1, 126.0, 126.5, 126.6, 127.4, 128.8, 130.6, 130.9, 131.3, 135.6, 168.9, 174.2; ESIHRMS: Found: *m/z* 300.9979. Calcd for $C_{14}H_{10}{}^{79}BrN_2O$: $(M+H)^+$ 300.9976.

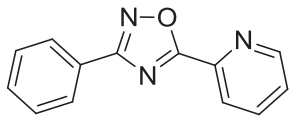
5-(1-methyl-1H-indol-5-yl)-3-phenyl-1,2,4-oxadiazole (3p):



Reaction time: 24 h.

Yield: 54%; White solid, mp: 169-171°C; IR (NaCl) 3053, 2985, 1616, 1593, 1553, 1483, 1421, 1361, 1155 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 3.81 (3H, s), 6.62 (1H, d, *J* = 3.2 Hz), 7.12 (1H, d, *J* = 3.2 Hz), 7.41 (1H, d, *J* = 8.8 Hz), 7.50-7.52 (3H, m), 8.06 (1H, dd, *J* = 1.2, 8.8 Hz), 8.17-8.21 (2H, m), 8.52 (1H, d, *J* = 1.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 33.0, 102.6, 109.7, 115.5, 121.4, 122.2, 127.4, 127.5, 128.4, 128.7, 130.6, 130.9, 138.8, 168.7, 177.1; ESIHRMS: Found: *m/z* 276.1142. Calcd for $C_{17}H_{14}N_3O$: $(M+H)^+$ 276.1137.

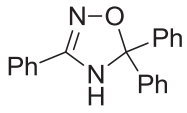
3-phenyl-5-(pyridin-2-yl)-1,2,4-oxadiazole (3q):



Reaction time: 24 h.

Yield: 54%; White solid, mp: 112-114°C; IR (NaCl) 3053, 2984, 1595, 1564, 1444, 1427, 1363, 1138 cm^{-1};^1H NMR (400 MHz, $CDCl_3$) δ 7.48-7.54 (4H, m), 7.90-7.95 (1H, m), 8.21-8.24 (2H, m), 8.29 (1H, d, *J* = 8.0 Hz), 8.86 (1H, d, *J* = 4.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 124.1, 126.5, 126.6, 127.5, 128.7, 131.3, 137.2, 143.6, 150.6, 169.1, 174.3; ESIHRMS: Found: *m/z* 224.0826. Calcd for $C_{13}H_9N_3O$: $(M+H)^+$ 224.0823.

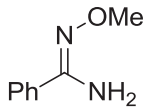
3,5,5-triphenyl-4,5-dihydro-1,2,4-oxadiazole (2r):



Reaction time: 19 h.

Yield: 33%; White solid, mp: 179-181°C; IR (NaCl) 3053, 2985, 2684, 1635, 1448, 1421, 1157 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$) δ 4.99 (1H, s), 7.34-7.45 (9H, m), 7.54-7.56 (4H, m), 7.77 (2H, d, *J* = 6.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 100.5, 125.6, 126.4, 126.5, 128.3, 128.5, 128.7, 130.8, 142.4, 154.6; ESIHRMS: Found: *m/z* 301.1347. Calcd for $C_{20}H_{17}N_2O$: $(M+H)^+$ 301.1341.

(*Z*)-*N*'-methoxybenzimidamide (1u'):[18]

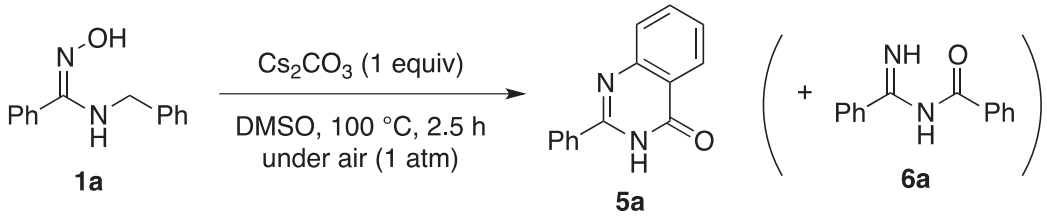


Reaction time: 100 ºC 24 h and 120 ºC 4 h.

Yield: 40%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.92 (3H, s), 4.79 (1H, s br), 7.37-7.39 (3H, m), 7.62 (2H, dd, *J* = 1.6, 7.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ 61.4, 125.8, 128.6, 129.9, 132.5, 151.8.

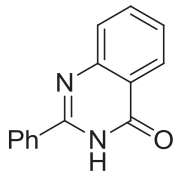
4. Synthesis of quinazolinones 5

A typical procedure for synthesis of **5a**:



To a solution of (*Z*)-*N*-benzyl-*N*′-hydroxybenzimidamide (113.3 mg, 0.501 mmol) in DMSO (5 mL) was added Cs_2CO_3 (163.1 mg, 0.501 mmol). The reaction mixture was then stirred for 2.5 h at 100 ºC under a dry air atmosphere. The resulting mixture was quenched with water and extracted four times with EtOAc. The combined organic extracts were washed with brine, dried over $MgSO_4$ and concentrated. Pure quinazolinone **5a** as a white solid was recrystallized from the crude material using hexane/ethyl acetate (57.1 mg, 0.257 mmol, 51% yield). The remaining residue was further purified by flash column chromatography (silica gel; hexane : ethyl acetate : triethyl amine = 75 : 25 : 1) afforded quinazolinone **5a** (15.0 mg, 0.067 mmol, 14% yield) as well as N-benzoly amidine **6a** (19.6 mg, 0.087 mmol, 17% yield) as a white solid. The combined yield of **5a** is 65% yield.

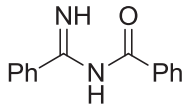
2-phenylquinazolin-4(3*H*)-one (5a):[19]



Reaction time: 2.5 h.

Yield: 65%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49-7.53 (1H, m), 7.57-7.60 (3H, m), 7.79-7.85 (2H, m), 8.15-8.17 (2H, m), 8.33 (1H, d, *J* = 7.6 Hz), 10.60 (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ 120.8, 126.4, 126.8, 127.3, 128.0, 129.1, 131.7, 132.8, 134.9, 149.5, 151.7, 163.7.

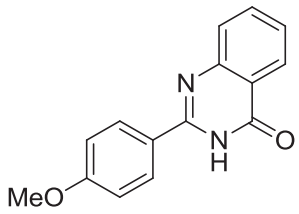
_N_-(imino(phenyl)methyl)benzamide (6a):



Reaction time: 2.5 h.

Yield: 17%; White solid, mp: 99-101°C; IR (NaCl) 3053, 2985, 1597, 1421, 1319, 1150 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$) δ 6.67 (1H, s br), 7.44-7.53 (5H, m), 7.59 (1H, t, *J* = 7.6 Hz), 8.04 (2H, d, *J* = 7.6 Hz), 8.38 (2H, d, *J* = 7.6 Hz), 10.75 (1H, s br); ^{13}C NMR (100 MHz, $CDCl_3$) δ 127.4, 128.1, 128.8, 129.7, 132.0, 132.4, 135.1, 137.7, 166.7, 180.5; ESIHRMS: Found: *m/z* 225.1023. Calcd for $C_{14}H_{12}N_2O$: $(M+H)^+$ 225.1027.

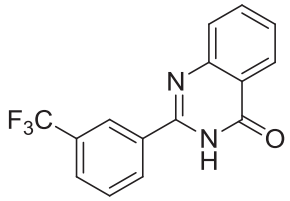
2-(4-methoxyphenyl)quinazolin-4(3*H*)-one (5c):[20]



Reaction time: 2 h.

Yield: 49%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.85 (3H, s), 7.09 (2H, d, *J* = 8.8 Hz), 7.48 (1H, dd, *J* = 7.2, 8.0 Hz), 7.70 (1H, d, *J* = 8.0 Hz), 7.79-7.83 (1H, m), 8.13 (1H, d, *J* = 8.0 Hz), 8.19 (2H, d, *J* = 8.8 Hz), 12.24 (1h, s br); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.4, 113.9, 120.6, 124.8, 125.8, 126.1, 127.1, 129.4, 134.5, 148.8, 151.9, 161.8, 162.3.

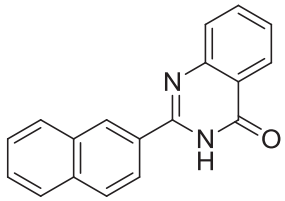
2-(3-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one (5f):



Reaction time: 2 h.

Yield: 51%; White solid, mp: 179-181°C; IR (NaCl) 3053, 2985, 1637, 1421, 1338, 1107 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.53-7.57 (1H, m), 7.80 (2H, dd, *J* = 8.0, 8.4 Hz), 7.84-7.88 (1H, m), 7.96 (1H, d, *J* = 8.0 Hz), 8.17 (1H, dd, *J* = 1.2, 8.0 Hz), 8.49 (1H, d, *J* = 7.6 Hz), 8.54 (1H, s), 12.75 (1H, s br); ^{13}C NMR (100 MHz, DMSO-d_6) δ 121.1, 123.9 (q, *J* = 270.0 Hz), 124.4 (q, *J* = 3.9 Hz), 125.8, 126.9, 127.5, 127.7 (q, *J* = 3.3 Hz), 129.4 (q, *J* = 32.0 Hz), 129.8, 131.7, 133.7, 134.6, 148.4, 151.0, 162.2; ESIHRMS: Found: *m/z* 291.0750. Calcd for $C_{15}H_{10}N_2OF_3$: $(M+H)^+$ 291.0745.

2-(naphthalen-2-yl)quinazolin-4(*3*H)-one (5g):

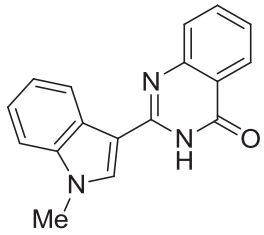


Reaction time: 2 h.

Yield: 53%; Pale yellow solid, mp: 285-287 ºC; IR (NaCl) 3053, 2985, 1647, 1421, 1153 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.55 (1H, dd, *J* = 7.2, 7.6 Hz), 7.61-7.67 (2H, m), 7.80 (1H, d, *J* = 8.0 Hz), 7.85-7.88 (1H, m), 8.01-8.09 (3H, m), 8.19 (1H, d, *J* = 7.6 Hz), 8.31 (1H, dd, *J* = 1.2, 8.4 Hz), 8.83 (1H, s), 12.67 (1H, s br); ^{13}C NMR

(100 MHz, DMSO-d_6) δ 121.0, 124.4, 125.8, 126.6, 126.8, 127.5, 127.6, 127.8, 128.0, 128.1, 128.9, 129.9, 132.2, 134.1, 134.5, 148.7, 152.1, 162.1; ESIHRMS: Found: *m/z* 273.1022. Calcd for $C_{18}H_{13}N_2O$: $(M+H)^+$ 273.1028.

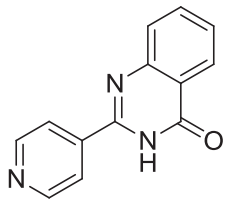
2-(1-methyl-1H-indol-3-yl)quinazolin-4(3*H*)-one (5h):



Reaction time: 2 h.

Yield: 44%; Pale yellow solid, mp: decompose, temperature: 290-295 ºC; IR (NaCl) 3053, 2985, 1680, 1651, 1595, 1377, 1157 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.89 (3H, s), 7.25-7.33 (2H, m), 7.39-7.43 (1H, m), 7.57 (1H, d, *J* = 8.0 Hz), 7.72 (1H, d, *J* = 7.6 Hz), 7.76-7.81 (1H, m), 8.10 (1H, dd, *J* = 0.8, 8.0 Hz), 8.52 (1H, s), 8.71 (1H, d, *J* = 7.6 Hz), 12.1 (1H, s br); ^{13}C NMR (100 MHz, DMSO-d_6) δ 33.3, 107.6, 110.5, 120.4, 121.2, 122.5, 122.7, 125.2, 125.8, 125.9, 126.9, 132.9, 134.4, 137.4, 149.7, 149.9, 162.1; ESIHRMS: Found: *m/z* 276.1131. Calcd for $C_{17}H_{14}N_3O$: $(M+H)^+$ 276.1137.

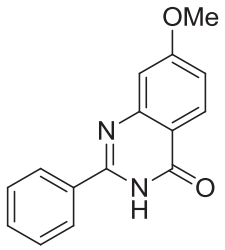
2-(pyridin-4-yl)quinazolin-4(3*H*)-one (5i):[21]



Reaction time: 3.5 h.

Yield: 49%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.58 (1H, dd, *J* = 7.2, 7.6 Hz), 7.79 (1H, d, *J* = 8.0 Hz), 7.88 (1H, dd, *J* = 7.2, 8.0 Hz), 8.11 (2H, d, *J* = 4.5 Hz), 8.18 (1H, d, *J* = 8.0 Hz), 8.79 (2H, d, *J* = 4.5 Hz), 12.77 (1H, s br); ^{13}C NMR (100 MHz, DMSO-d_6) δ 121.46, 121.55, 125.9, 127.4, 127.7, 134.7, 139.9, 148.2, 150.2, 150.5, 162.0.

7-methoxy-2-phenylquinazolin-4(3*H*)-one (5n):[22]



Reaction time: 2.5 h.

Yield: 58%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 3.89 (3H, s), 7.44 (1H, dd, J = 2.7, 7.5 Hz), 7.53-7.55 (4H, m), 7.70 (1H, d, J = 8.8 Hz), 8.16 (2H, d, J = 6.6 Hz), 12.51 (1H, s br); ^{13}C NMR (100 MHz, DMSO-d_6) δ 55.6, 105.8, 121.8, 124.1, 127.5, 128.6, 129.2, 131.0, 132.8, 143.2, 150.1, 157.7, 162.1.

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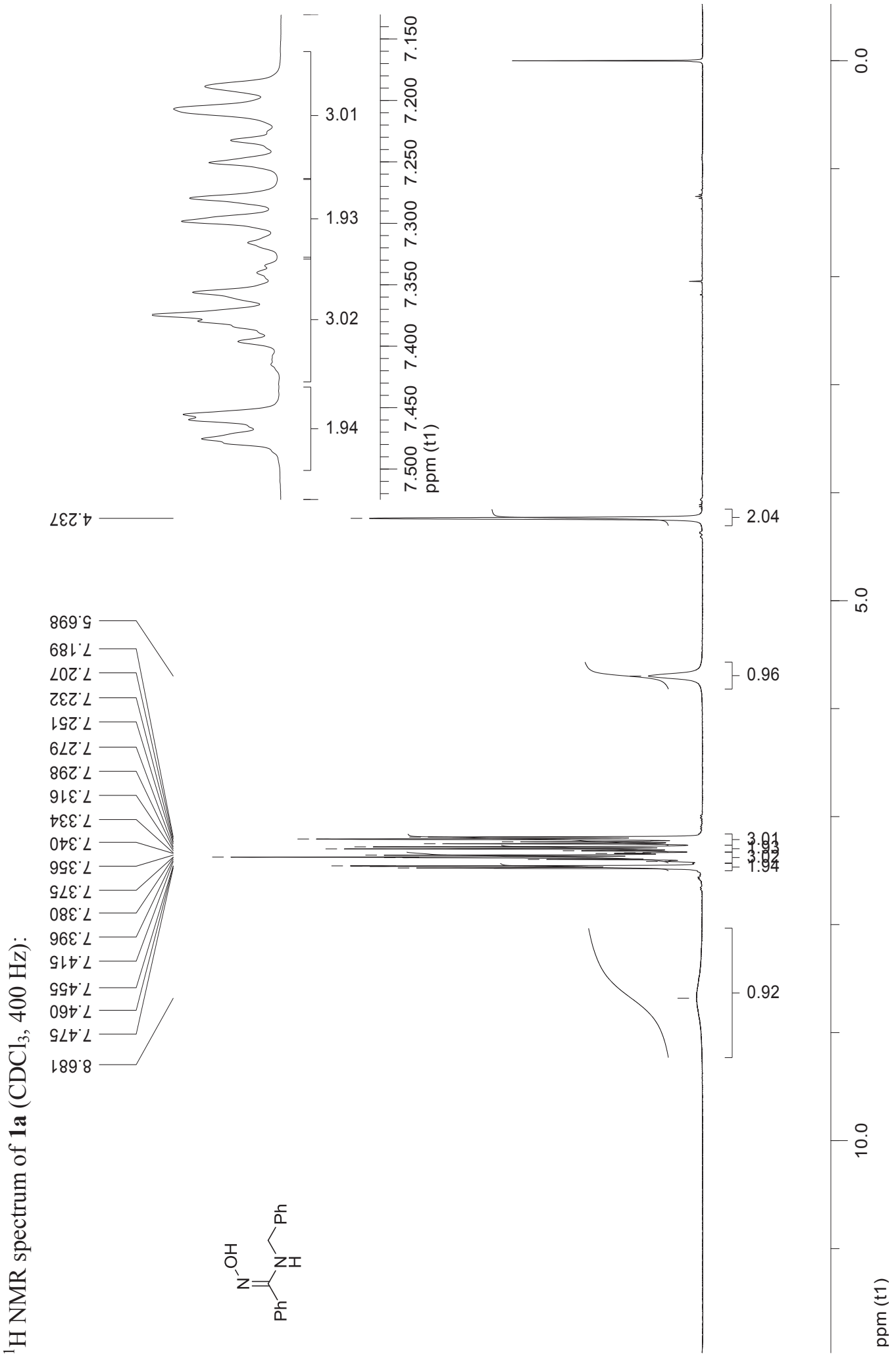
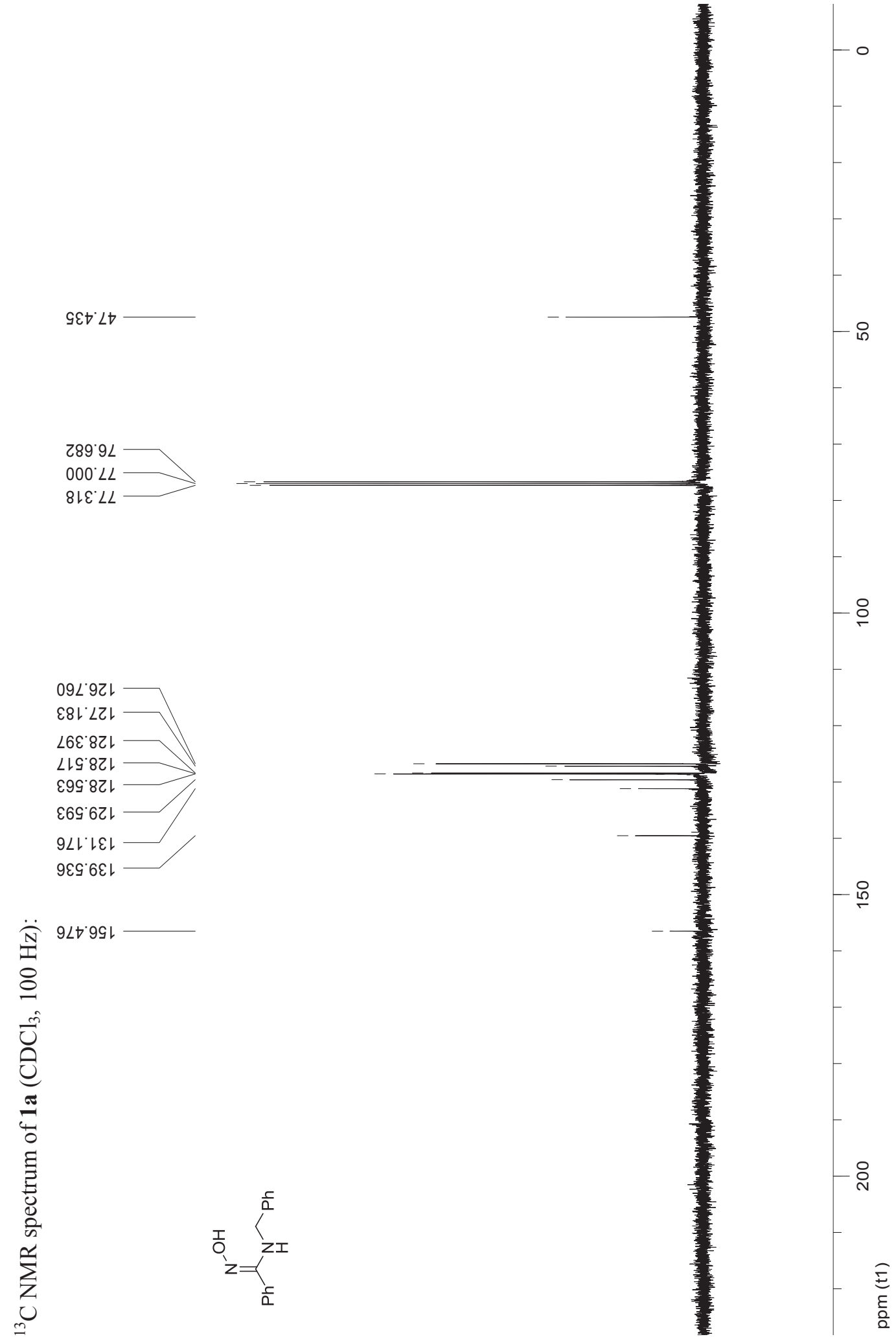
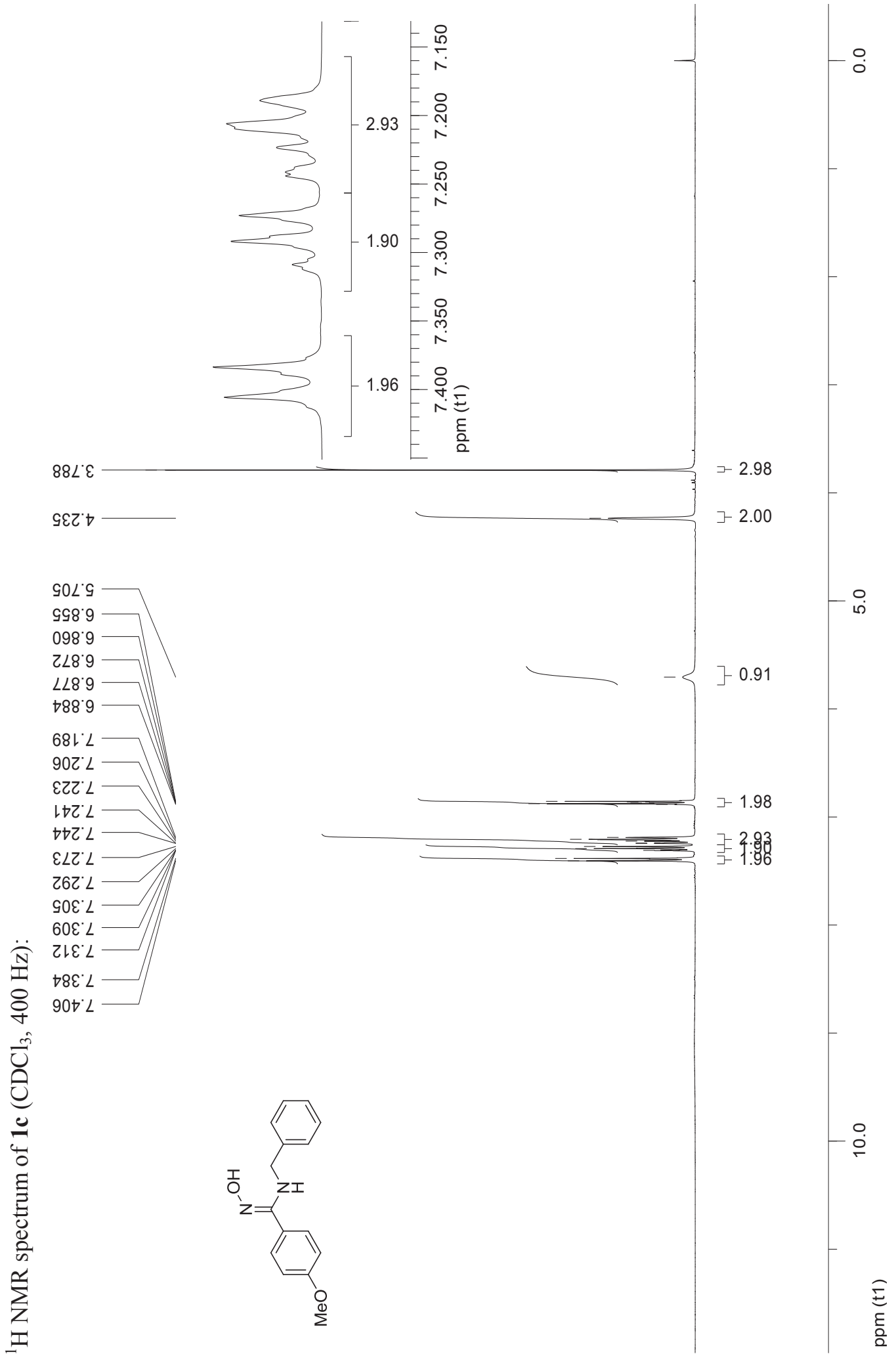
^{1}H NMR spectrum of **1a** ($CDCl_3$, 400 Hz):



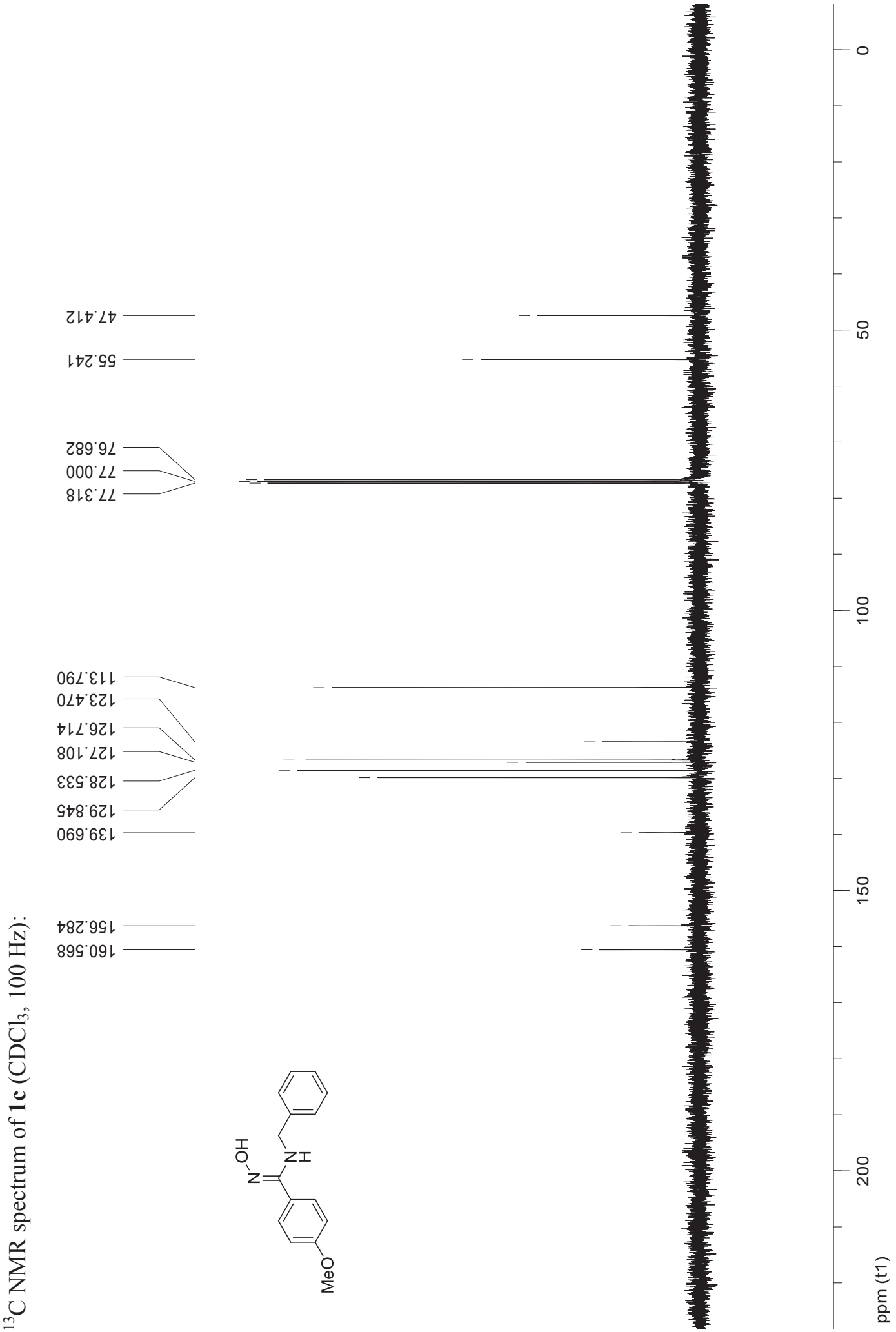
^{13}C NMR spectrum of **1a** ($CDCl_3$, 100 Hz):



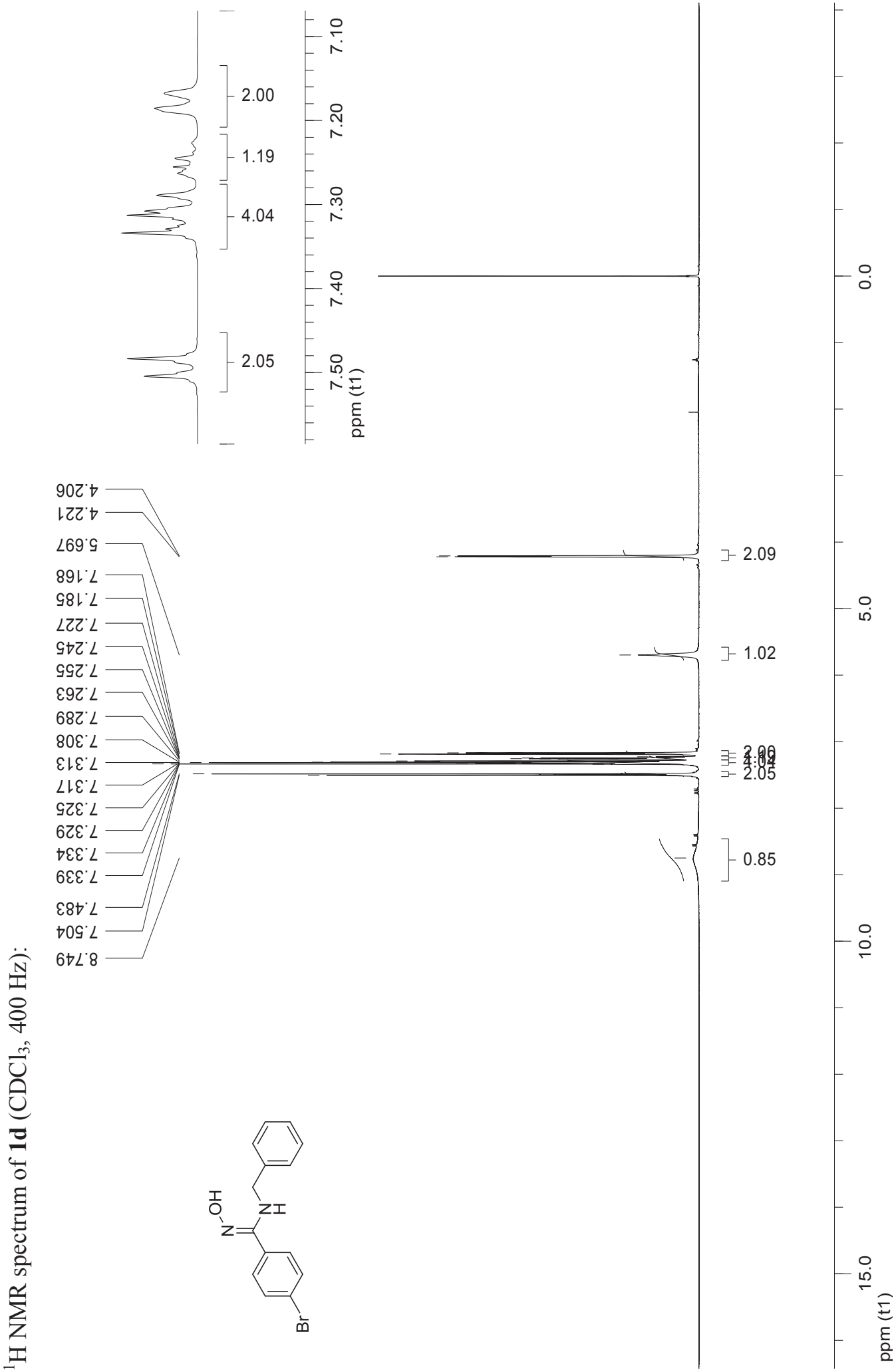
^{1}H NMR spectrum of **1c** ($CDCl_3$, 400 Hz):



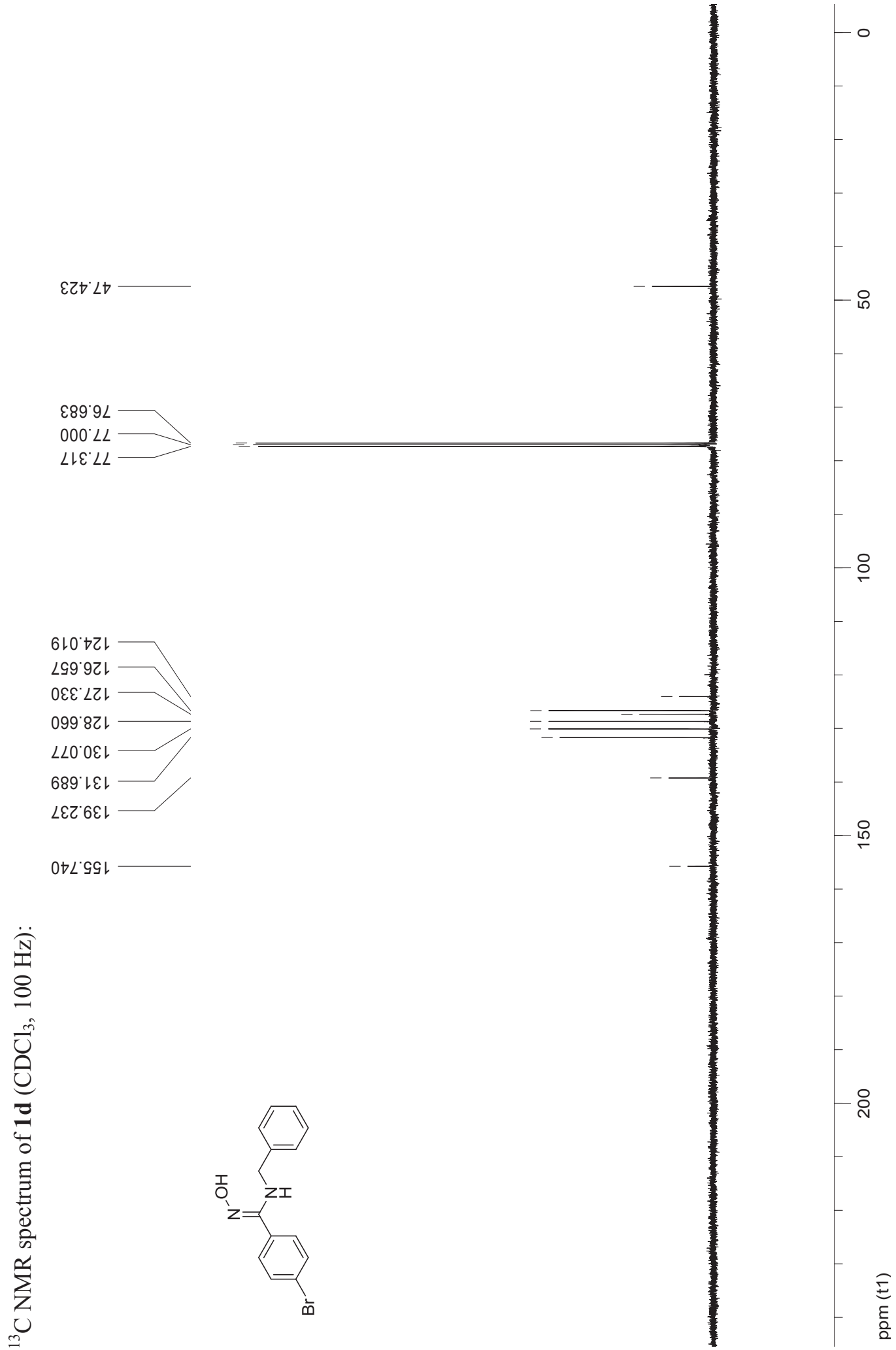
^{13}C NMR spectrum of **1c** ($CDCl_3$, 100 Hz):



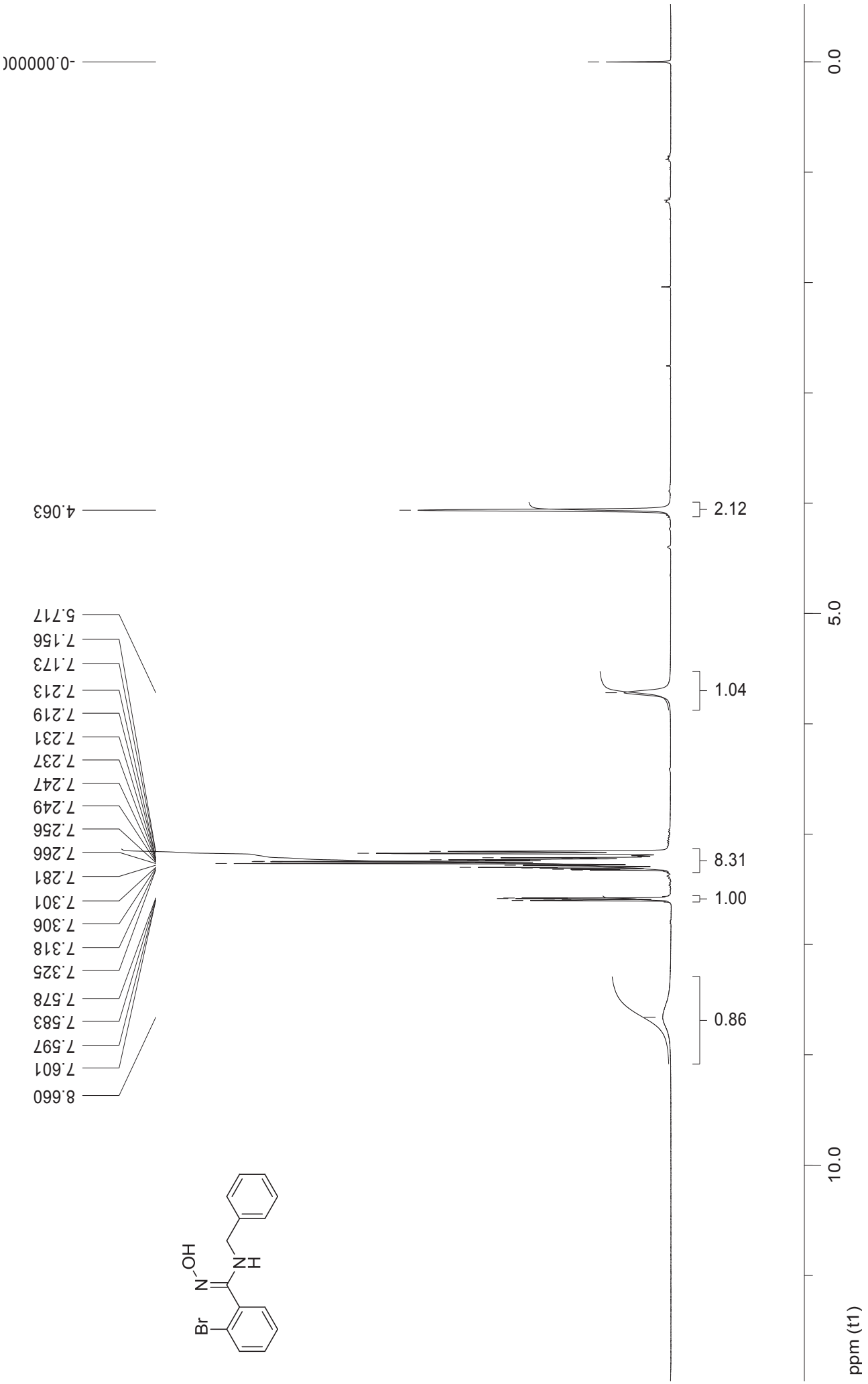
^{1}H NMR spectrum of **1d** ($CDCl_3$, 400 Hz):



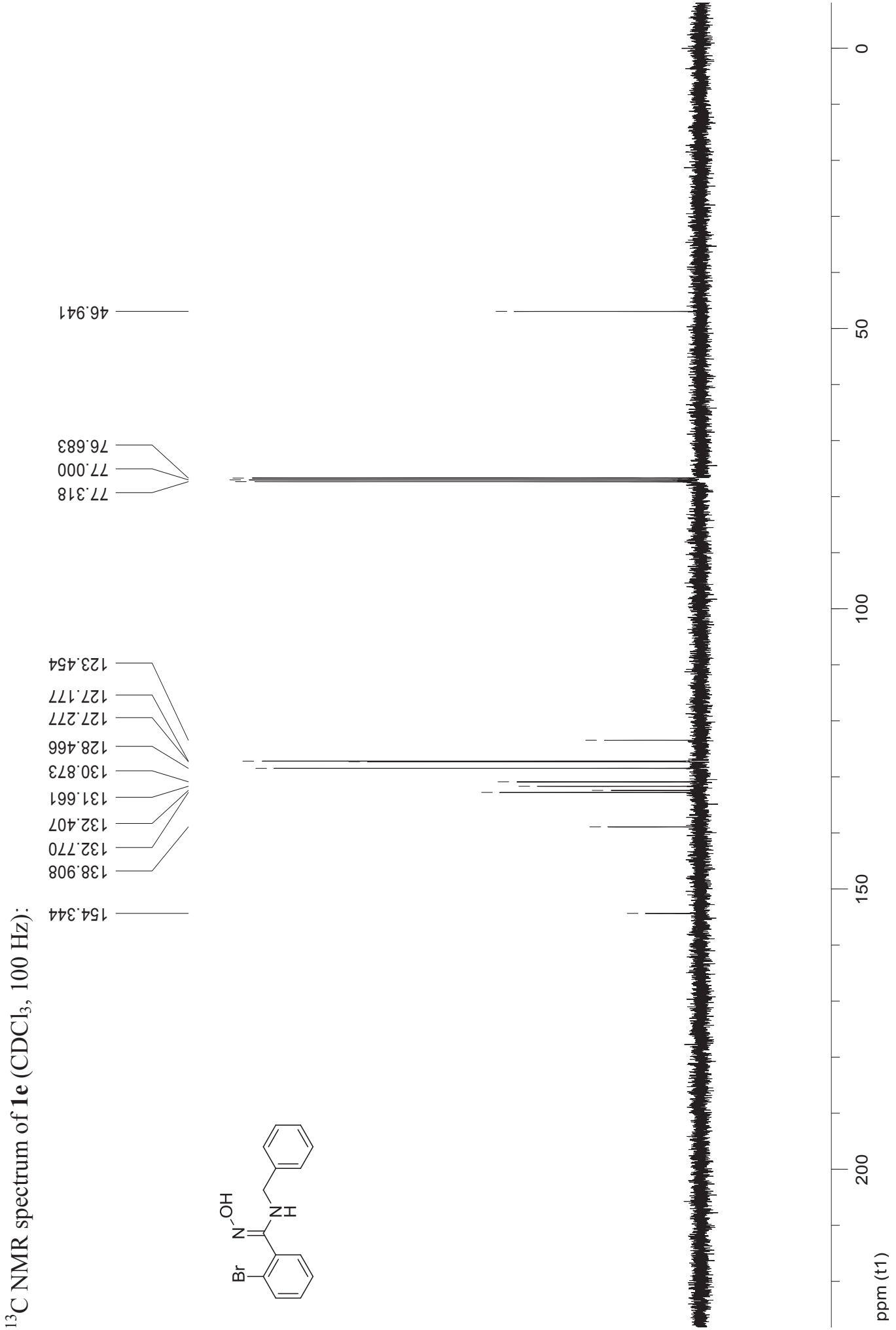
^{13}C NMR spectrum of **1d** ($CDCl_3$, 100 Hz):



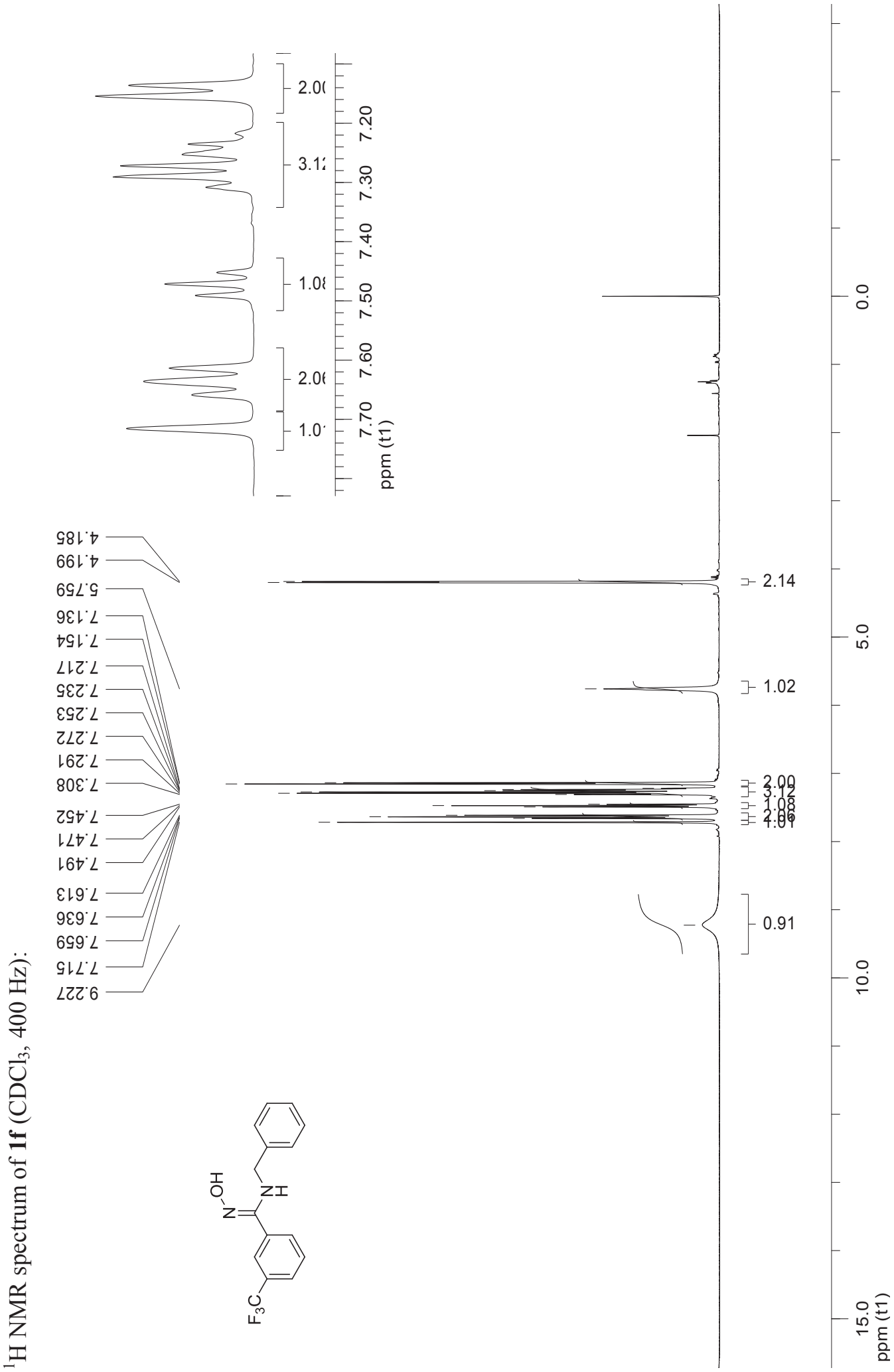
^{1}H NMR spectrum of **1e** ($CDCl_3$, 400 Hz):



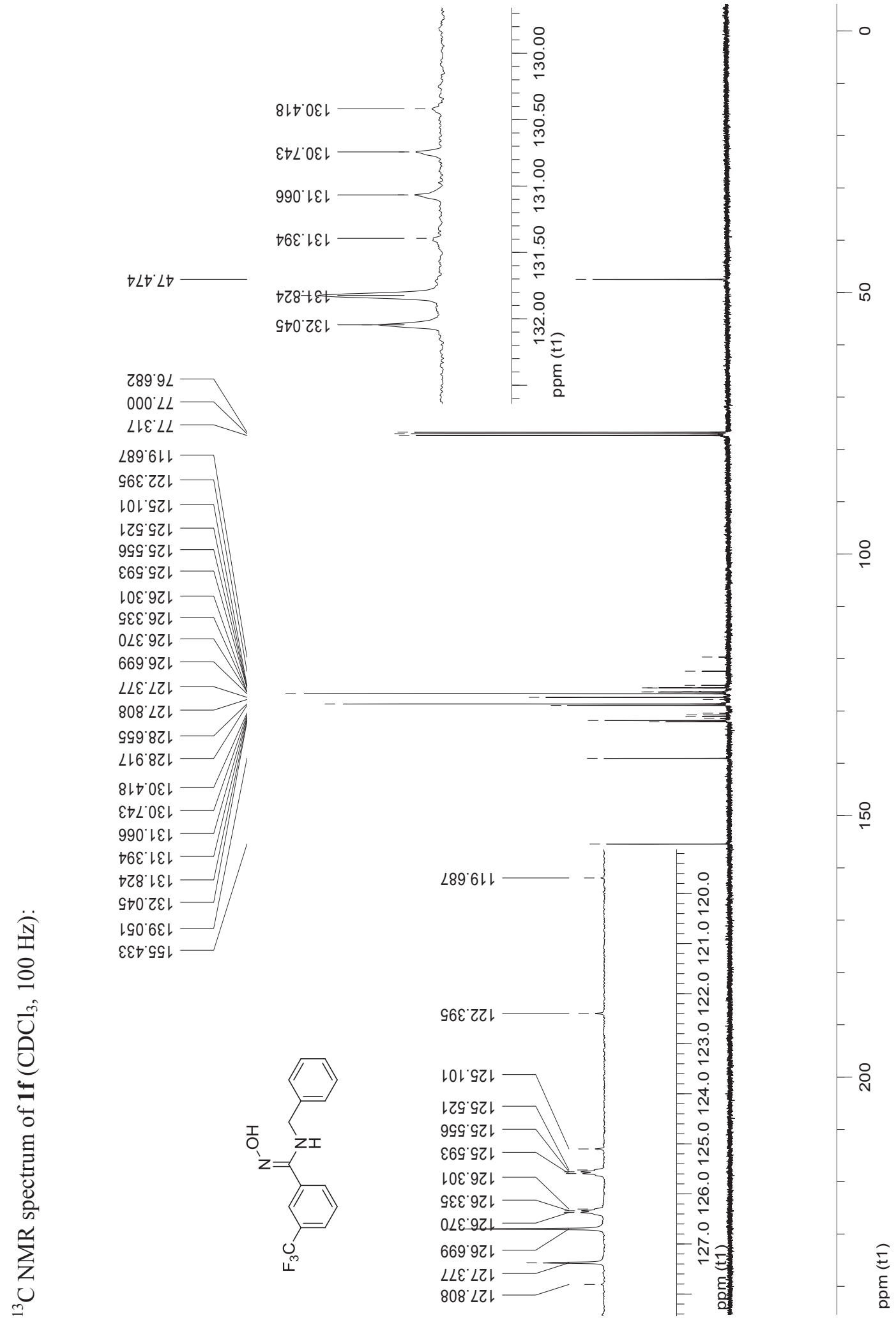
^{13}C NMR spectrum of **1e** ($CDCl_3$, 100 Hz):



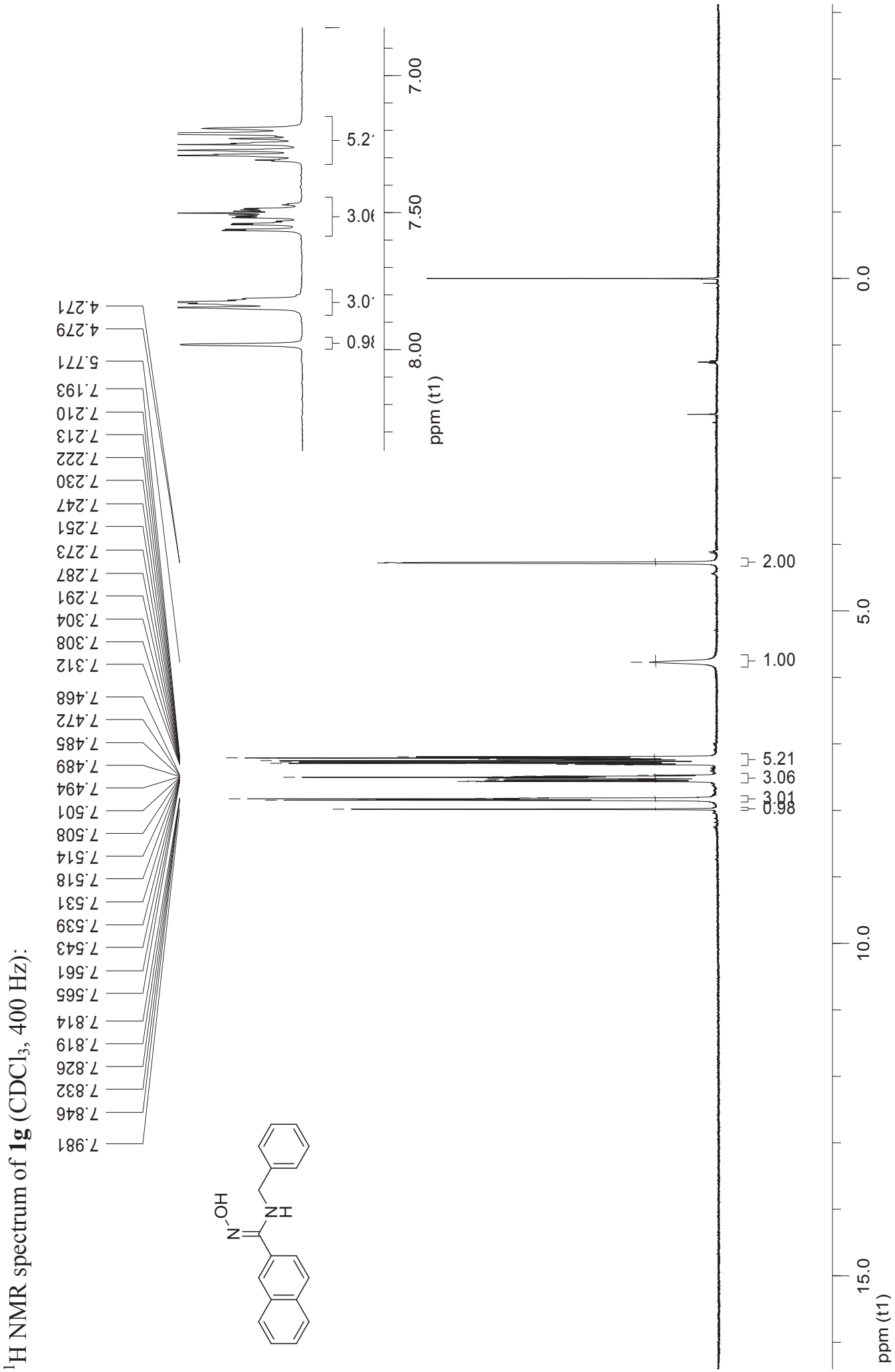
^{1}H NMR spectrum of **1f** ($CDCl_3$, 400 Hz):



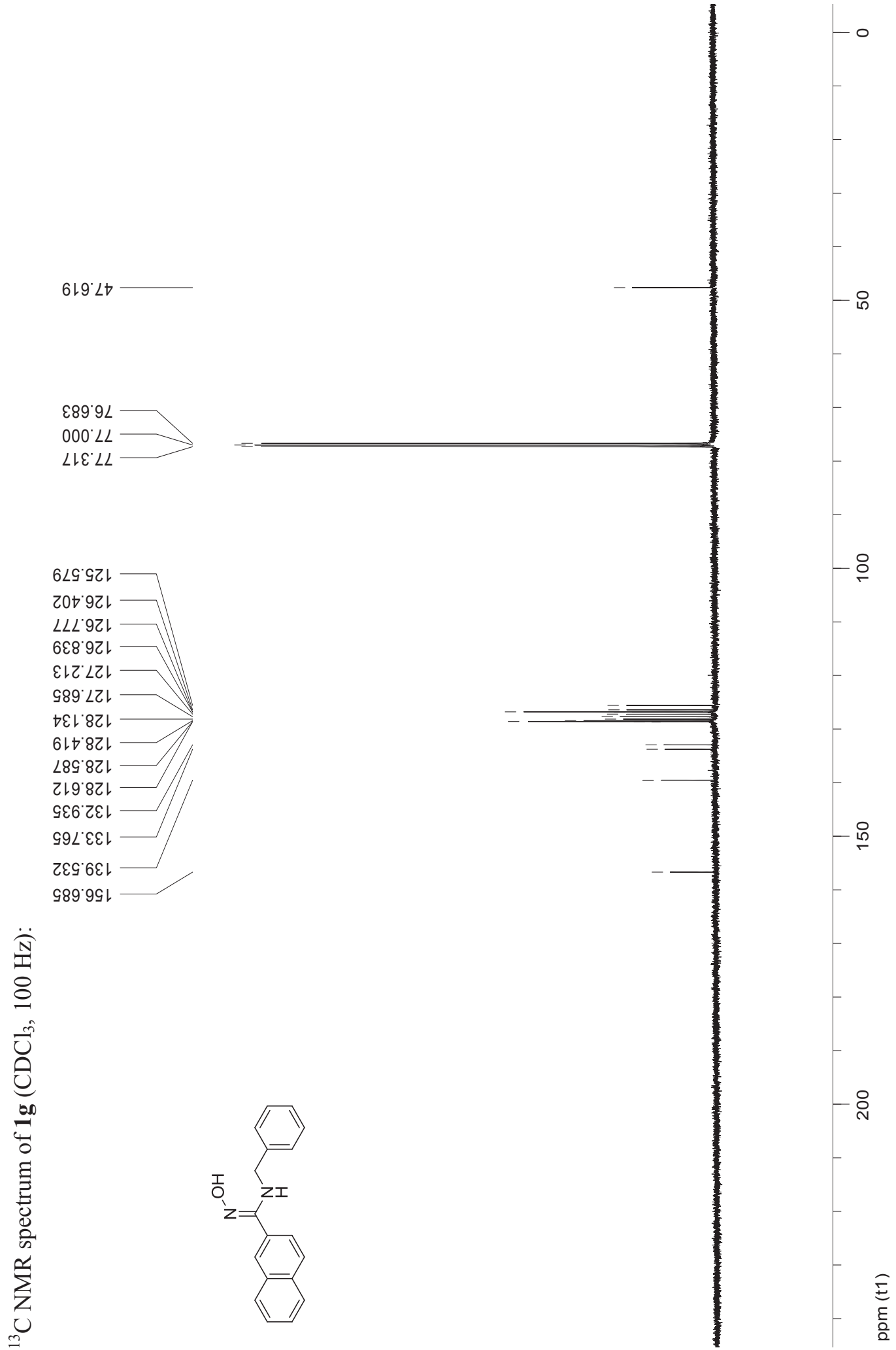
^{13}C NMR spectrum of **1f** ($CDCl_3$, 100 Hz):



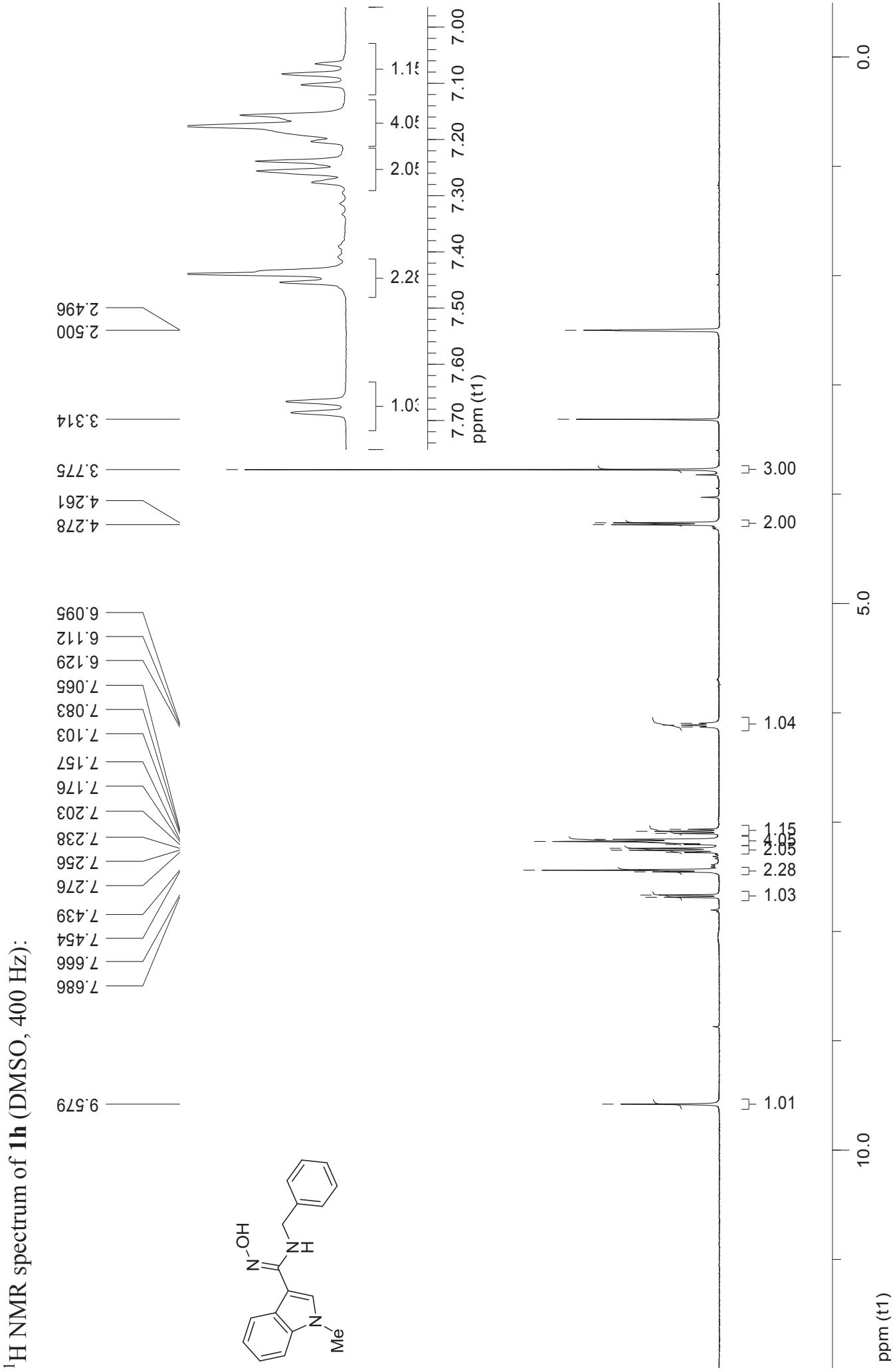
^{1}H NMR spectrum of **1g** ($CDCl_3$, 400 Hz):



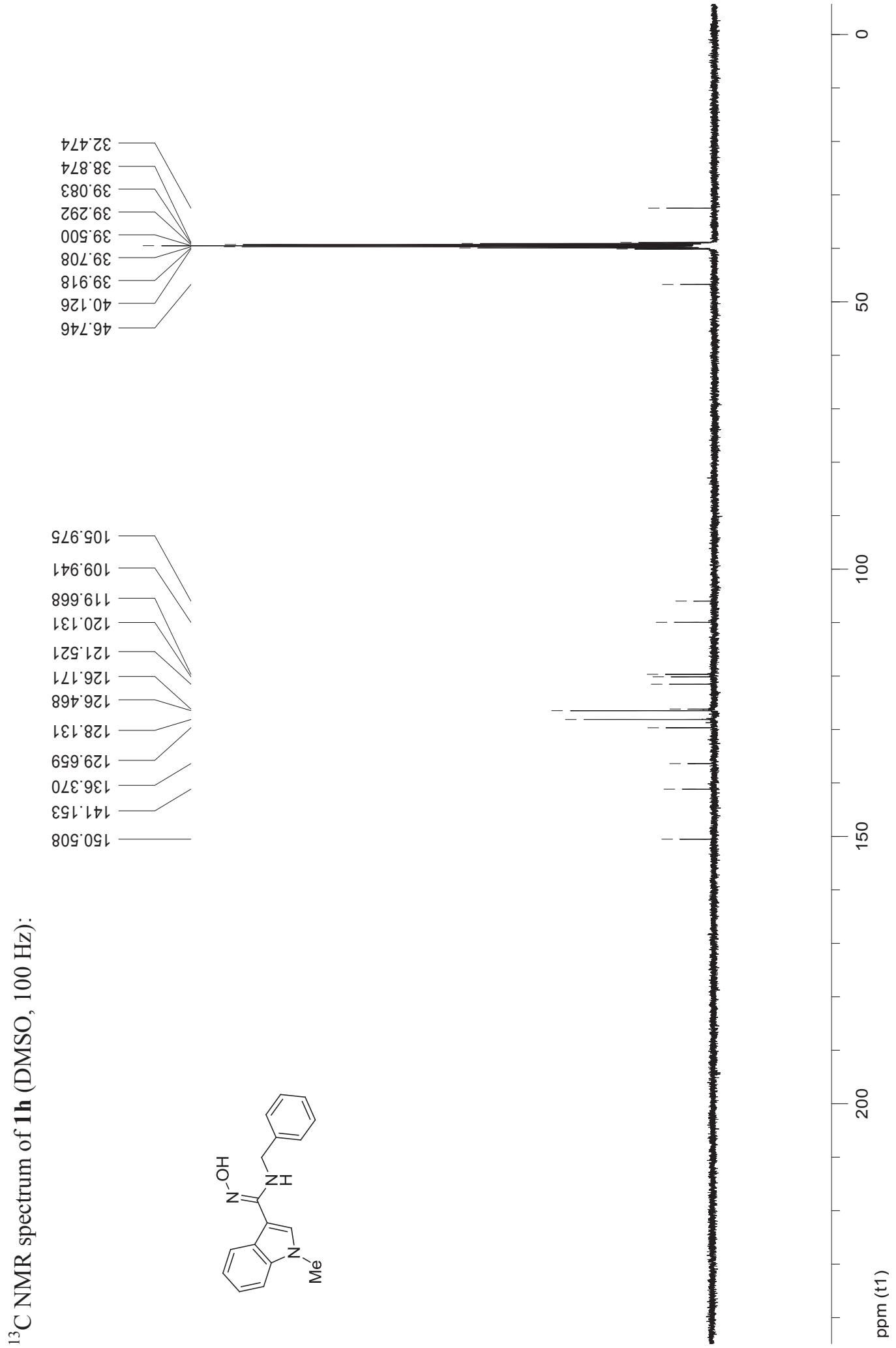
^{13}C NMR spectrum of **1g** ($CDCl_3$, 100 Hz):



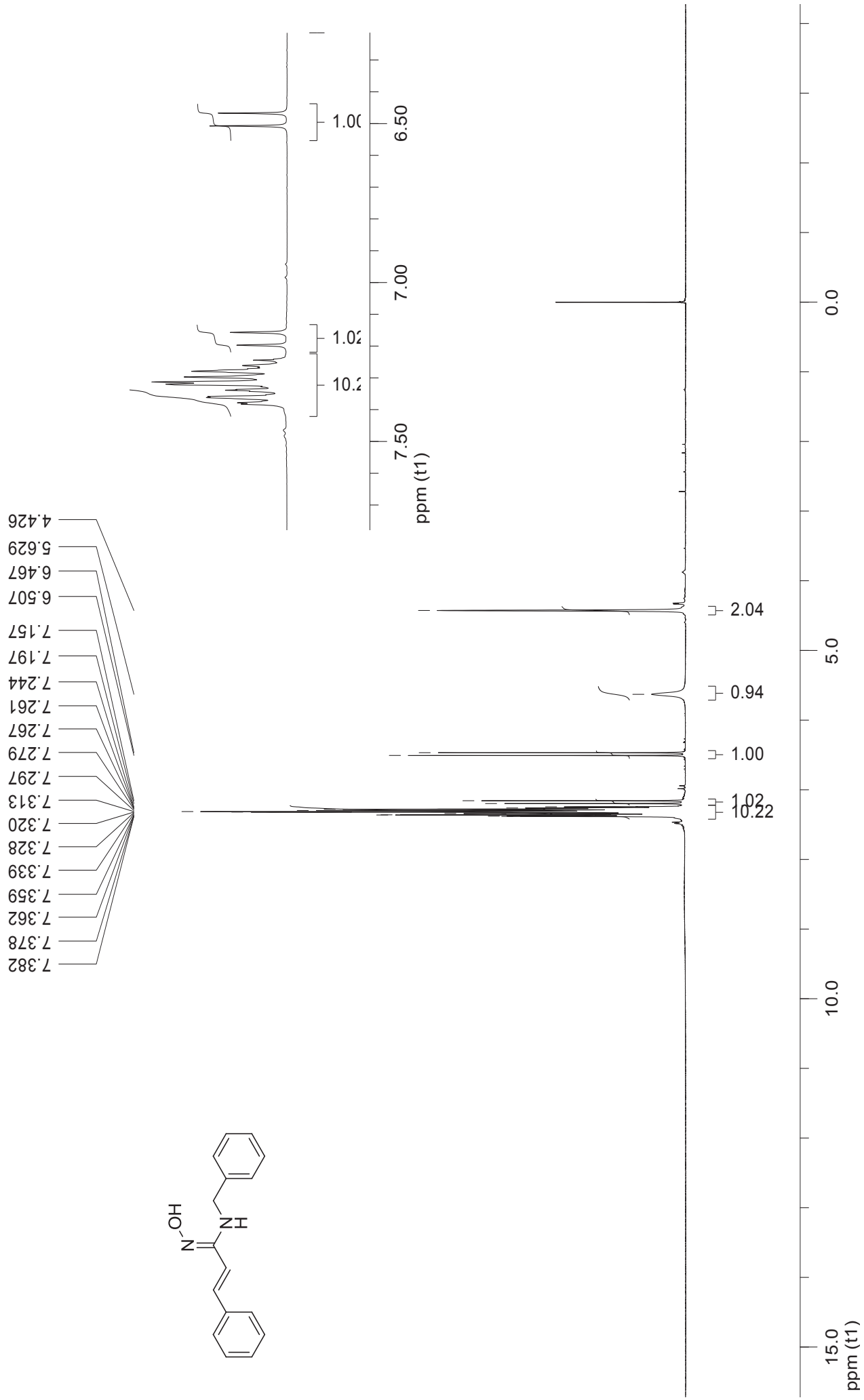
^{1}H NMR spectrum of **1h** (DMSO, 400 Hz):



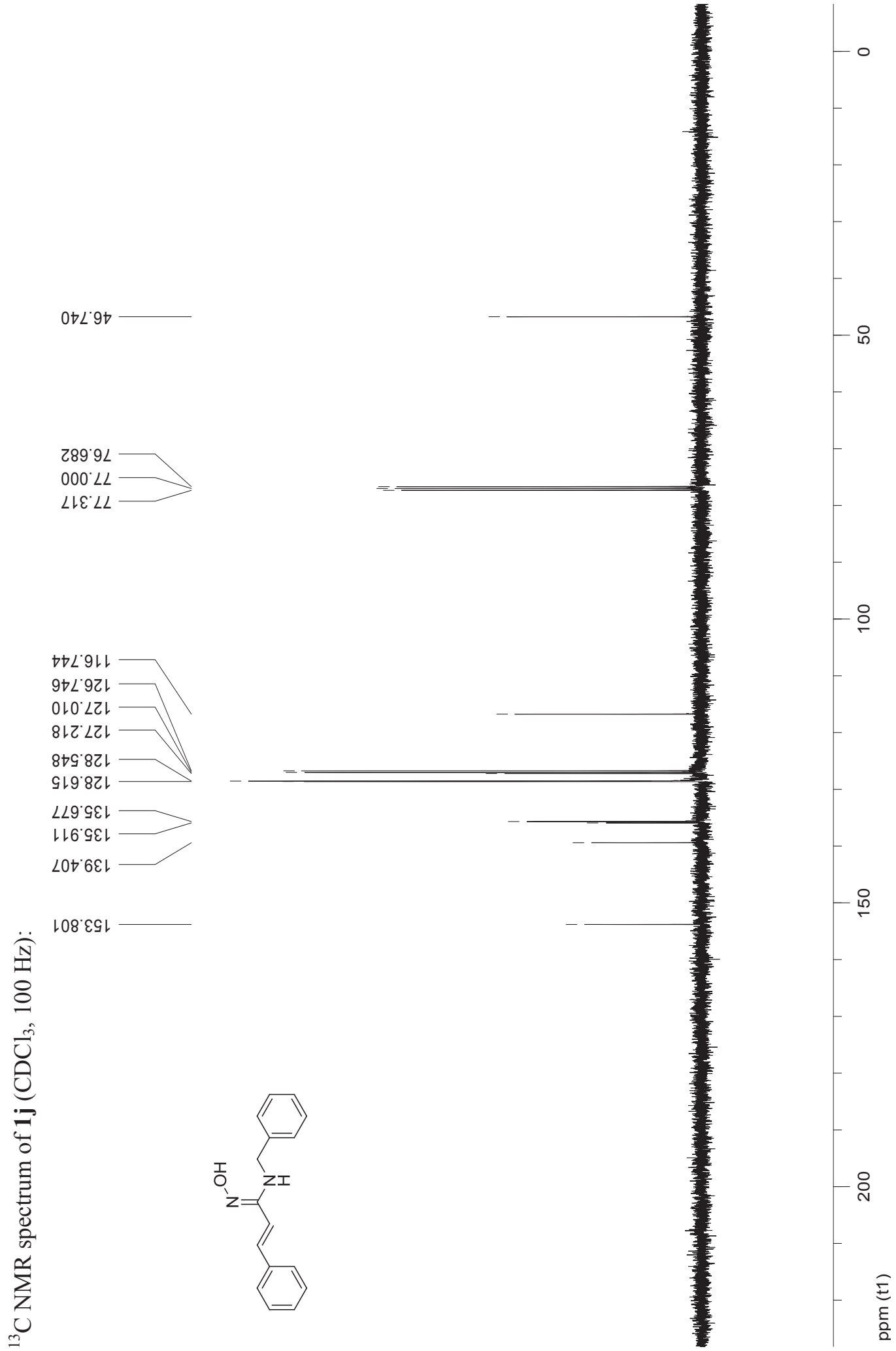
^{13}C NMR spectrum of **1h** (DMSO, 100 Hz):



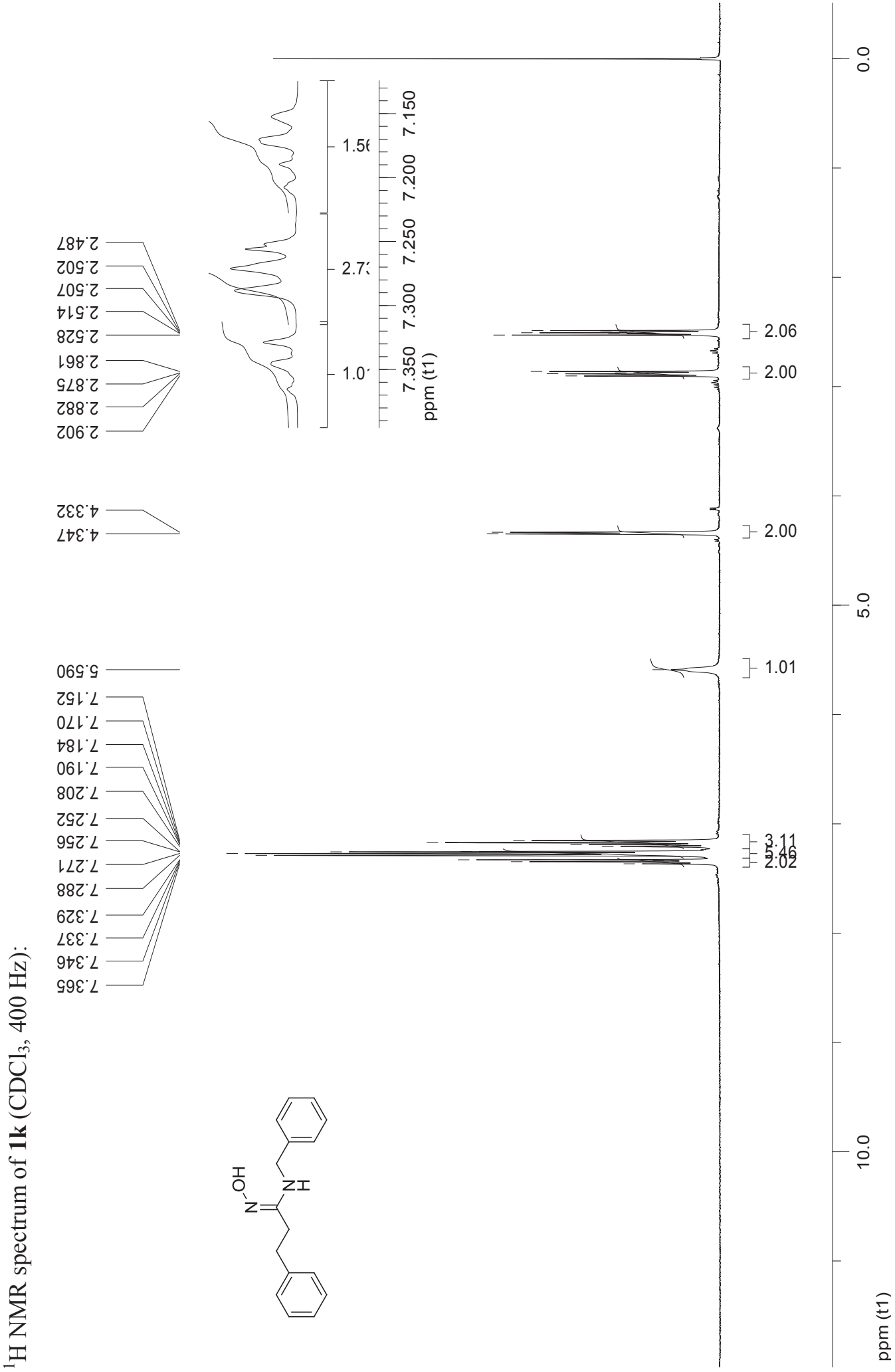
^{1}H NMR spectrum of **1j** ($CDCl_3$, 400 Hz):



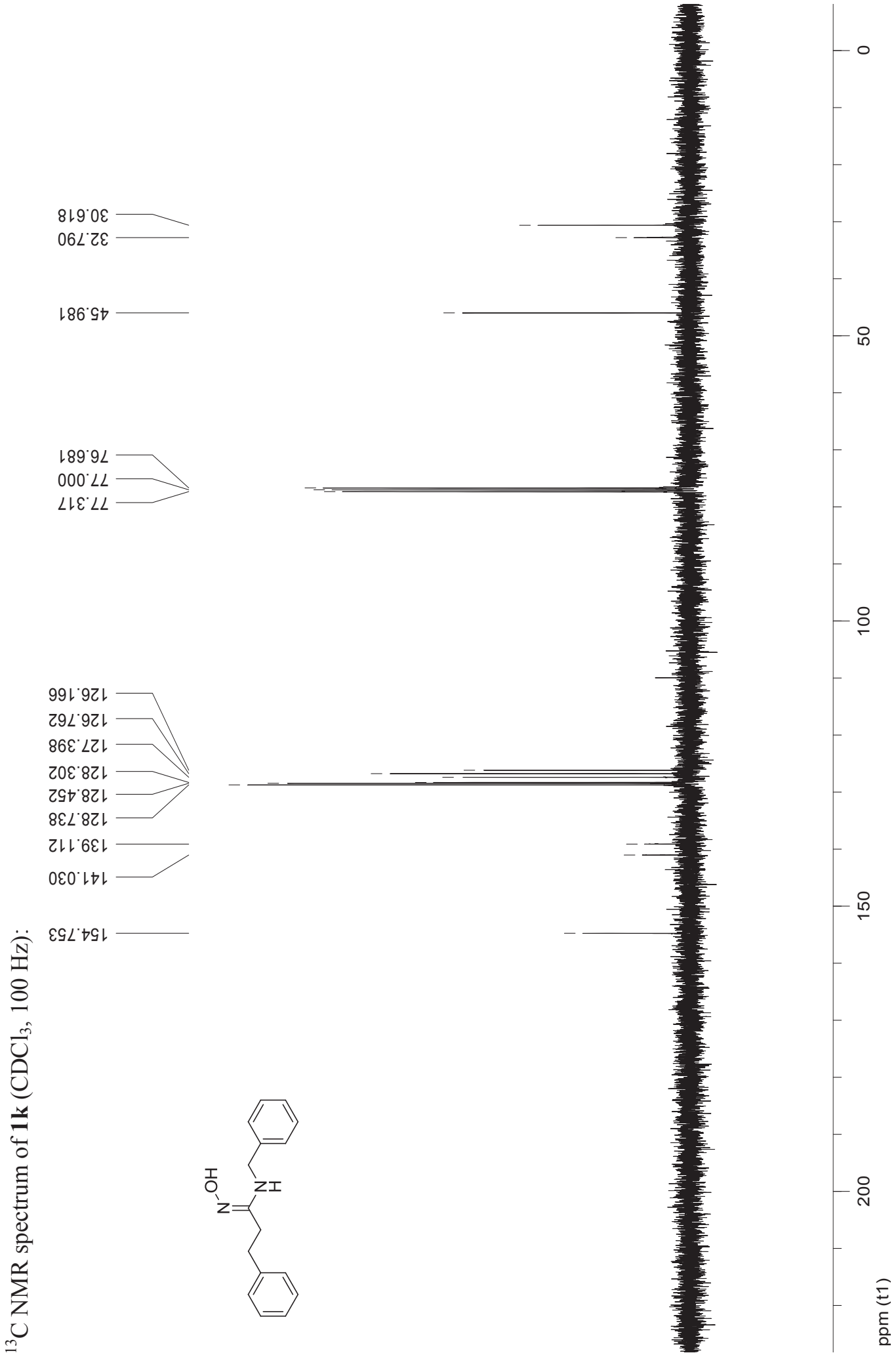
^{13}C NMR spectrum of **1j** ($CDCl_3$, 100 Hz):



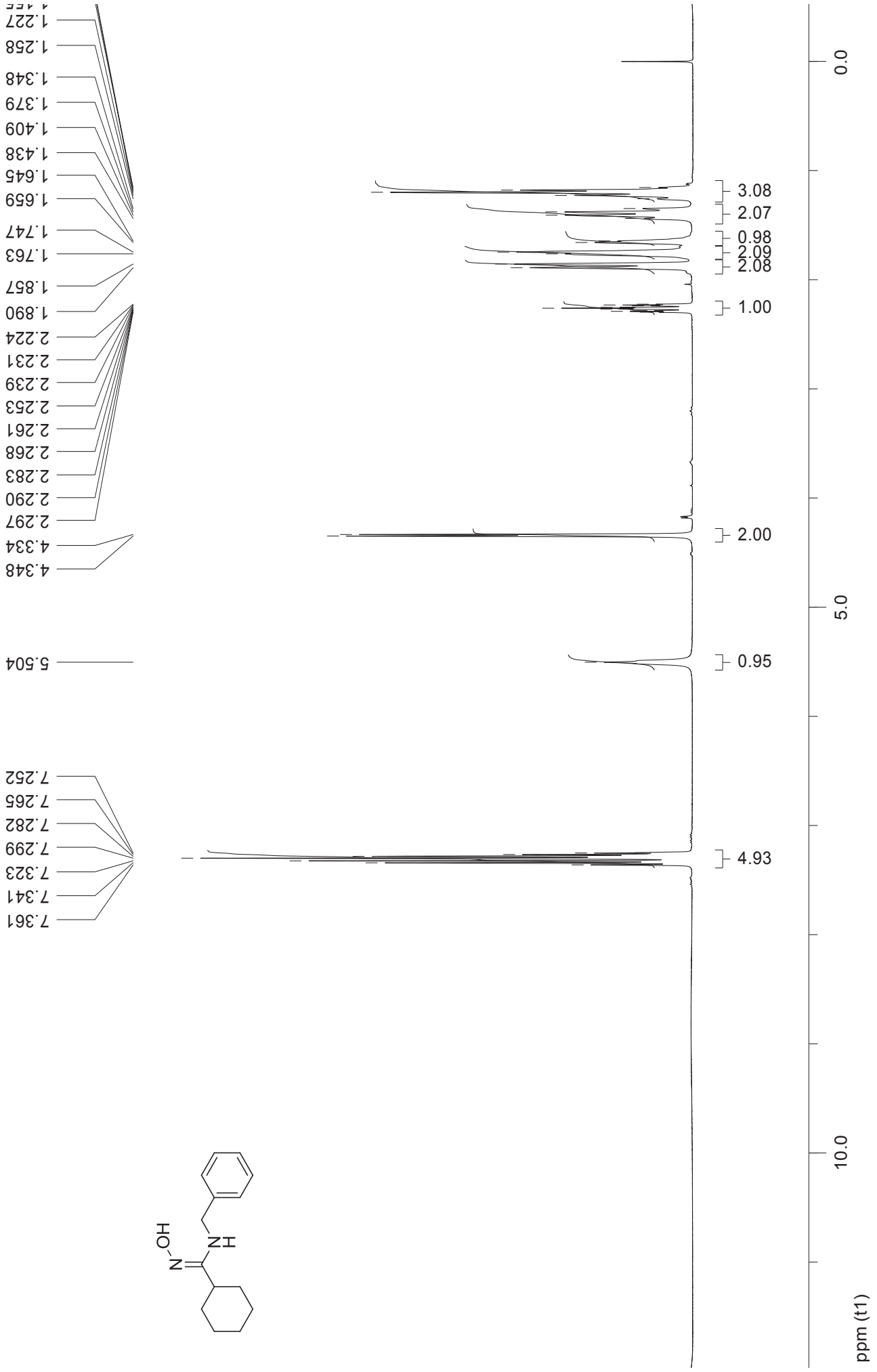
^{1}H NMR spectrum of **1k** ($CDCl_3$, 400 Hz):



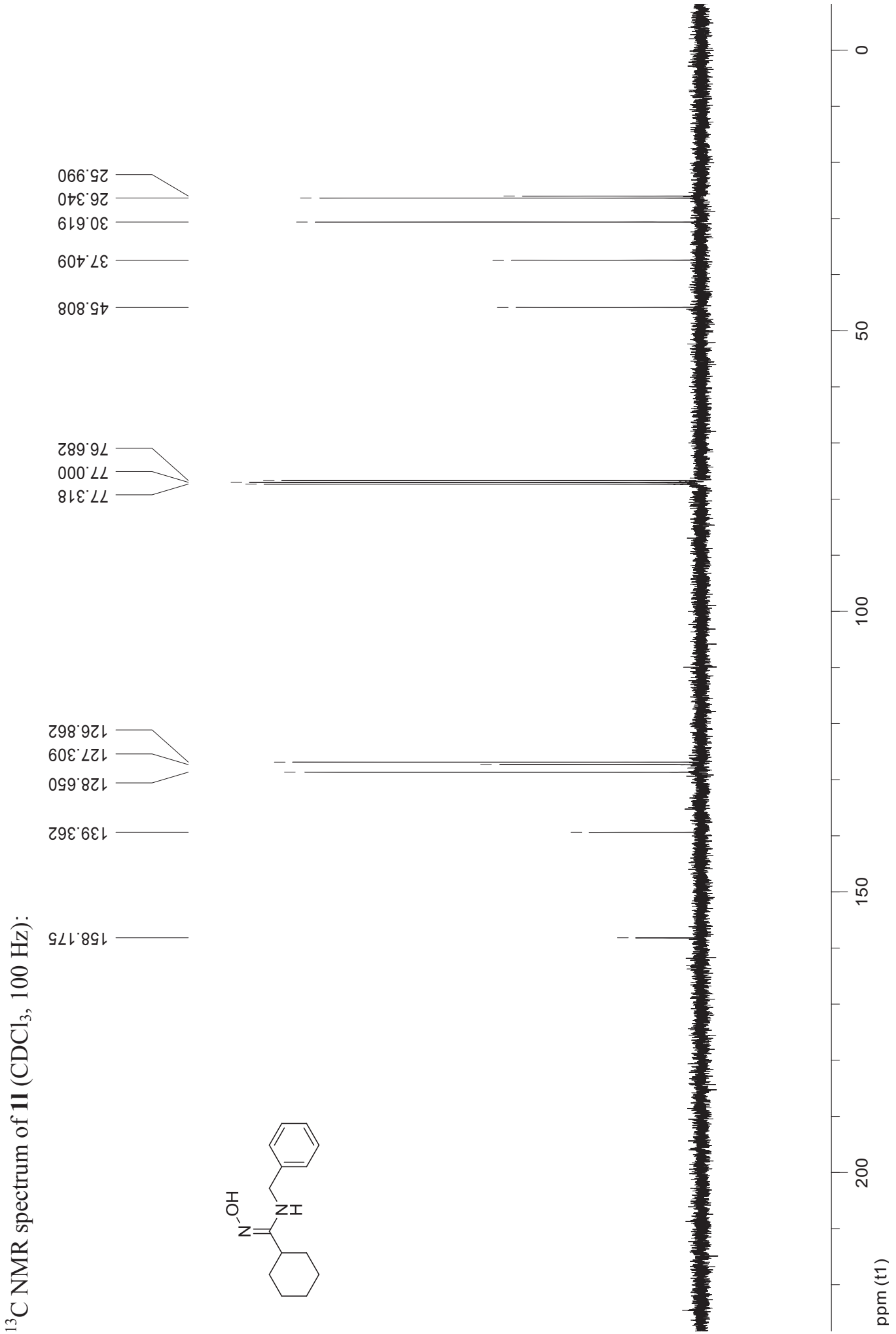
^{13}C NMR spectrum of **1k** ($CDCl_3$, 100 Hz):



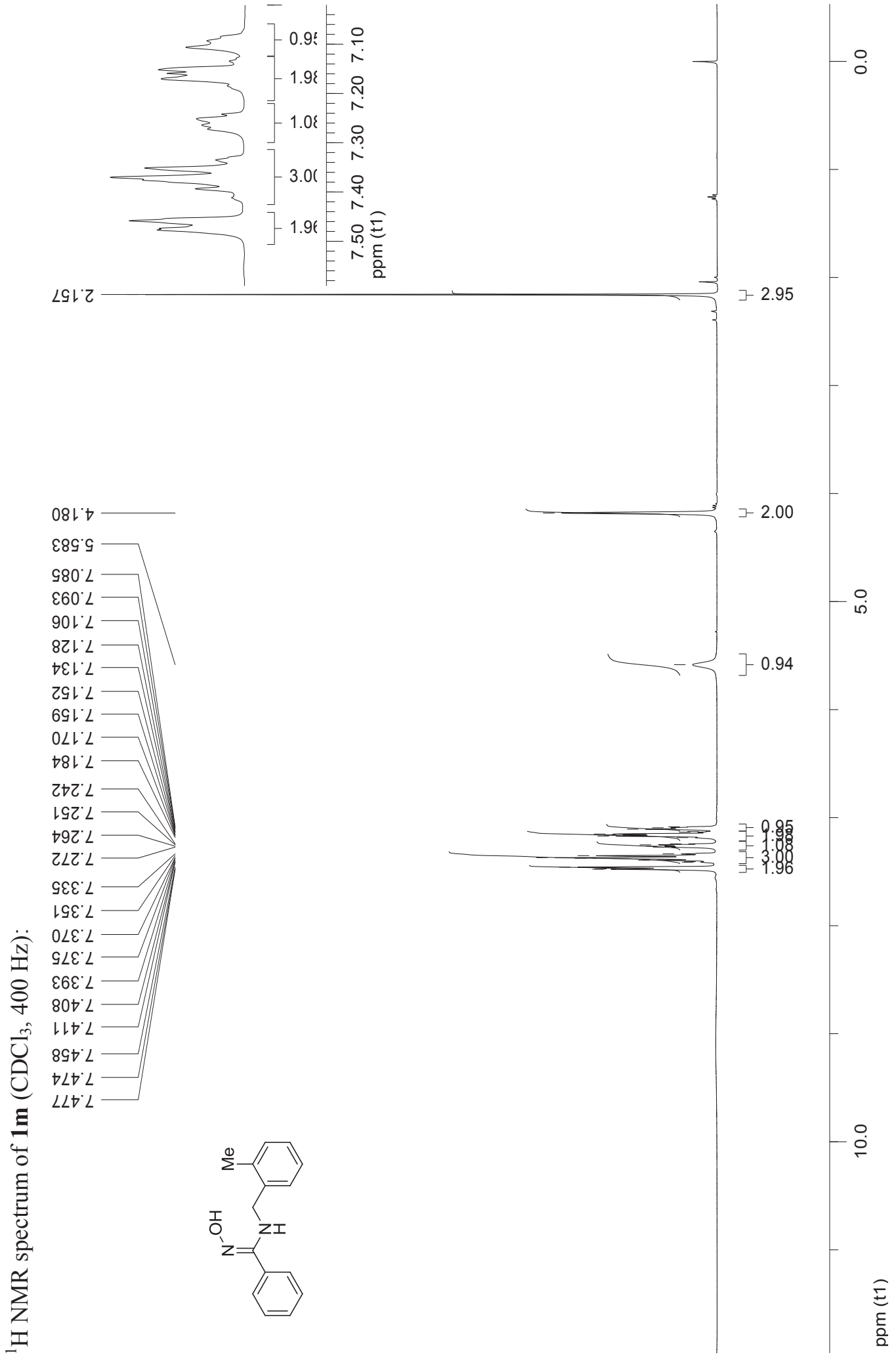
^{1}H NMR spectrum of **11** ($CDCl_3$, 400 Hz):



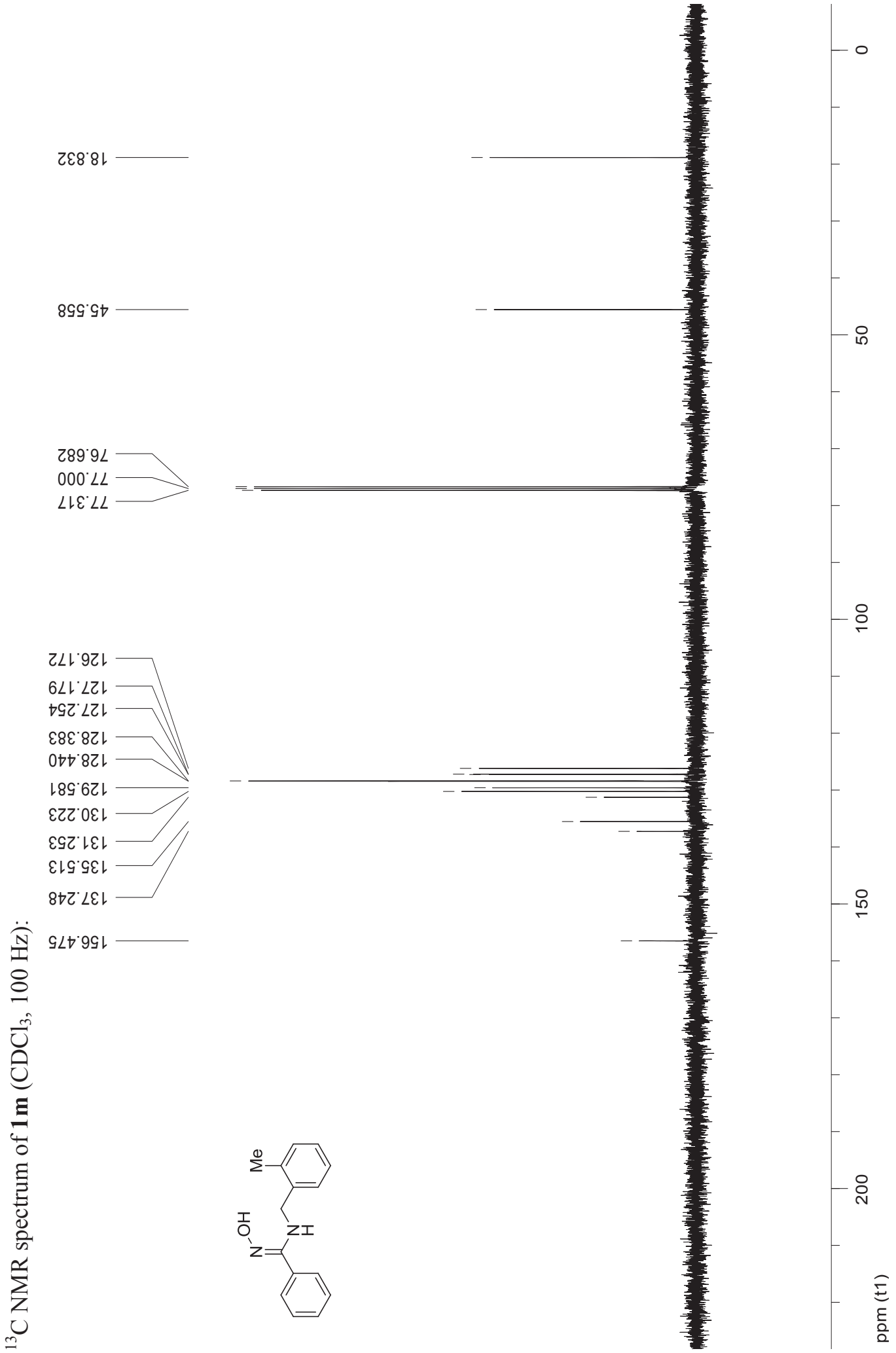
^{13}C NMR spectrum of **11** ($CDCl_3$, 100 Hz):



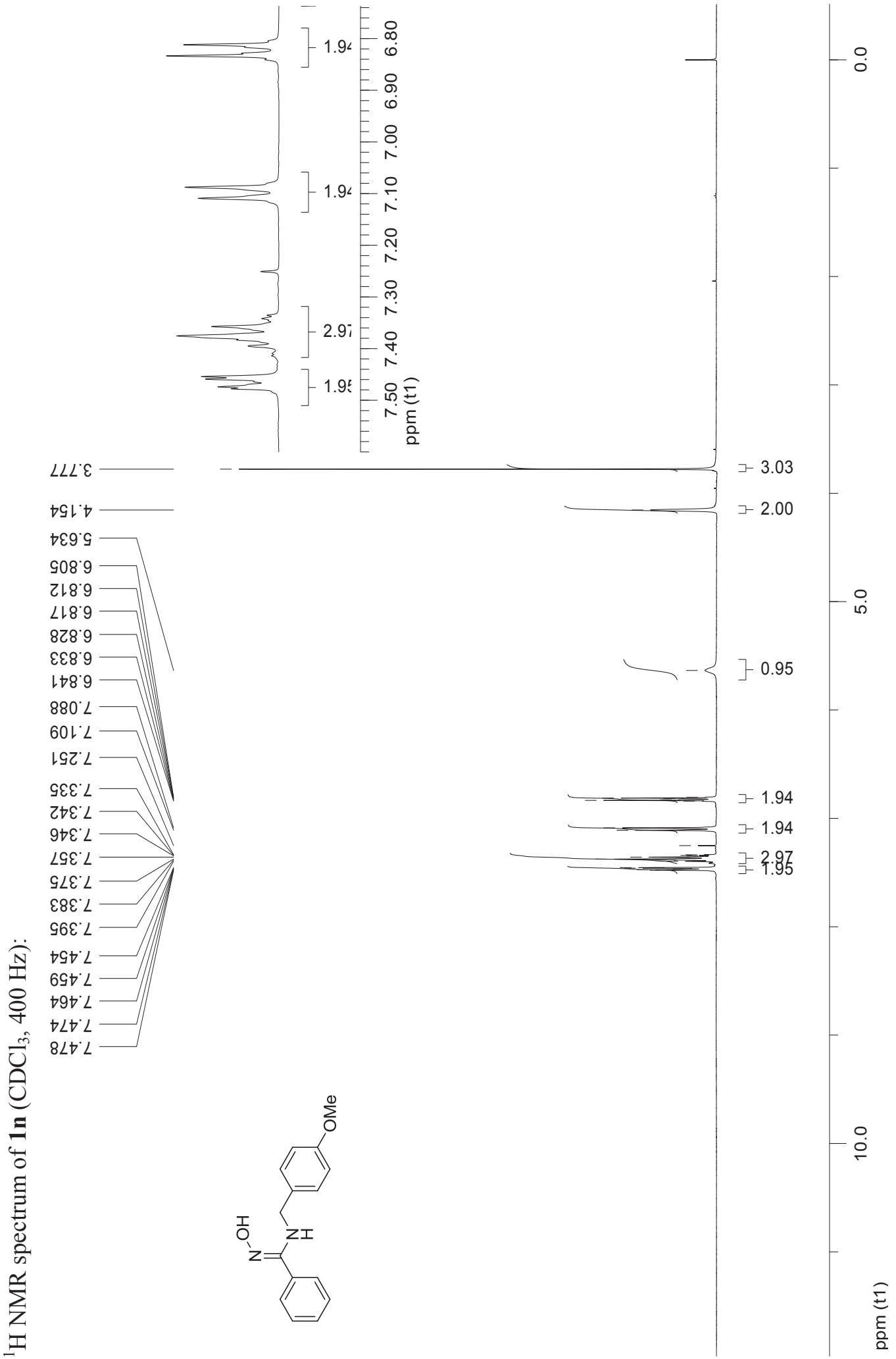
^{1}H NMR spectrum of **1m** ($CDCl_3$, 400 Hz):



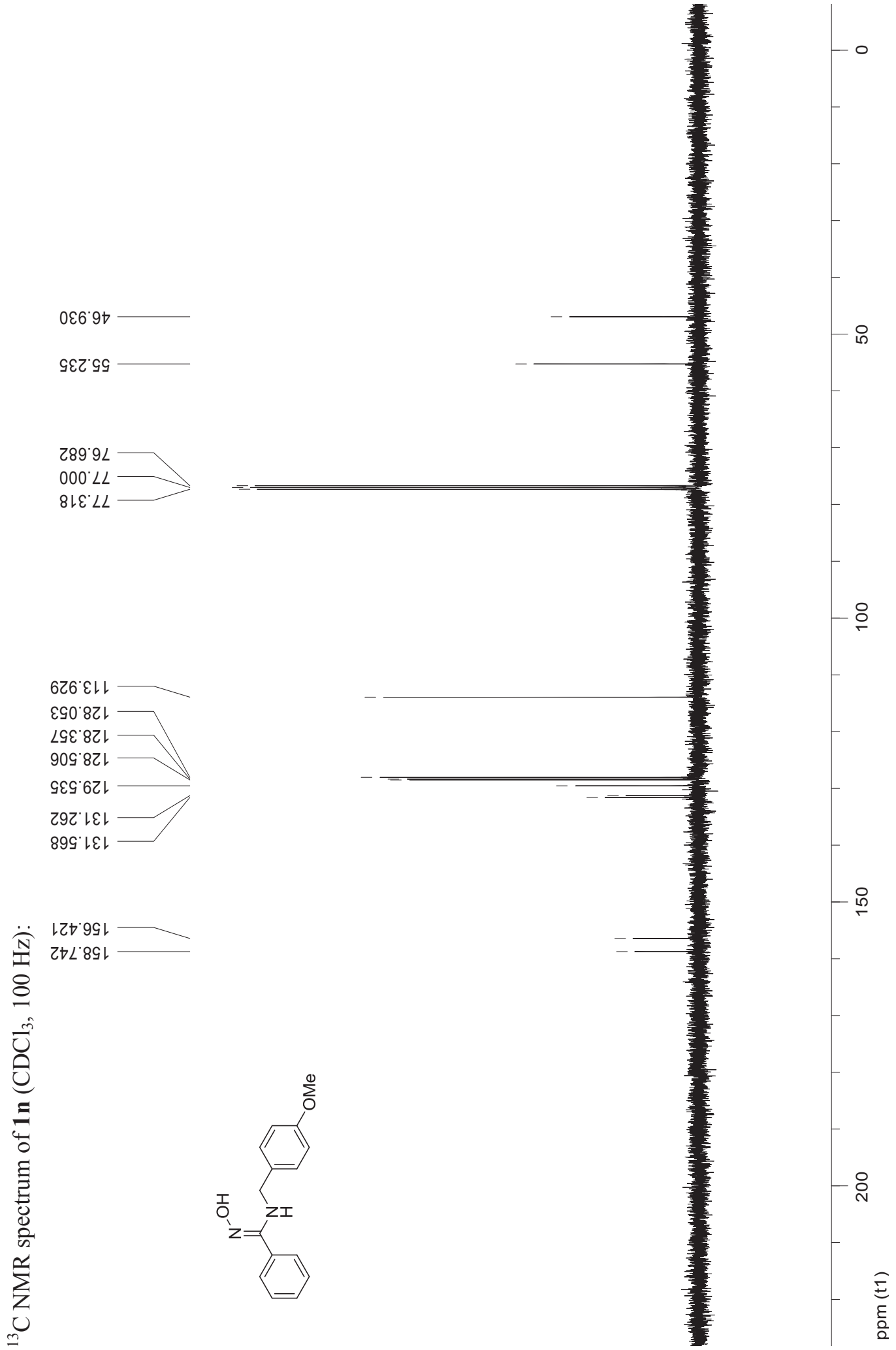
^{13}C NMR spectrum of **1m** ($CDCl_3$, 100 Hz):



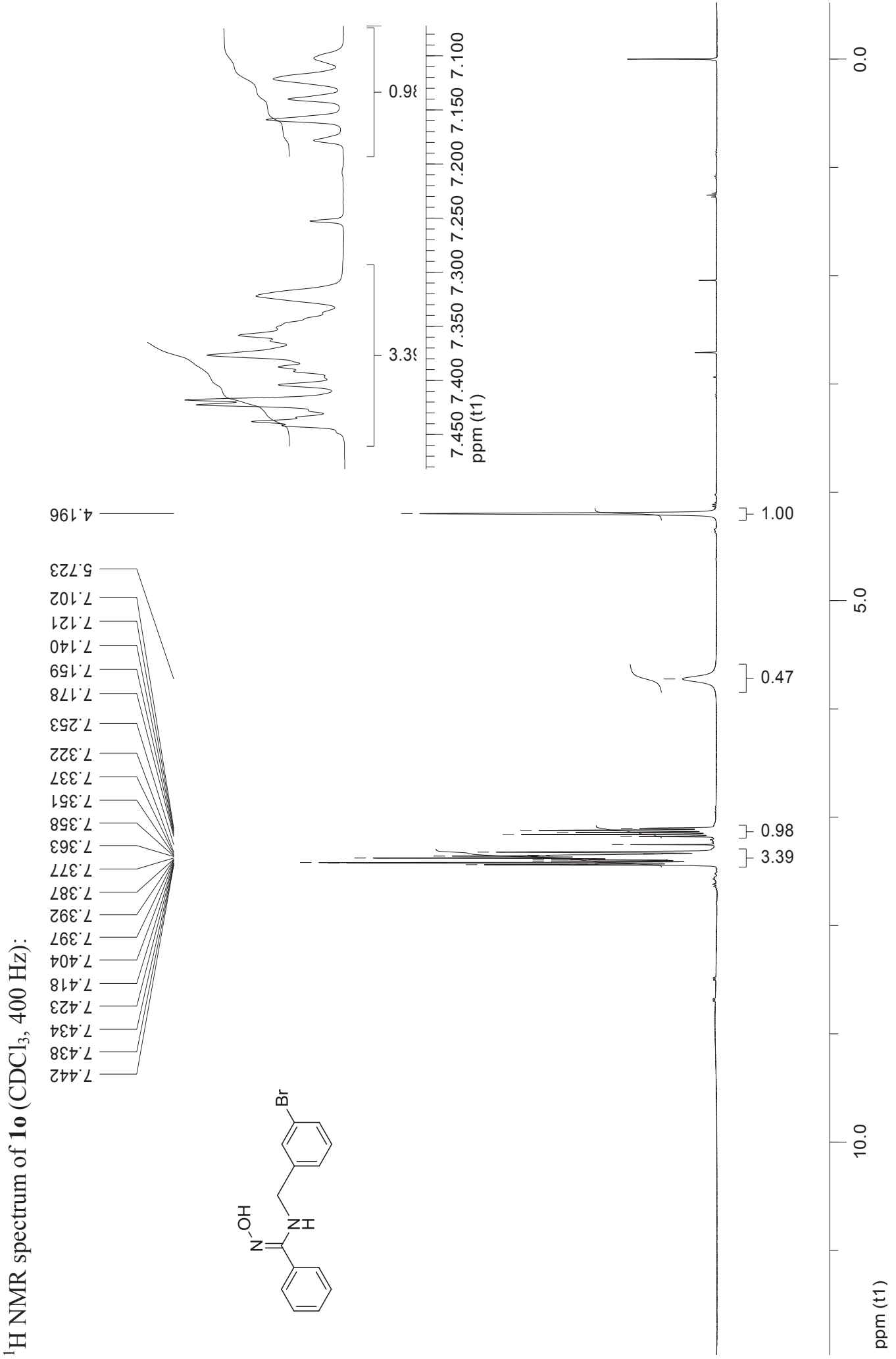
^{1}H NMR spectrum of **1n** ($CDCl_3$, 400 Hz):



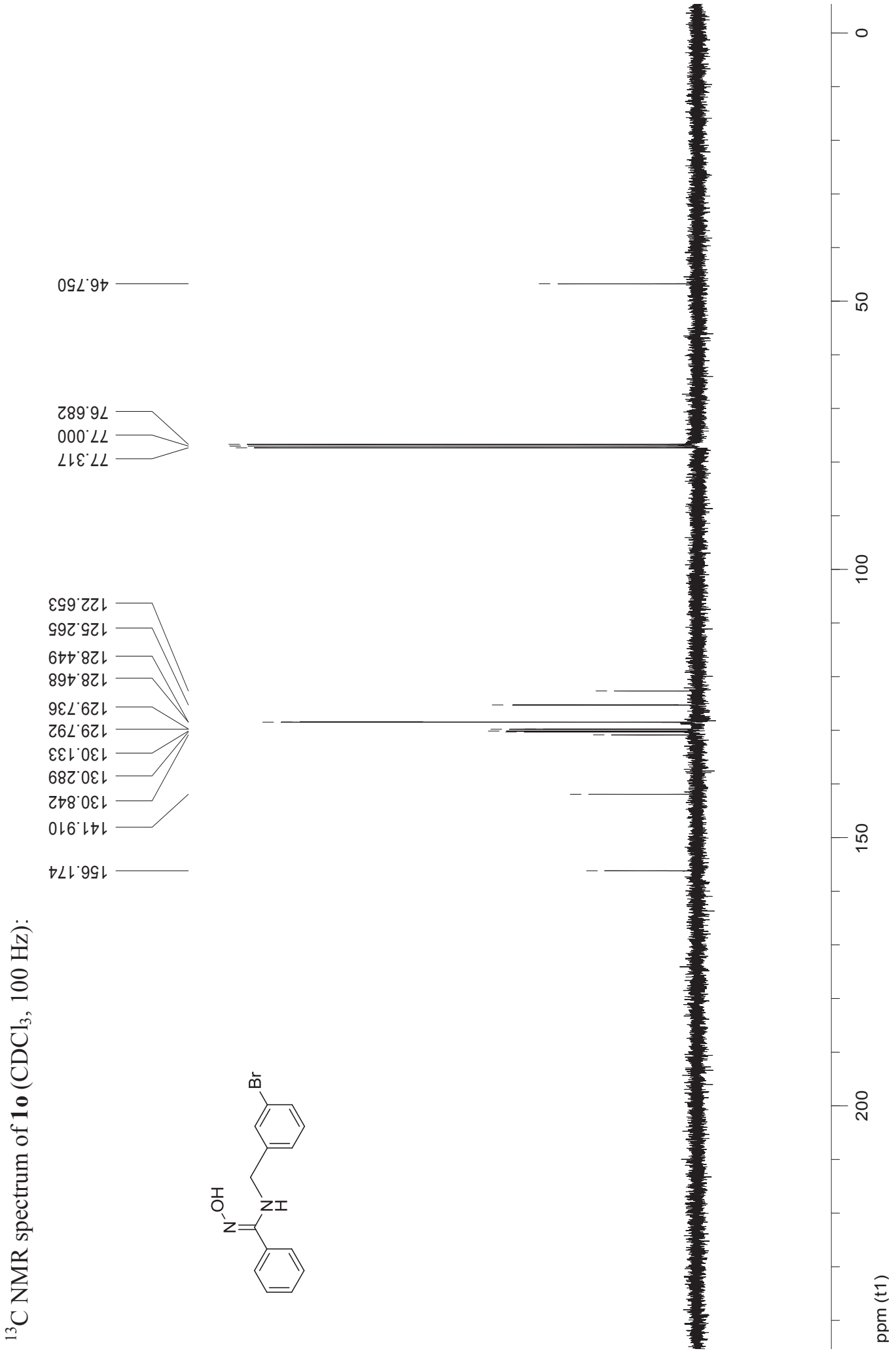
^{13}C NMR spectrum of **1n** ($CDCl_3$, 100 Hz):



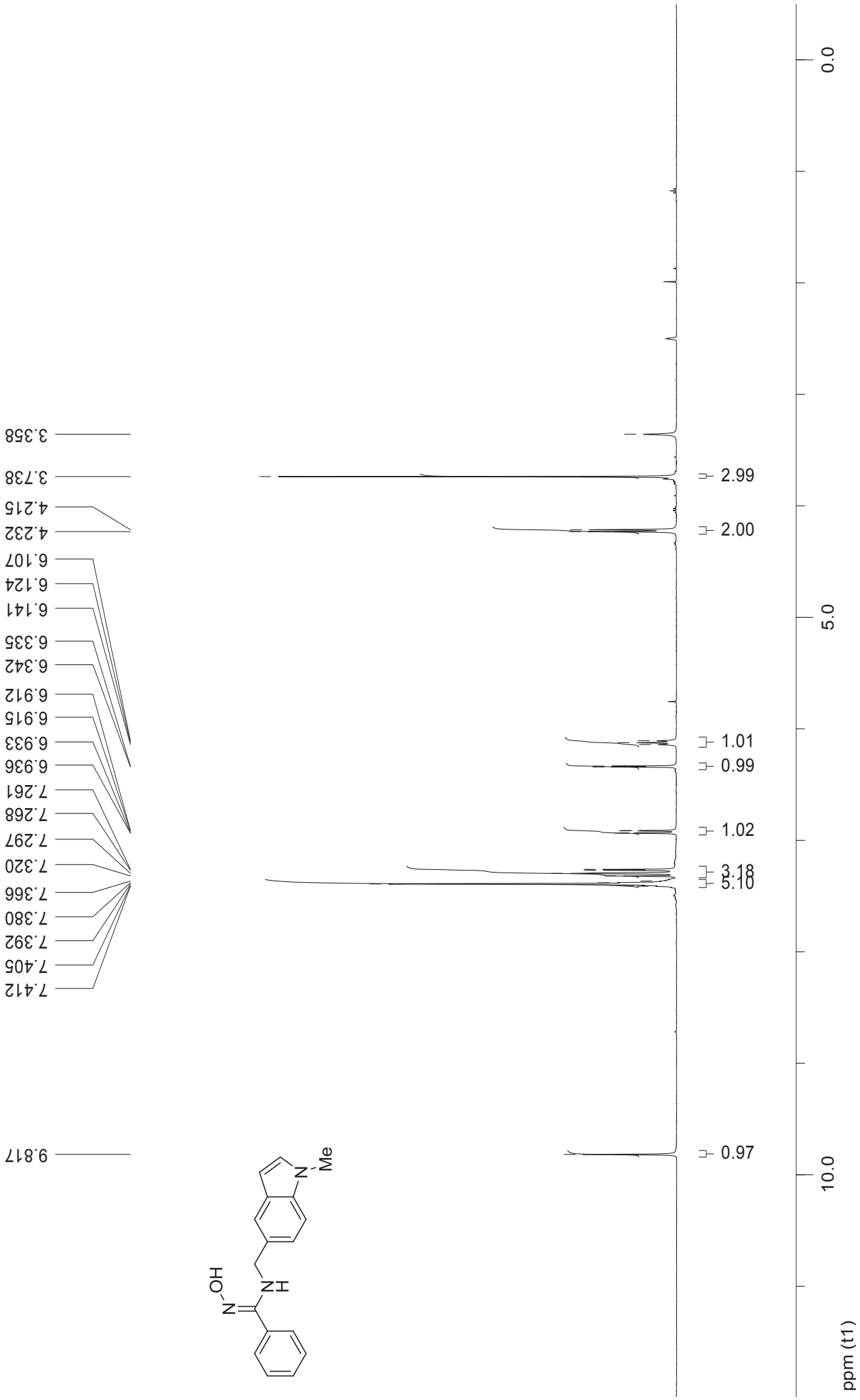
^{1}H NMR spectrum of **1o** ($CDCl_3$, 400 Hz):



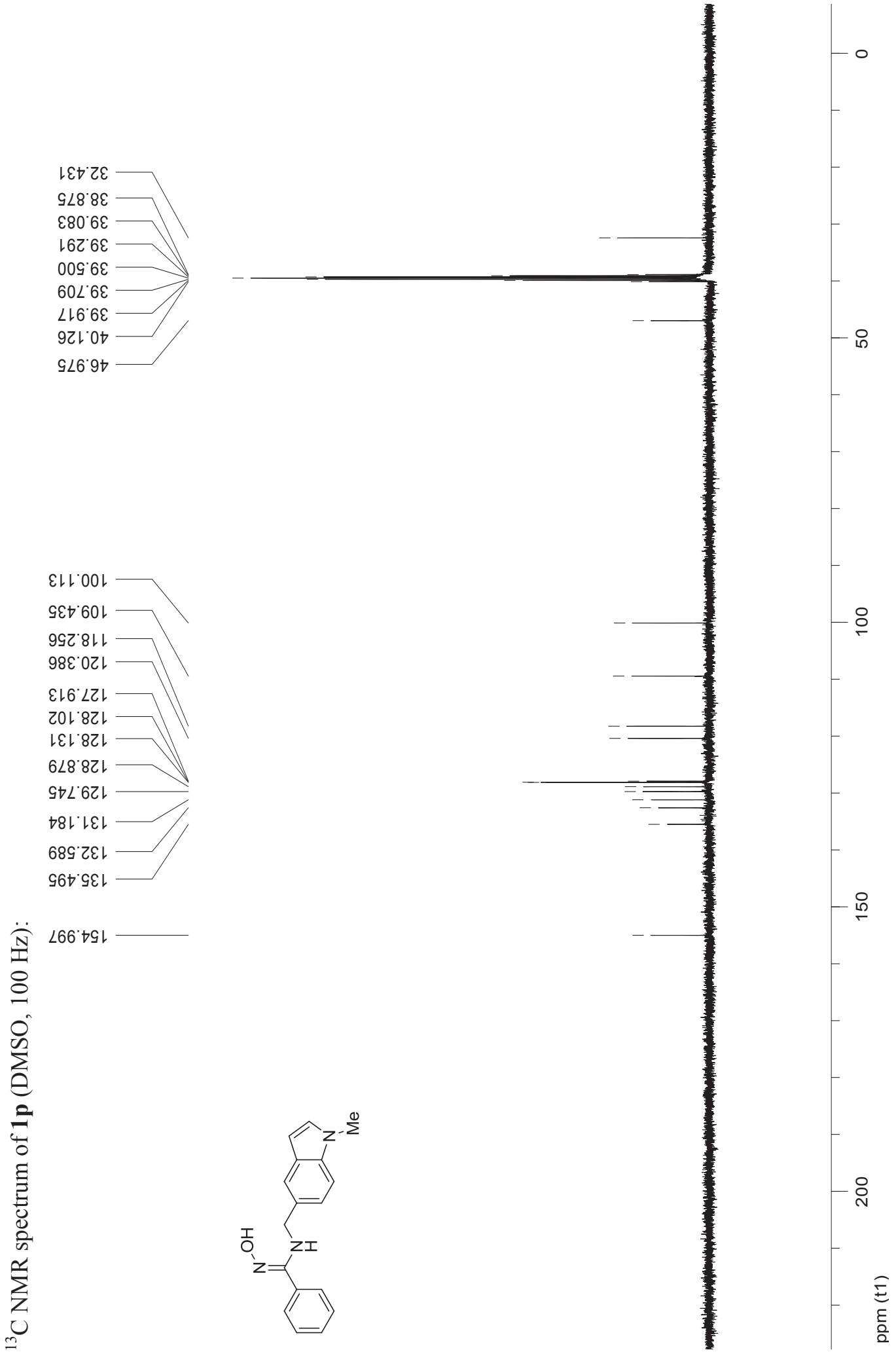
^{13}C NMR spectrum of **1o** ($CDCl_3$, 100 Hz):



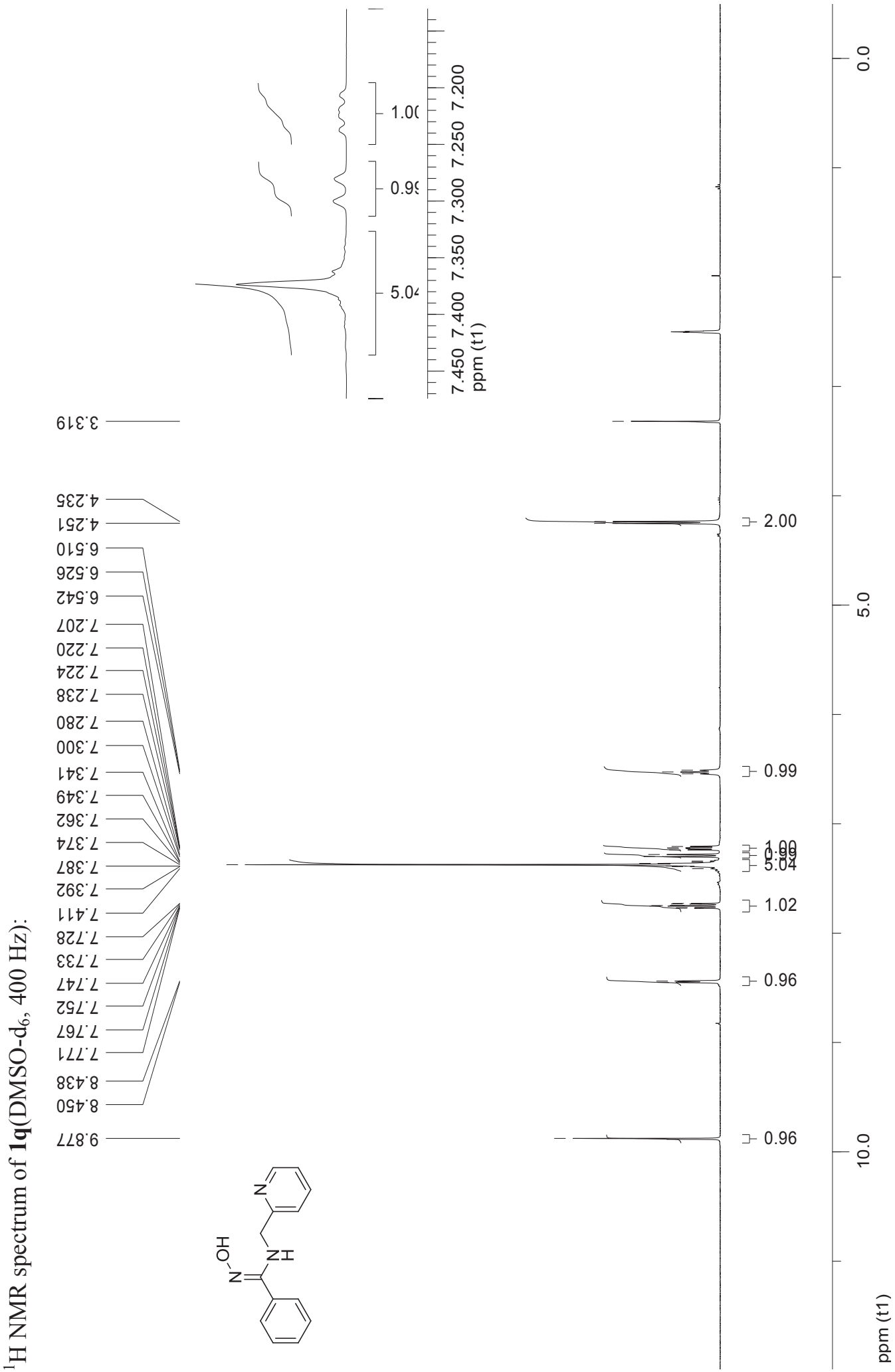
^{1}H NMR spectrum of **1p** (DMSO, 400 Hz):



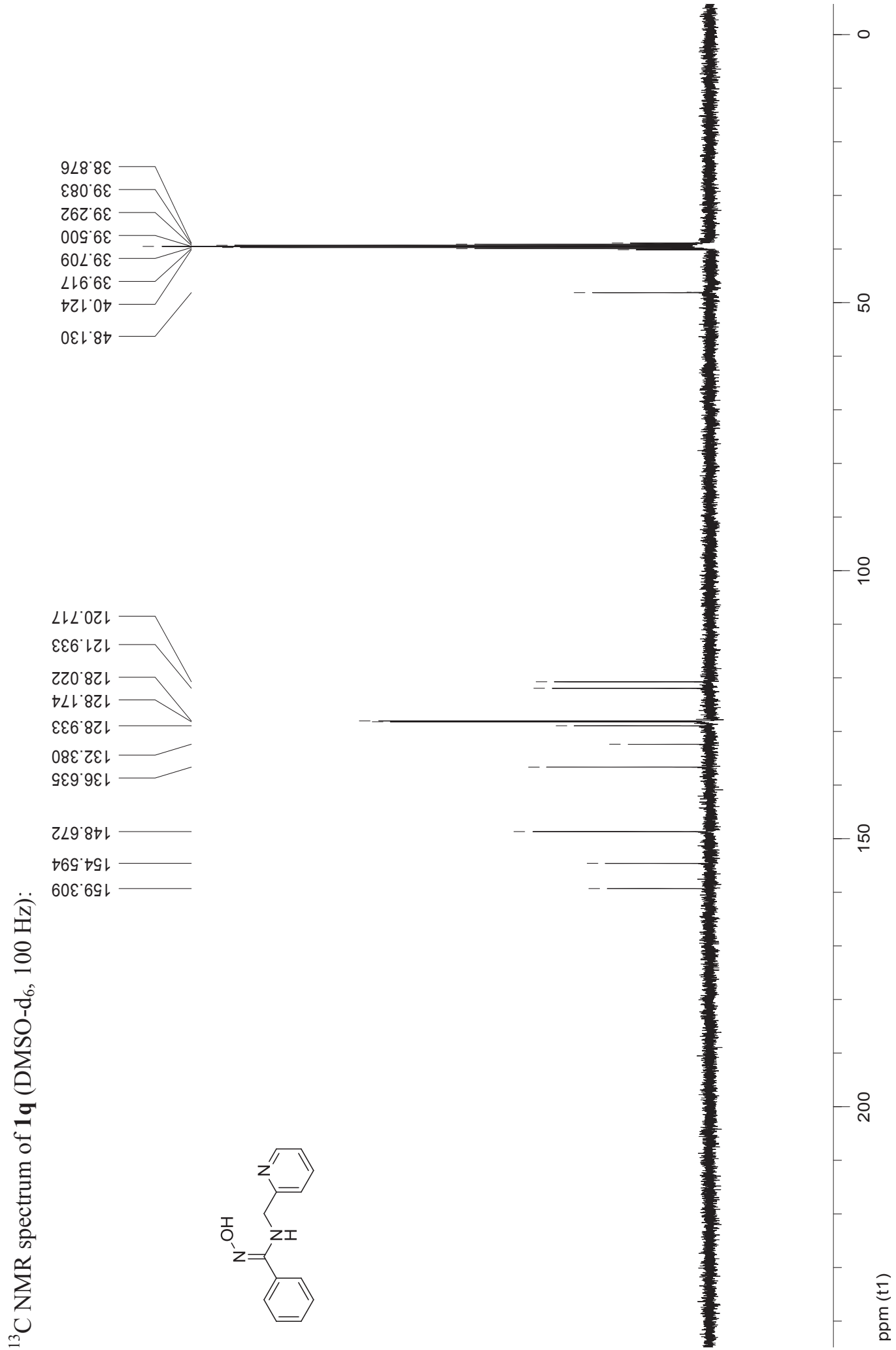
^{13}C NMR spectrum of **1p** (DMSO, 100 Hz):



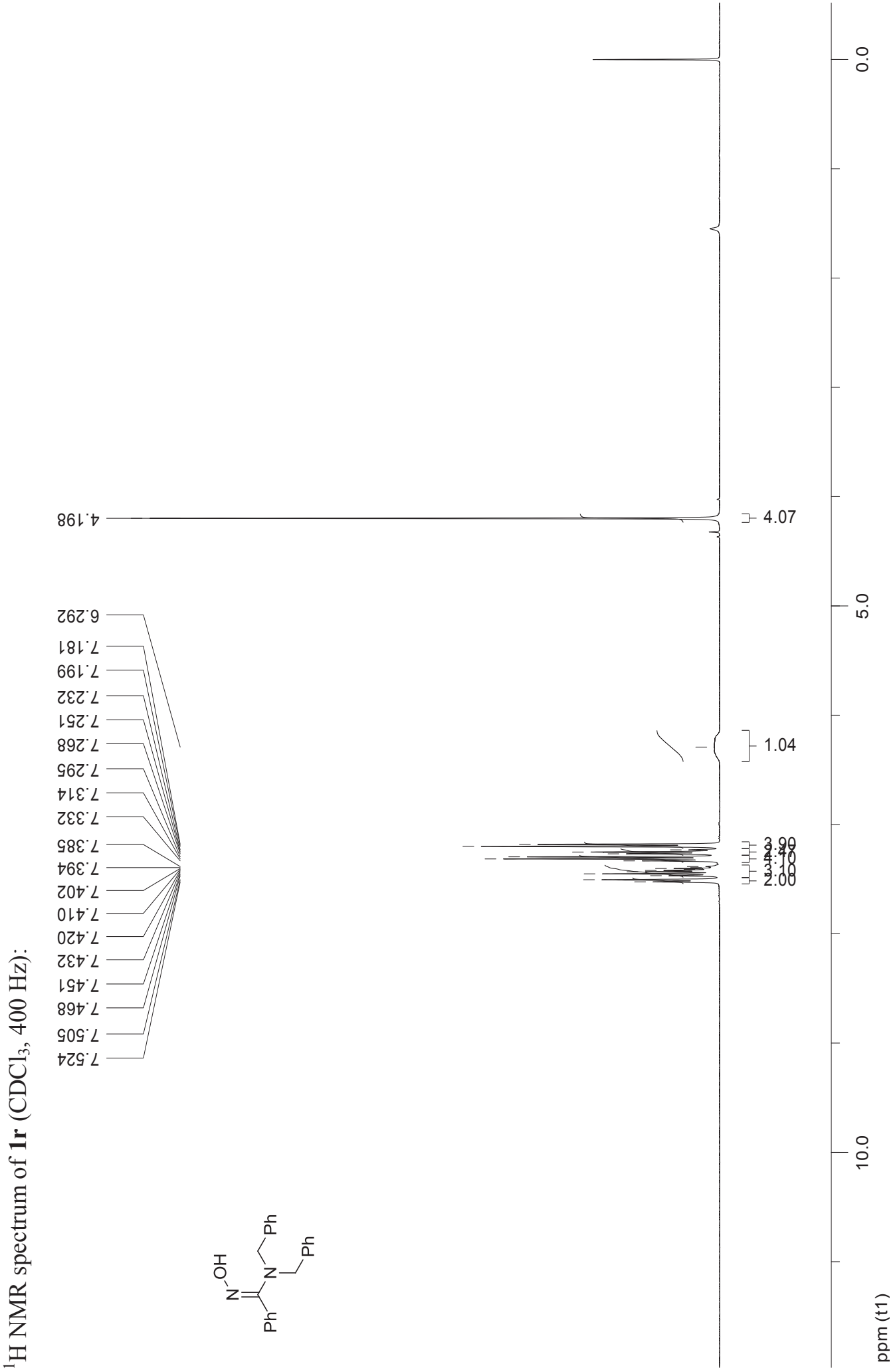
^{1}H NMR spectrum of **1q**(DMSO-d_6, 400 Hz):



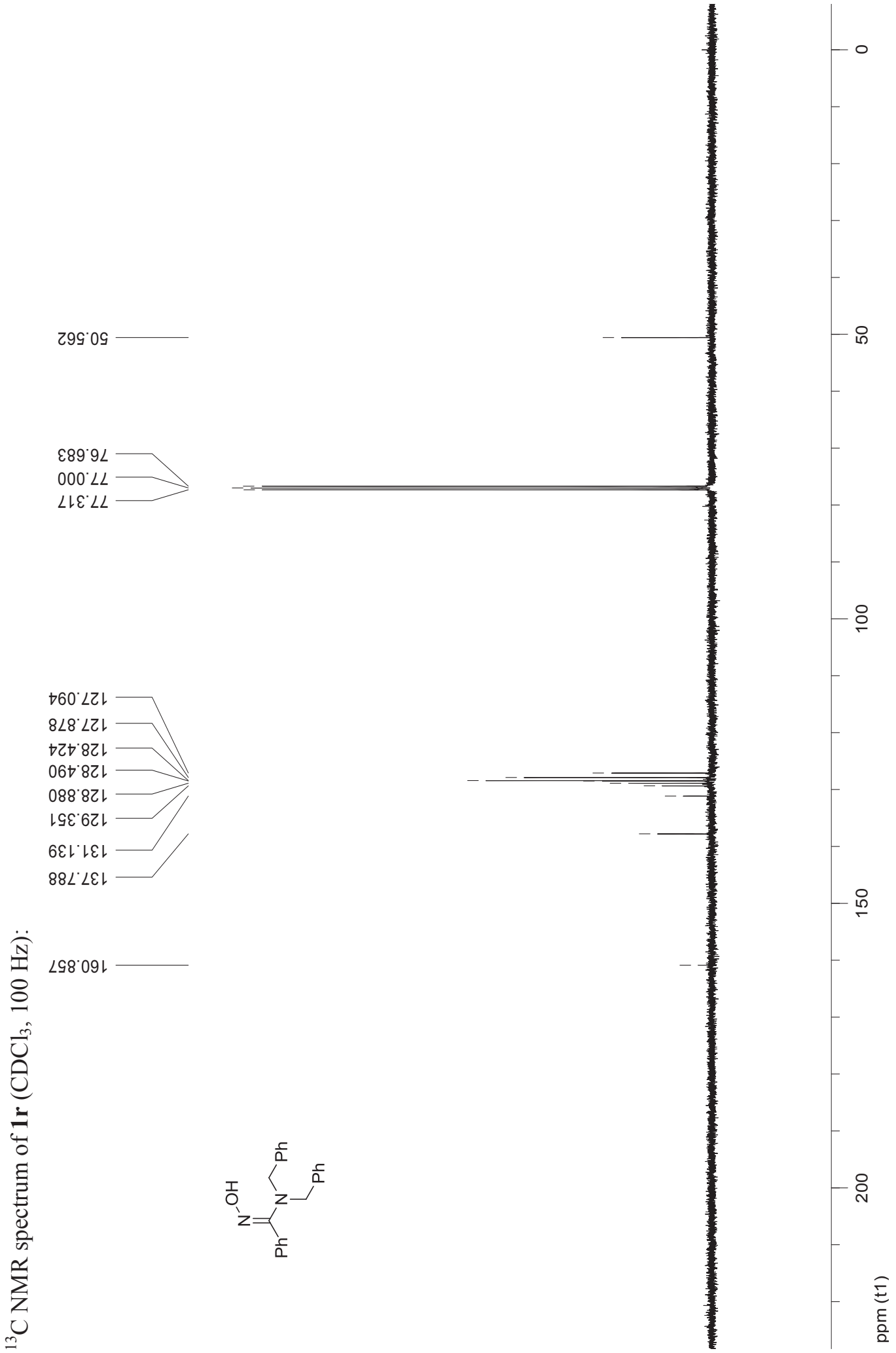
^{13}C NMR spectrum of **1q** (DMSO-d$_6$, 100 Hz):



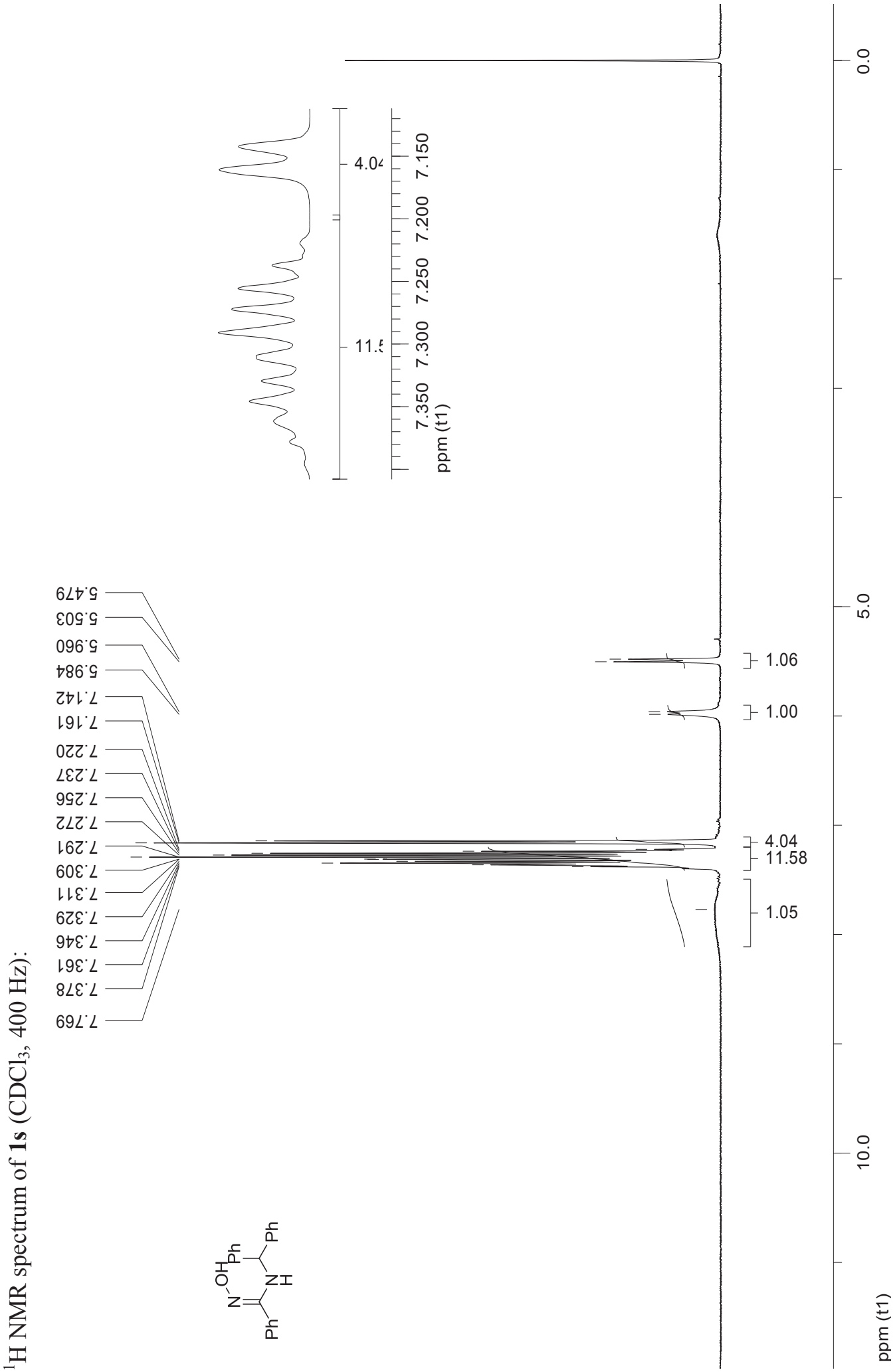
^{1}H NMR spectrum of **1r** ($CDCl_3$, 400 Hz):



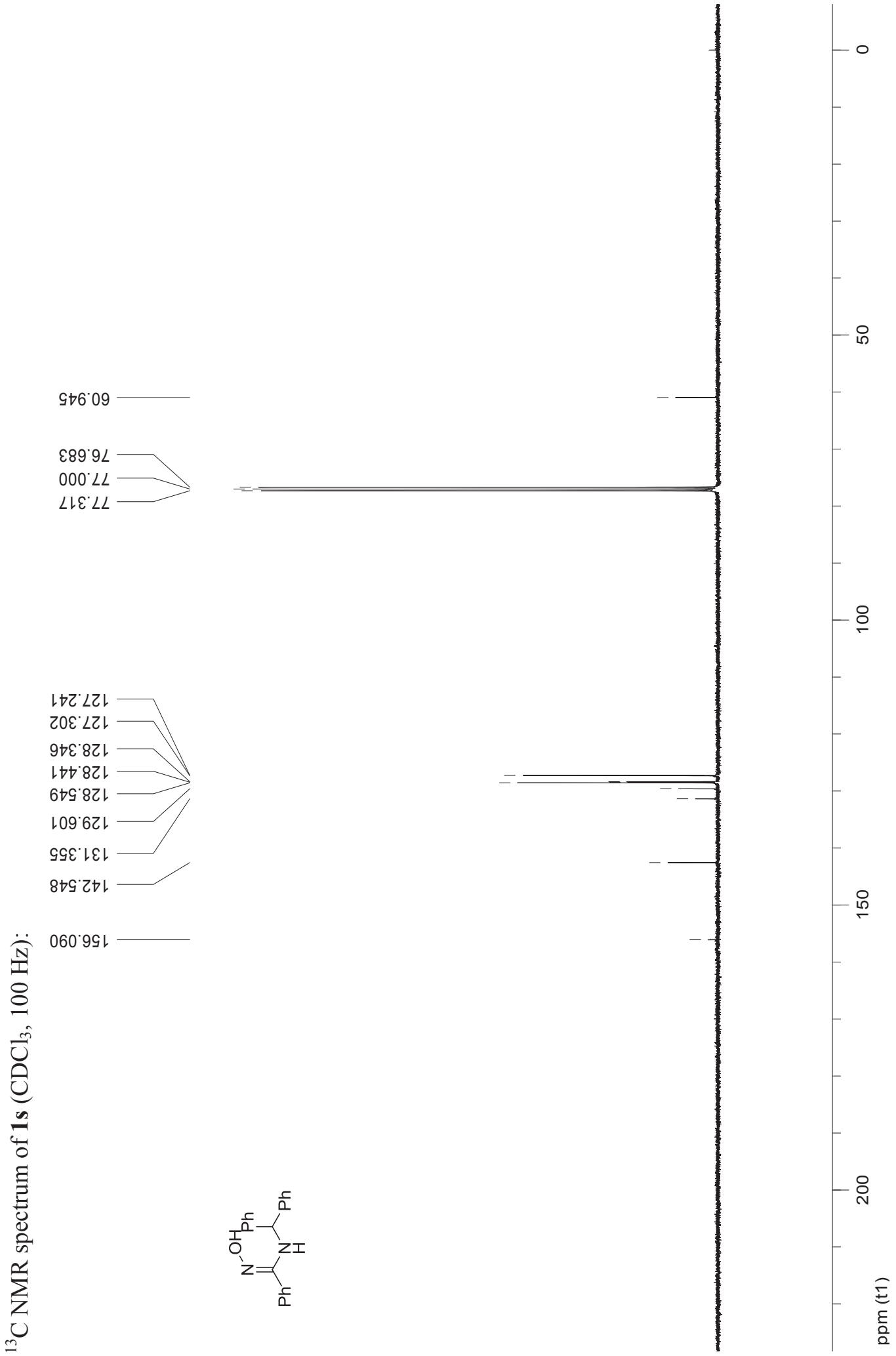
^{13}C NMR spectrum of **1r** ($CDCl_3$, 100 Hz):



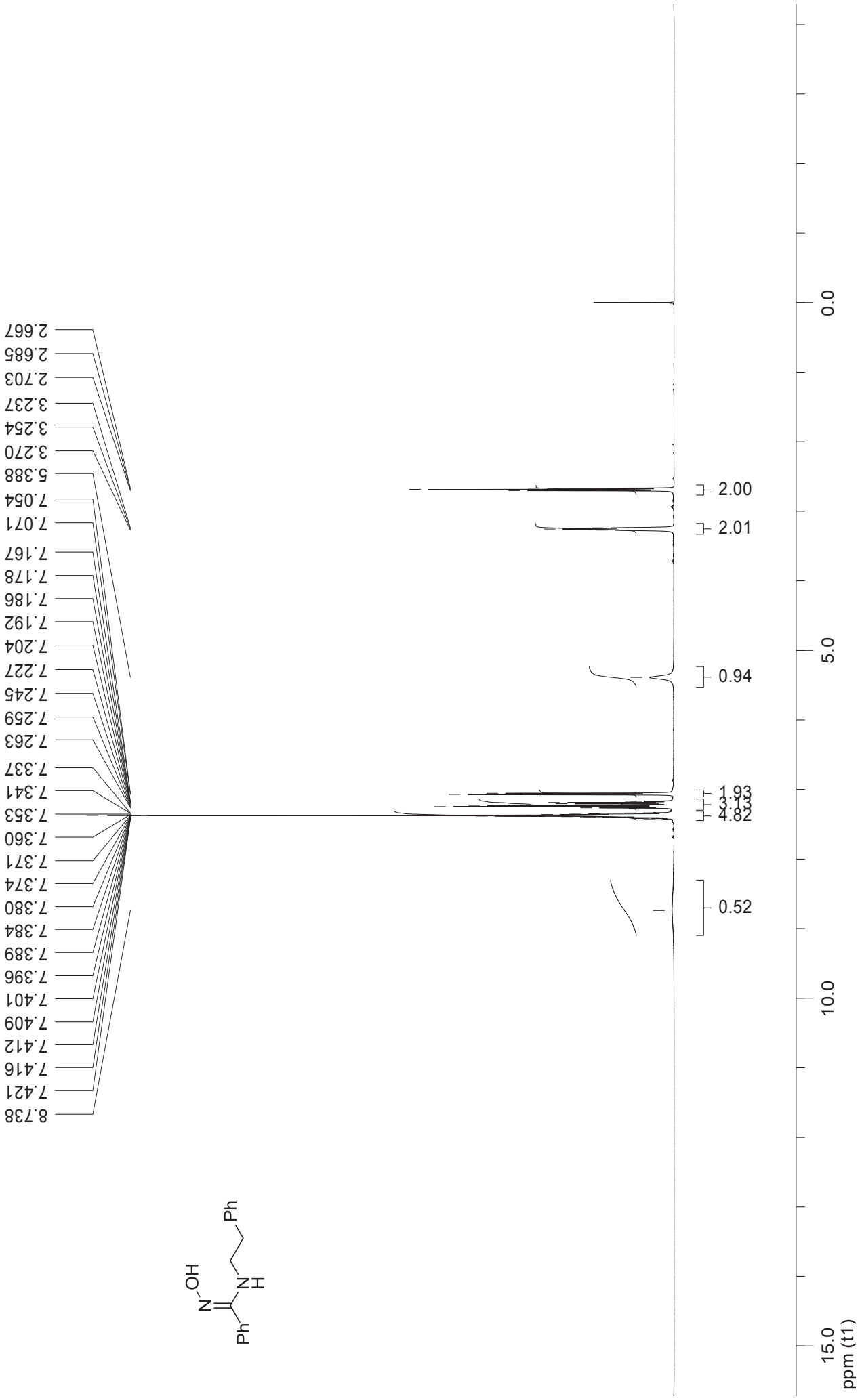
^{1}H NMR spectrum of **1s** ($CDCl_3$, 400 Hz):



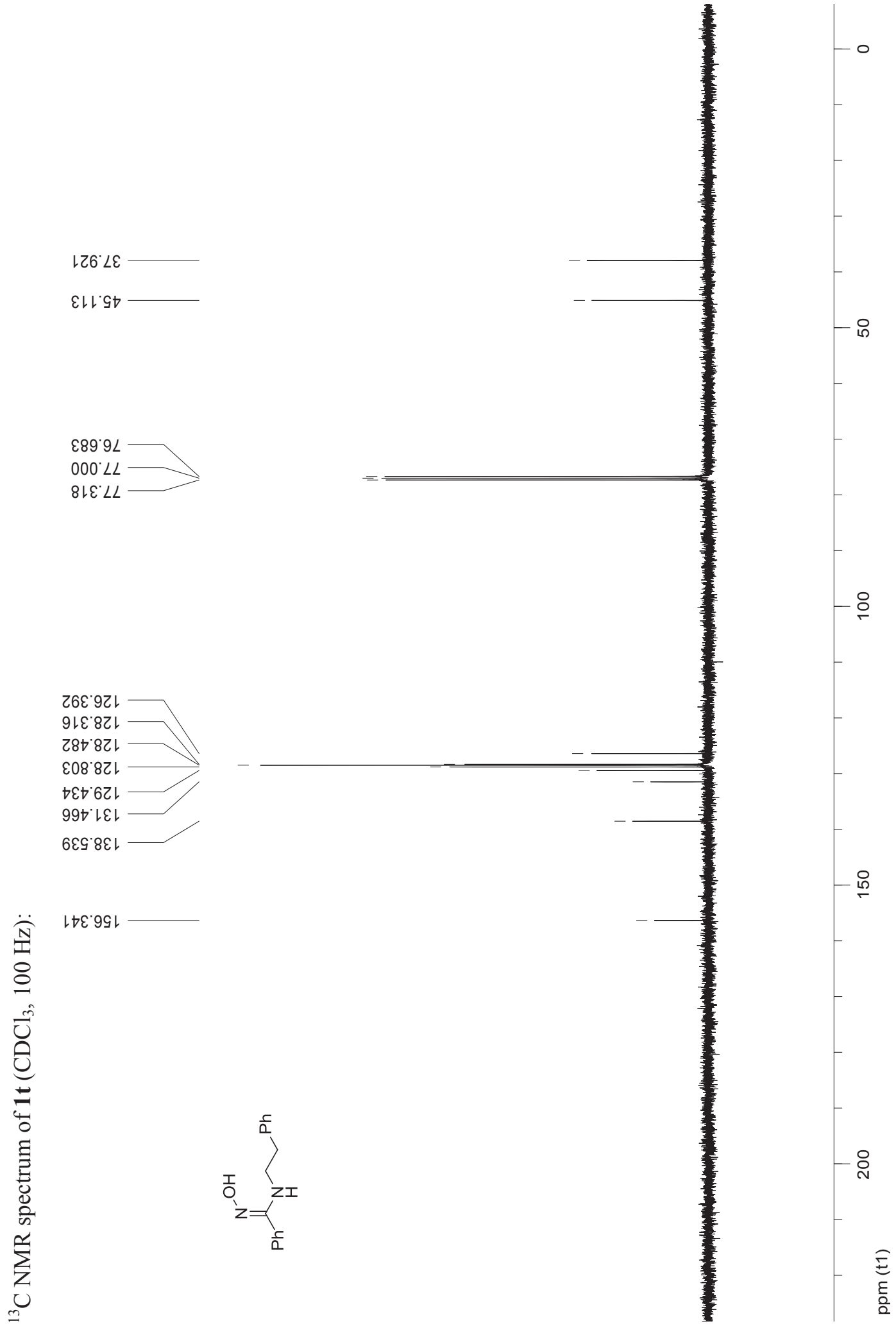
^{13}C NMR spectrum of **1s** ($CDCl_3$, 100 Hz):



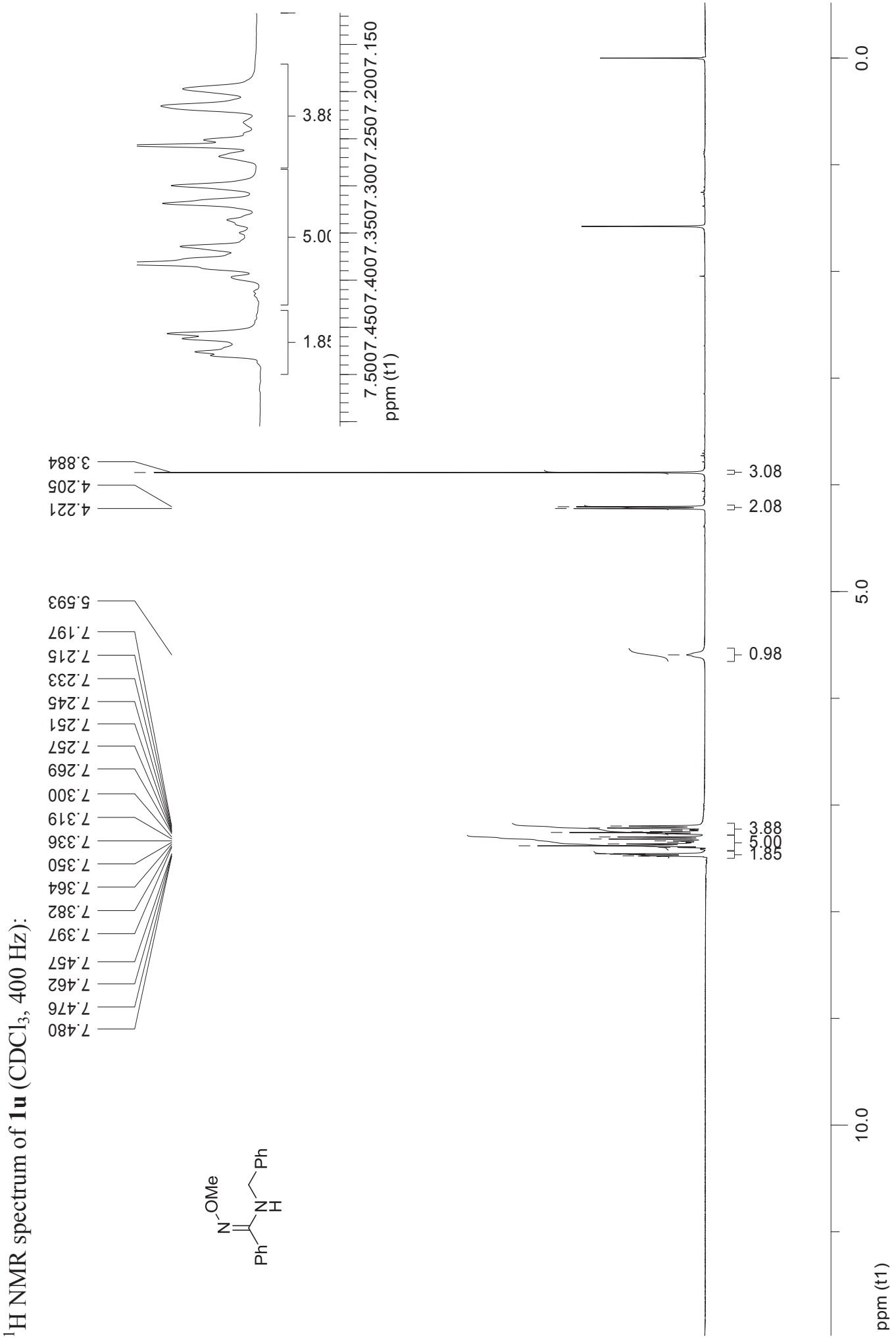
^{1}H NMR spectrum of **1t** ($CDCl_3$, 400 Hz):



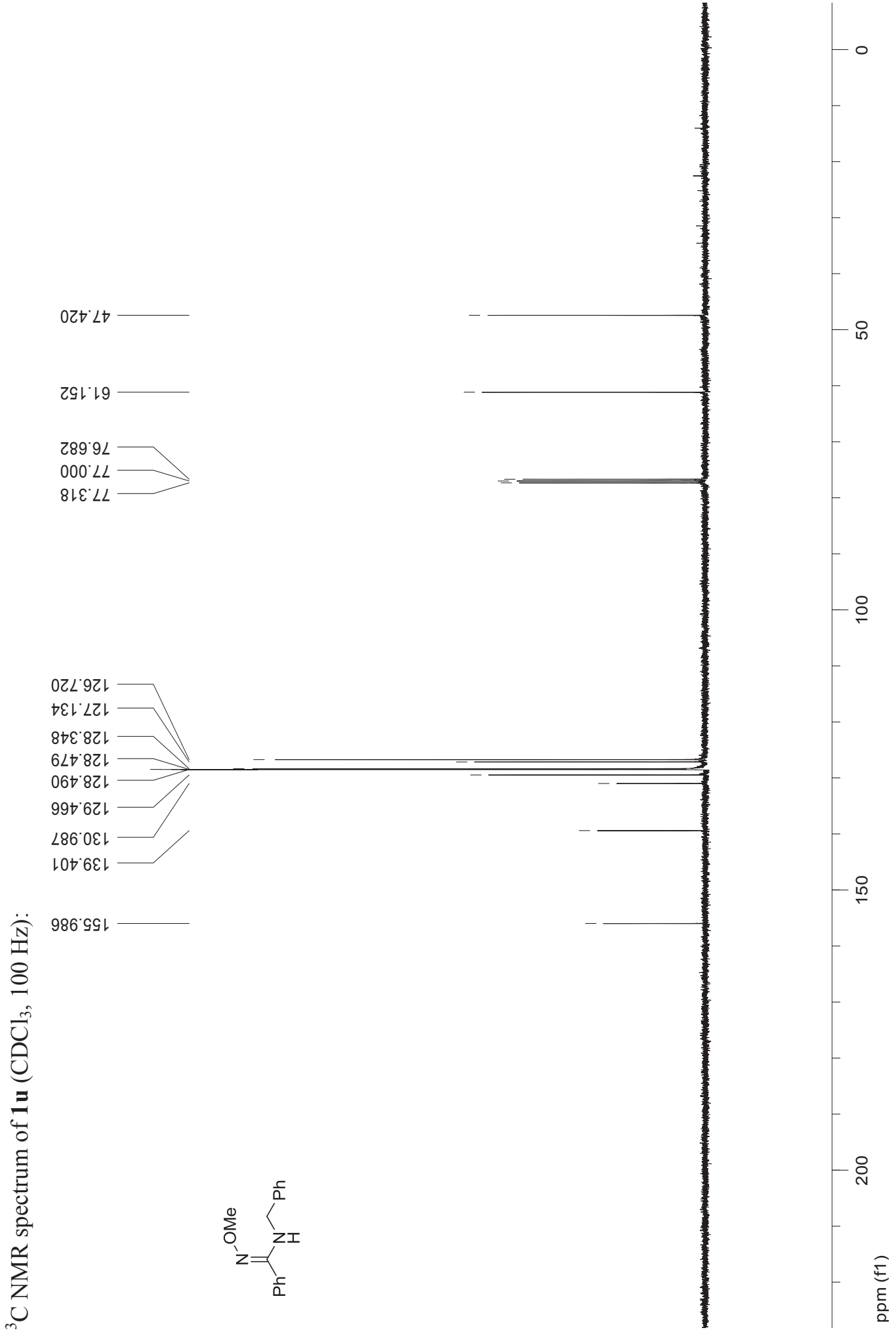
^{13}C NMR spectrum of **1t** ($CDCl_3$, 100 Hz):



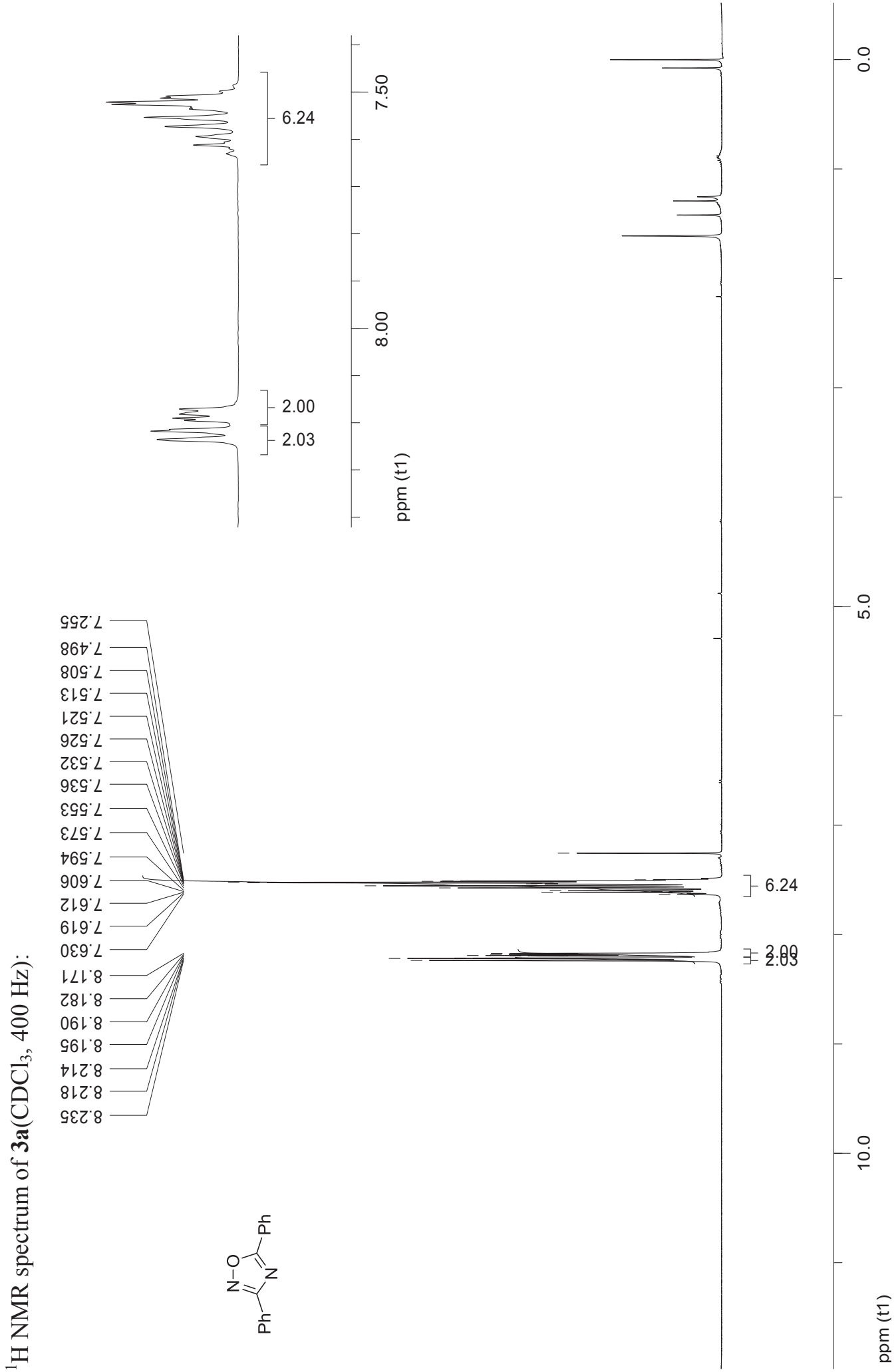
^{1}H NMR spectrum of **1u** ($CDCl_3$, 400 Hz):



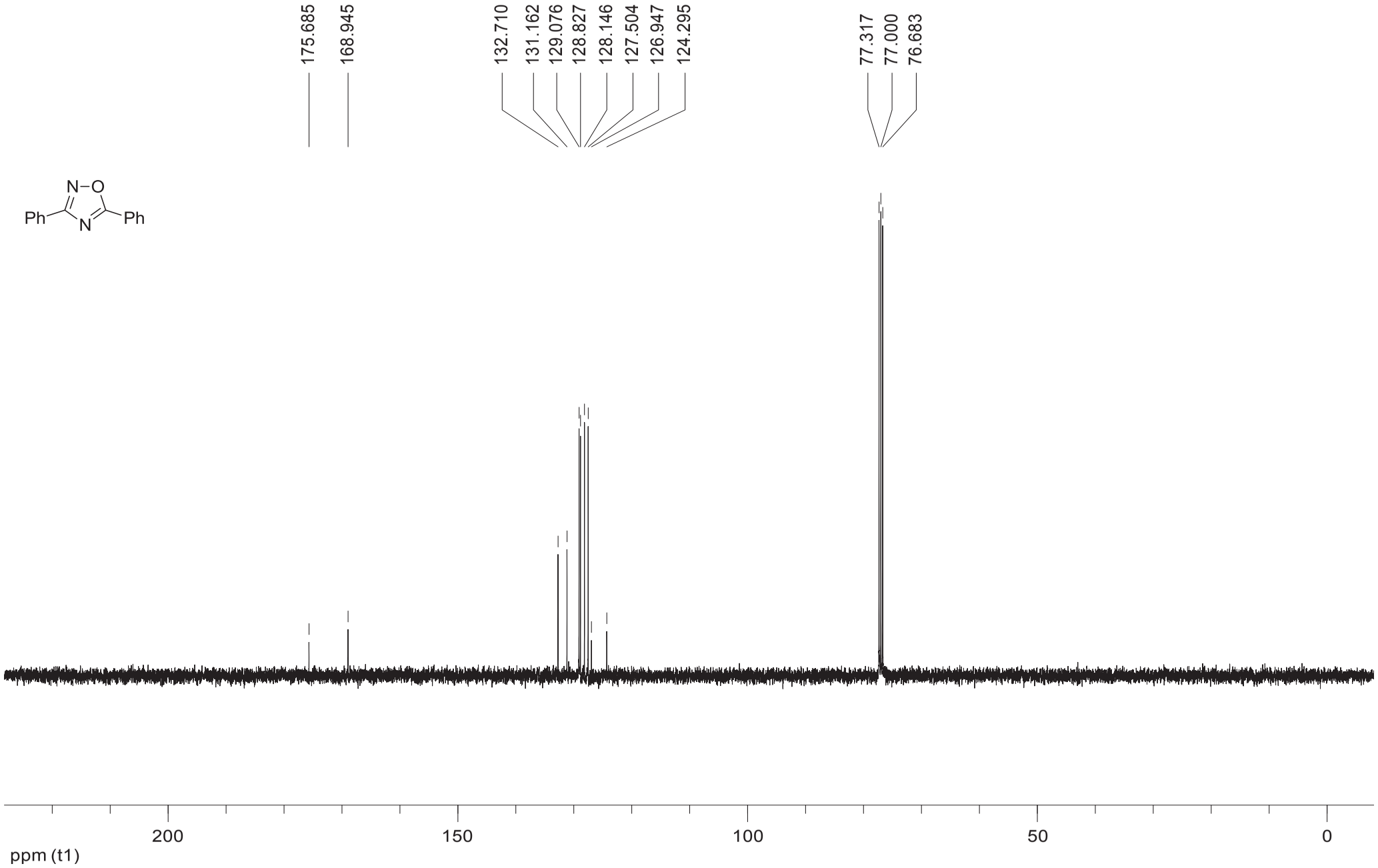
^{13}C NMR spectrum of **1u** ($CDCl_3$, 100 Hz):



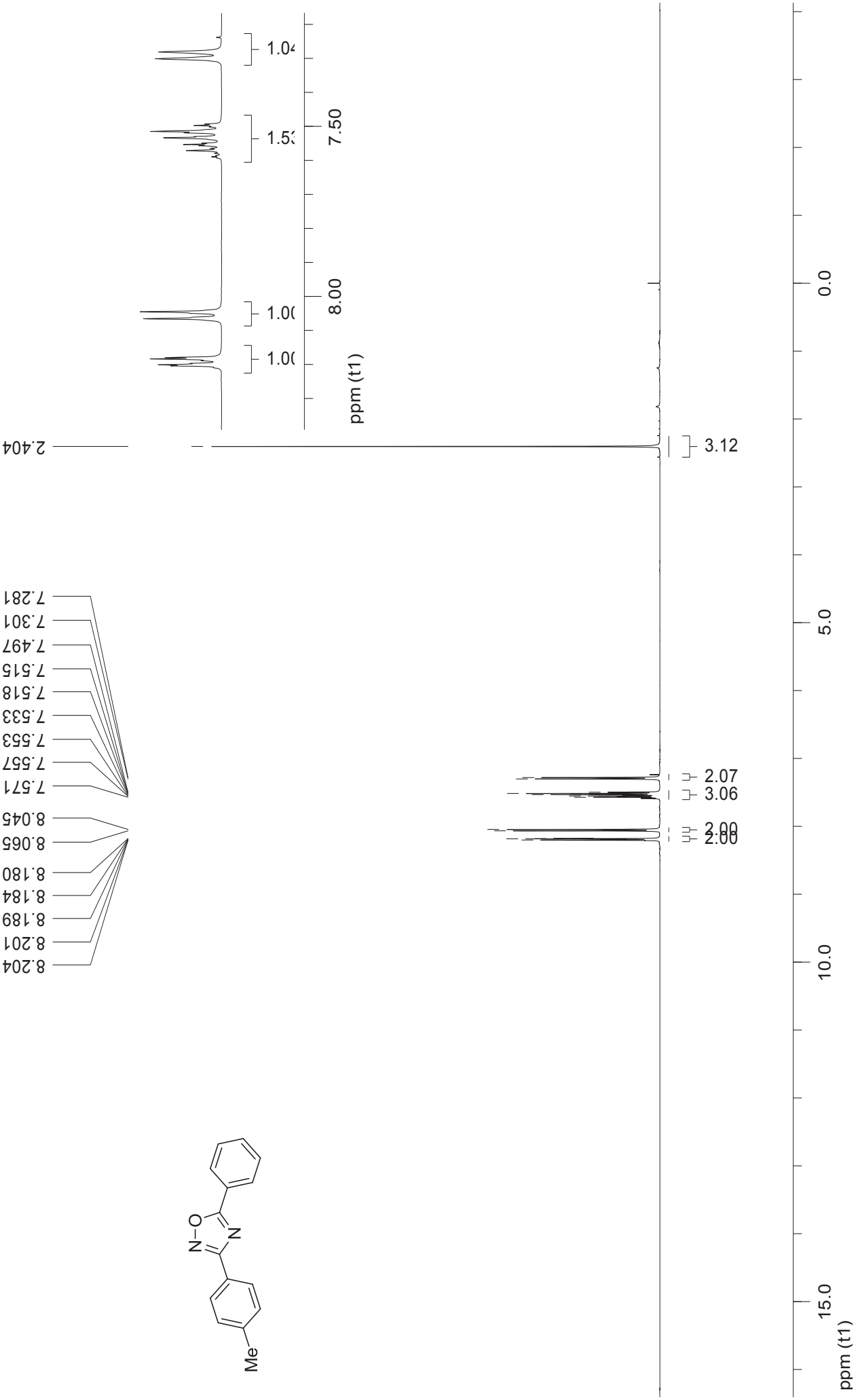
^{1}H NMR spectrum of **3a**($CDCl_3$, 400 Hz):



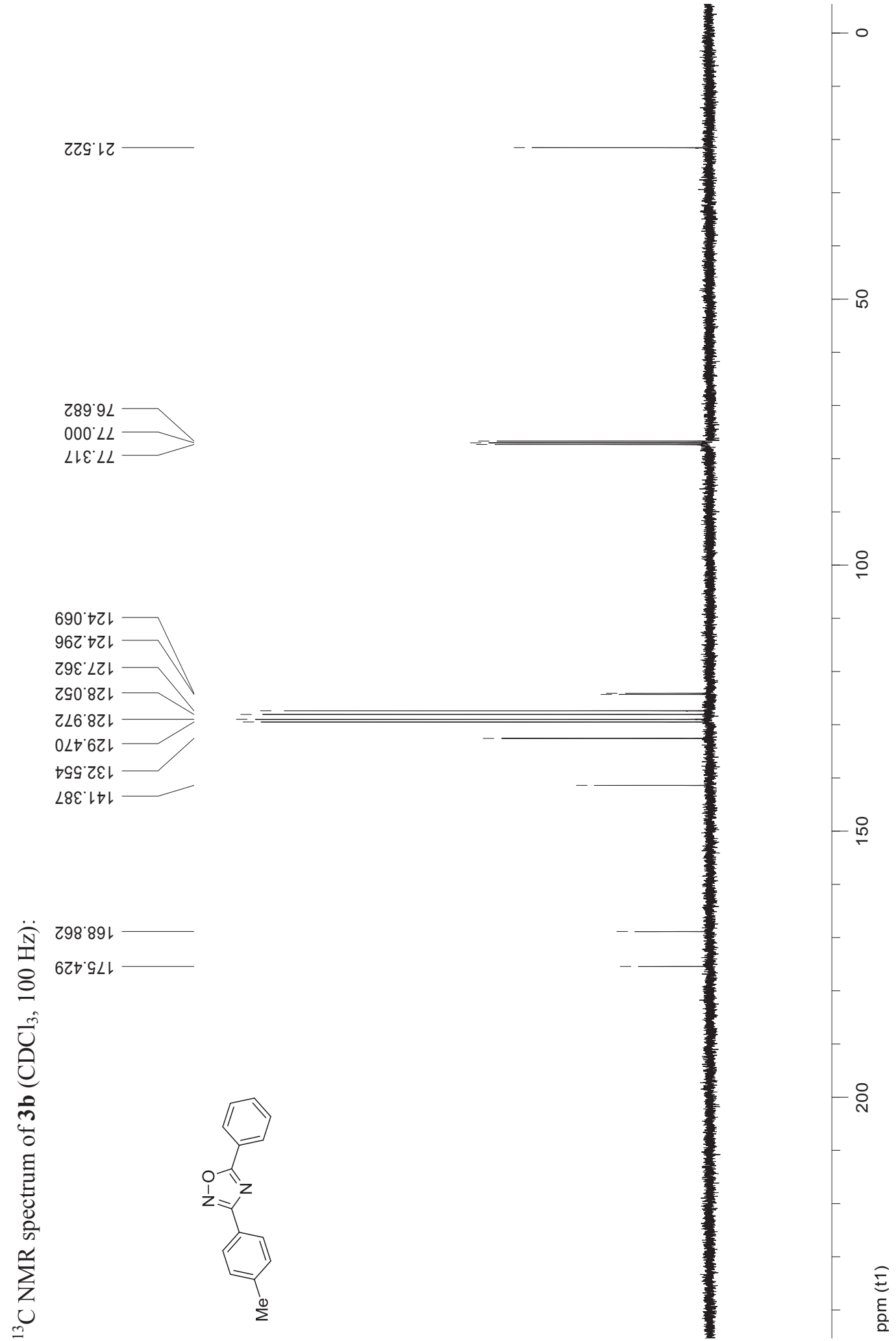
^{13}C NMR spectrum of **3a**($CDCl_3$, 100 Hz):



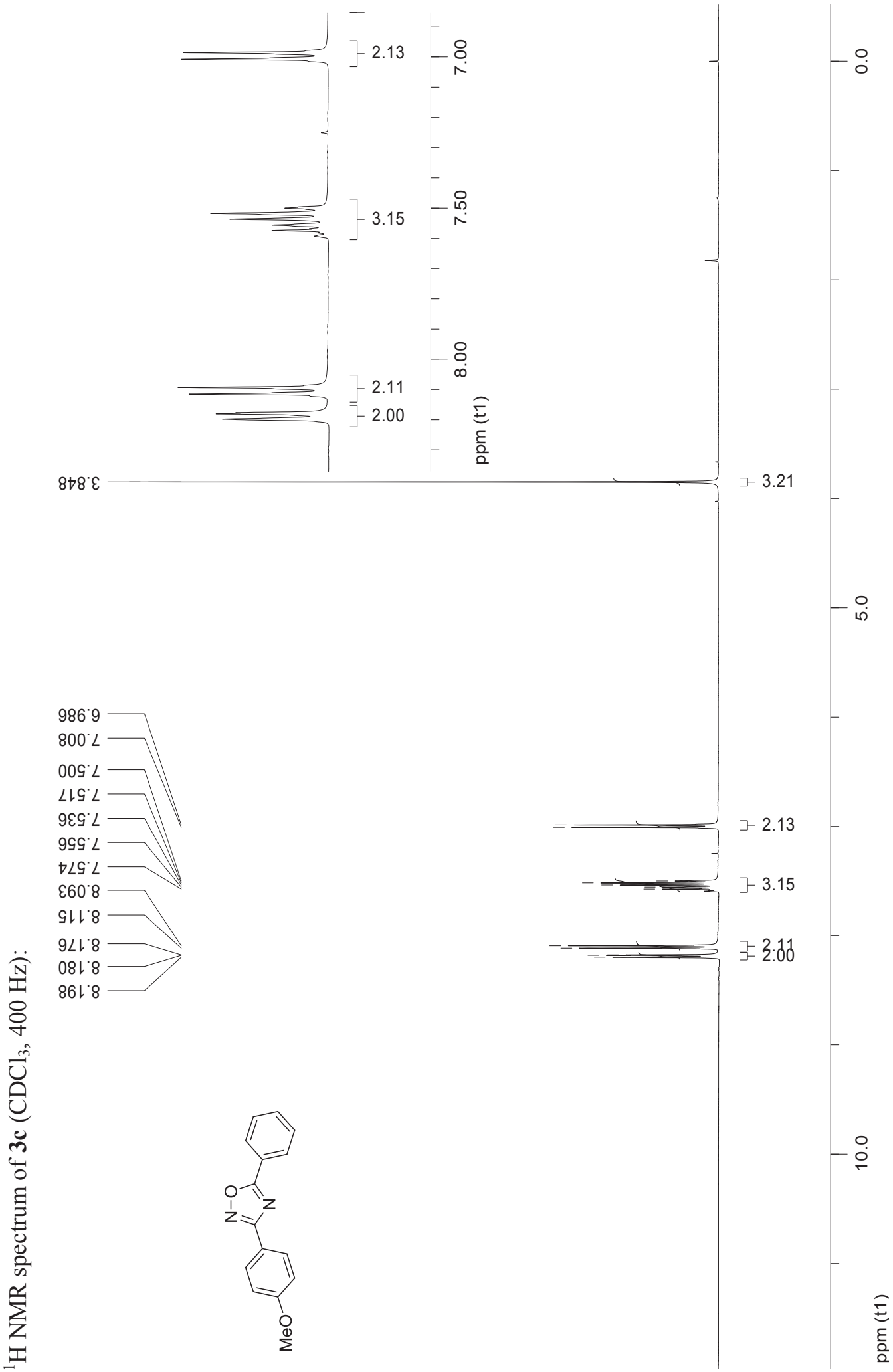
^{1}H NMR spectrum of **3b** ($CDCl_3$, 400 Hz):



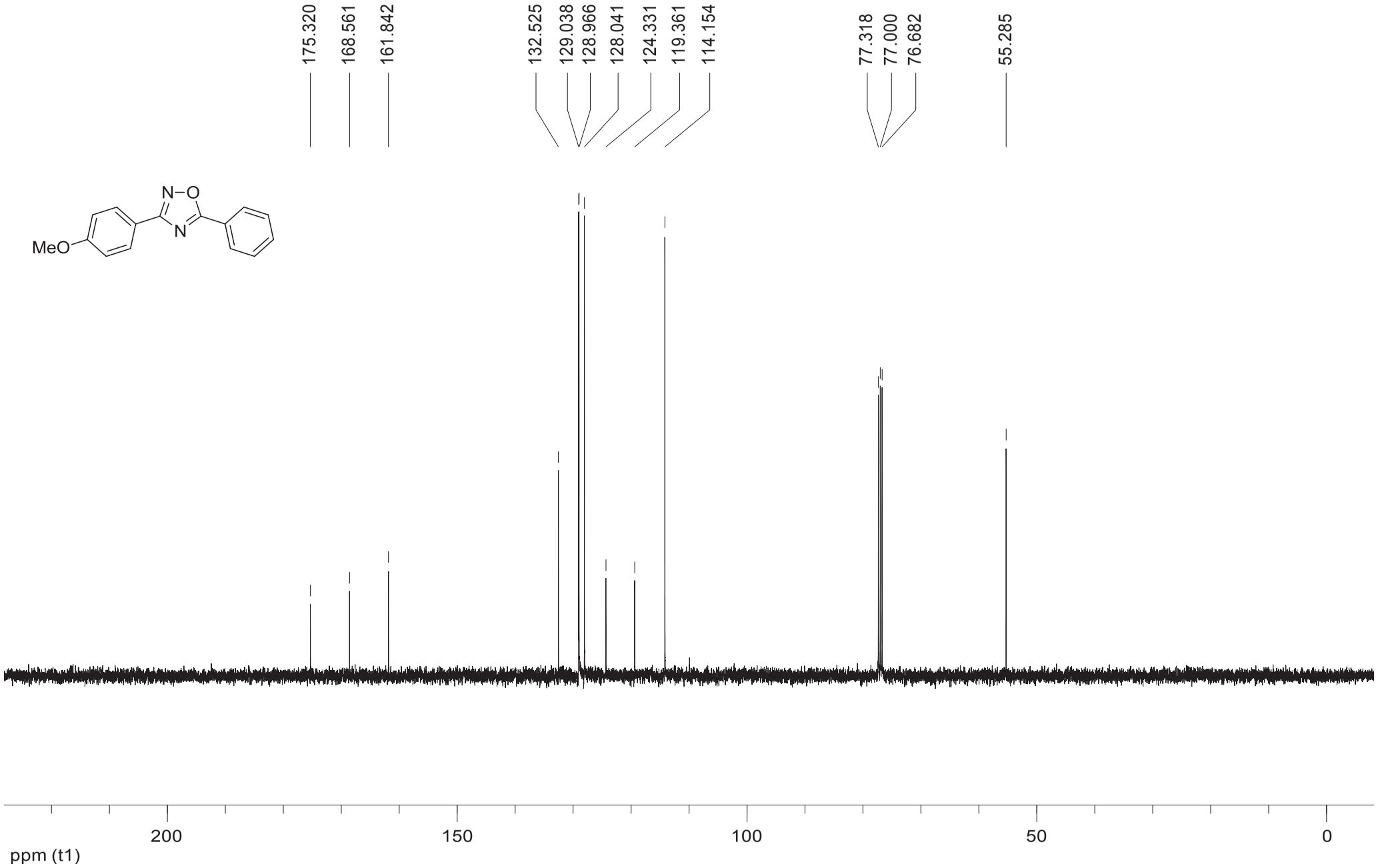
^{13}C NMR spectrum of **3b** ($CDCl_3$, 100 Hz):



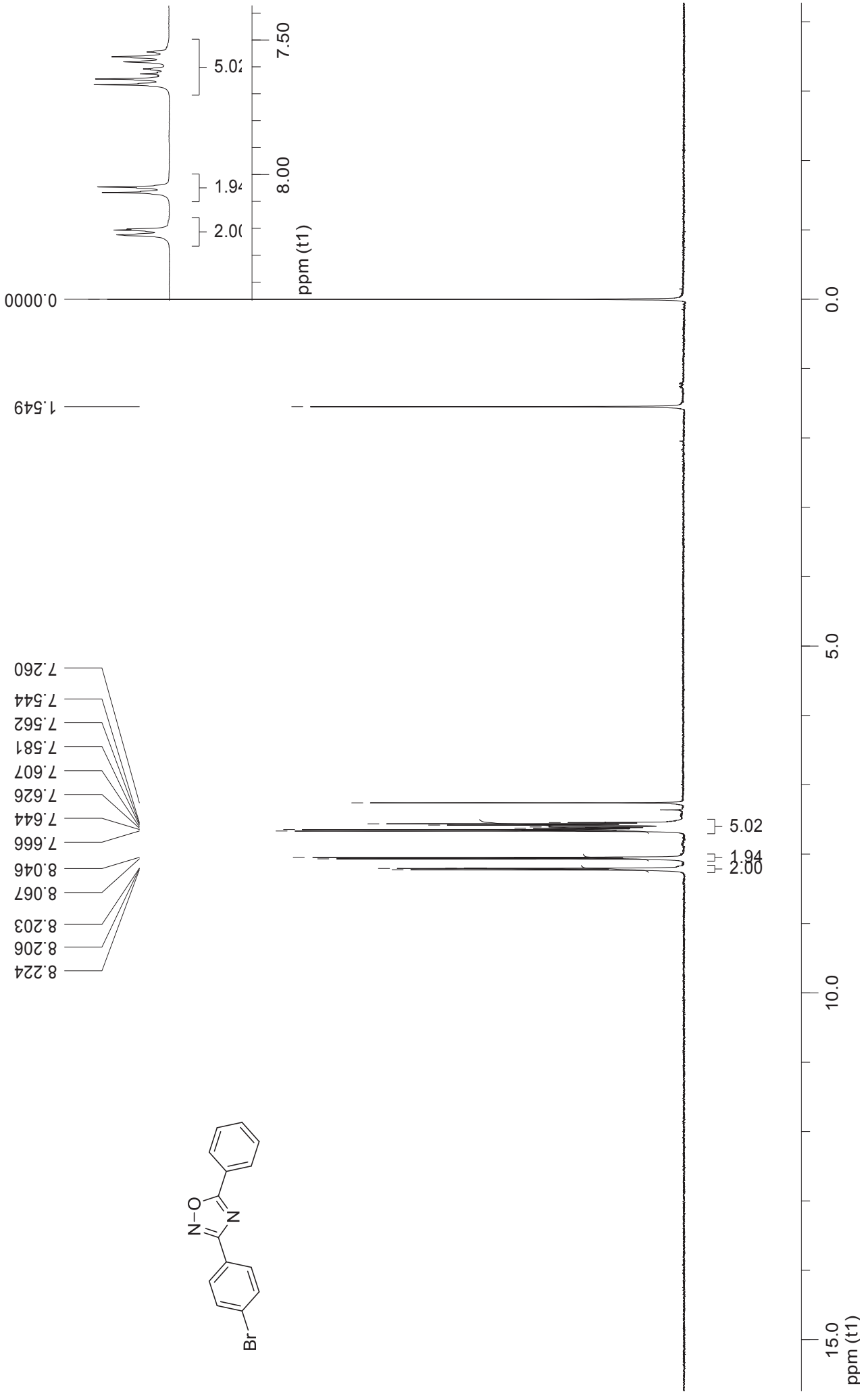
^{1}H NMR spectrum of **3c** ($CDCl_3$, 400 Hz):



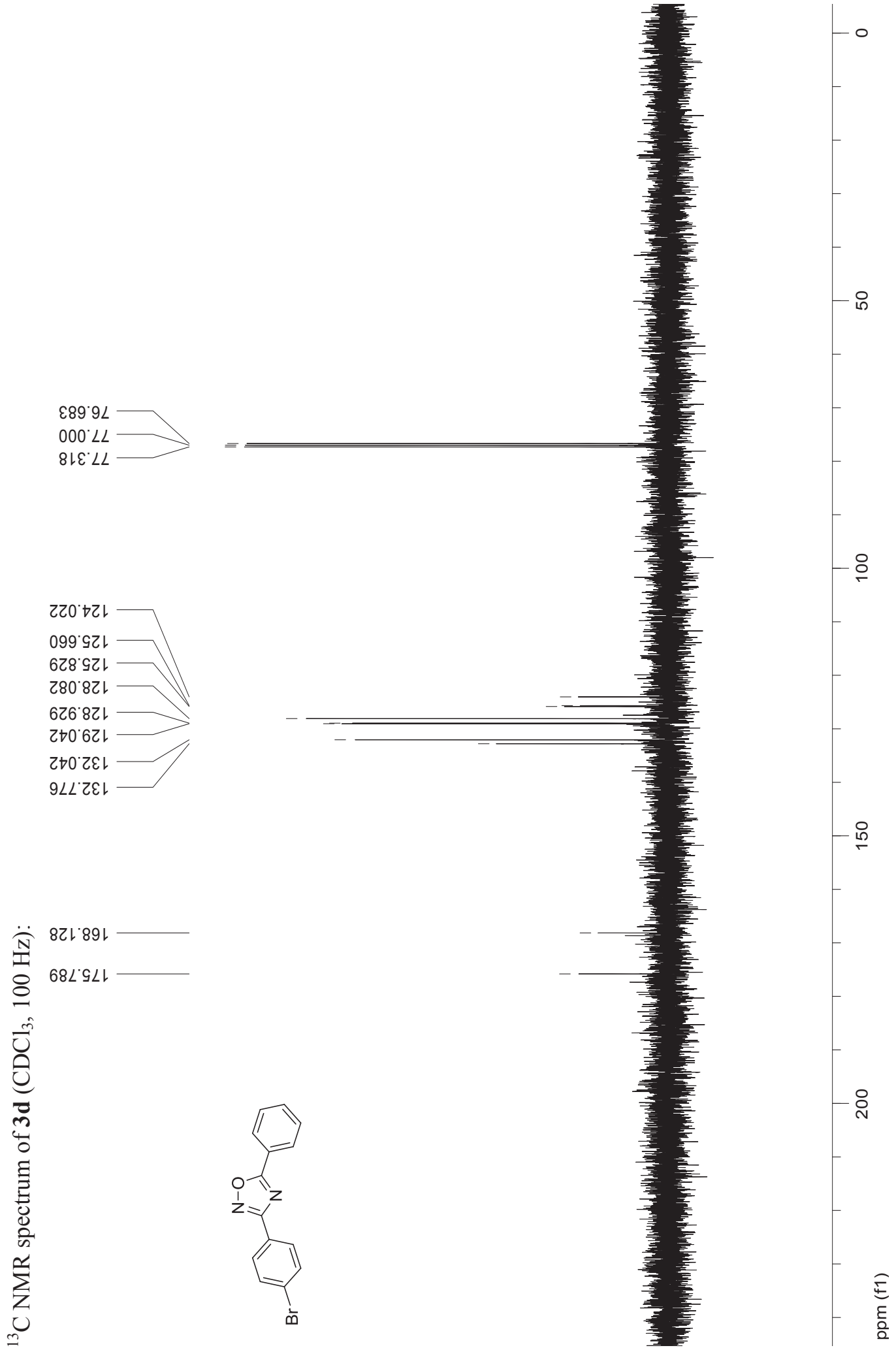
^{13}C NMR spectrum of **3c** ($CDCl_3$, 100 Hz):



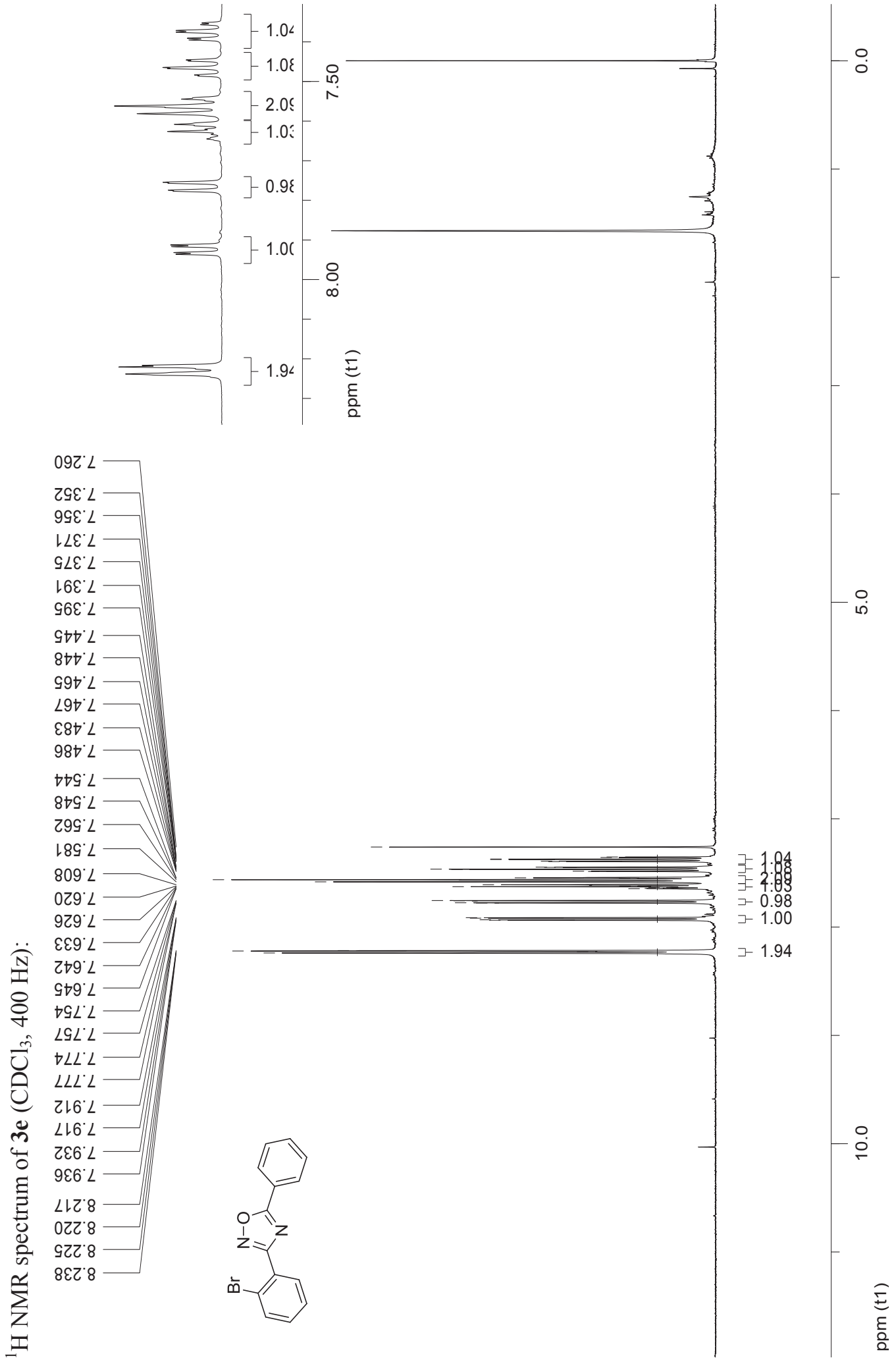
^{1}H NMR spectrum of **3d** ($CDCl_3$, 400 Hz):



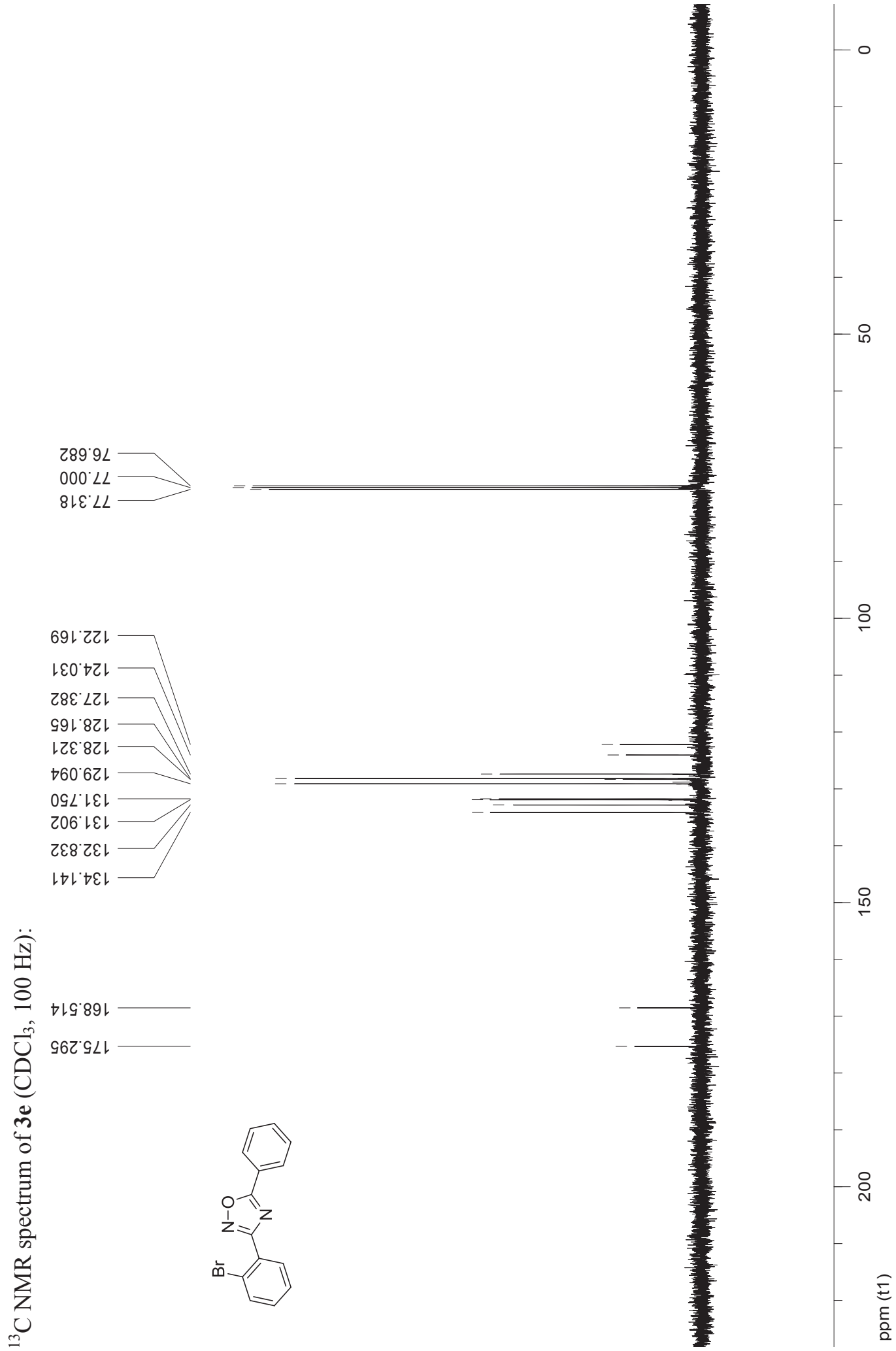
^{13}C NMR spectrum of **3d** ($CDCl_3$, 100 Hz):



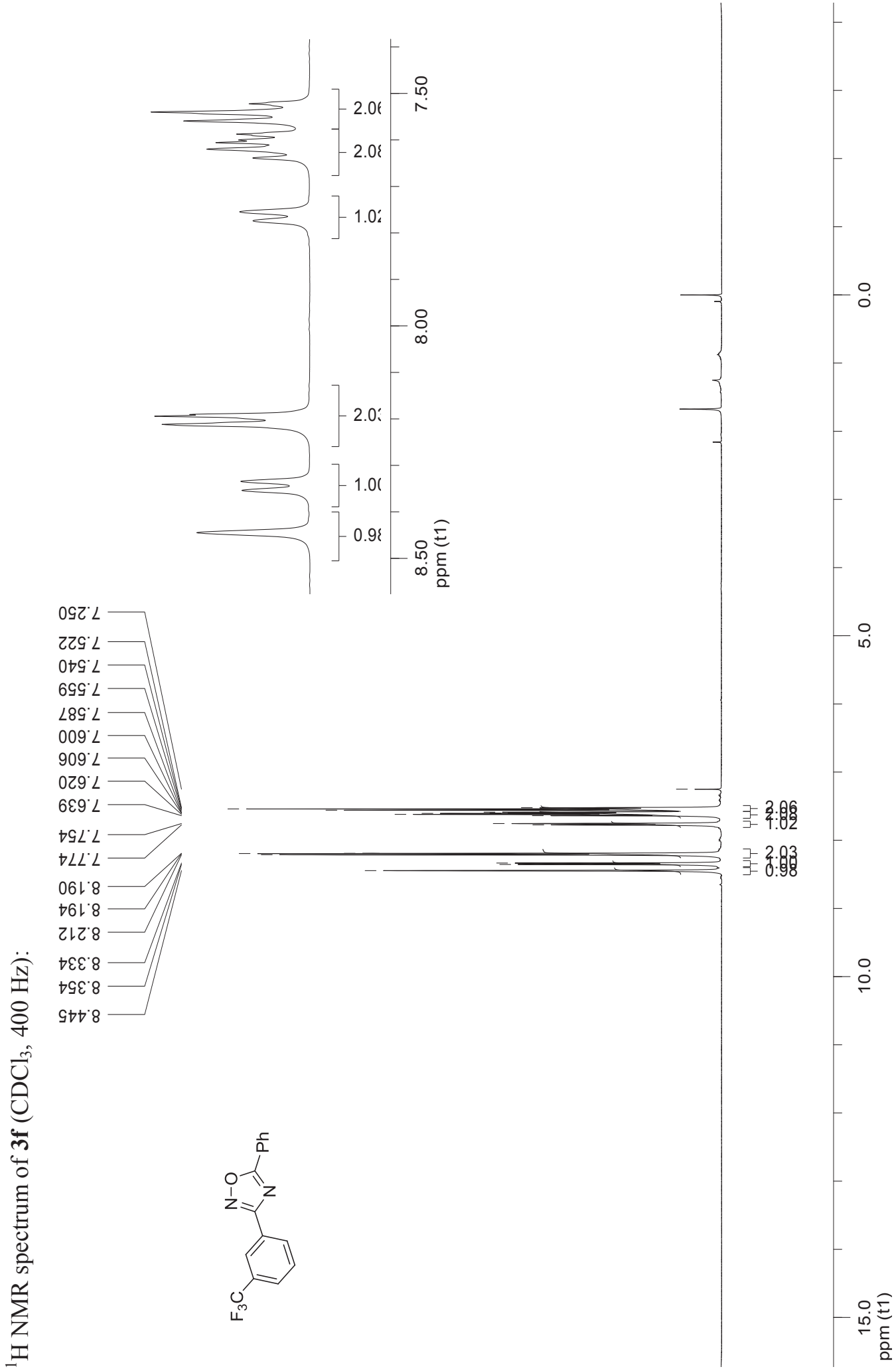
^{1}H NMR spectrum of **3e** ($CDCl_3$, 400 Hz):



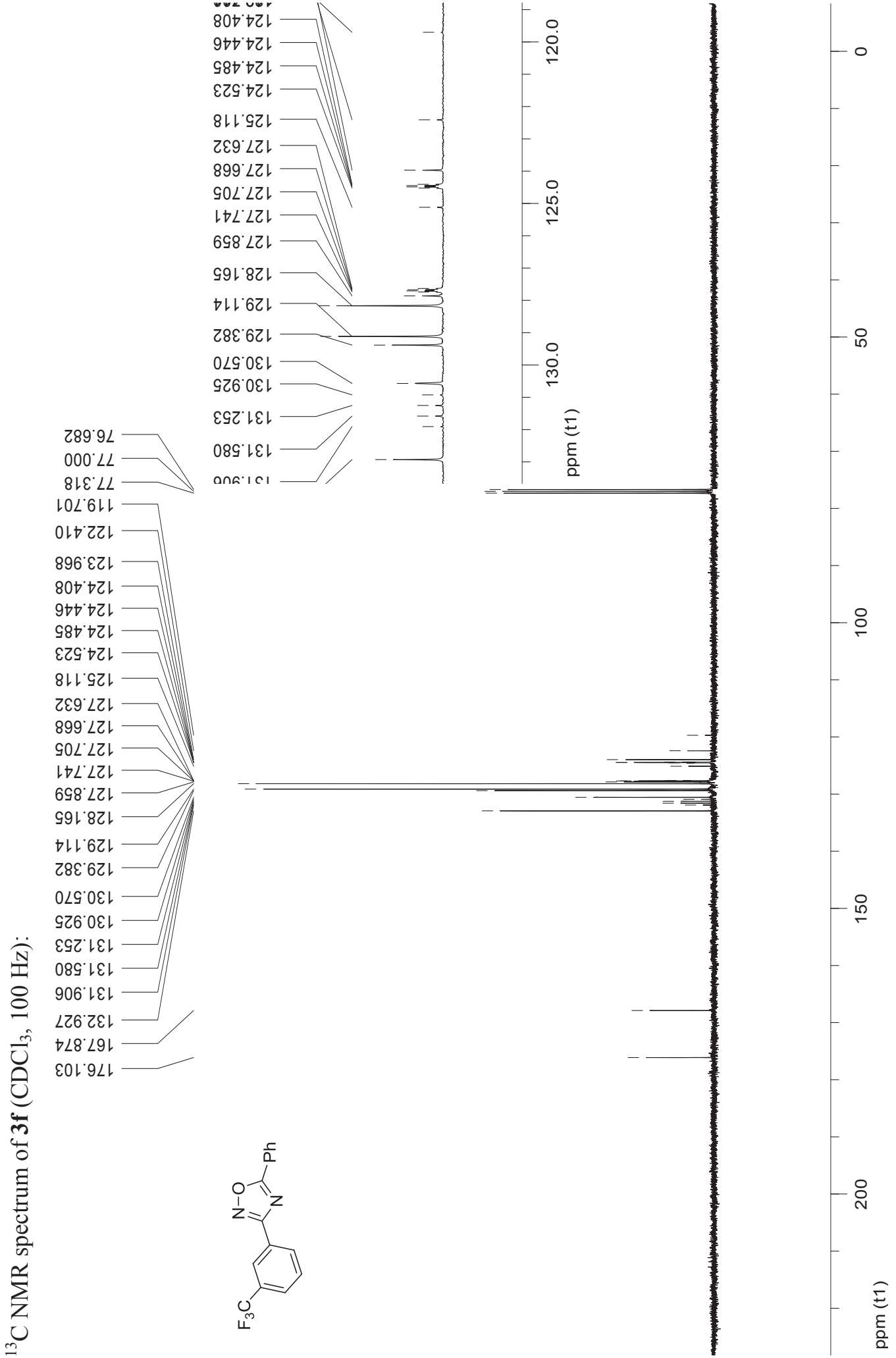
^{13}C NMR spectrum of **3e** ($CDCl_3$, 100 Hz):



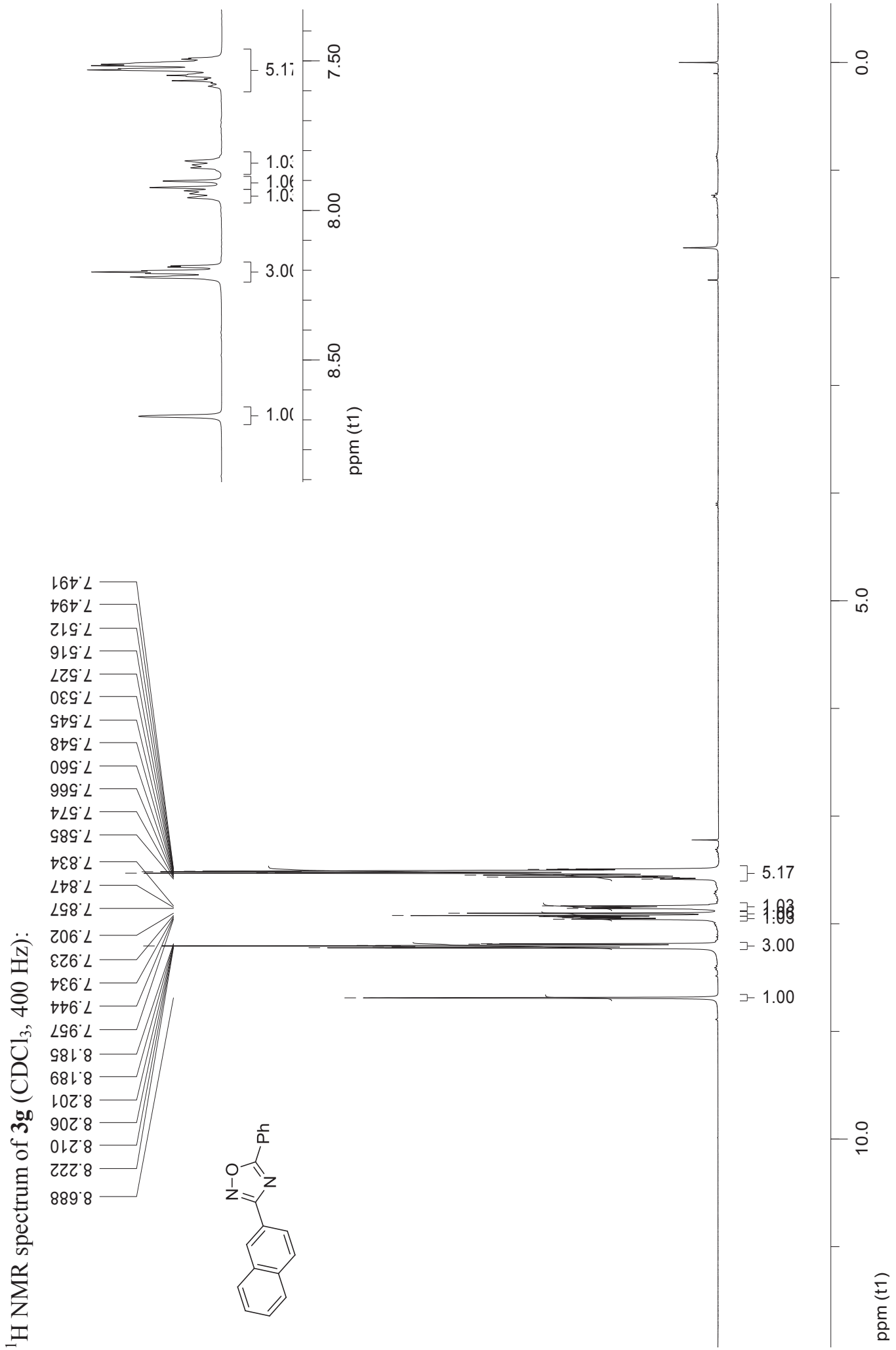
^{1}H NMR spectrum of **3f** ($CDCl_3$, 400 Hz):



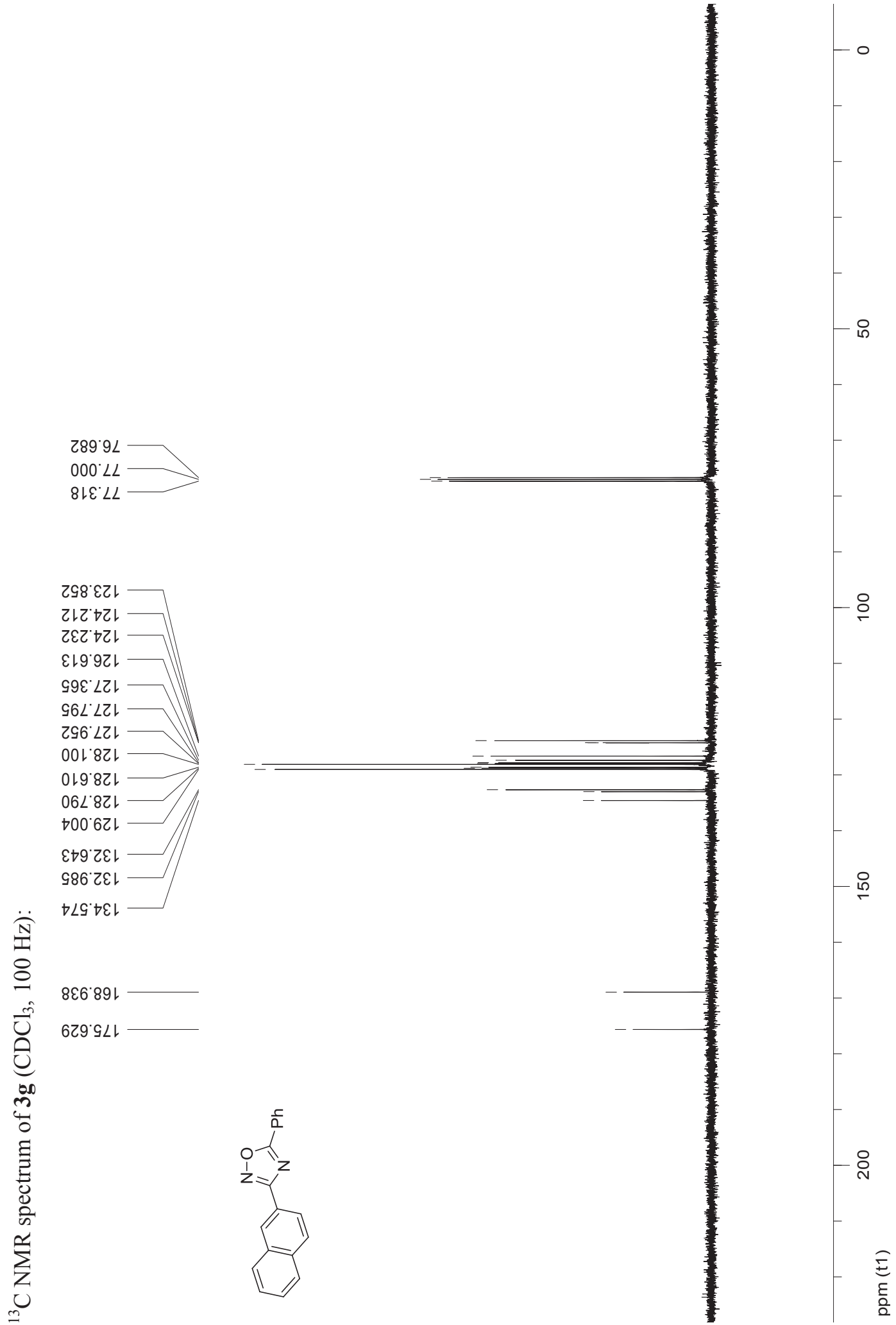
^{13}C NMR spectrum of **3f** ($CDCl_3$, 100 Hz):



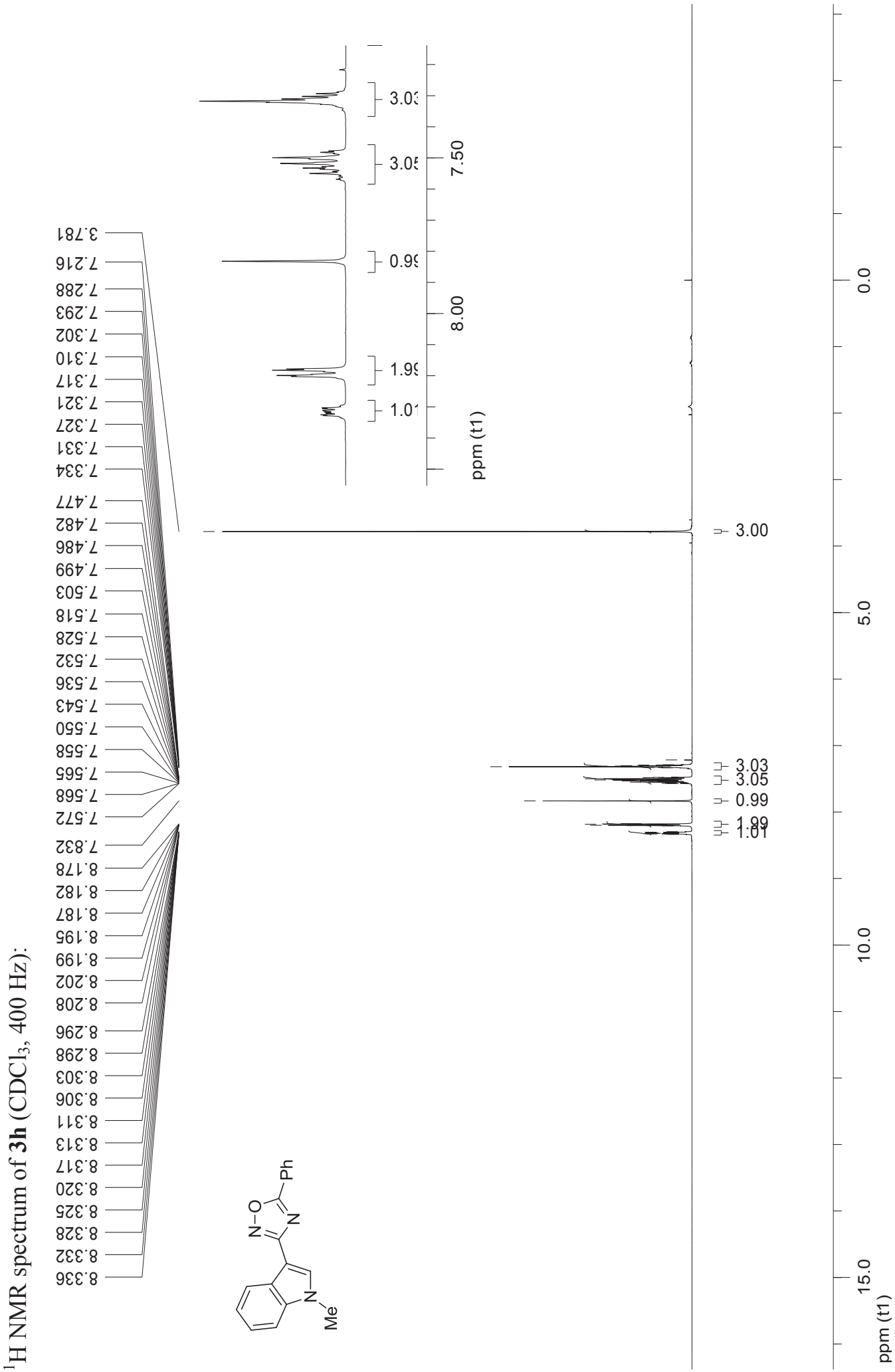
^{1}H NMR spectrum of **3g** ($CDCl_3$, 400 Hz):



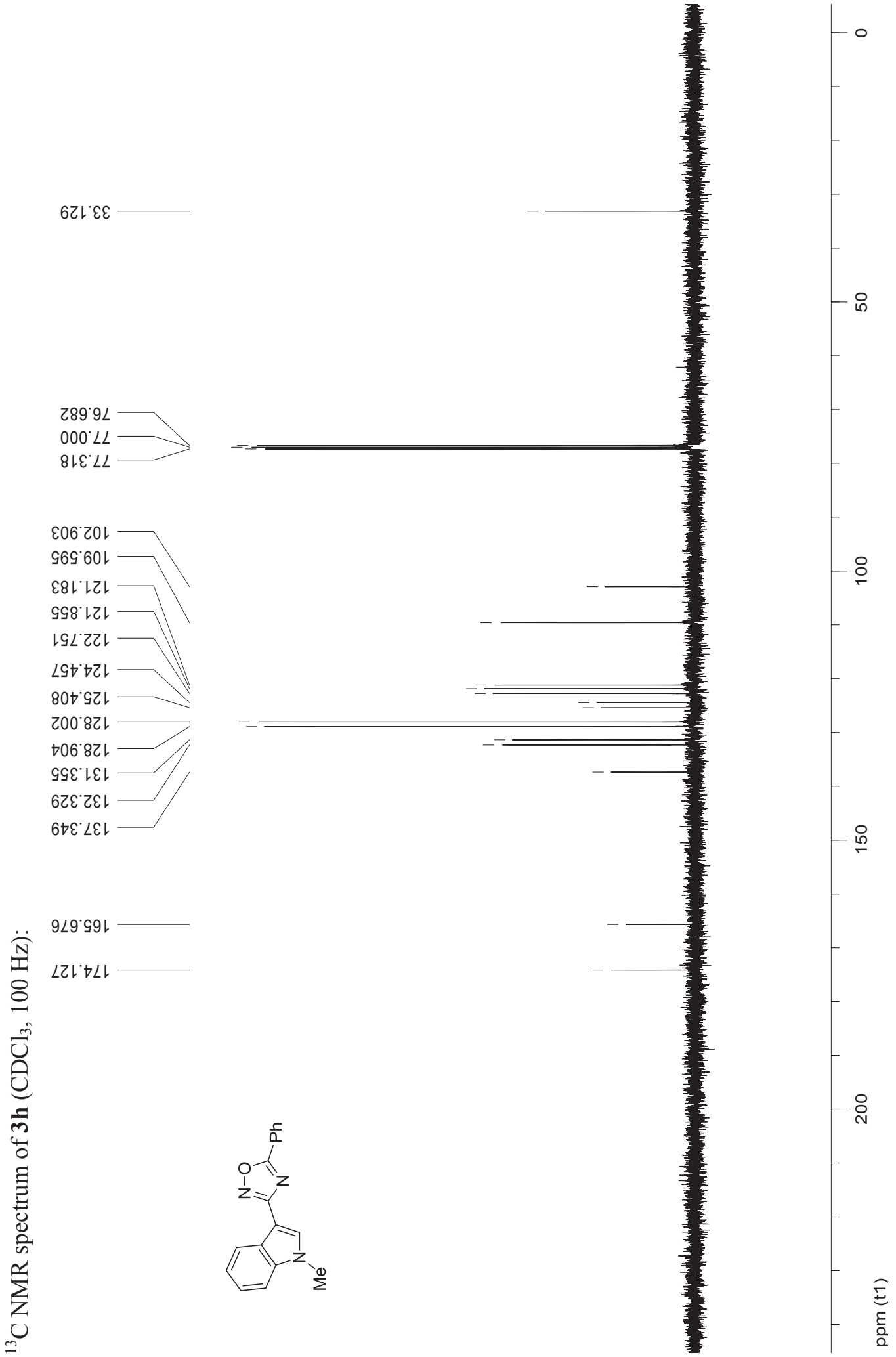
^{13}C NMR spectrum of **3g** ($CDCl_3$, 100 Hz):



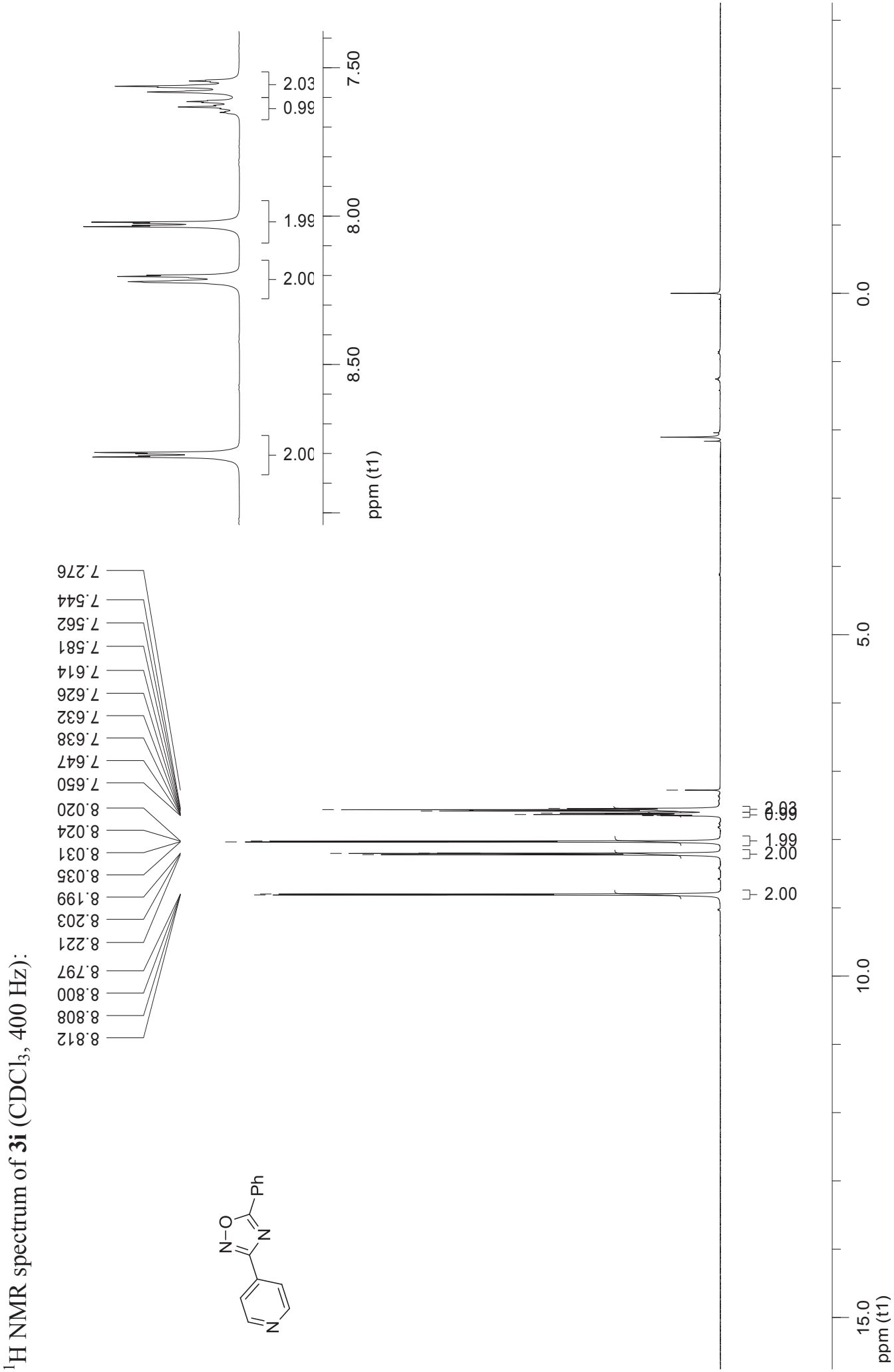
^{1}H NMR spectrum of **3h** ($CDCl_3$, 400 Hz):



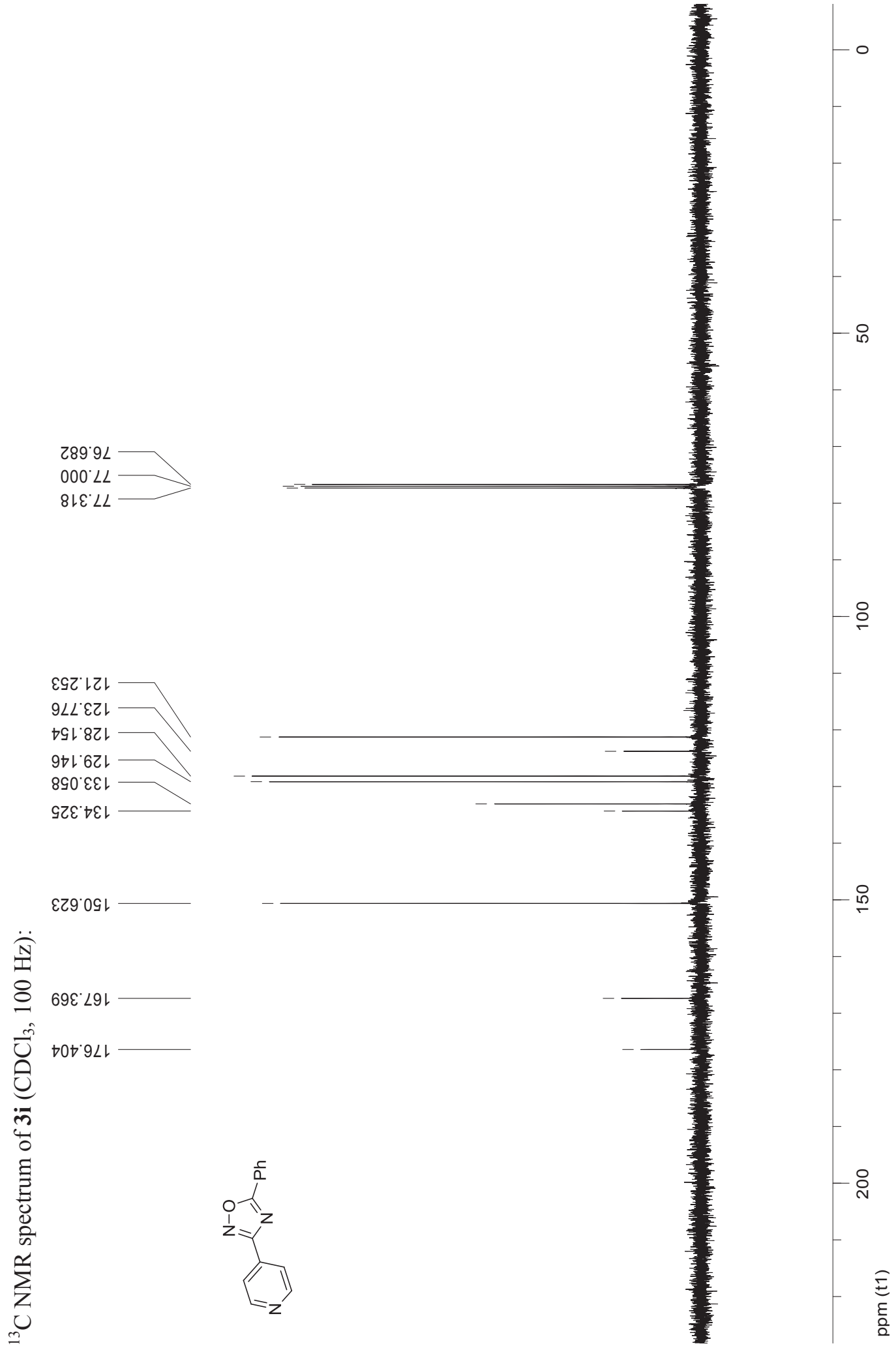
^{13}C NMR spectrum of **3h** ($CDCl_3$, 100 Hz):



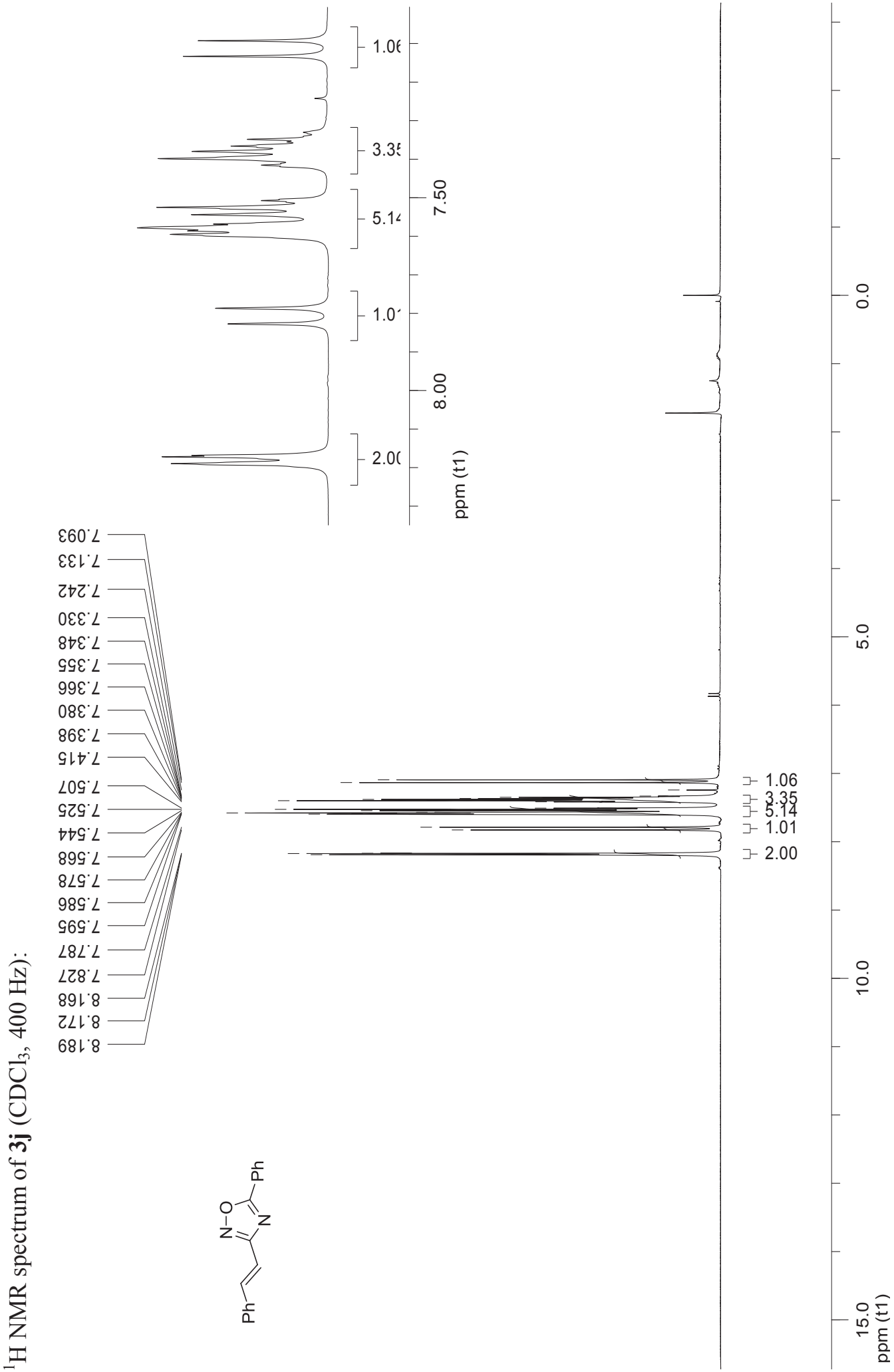
^{1}H NMR spectrum of **3i** ($CDCl_3$, 400 Hz):



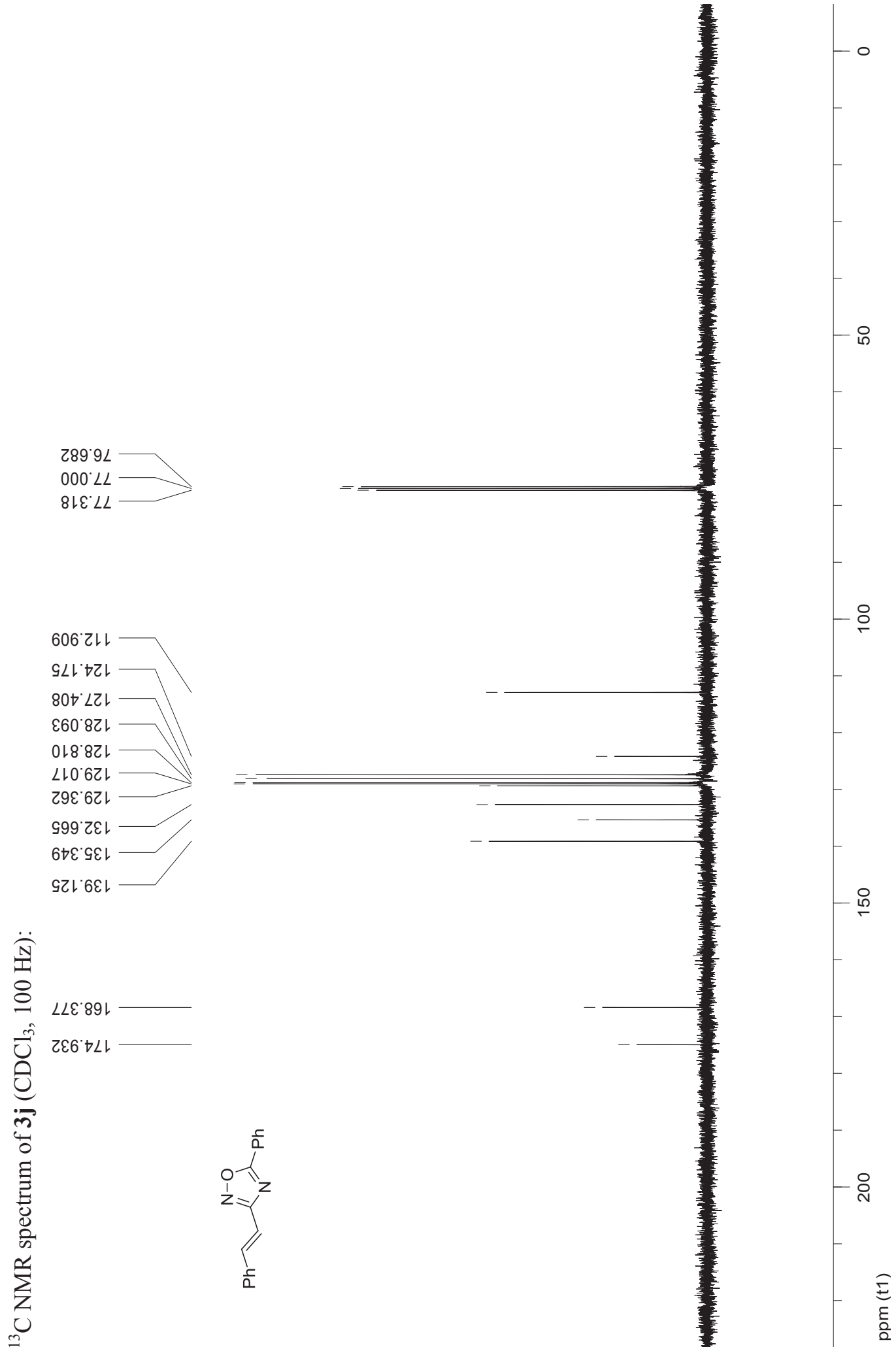
^{13}C NMR spectrum of **3i** ($CDCl_3$, 100 Hz):



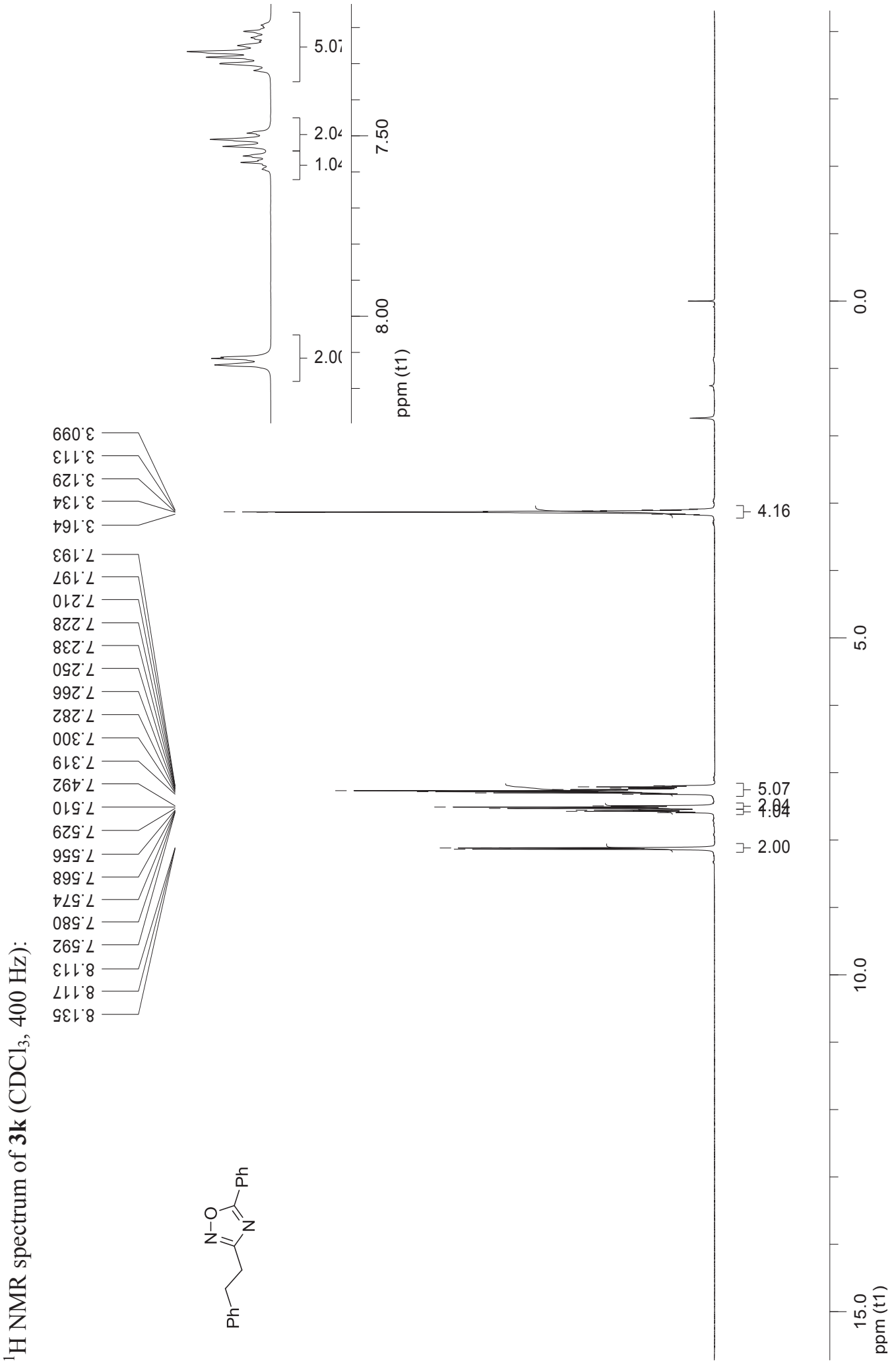
^{1}H NMR spectrum of **3j** ($CDCl_3$, 400 Hz):



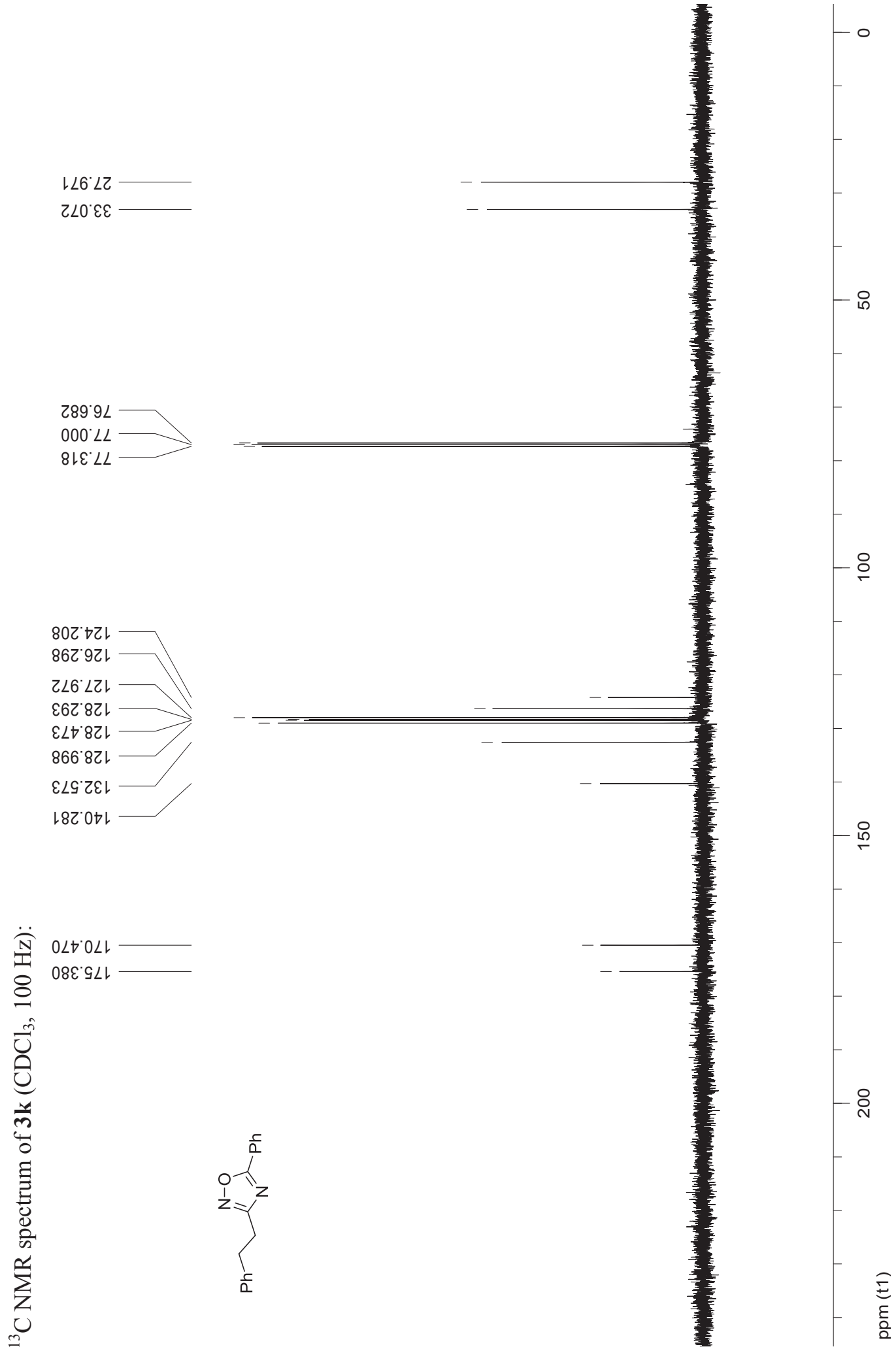
^{13}C NMR spectrum of **3j** ($CDCl_3$, 100 Hz):



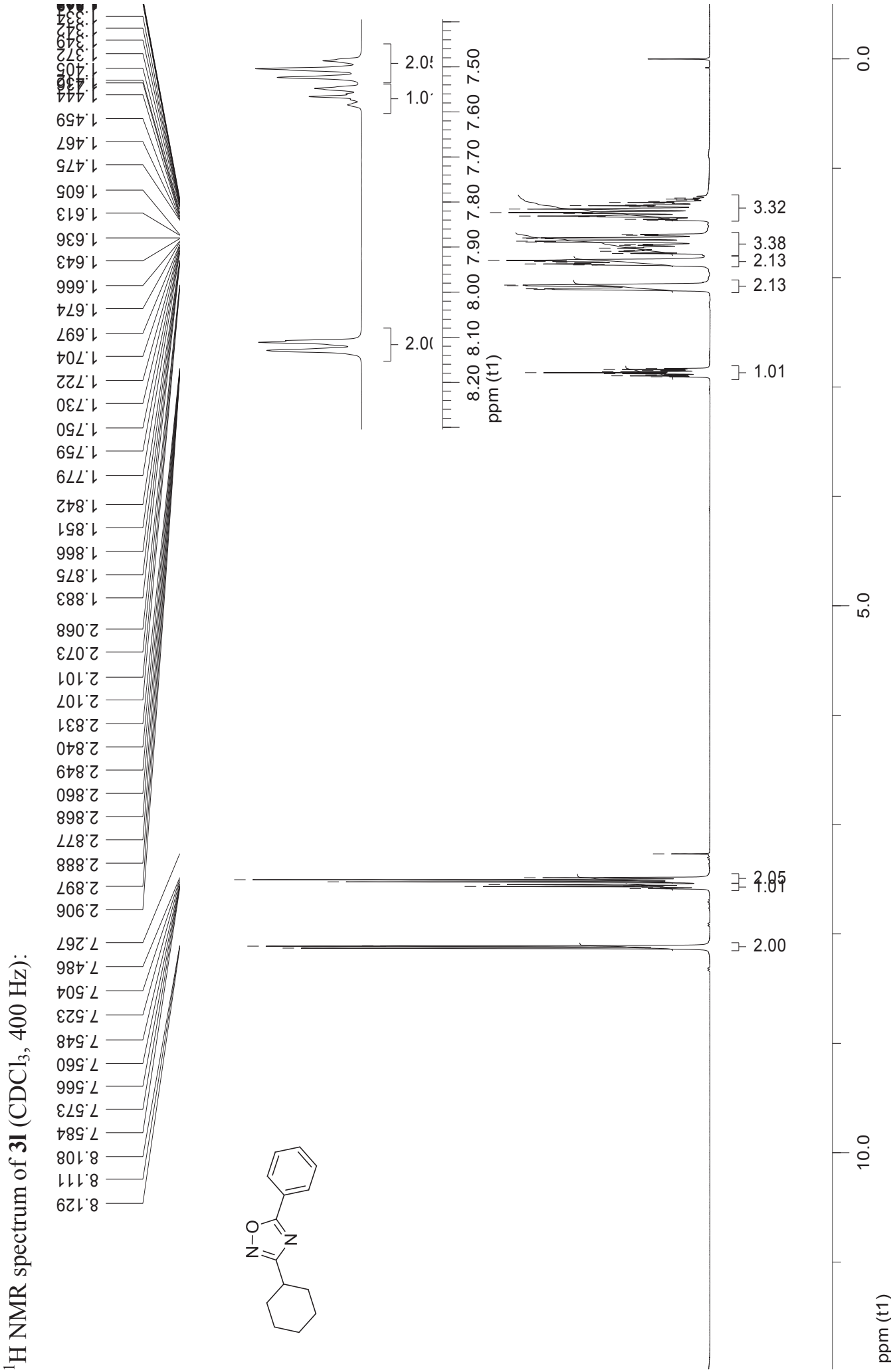
^{1}H NMR spectrum of **3k** ($CDCl_3$, 400 Hz):



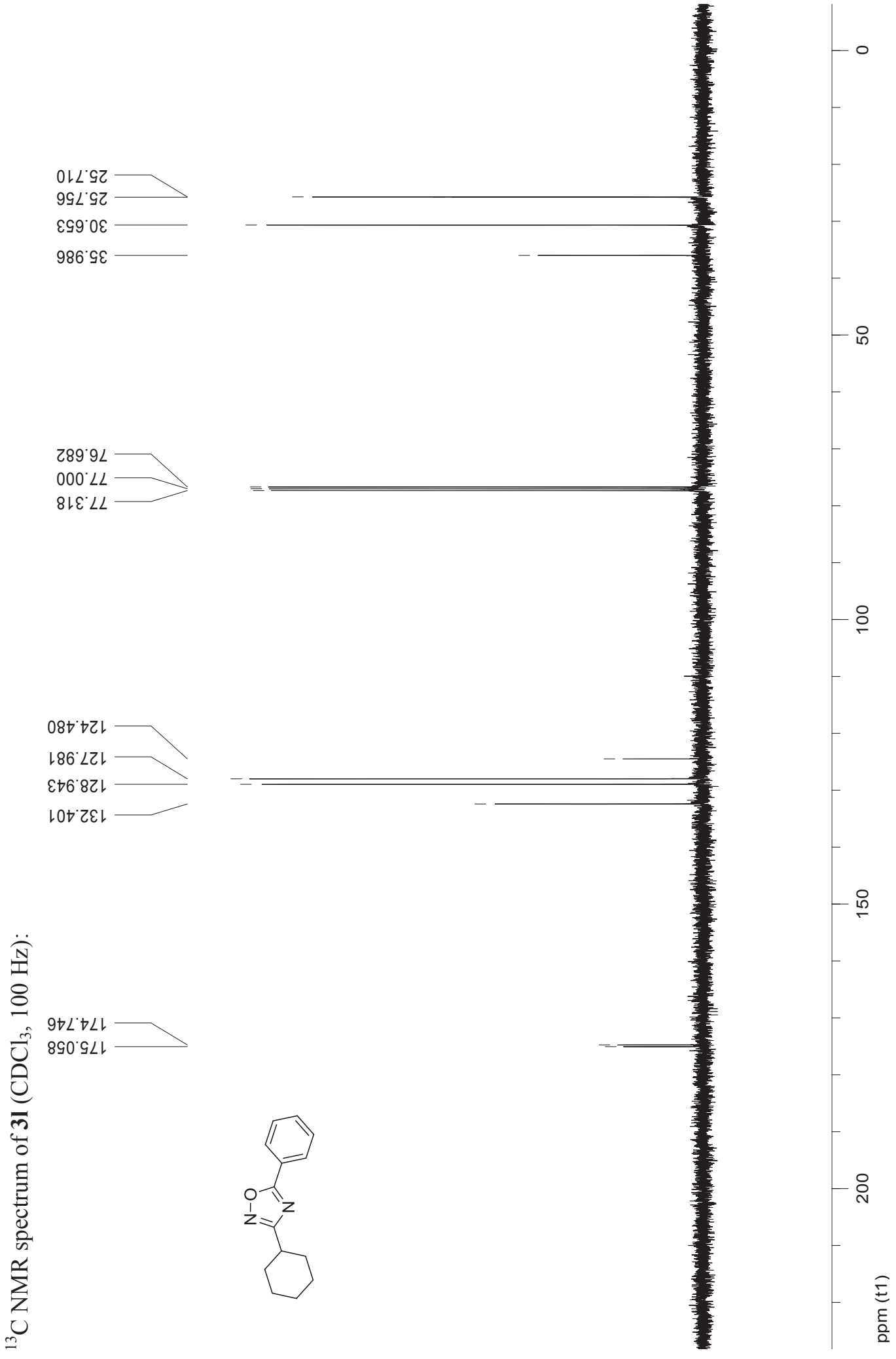
^{13}C NMR spectrum of **3k** ($CDCl_3$, 100 Hz):



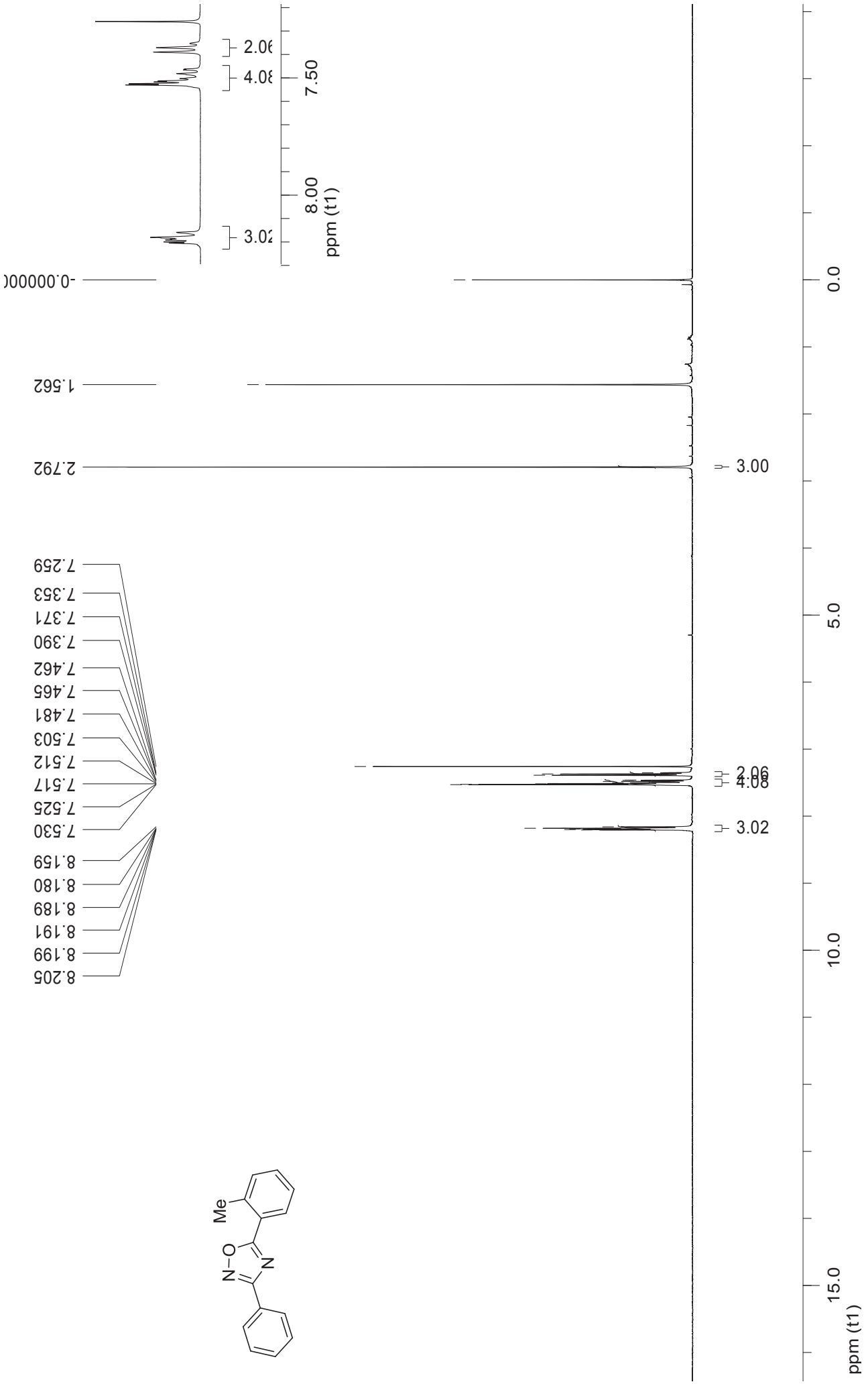
^{1}H NMR spectrum of **3l** ($CDCl_3$, 400 Hz):



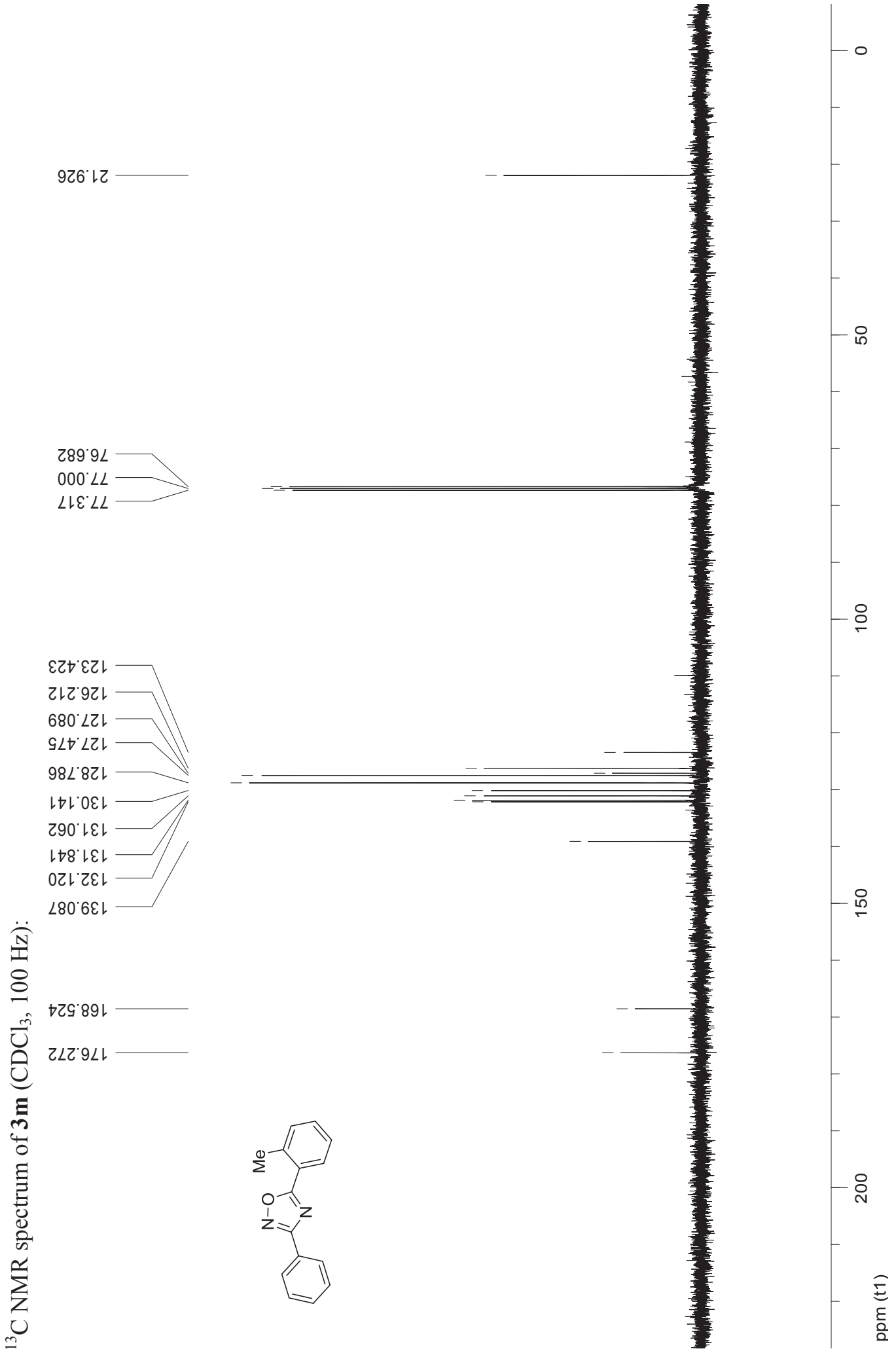
^{13}C NMR spectrum of **3l** ($CDCl_3$, 100 Hz):



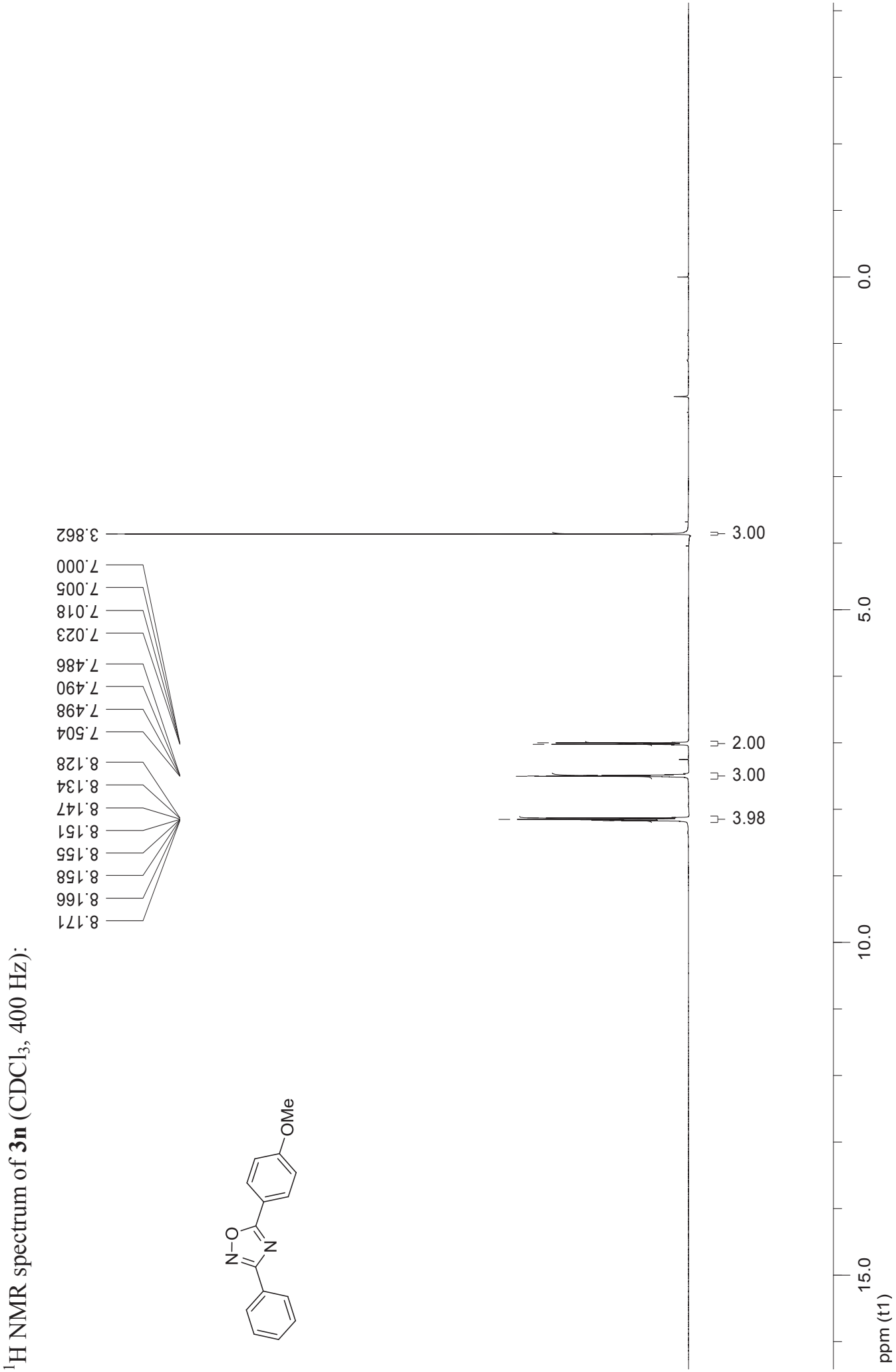
^{1}H NMR spectrum of **3m** ($CDCl_3$, 400 Hz):



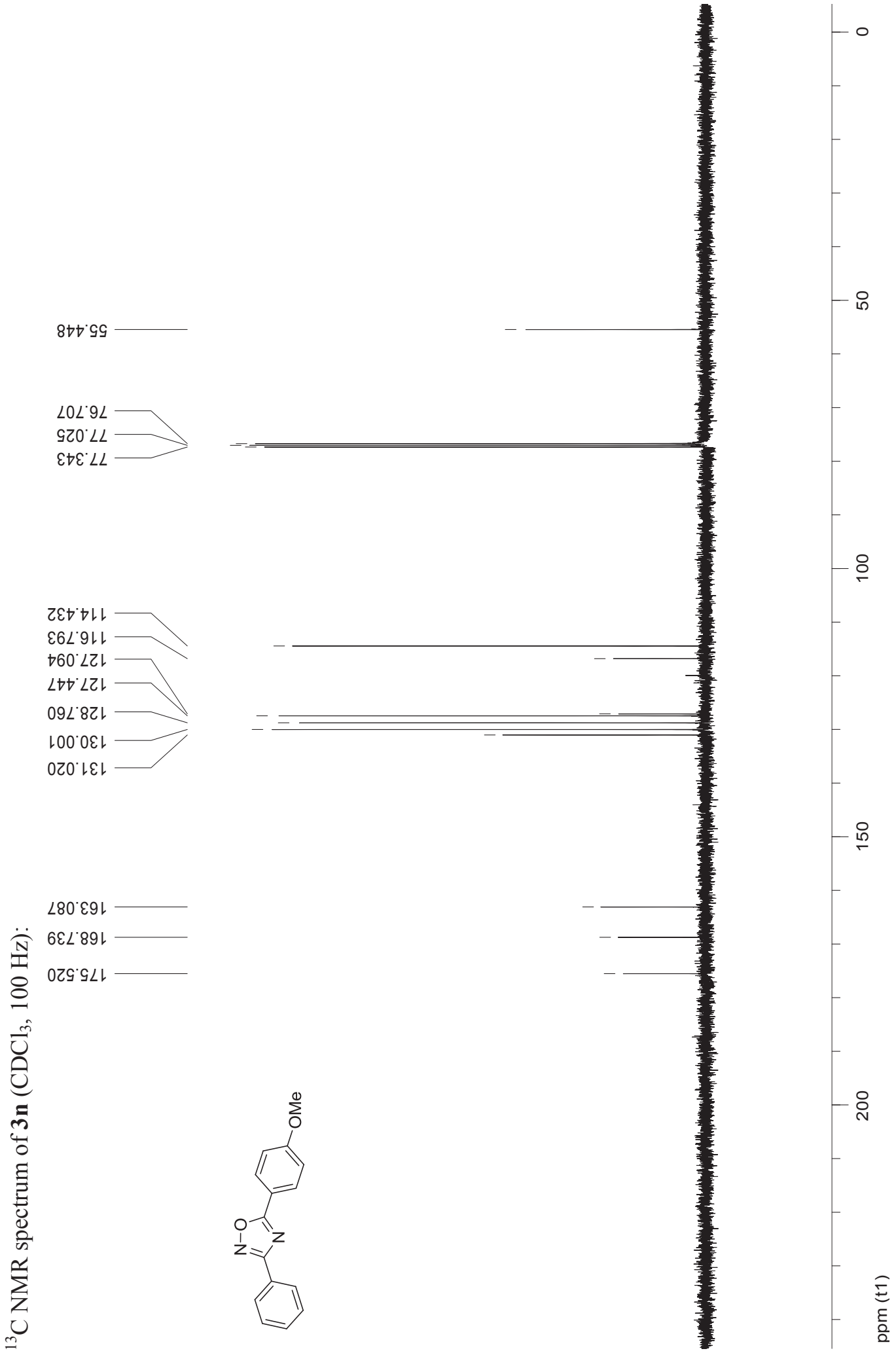
^{13}C NMR spectrum of **3m** ($CDCl_3$, 100 Hz):



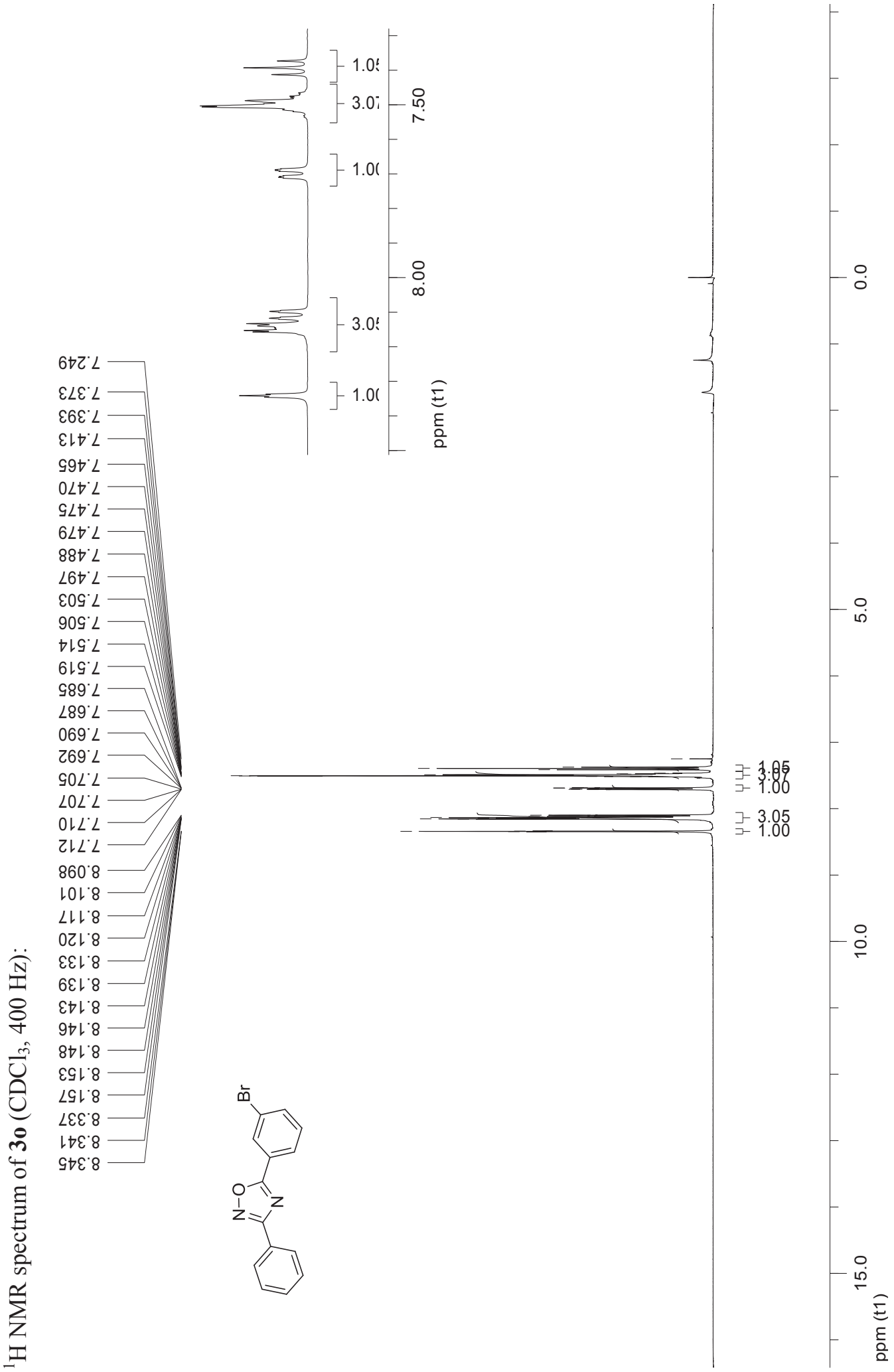
^{1}H NMR spectrum of **3n** ($CDCl_3$, 400 Hz):



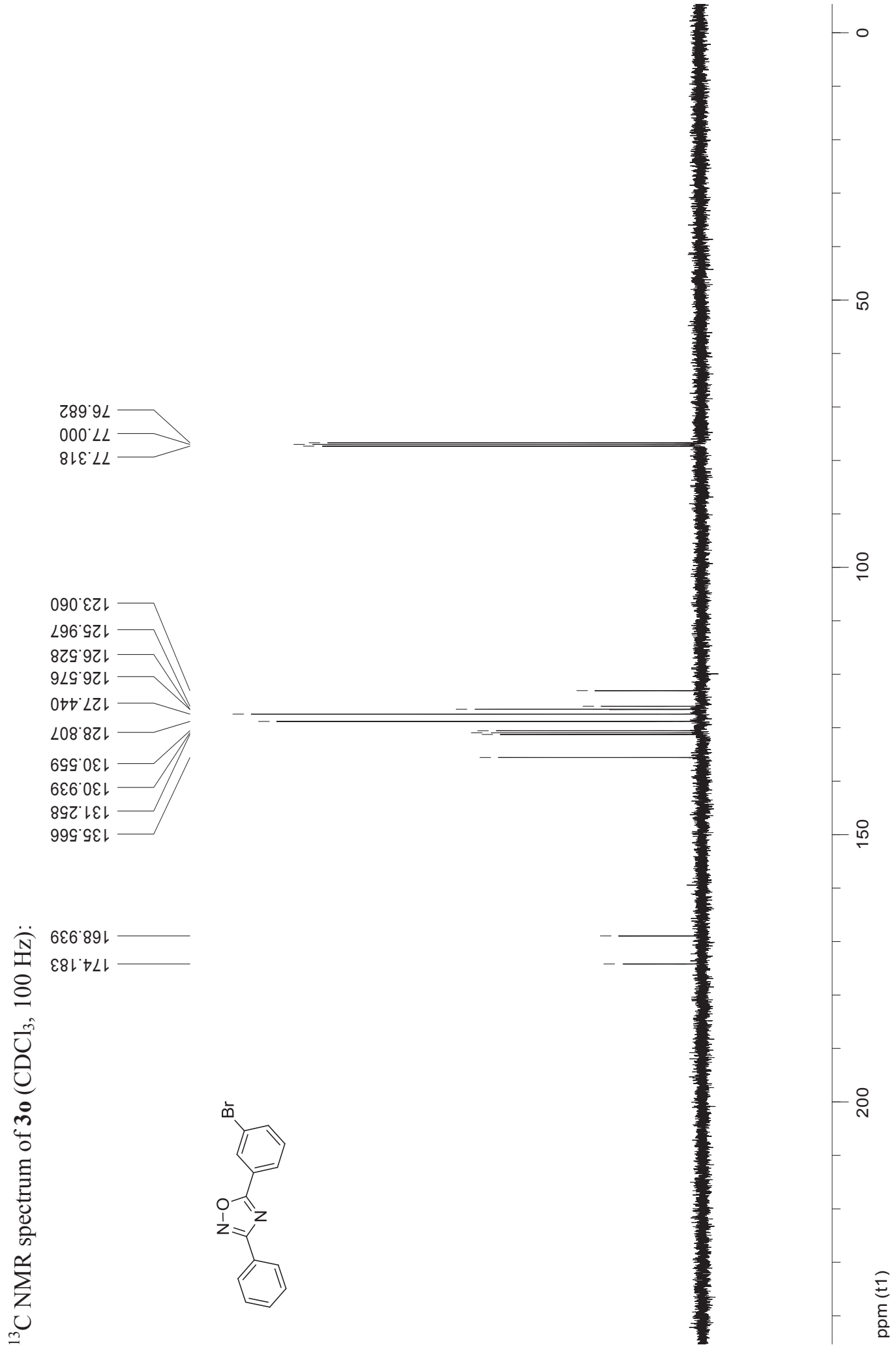
^{13}C NMR spectrum of **3n** ($CDCl_3$, 100 Hz):



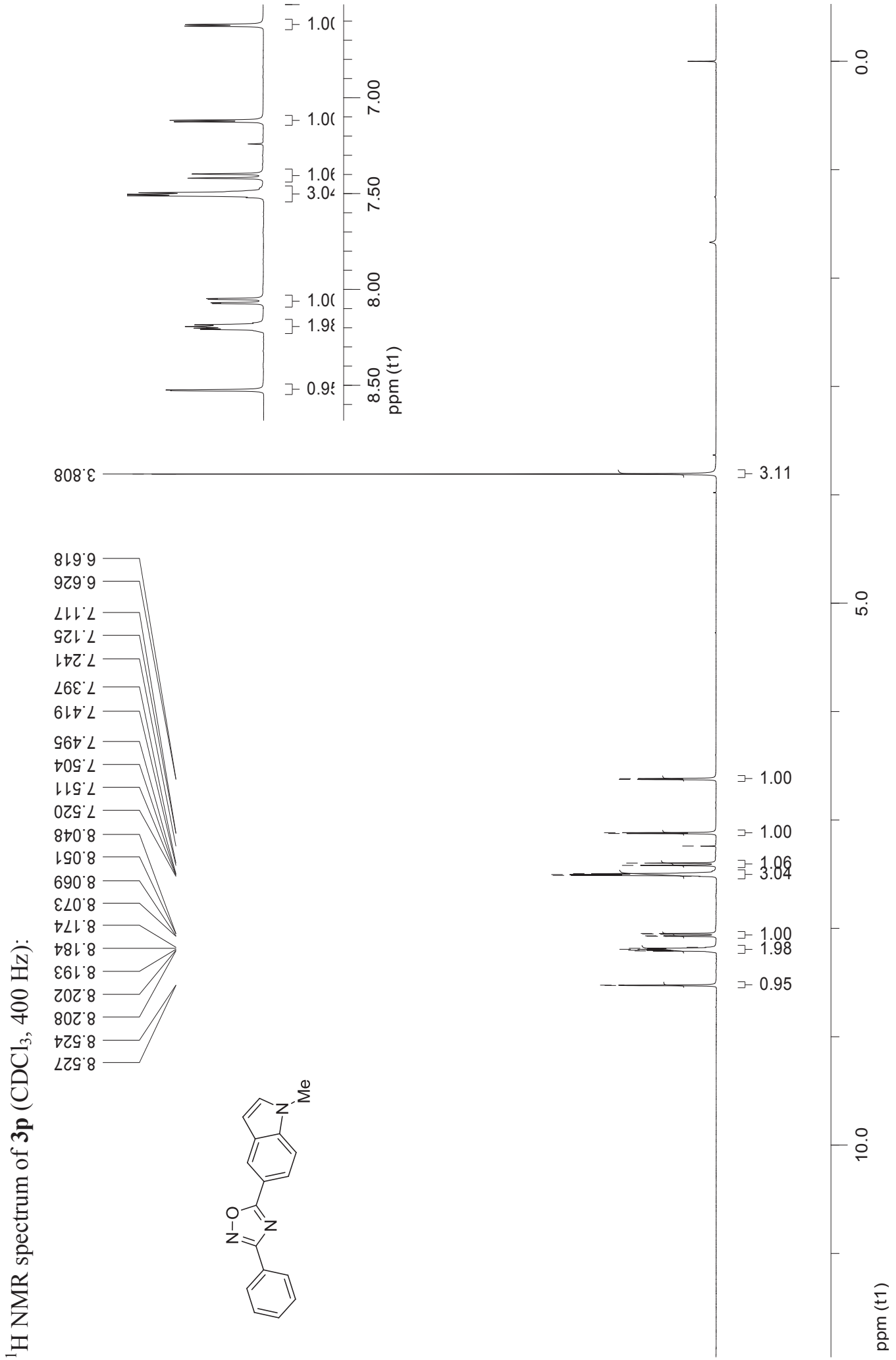
^{1}H NMR spectrum of **3o** ($CDCl_3$, 400 Hz):



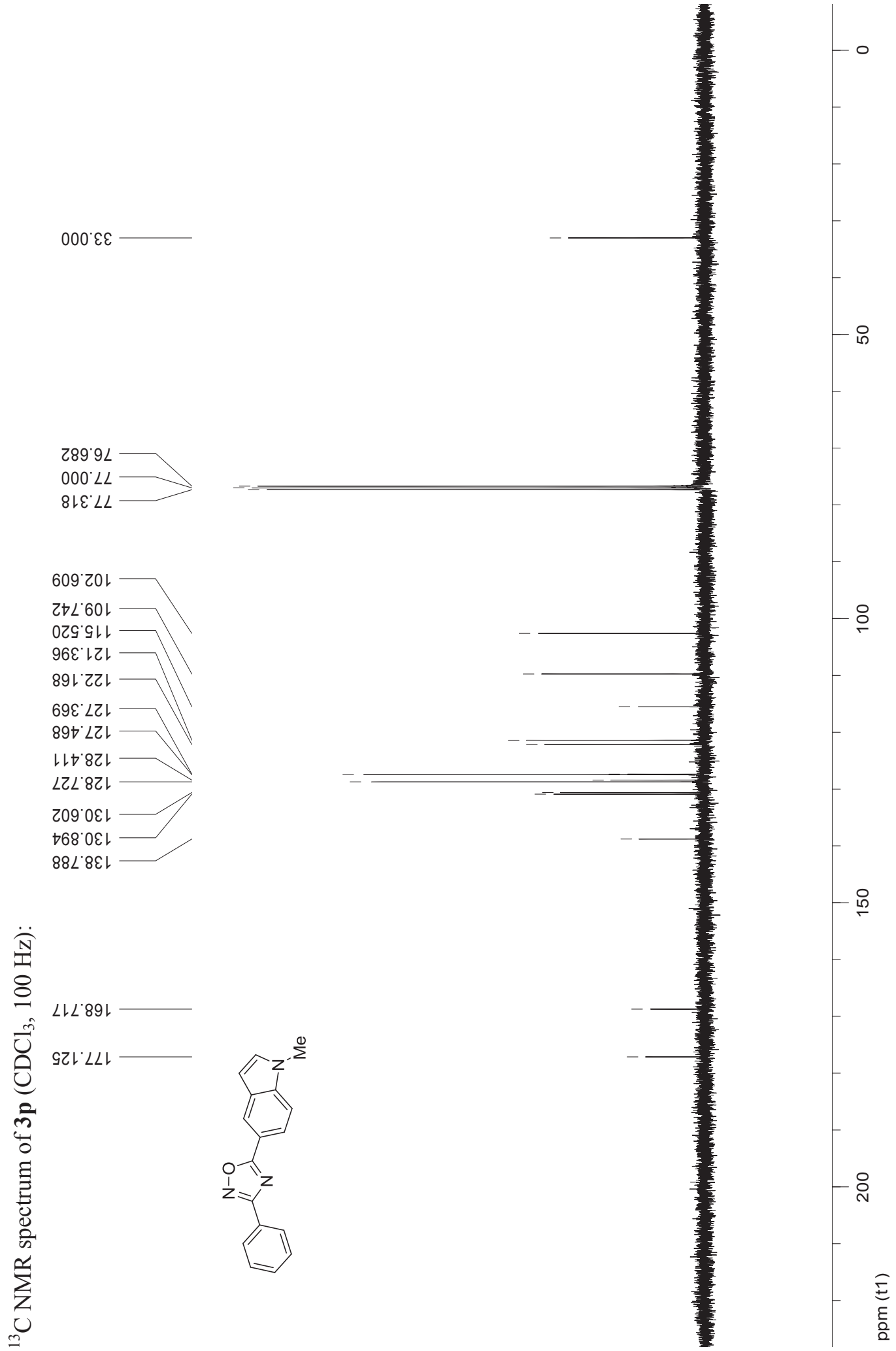
^{13}C NMR spectrum of **3o** ($CDCl_3$, 100 Hz):



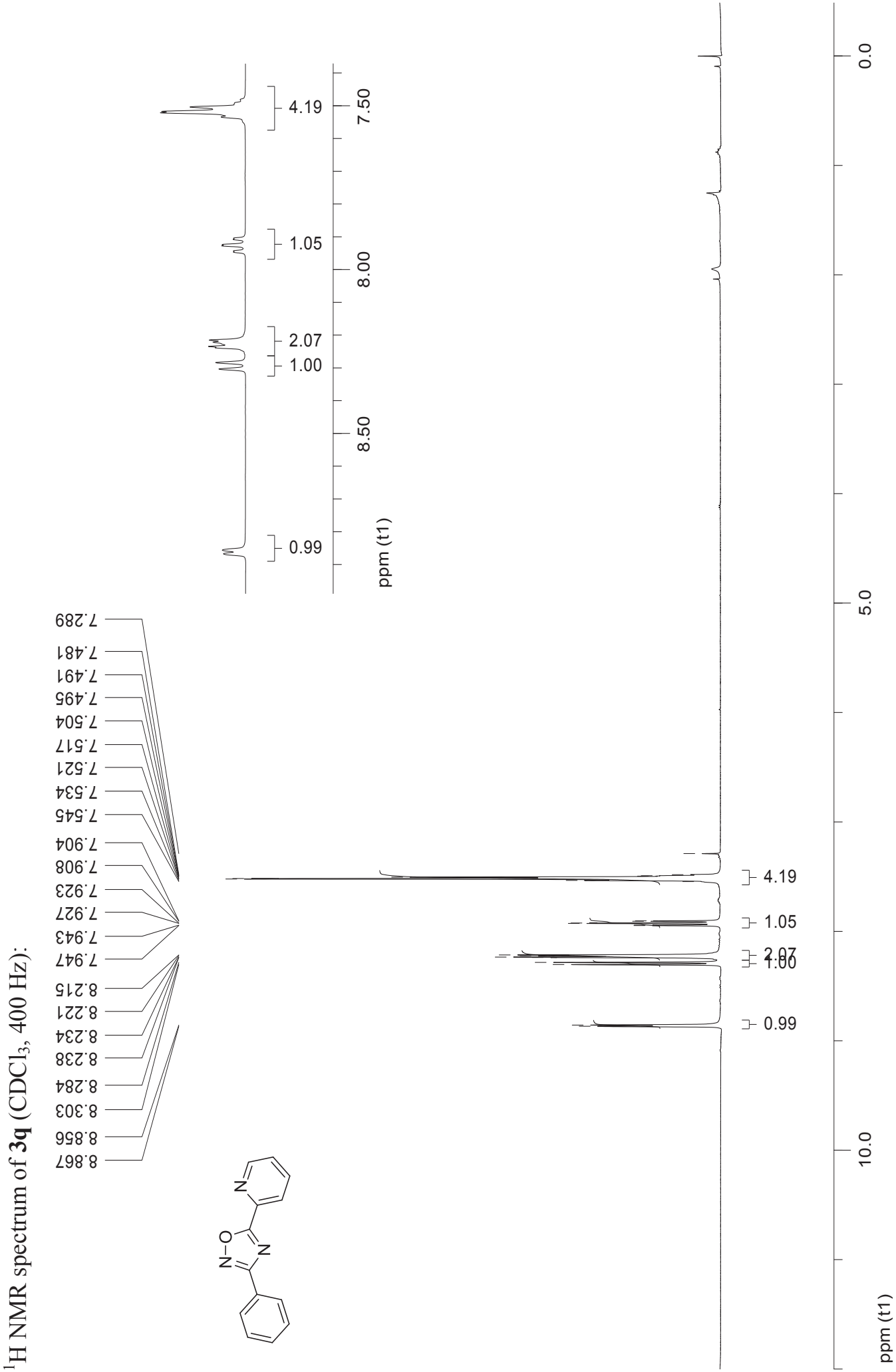
^{1}H NMR spectrum of **3p** ($CDCl_3$, 400 Hz):



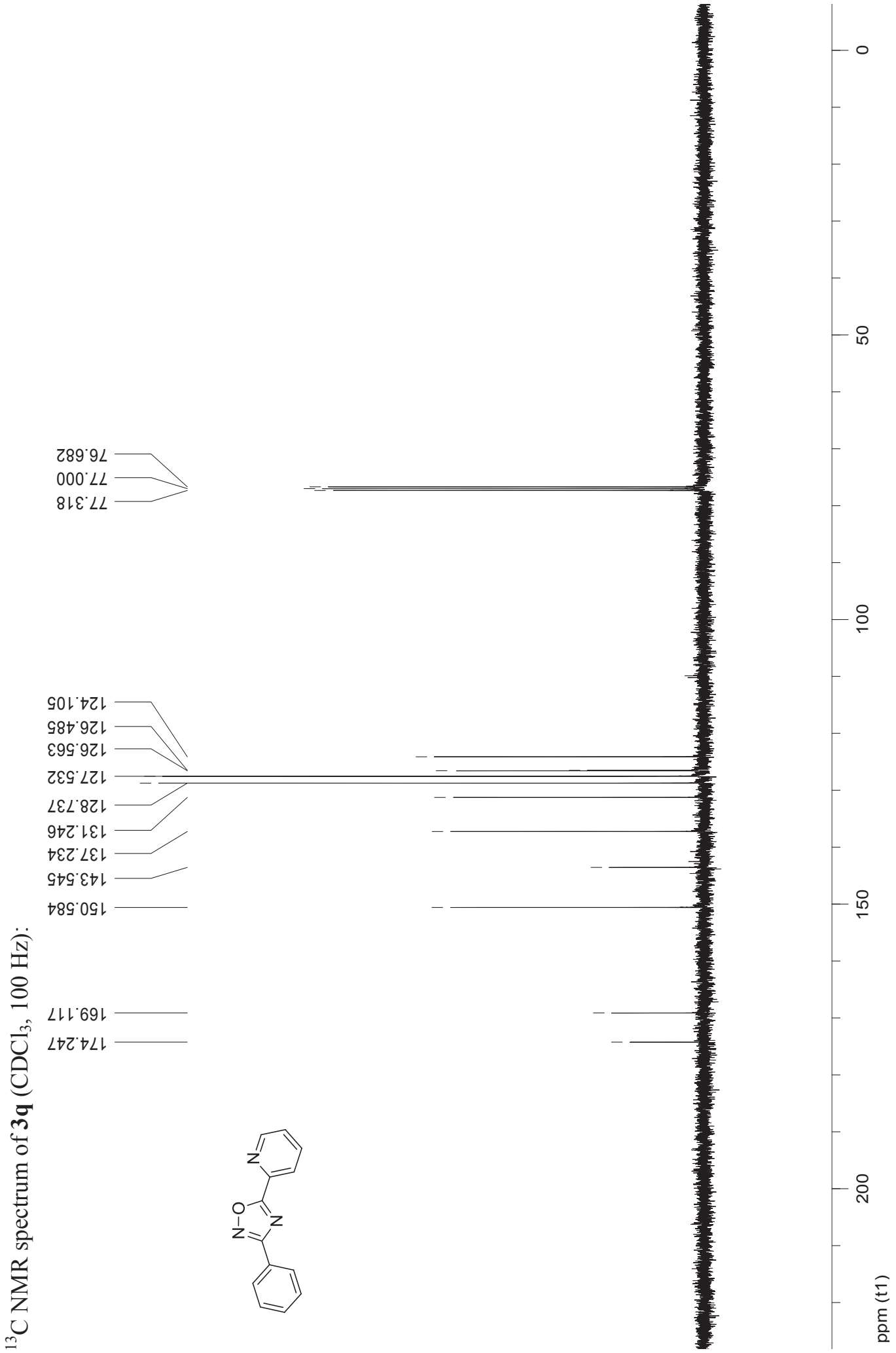
^{13}C NMR spectrum of **3p** ($CDCl_3$, 100 Hz):



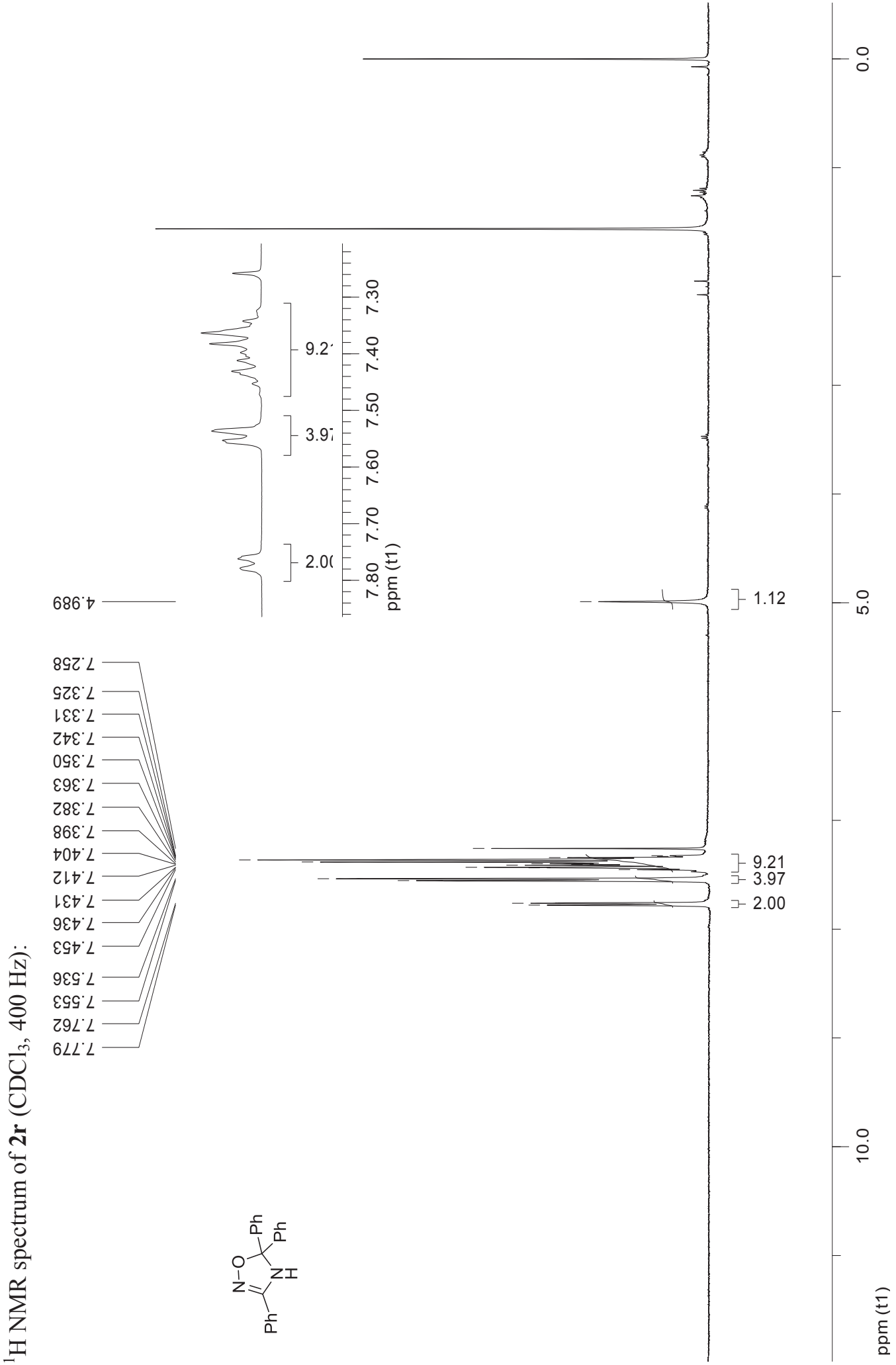
^{1}H NMR spectrum of **3q** ($CDCl_3$, 400 Hz):



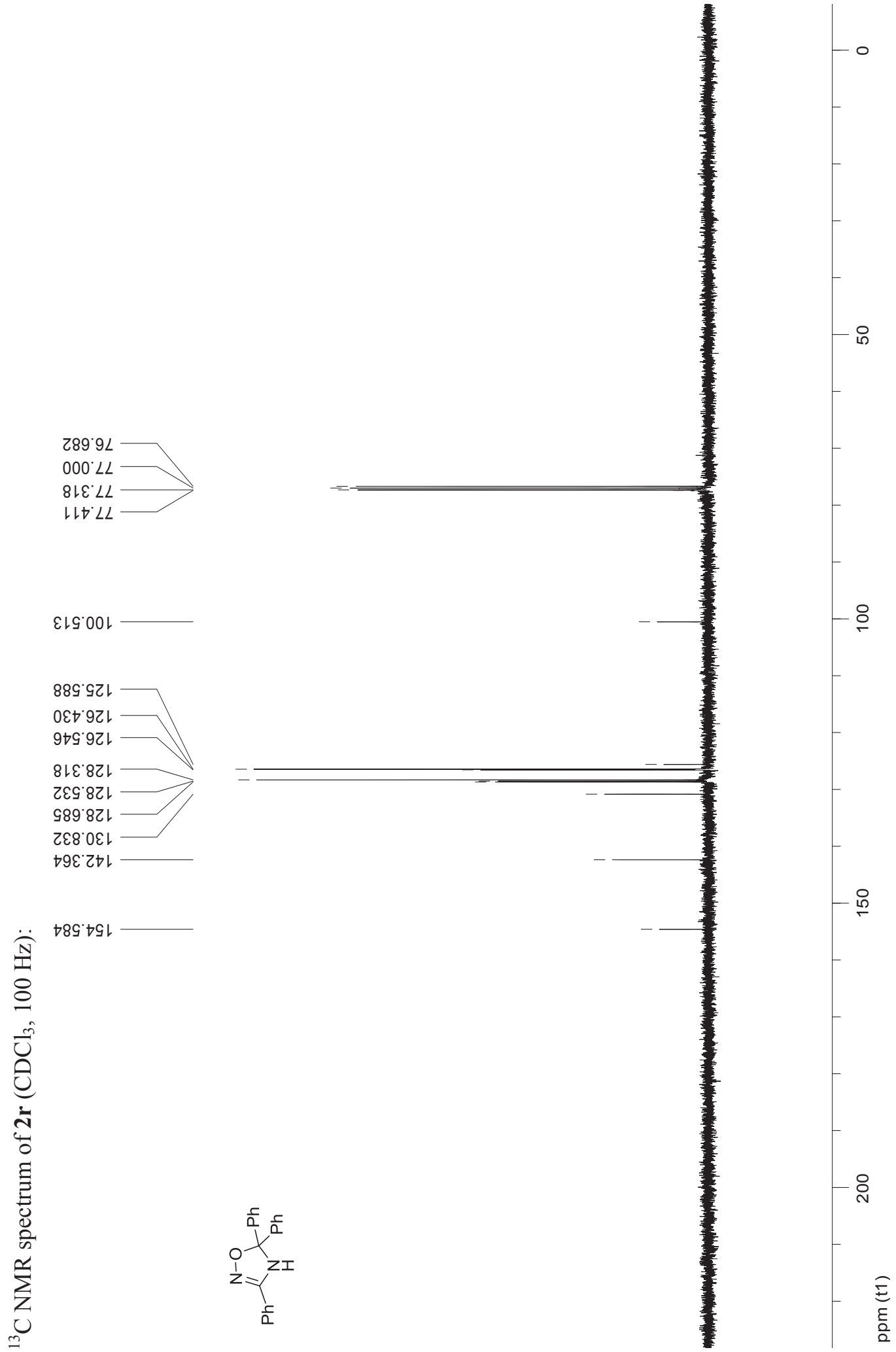
^{13}C NMR spectrum of **3q** ($CDCl_3$, 100 Hz):



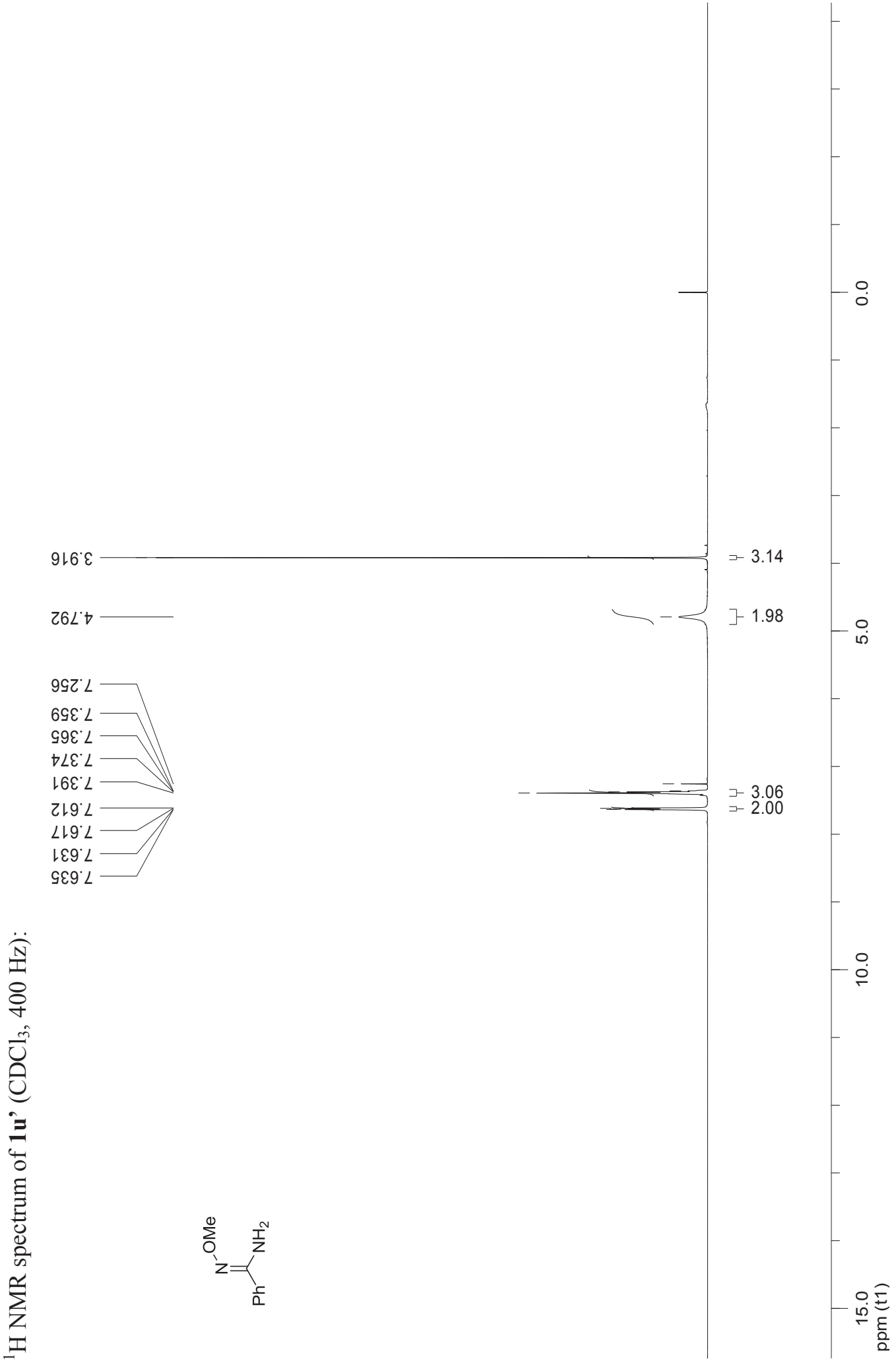
^{1}H NMR spectrum of **2r** ($CDCl_3$, 400 Hz):



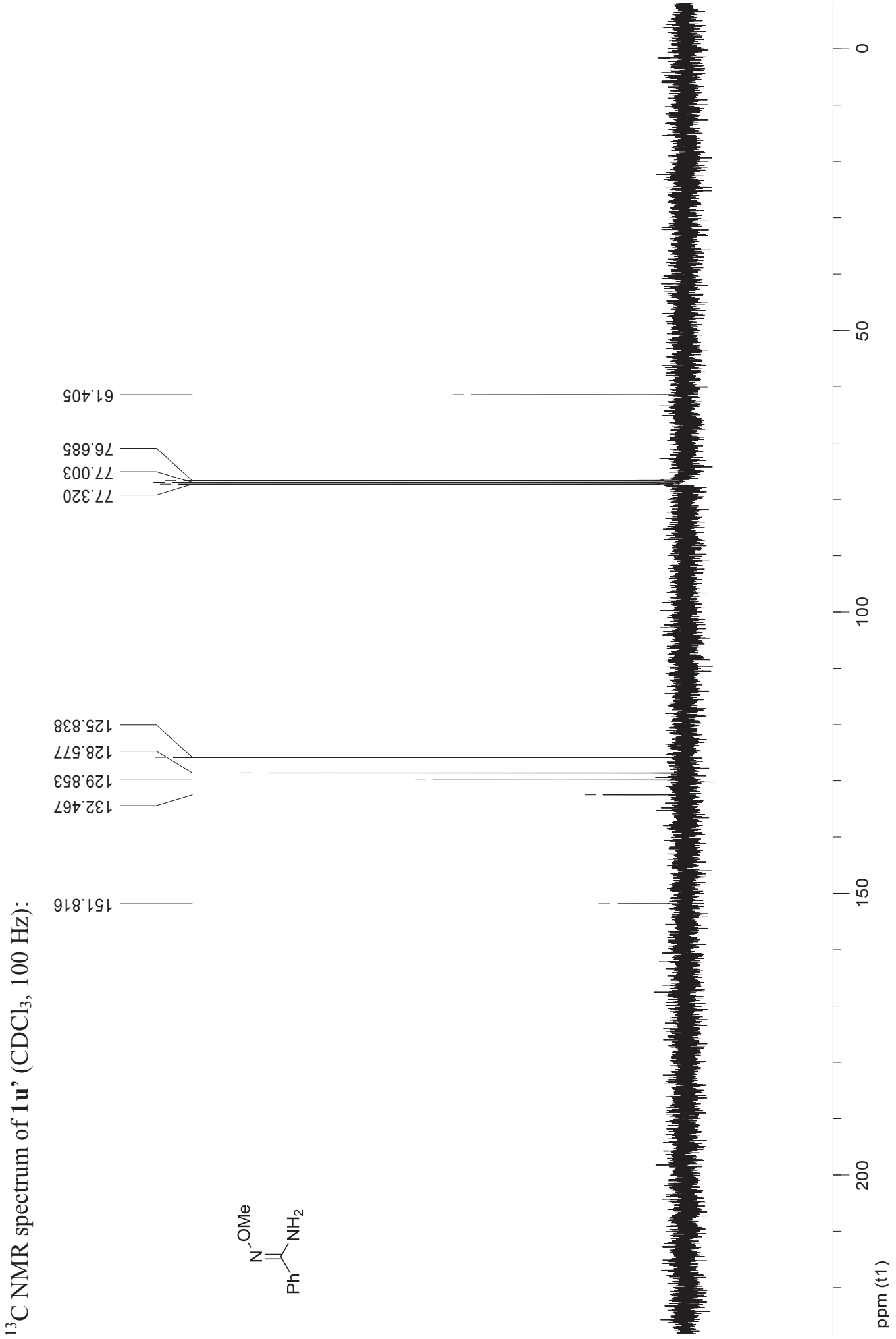
^{13}C NMR spectrum of **2r** ($CDCl_3$, 100 Hz):



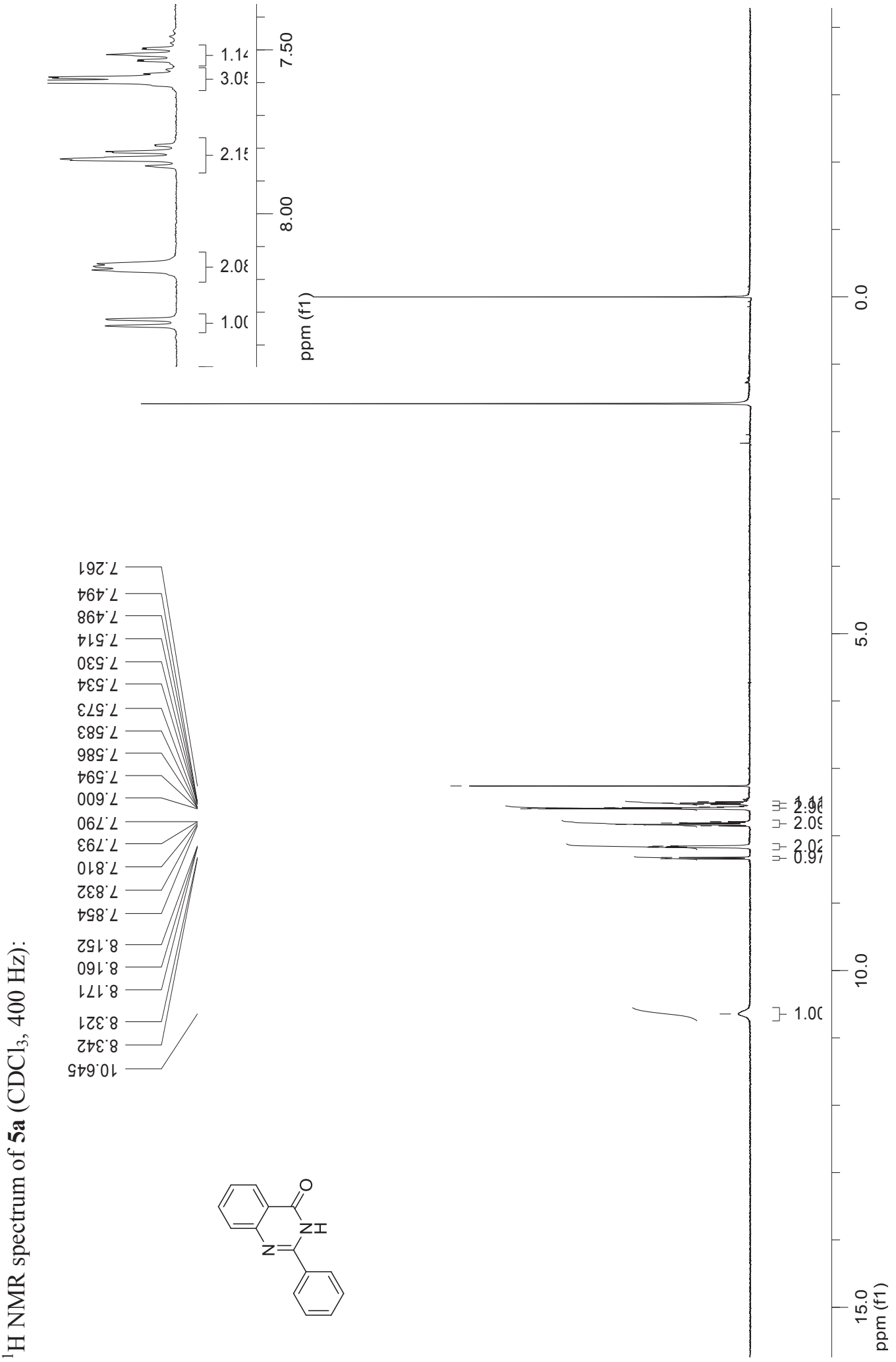
^{1}H NMR spectrum of **1u'** ($CDCl_3$, 400 Hz):



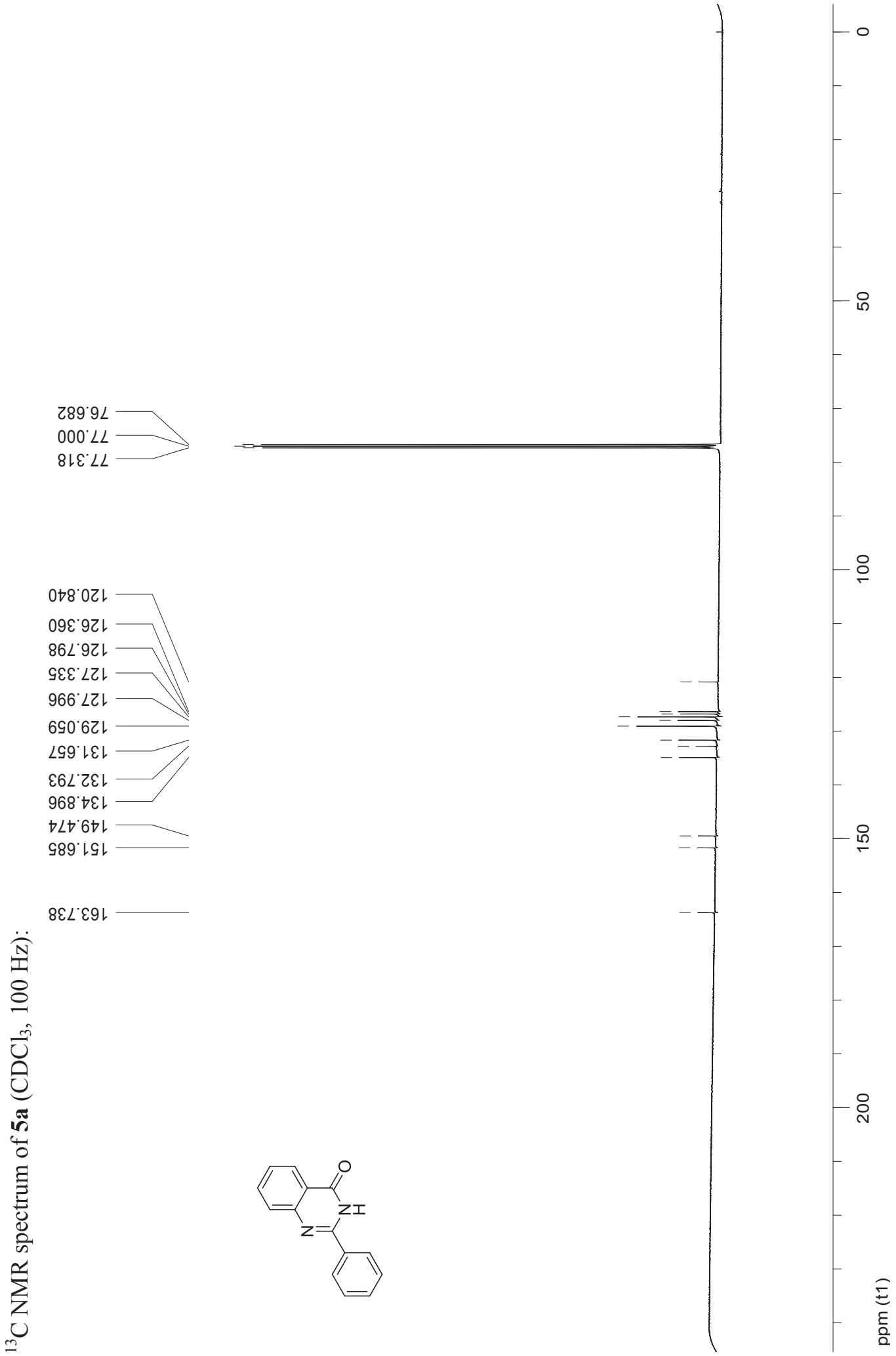
^{13}C NMR spectrum of **1u'** ($CDCl_3$, 100 Hz):



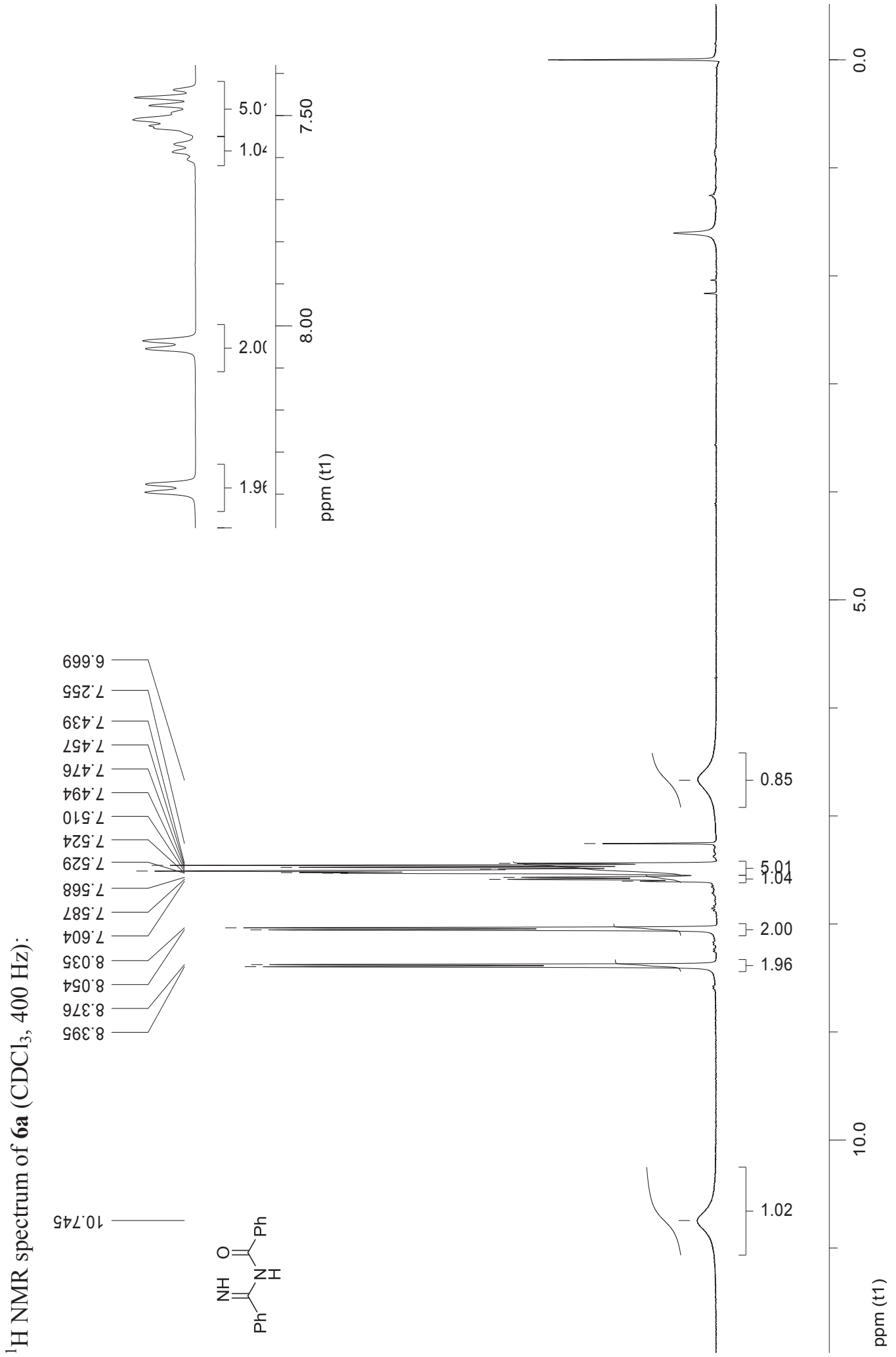
^{1}H NMR spectrum of **5a** ($CDCl_3$, 400 Hz):



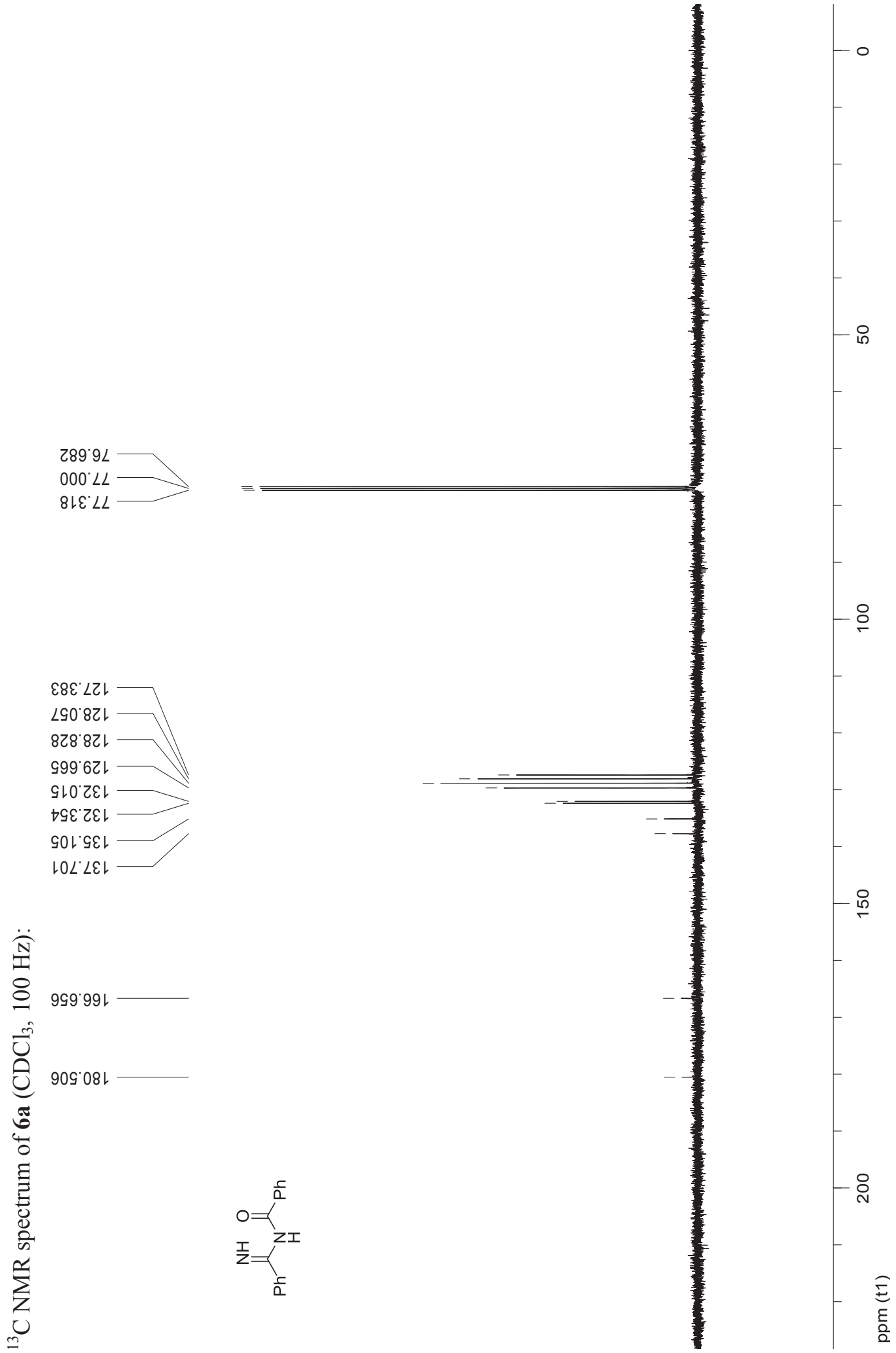
^{13}C NMR spectrum of **5a** ($CDCl_3$, 100 Hz):



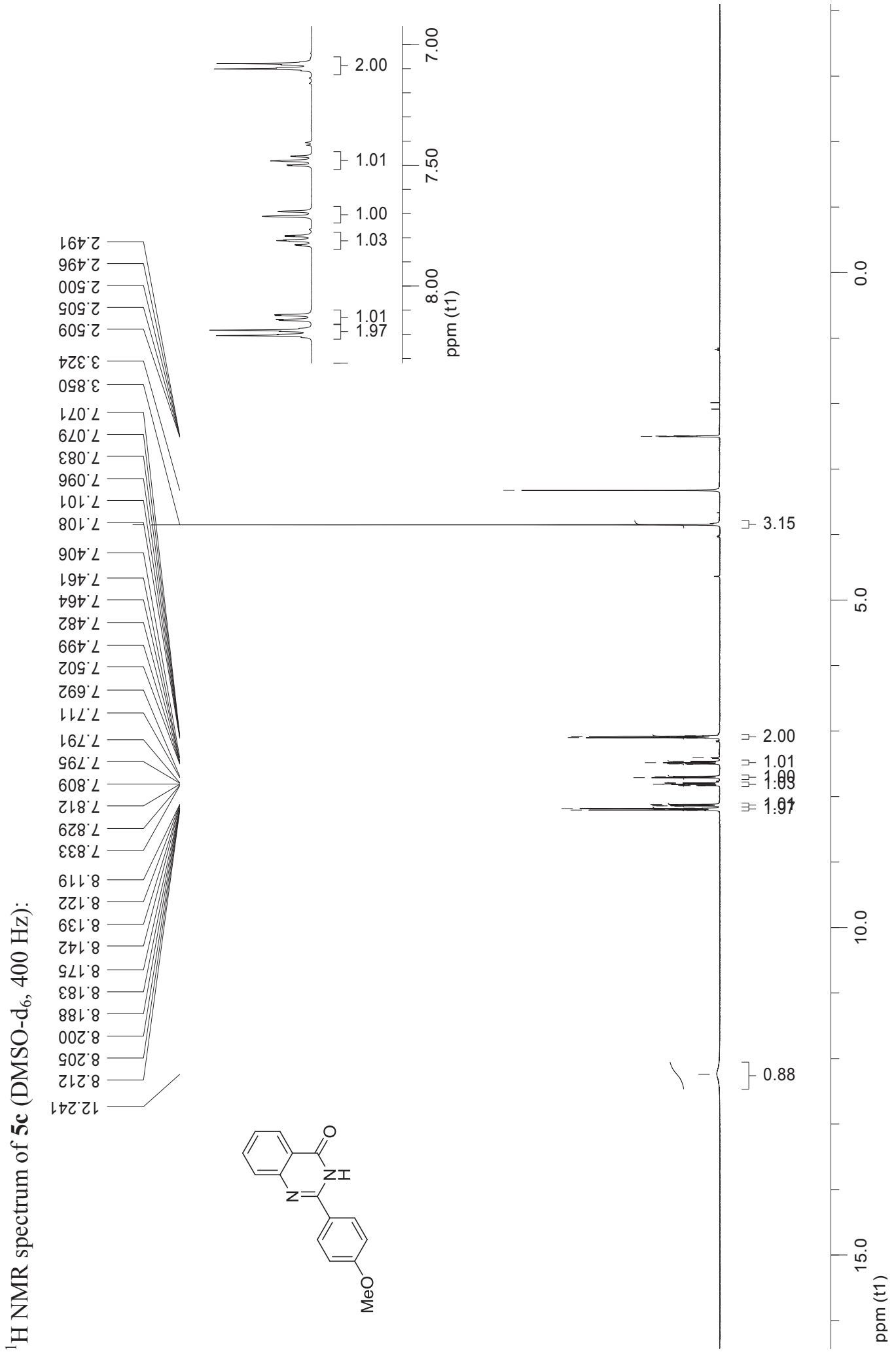
^{1}H NMR spectrum of **6a** ($CDCl_3$, 400 Hz):



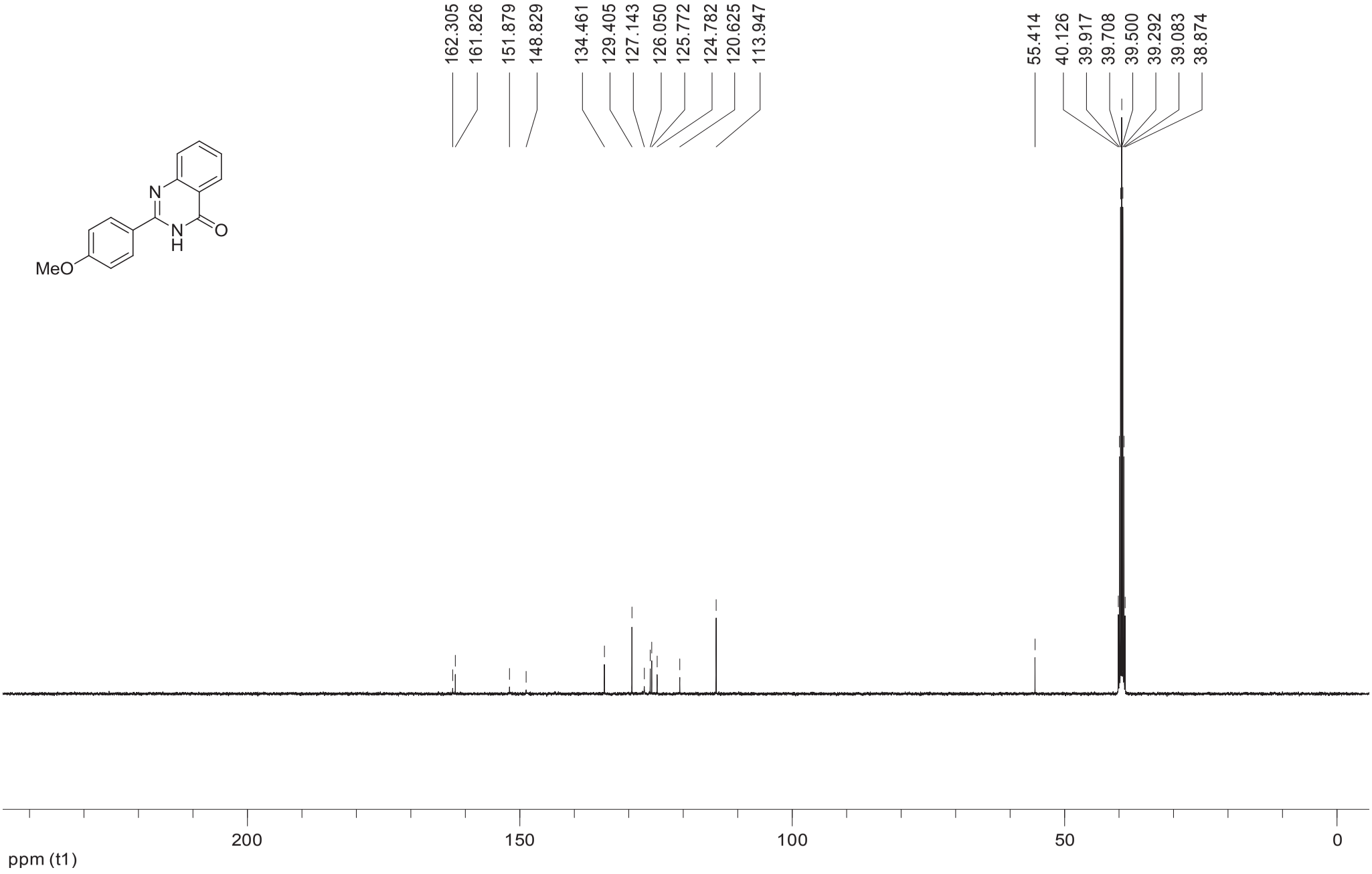
^{13}C NMR spectrum of **6a** ($CDCl_3$, 100 Hz):



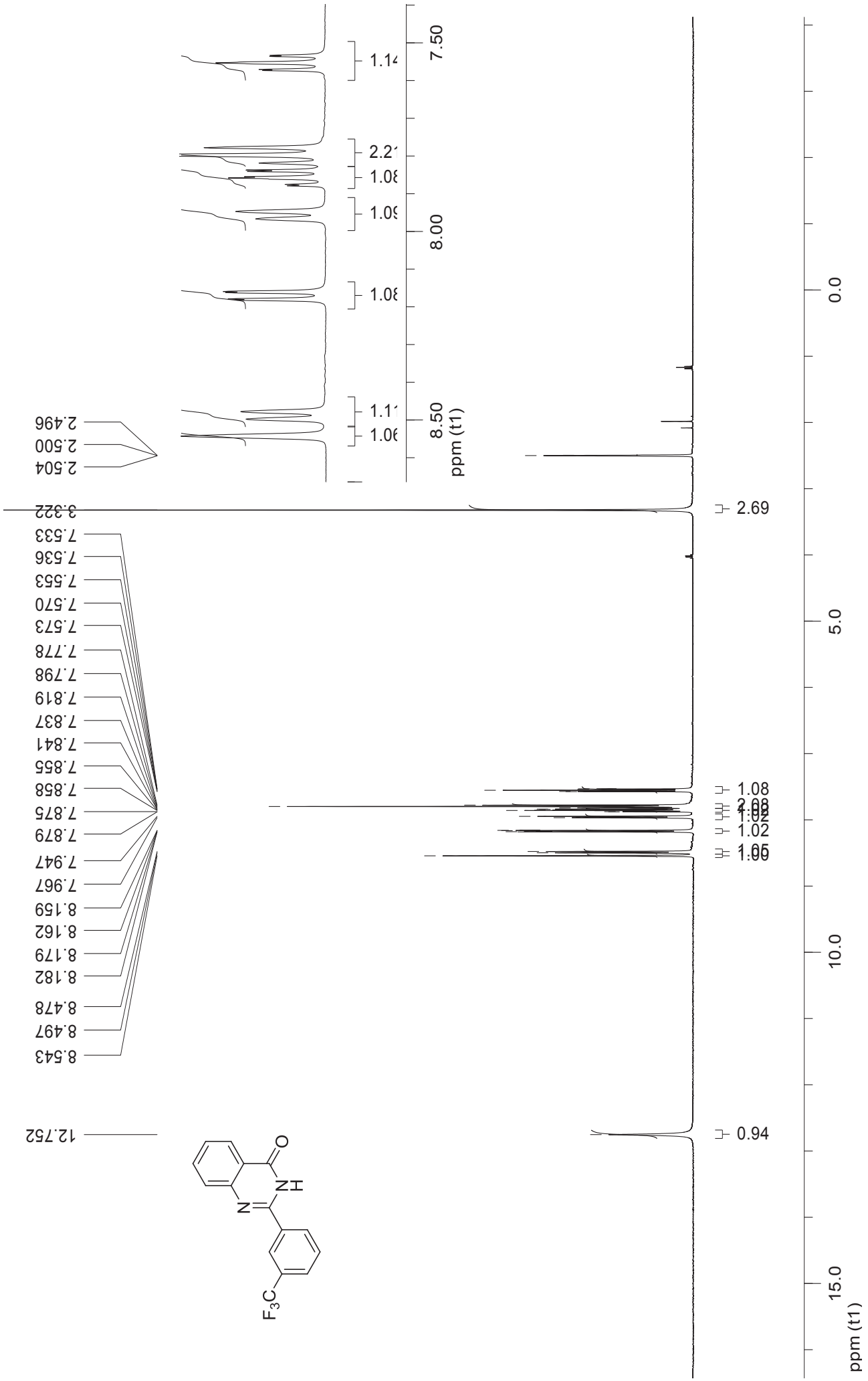
^{1}H NMR spectrum of **5c** (DMSO-d_6, 400 Hz):



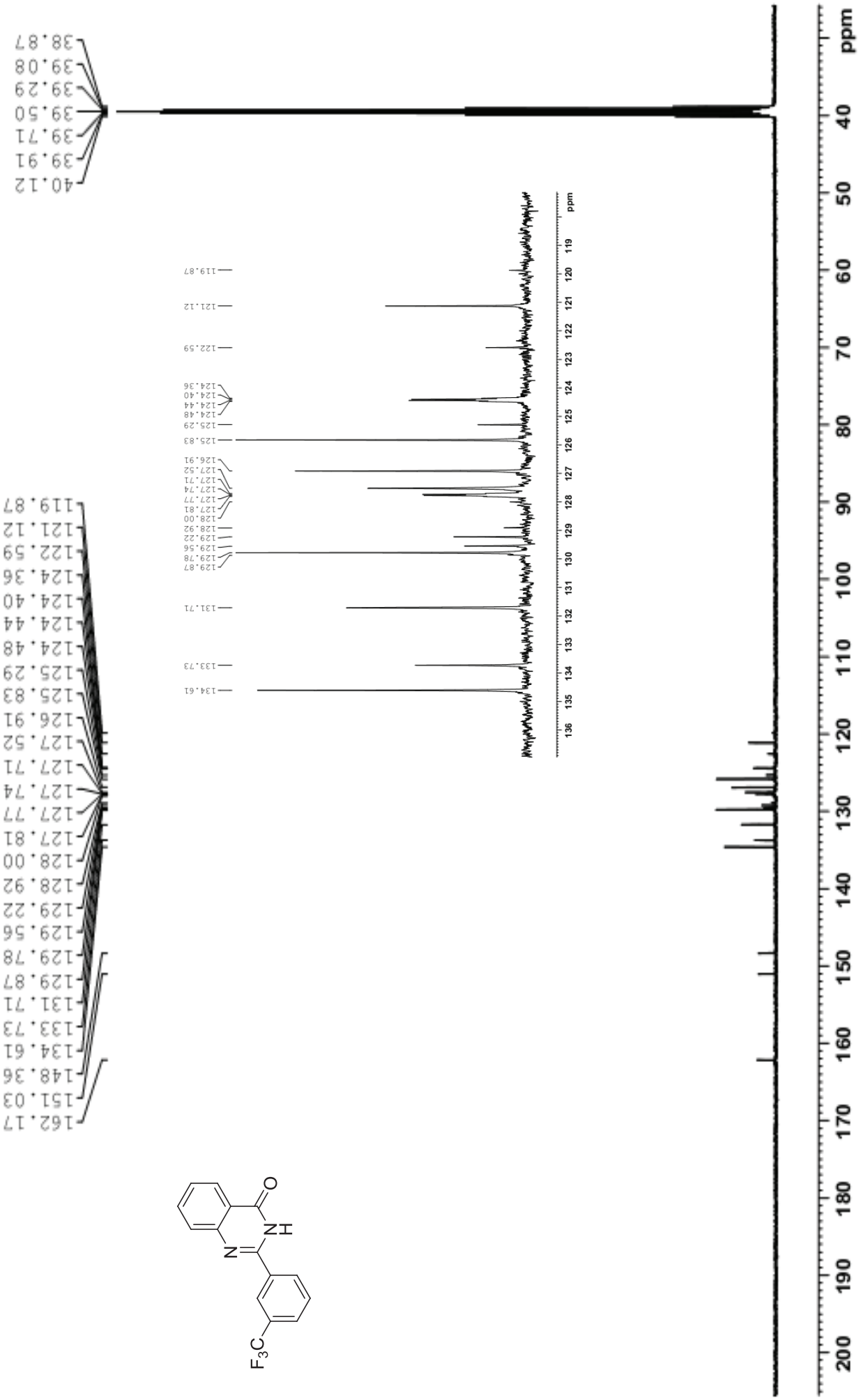
^{13}C NMR spectrum of **5c** (DMSO-d_6, 100 Hz):



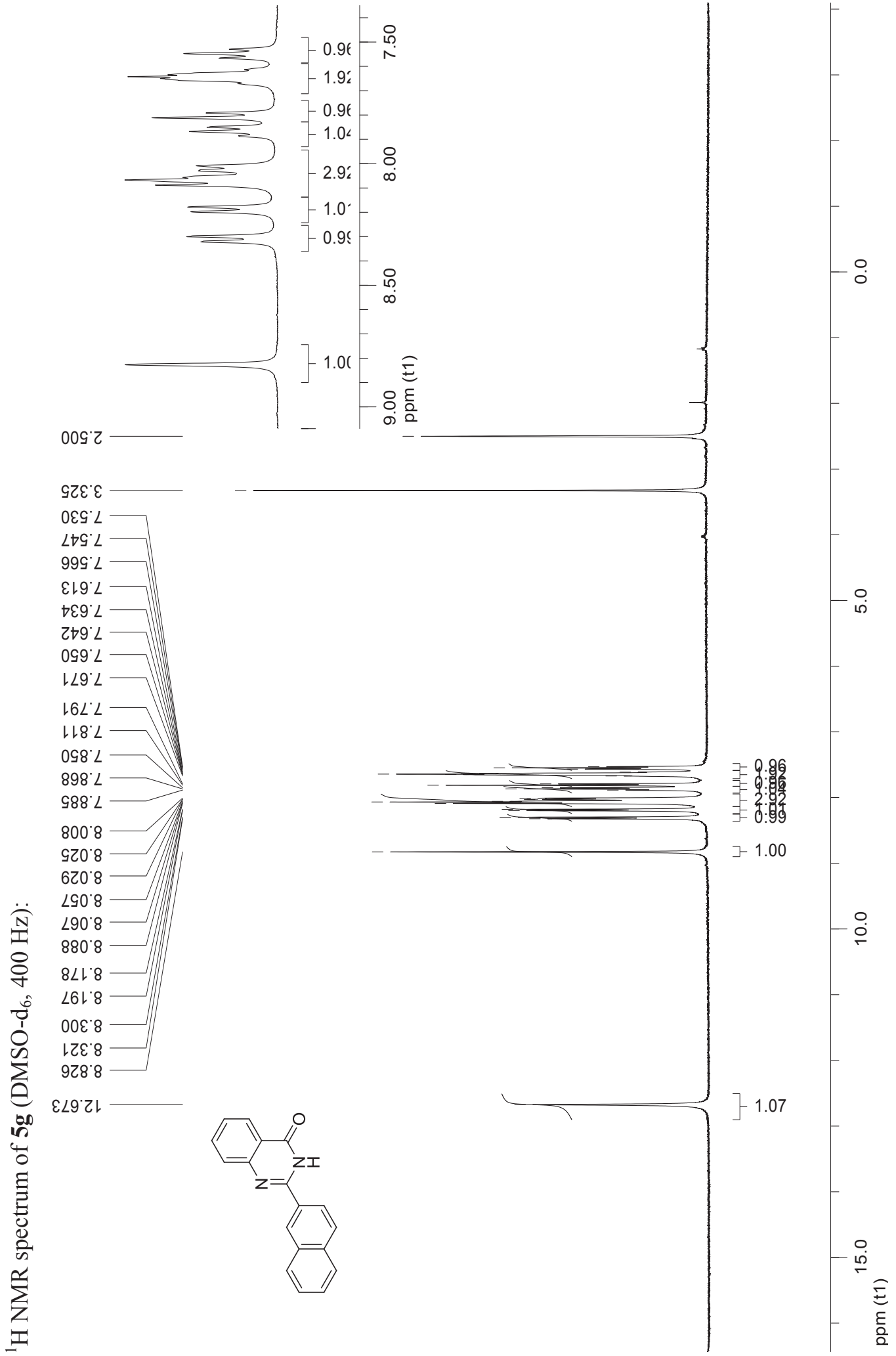
^{1}H NMR spectrum of **5f** (DMSO-d_6, 400 Hz):



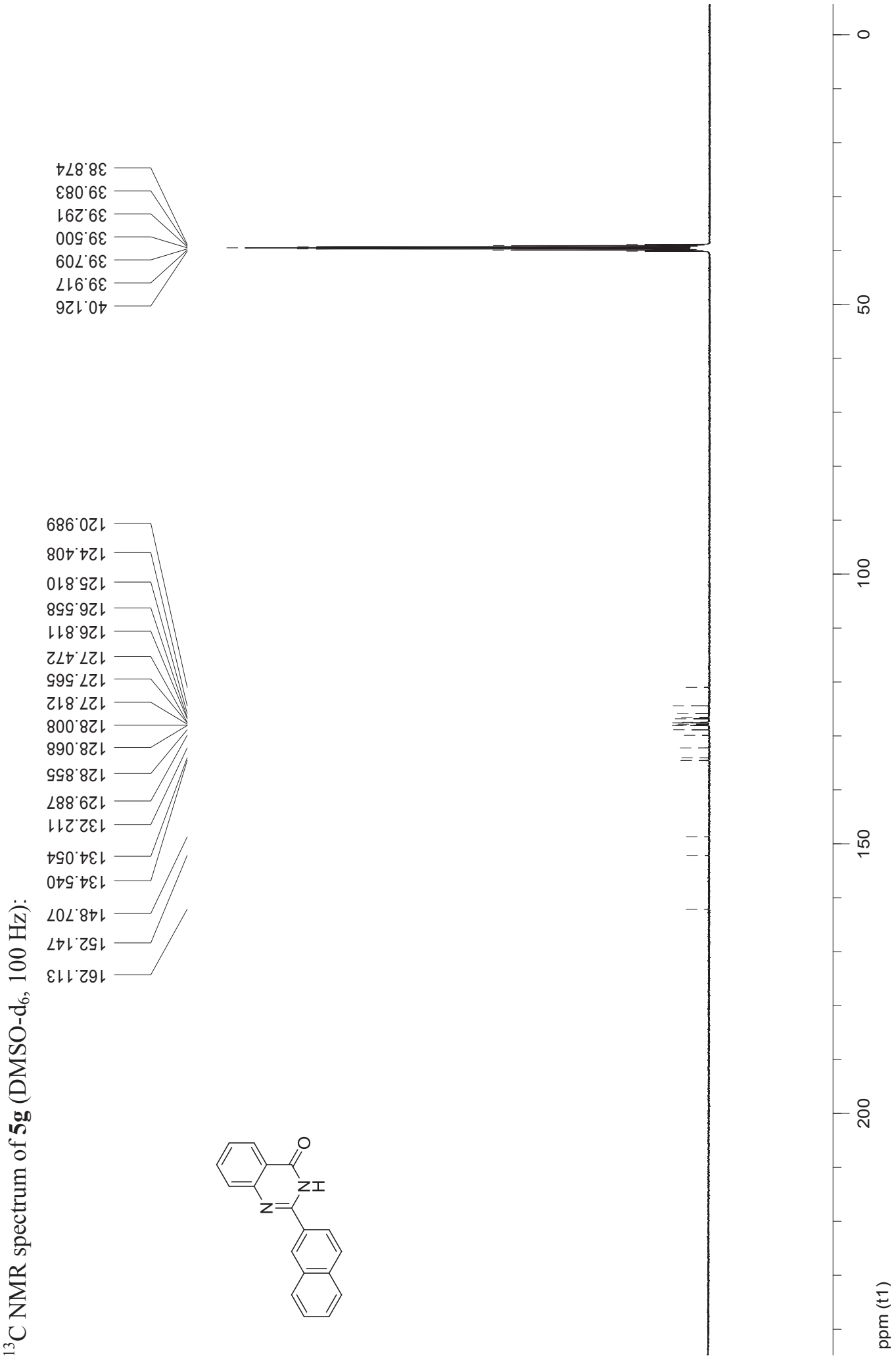
^{13}C NMR spectrum of **5f** (DMSO-d_6, 100 Hz):



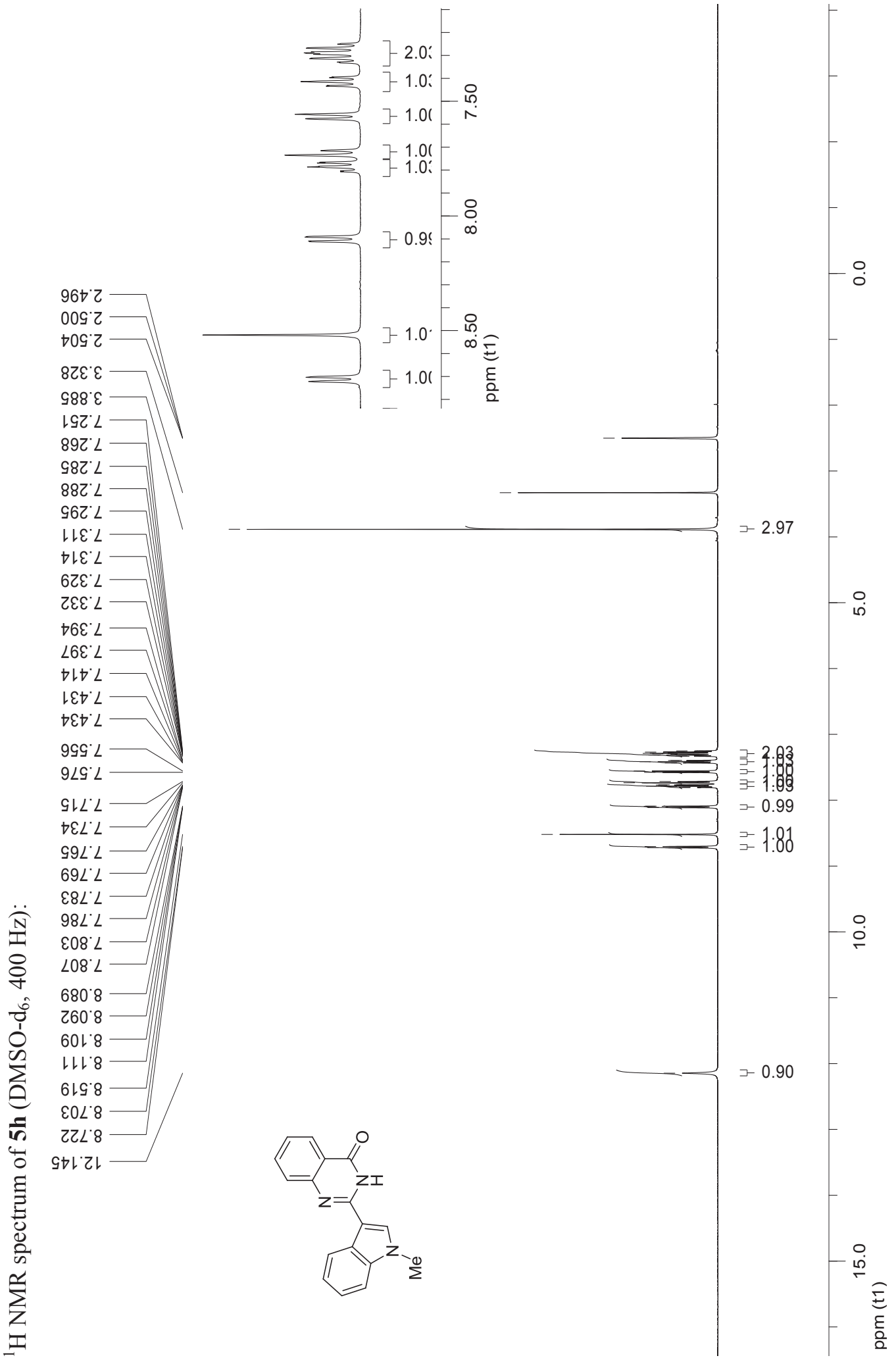
^{1}H NMR spectrum of **5g** (DMSO-d_6, 400 Hz):



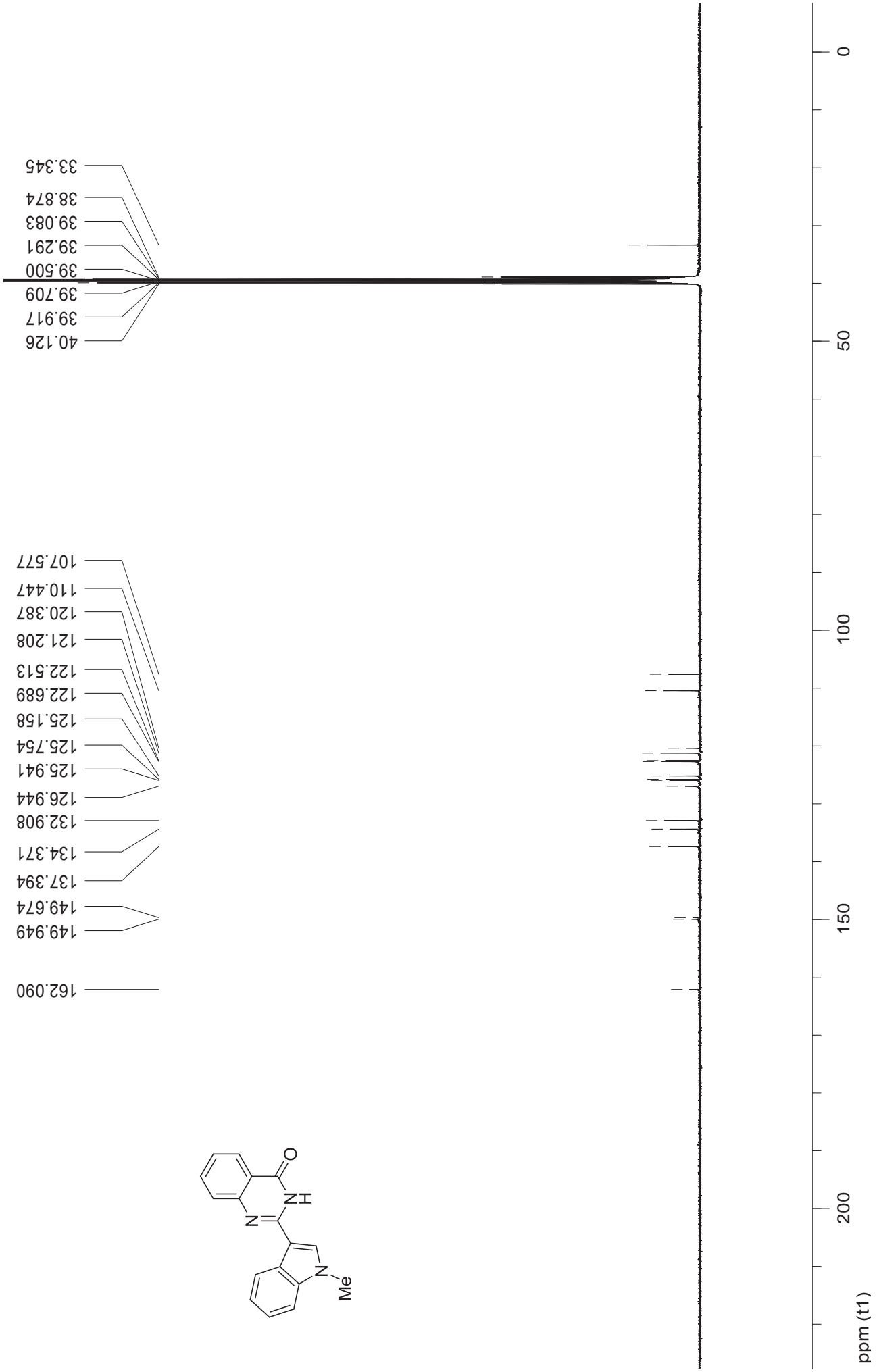
^{13}C NMR spectrum of **5g** (DMSO-d_6, 100 Hz):



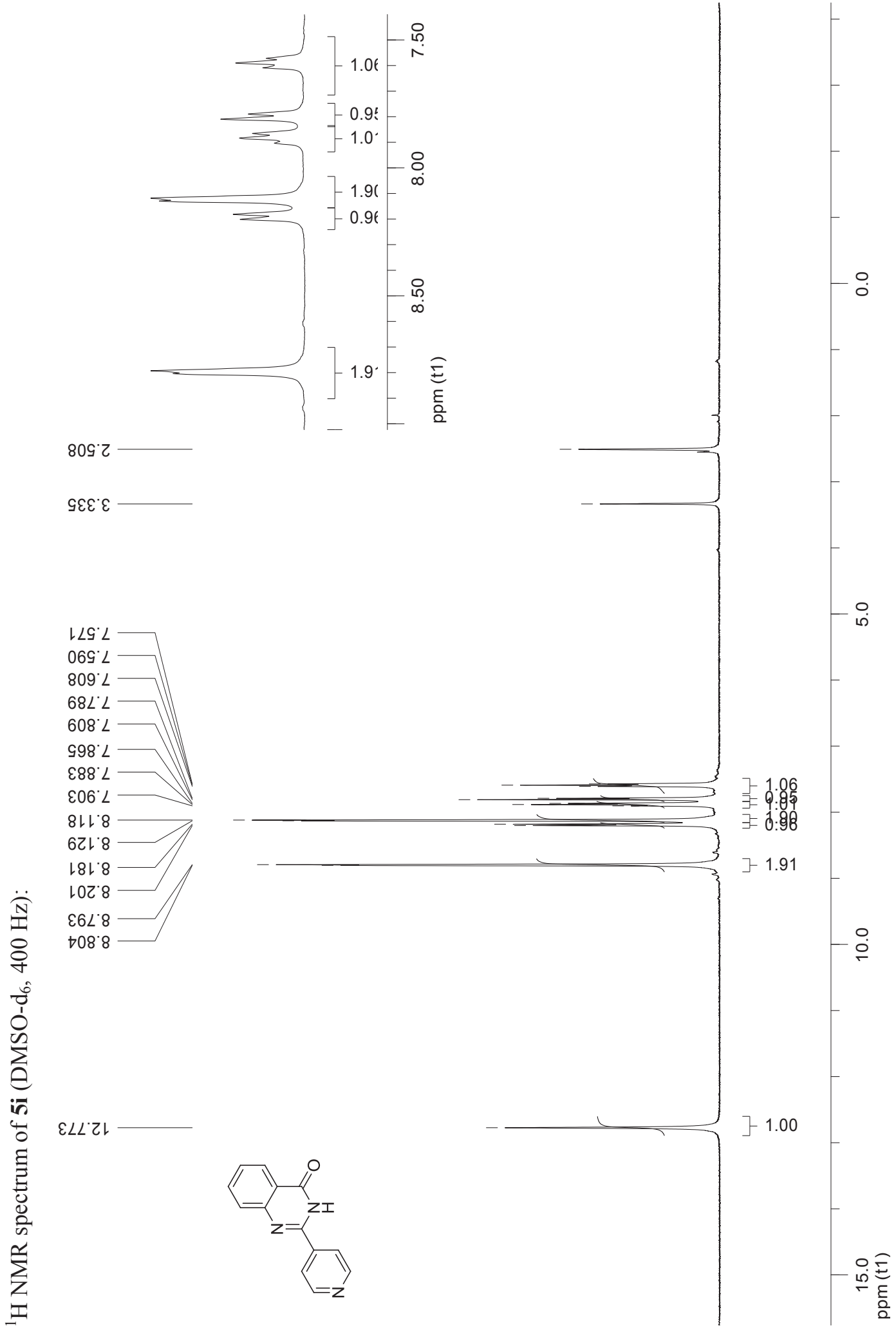
^{1}H NMR spectrum of **5h** (DMSO-d_6, 400 Hz):



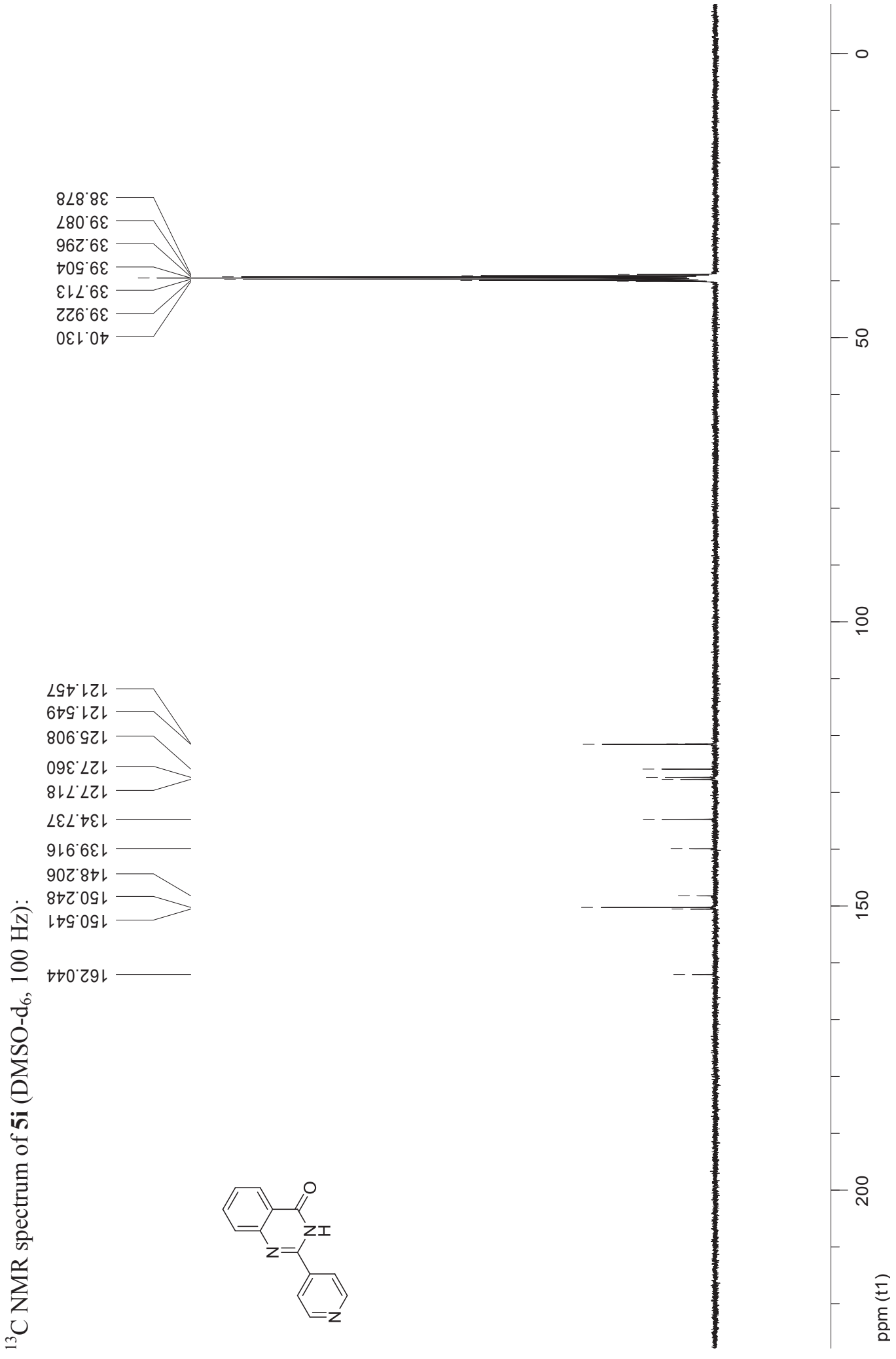
^{13}C NMR spectrum of **5h** (DMSO-d_6, 100 Hz):



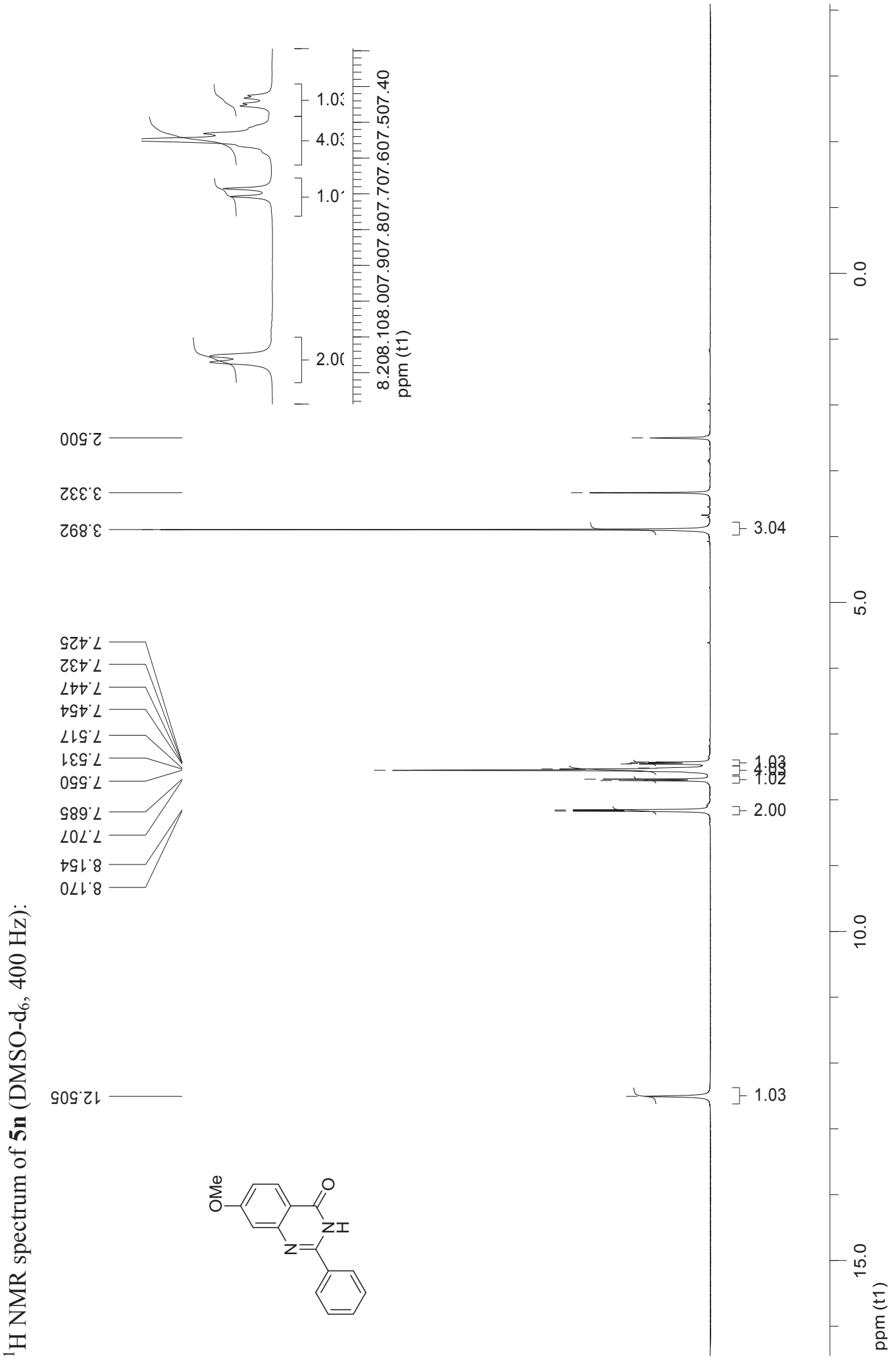
^{1}H NMR spectrum of **5i** (DMSO-d_6, 400 Hz):



^{13}C NMR spectrum of **5i** (DMSO-d_6, 100 Hz):



^{1}H NMR spectrum of **5n** (DMSO-d_6, 400 Hz):



^{13}C NMR spectrum of **5n** (DMSO-d$_6$, 100 Hz):