Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Supporting information

for

$Pd(OAc)_2$-Catalysed Regioselective Alkoxylation of Aryl (β-carbolin-1-yl) methanones via β-Carboline directed *ortho*-C(sp2)-H activation of aryl ring

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Contents :

1. General conditions S-1
2. Spectroscopic data for starting Aryl (β-carbolin-1-yl) methanones S-2
3. References S-5
4. Copies of ^1H and ^{13}C NMR spectra S-6

General Conditions:

Thin layer chromatography (TLC) was used to monitor all experiments. TLC was performed on pre-coated silica gel plates. After elution, plate was visualized under UV illumination at 254 nm. The melting points were recorded on a hot stage apparatus using silicone oil and are uncorrected. IR spectra were recorded using a FTIR spectrophotometer. ^{1}H NMR and ^{13}C NMR spectra were recorded on 400 and 500 MHz spectrometers, using TMS as an internal standard (chemical shifts in δ). Peak multiplicities of NMR signals were designated as s (singlet), bs (broad singlet), d (doublet), dd (doublet of doublet), t (triplet), m (multiplet) etc. The ESI-MS were recorded on Ion Trap Mass spectrometer and the HRMS spectra were recorded as ESI-HRMS on a Q-TOF LC-MS/MS mass spectrometer. Commercial grade reagents and solvents were used without further purification.

2. The aryl (β-carbolin-1-yl) methanones were prepared according to the literature procedure.[24]

Phenyl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1a), MP 132-134 ^{o}C**.**[1]

(9*H*-Pyrido[3,4-*b*]indol-1-yl)(p-tolyl)methanone (1b), MP 156-158 ^{o}C**.**[1]

(4-Methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1c), MP 172-174 ^{o}C**.**[1]

[1,1'-Biphenyl]-4-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1d), MP 184-186 ^{o}C**.**[1]

(4-Chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1e), MP 160-162 ^{o}C**.**[1]

(4-Bromophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1f), MP 182-184 ^{o}C**.**[1]

(4-Nitrophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1g), MP 246-248 ^{o}C**.**[1]

(3-Chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1h). Yield: 85% as a yellow solid, mp 166-168 ^{o}C; R_f = 0.61 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 662, 1119, 1411, 1617, 3381 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.34-7.38 (m, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.56-7.59 (m, 1H), 7.59-7.63 (m, 2H), 8.17 (s, 1H), 8.18 (s, 1H), 8.22-8.25 (m, 1H), 8.34 (t, J = 1.7 Hz, 1H), 8.61 (d, J = 4.9 Hz, 1H), 10.42 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 112.2, 118.9, 120.9, 121.1, 121.9, 129.4, 129.5, 131.4, 131.9, 132.4,

134.2, 135.9, 137.5, 138.3, 139.2, 141.2, 193.9. MS (ESI+) m/z = 307.1. ESI-HRMS calculated for $C_{18}H_{11}ClN_2O$ $[MH]^+$: 307.0638, found: 307.0640.

(2,4-Dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1i). Yield: 81% as a yellow solid, mp 152-154 ^oC; R_f = 0.64 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 756, 1185, 1277, 1520, 1614, 3455 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) = 2.32 (s, 6H), 7.06 (t, J = 3.0 Hz, 2H), 7.25-7.32 (m, 1H), 7.48-7.56 (m, 3H), 8.06 (d, J = 4.7 Hz, 1H), 8.09-8.11 (m, 1H), 8.49 (t, J = 5.2 Hz, 1H), 10.42 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 20.4, 21.6, 112.1, 118.7, 120.9, 121.9, 125.8, 129.4, 130.4, 131.7, 131.9, 135.5, 136.7, 137.1, 137.5, 137.6, 138.6, 140.9, 141.3, 200.2. MS (ESI+) m/z = 301.1. ESI-HRMS calculated for $C_{20}H_{16}N_2O$ $[MH]^+$: 301.1341, found: 301.1345

(9*H*-pyrido[3,4-*b*]indol-1-yl)(thiophen-2-yl)methanone (1k), MP 226-228 ^oC**.**[24]

Pyridin-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1l). Yield: 82% as a yellow solid, mp 188-190 ^oC; R_f = 0.22 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 764, 1259, 1423, 1618, 3397 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.27-7.31 (m, 1H), 7.41-7.44 (m, 1H), 7.53-7.59 (m, 2H), 7.82-7.86 (m, 1H), 8.09 (d, J = 0.4 Hz, 1H), 8.11 (dd, J_1 = 2.4 Hz, J_2 = 0.8 Hz, 1H), 8.16-8.18 (m, 1H), 8.54 (d, J = 4.9 Hz, 1H), 8.79-8.81 (m, 1H), 10.38 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 112.3, 119.0, 120.8, 120.9, 121.9, 125.8, 126.4, 129.5, 131.9, 135.6, 136.3, 137.6, 138.6, 141.2, 149.8, 155.1, 194.5. MS (ESI+) m/z = 274.1. ESI-HRMS calculated for $C_{17}H_{11}N_3O$ $[MH]^+$: 274.0980, found: 274.0984.

Pyridin-4-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1m). Yield: 84% as a yellow solid, mp 182-184 ^oC; R_f = 0.21 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 785, 1245, 1484, 1614, 3385 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.28-7.32 (m, 1H), 7.54-7.59 (m, 2H), 8.03 (d, J = 1.6 Hz, 1H), 8.04 (d, J = 1.6 Hz, 1H), 8.11-8.14 (m, 2H), 8.53 (d, J = 4.9 H, 1H), 8.78 (d, J = 1.6 Hz, 1H), 8.79 (d, J = 1.6 Hz, 1H), 10.37 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 112.2, 119.4, 120.8, 121.3, 122.0, 124.4, 129.7, 132.1, 135.3, 137.4, 138.5, 141.2, 144.2, 150.1, 194.4. MS (ESI+) m/z = 274.1. ESI-HRMS calculated for $C_{17}H_{11}N_3O$ $[MH]^+$: 274.0980, found: 274.0983.

Benzofuran-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (1n).[1] MP 202-204 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) = 7.25-7.29 (m, 2H), 7.41-7.46 (m, 1H), 7.52-7.58 (m, 2H), 7.62 (d, J = 8.4 Hz, 1H), 7.75 (d, J = 7.8 Hz, 1H), 8.11 (t, J = 5.2 Hz, 2H), 8.57 (d, J = 4.9 Hz, 1H), 8.81 (d, J = 0.8 Hz, 1H), 10.44 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 112.3,

112.5, 119.0, 120.6, 120.8, 120.9, 121.9, 123.8, 124.0, 127.9, 128.6, 129.5, 131.9, 135.8, 137.0, 138.3, 141.2, 151.3, 155.8, 182.5. MS (ESI+) m/z = 313.1.

Methyl 1-benzoyl-9*H*-pyrido[3,4-*b*]indole-3-carboxylate (2), MP 238-240 ^{o}C**.**[24]

Ethyl 1-benzoyl-9*H*-pyrido[3,4-*b*]indole-3-carboxylate (3). Yield: 74% as a yellow solid, mp 142-144 ^{o}C; R_f = 0.62 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 760, 1125, 1262, 1400, 1620, 1716, 3429 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.45 (t, J = 7.1 Hz, 3H), 4.45 (q, J = 7.1 Hz, 2H), 7.32-7.36 (m, 1H), 7.47-7.50 (m, 2H), 7.54-7.59 (m, 3H), 8.17 (d, J = 7.8 Hz, 1H), 8.61 (t, J = 7.2 Hz, 2H), 8.97 (s, 1H), 10.63 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.5, 61.7, 112.5, 120.5, 121.3, 121.7, 122.1, 128.2, 129.8, 132.2, 133.1, 135.7, 136.8, 136.9, 138.3, 141.4, 165.8, 193.6. MS (ESI+) m/z = 345.1. ESI-HRMS calculated for $C_{21}H_{16}N_2O_3$ $[MH]^+$: 345.1239, found: 345.1243.

(9-Methyl-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone (9).Yield: 94% as a yellow solid, mp 122-124 ^{o}C; R_f = 0.52 (Hexanes: EtOAc, 8:2, v/v). IR (KBr) ν_{max}: 761, 1156, 1352, 1455 1618 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 3.78 (s, 3H), 7.33-7.37 (m, 1H), 7.49-7.53 (m, 3H), 7.61-7.68 (m, 2H), 8.05 (d, J = 1.4 Hz, 1H), 8.07 (d, J = 2.7 Hz, 1H), 8.13 (d, J = 5.0 Hz, 1H), 8.19 (d, J = 7.8 Hz, 1H), 8.52 (d, J = 5.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 32.9, 109.9, 116.5, 120.4, 120.9, 121.7, 128.6, 129.2, 131.2, 131.4, 133.7, 135.9, 137.2, 137.4, 140.1, 142.9, 194.5. MS (ESI+) m/z = 287.1. ESI-HRMS calculated for $C_{19}H_{14}N_2O$ $[MH]^+$: 287.1184, found: 287.1180.

Methyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate (7).[2] Yield: 74% (0.165 g from 0.312 g); a yellow solid, mp 166-168 ^{o}C; R_f = 0.38 (Hexanes: EtOAc, 6:4, v/v). IR (KBr) ν_{max}: 765, 1256, 1410, 1616, 1720 3395 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 4.06 (s, 3H), 7.25-7.28 (m, 1H), 7.49-7.57 (m, 2H), 8.07-8.09 (m, 2H), 8.51 (d, J = 4.9 Hz, 1H), 9.83 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 52.9, 111.9, 118.8, 120.8, 120.9, 122.0, 129.6, 131.6, 137.3, 139.0, 140.9, 167.4. MS (ESI+) m/z = 227.1. ESI-HRMS calculated for $C_{13}H_{10}N_2O_2$ $[MH]^+$: 227.0821, found: 227.0823.

Ethyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate (8).[2] Yield: 76% (0.181 g from 0.312 g); a yellow solid, mp 146-148 ^{o}C; R_f = 0.42 (Hexanes: EtOAc, 6:4, v/v). IR (KBr) ν_{max}: 758, 1225, 1484, 1613, 1719 3378 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.47 (t, J = 7.1 Hz, 3H), 4.54 (q, J = 7.1 Hz, 2H), 7.24-7.28 (m, 1H), 7.49-7.56 (m, 2H), 8.08 (t, J = 6.9 Hz, 2H), 8.53 (d, J = 5.0 Hz, 1H), 9.87 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ (ppm) = 14.6,

62.1, 111.9, 118.7, 120.8, 120.9, 122.0, 129.5, 129.9, 131.6, 137.3, 139.0, 140.9, 167.0. MS (ESI+) m/z = 241.1. ESI-HRMS calculated for $C_{14}H_{12}N_2O_2$ $[MH]^+$: 241.0977, found: 241.0973.

References:

1 Y. P Zhu, M. C Liu, Q Cai, F. C Jia and A. X. Wu, *Chem. Eur. J*., 2013, **19**, 10132.

2. T. H. Trieu, J. Dong, Q. Zhang, B. Zheng, T. Z. Meng, X. Lu and X. Shi, *Eur. J. Org. Chem.*, 2013, 3271.

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

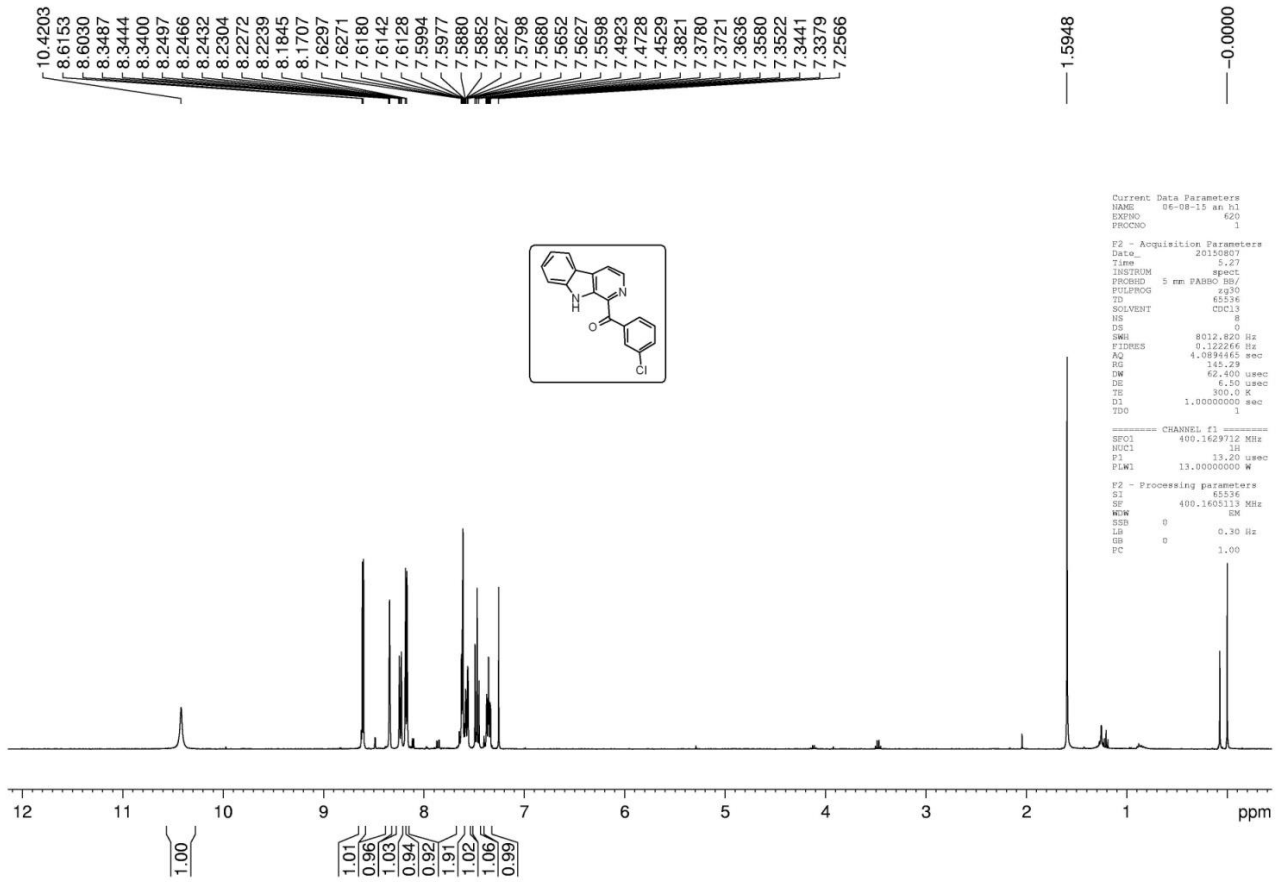

Figure. S-1: ^{1}H-NMR spectrum of (3-Chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1h)**.

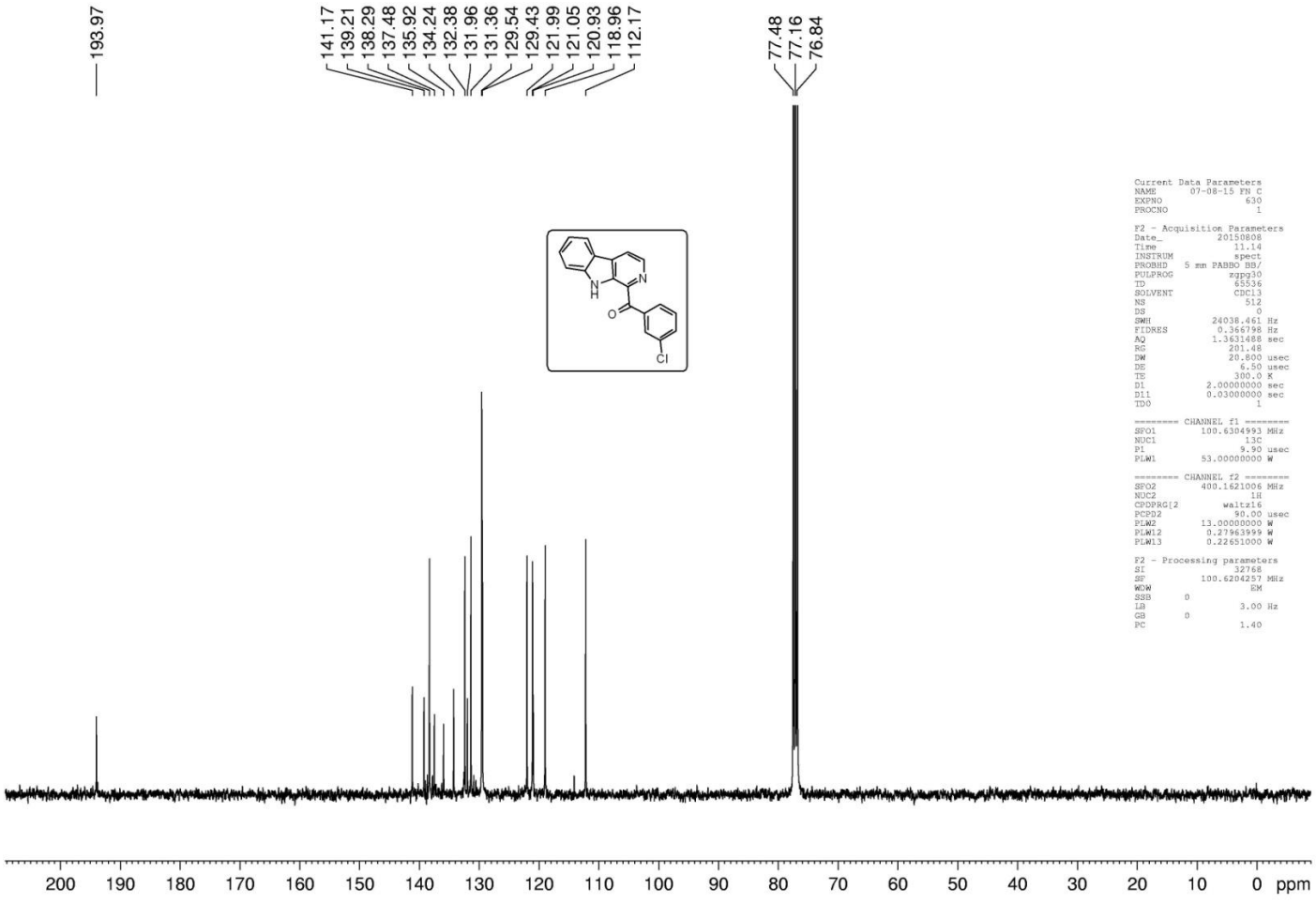

Figure. S-2: ^{13}C-NMR spectrum of (3-Chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1h)**.

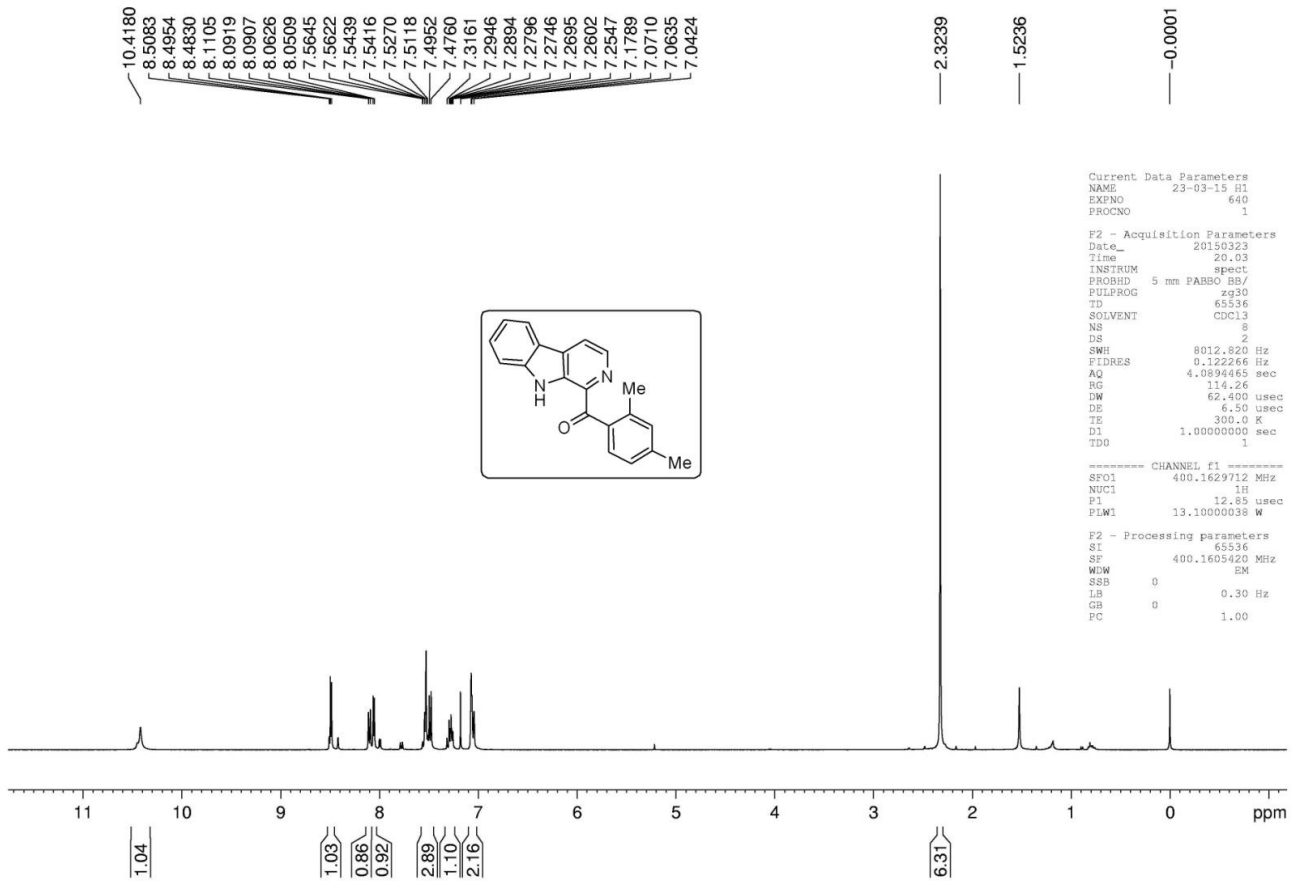

Figure. S-3: ^{1}H-NMR spectrum of (2,4-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1i)**.

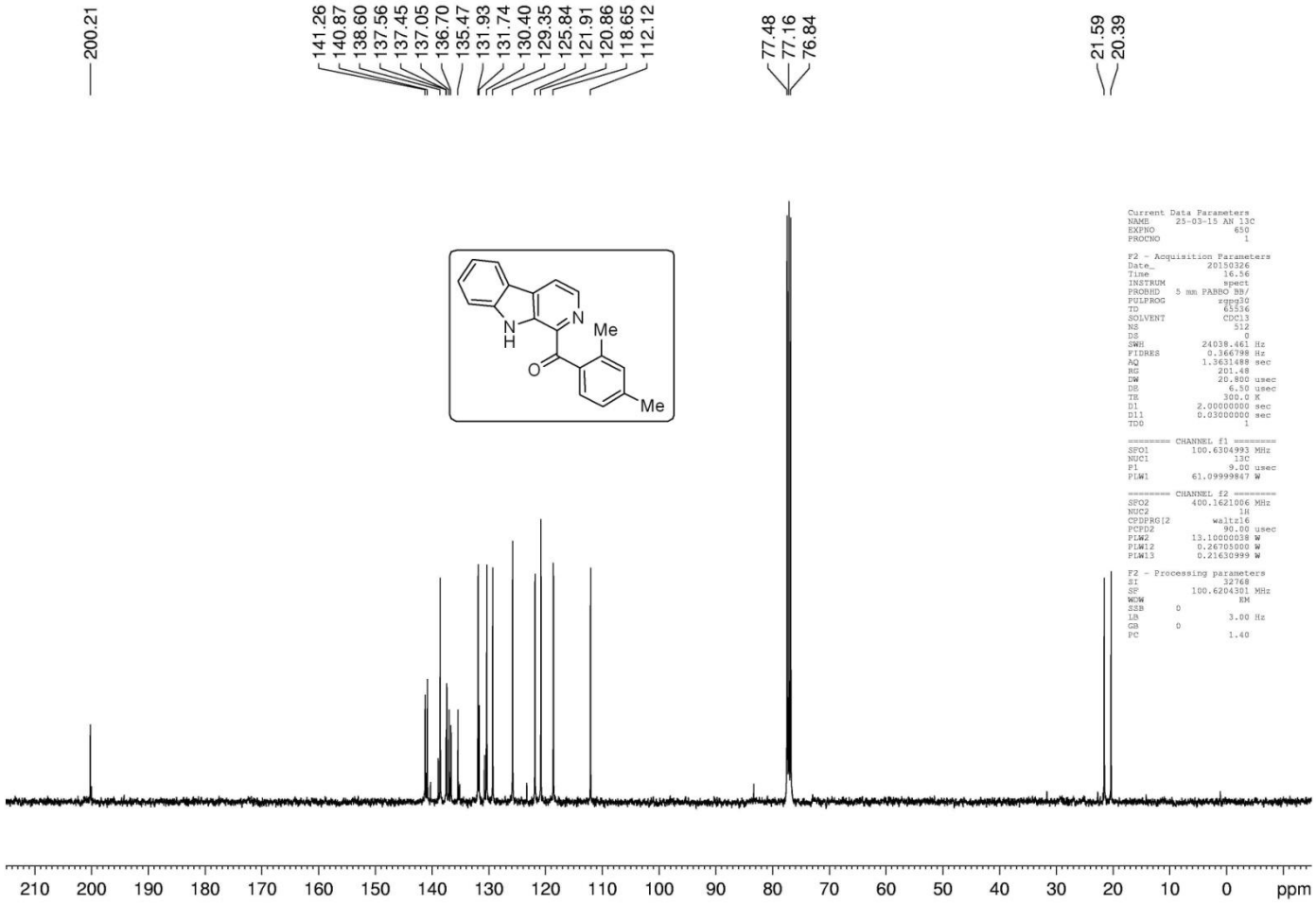

Figure. S-4: ^{13}C-NMR spectrum of (2,4-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1i)**.

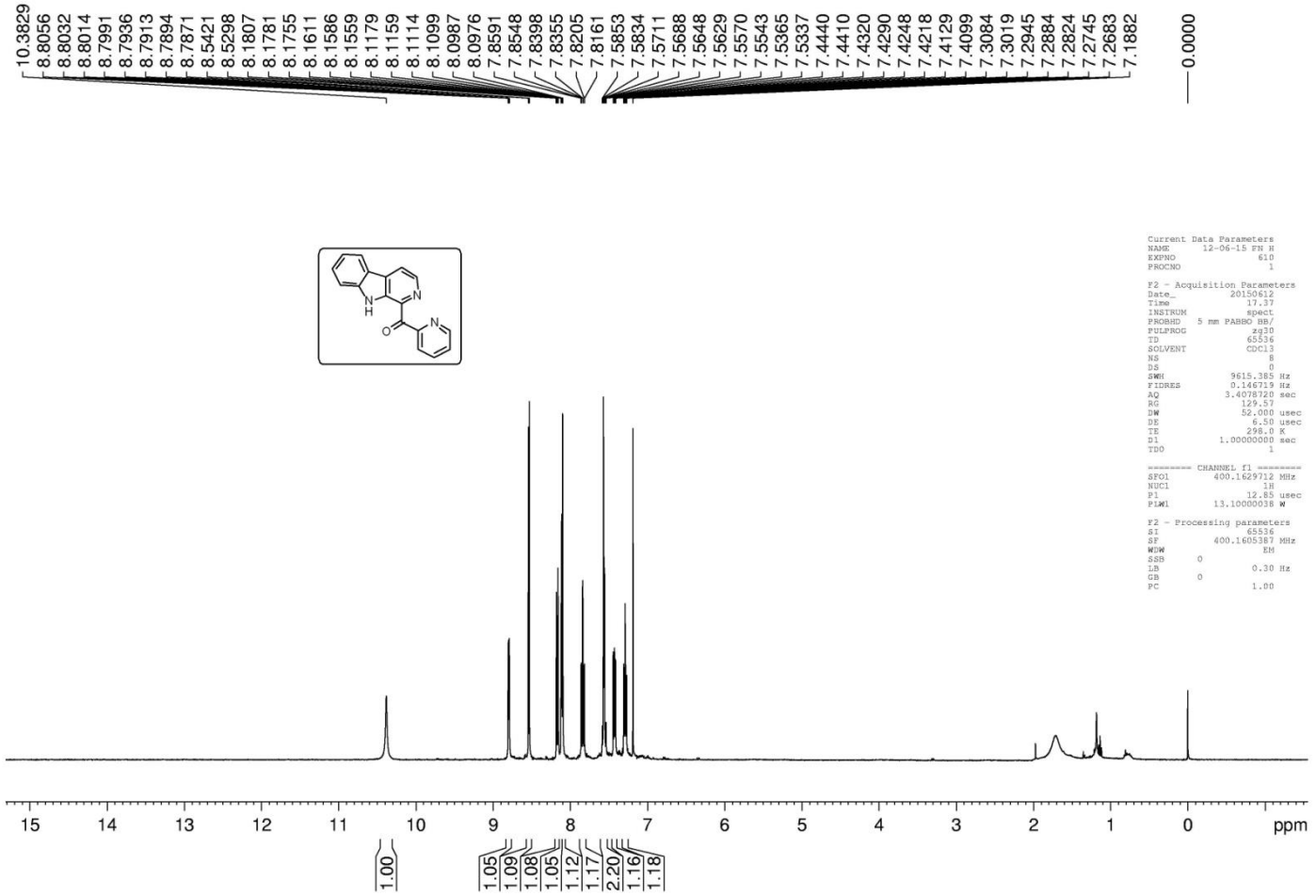

Figure. S-5: ^{1}H-NMR spectrum of pyridin-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1l).**

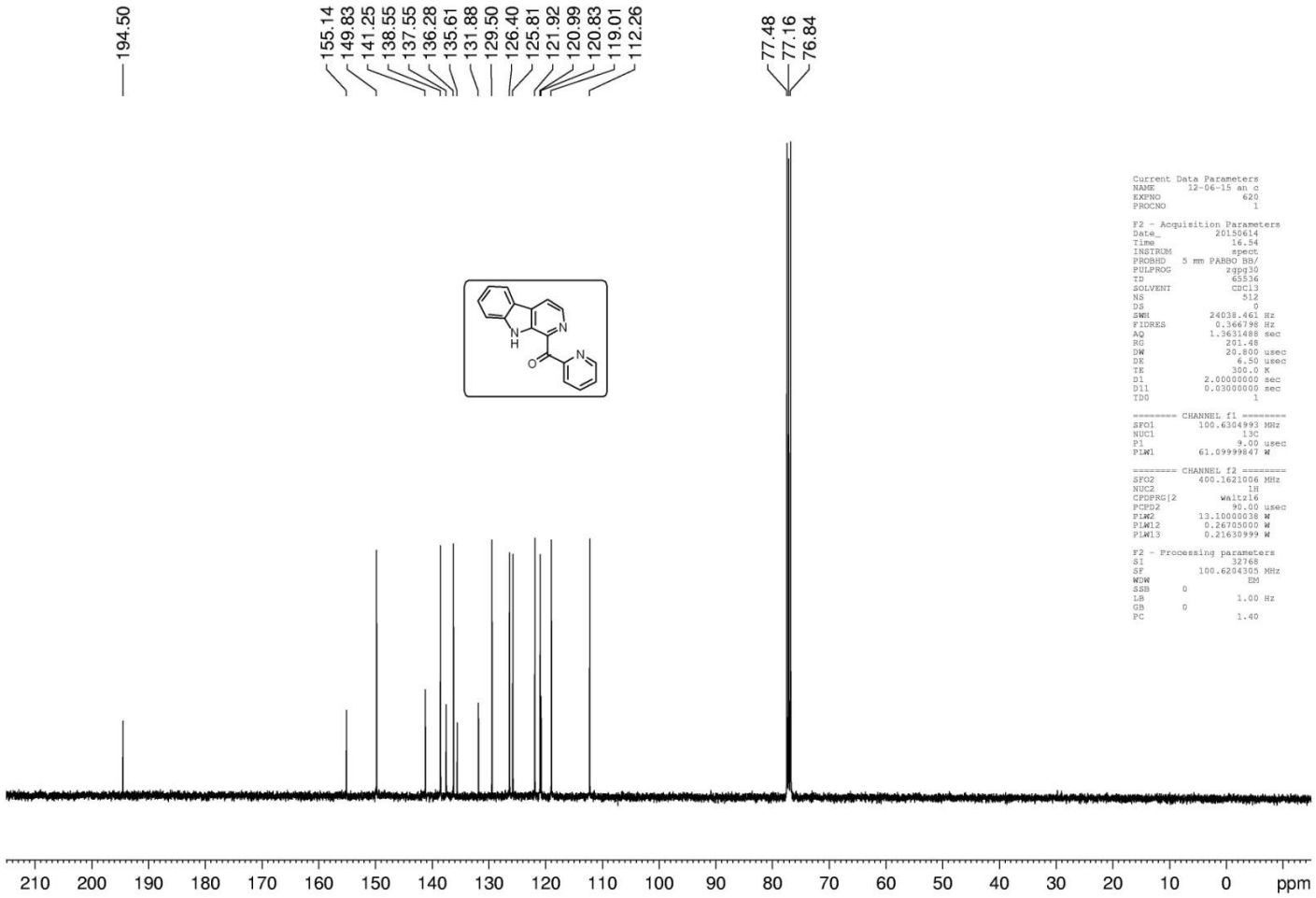

Figure. S-6: ^{13}C-NMR spectrum of pyridin-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1l).**

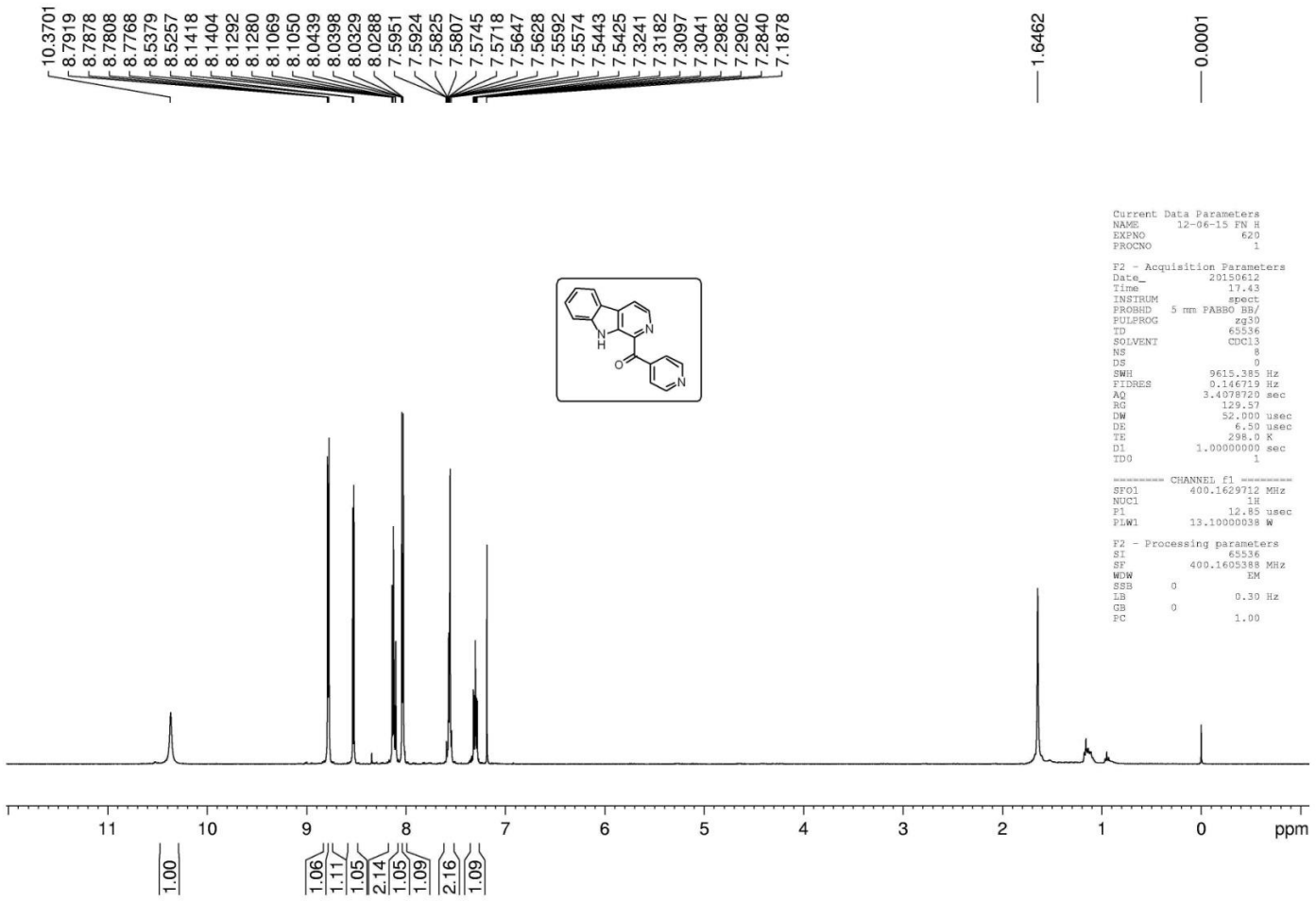

Figure. S-7: ^{1}H-NMR spectrum of pyridin-4-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1m).**

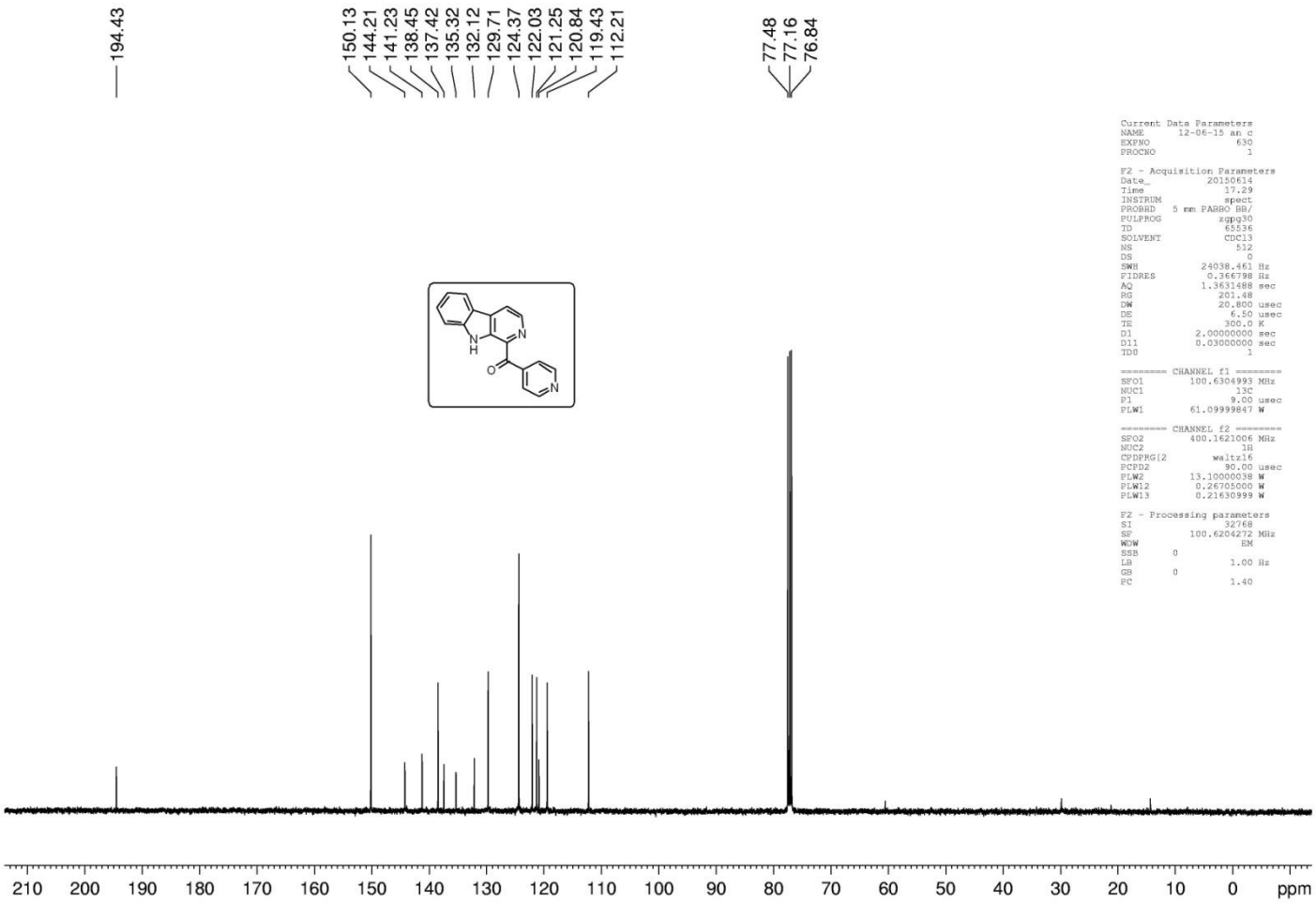

Figure. S-8: ^{13}C-NMR spectrum of pyridin-4-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1m).**

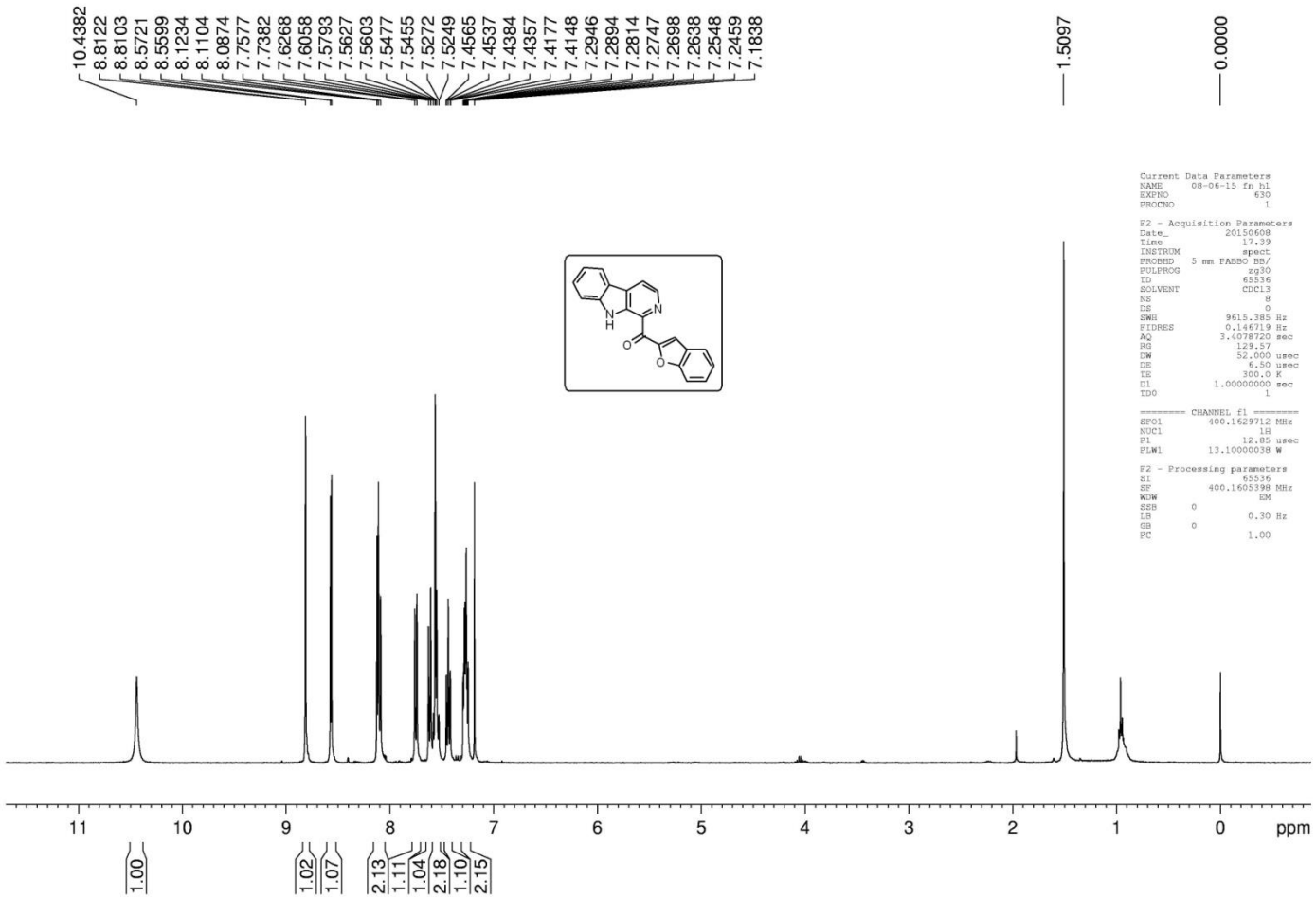

Figure. S-9: ^{1}H-NMR spectrum of benzofuran-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1n)**.

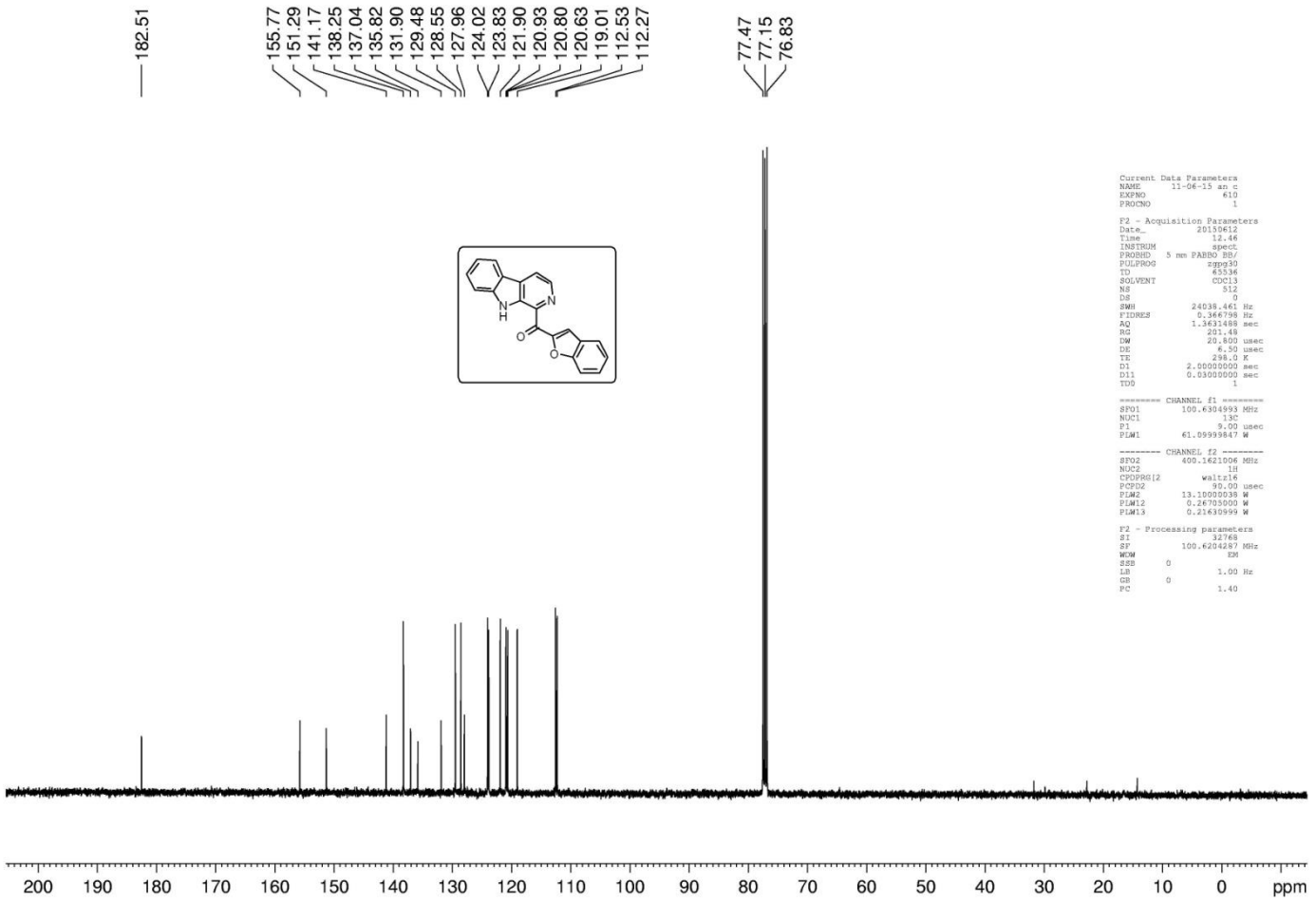

Figure. S-10: ^{13}C-NMR spectrum of benzofuran-2-yl(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(1n).**

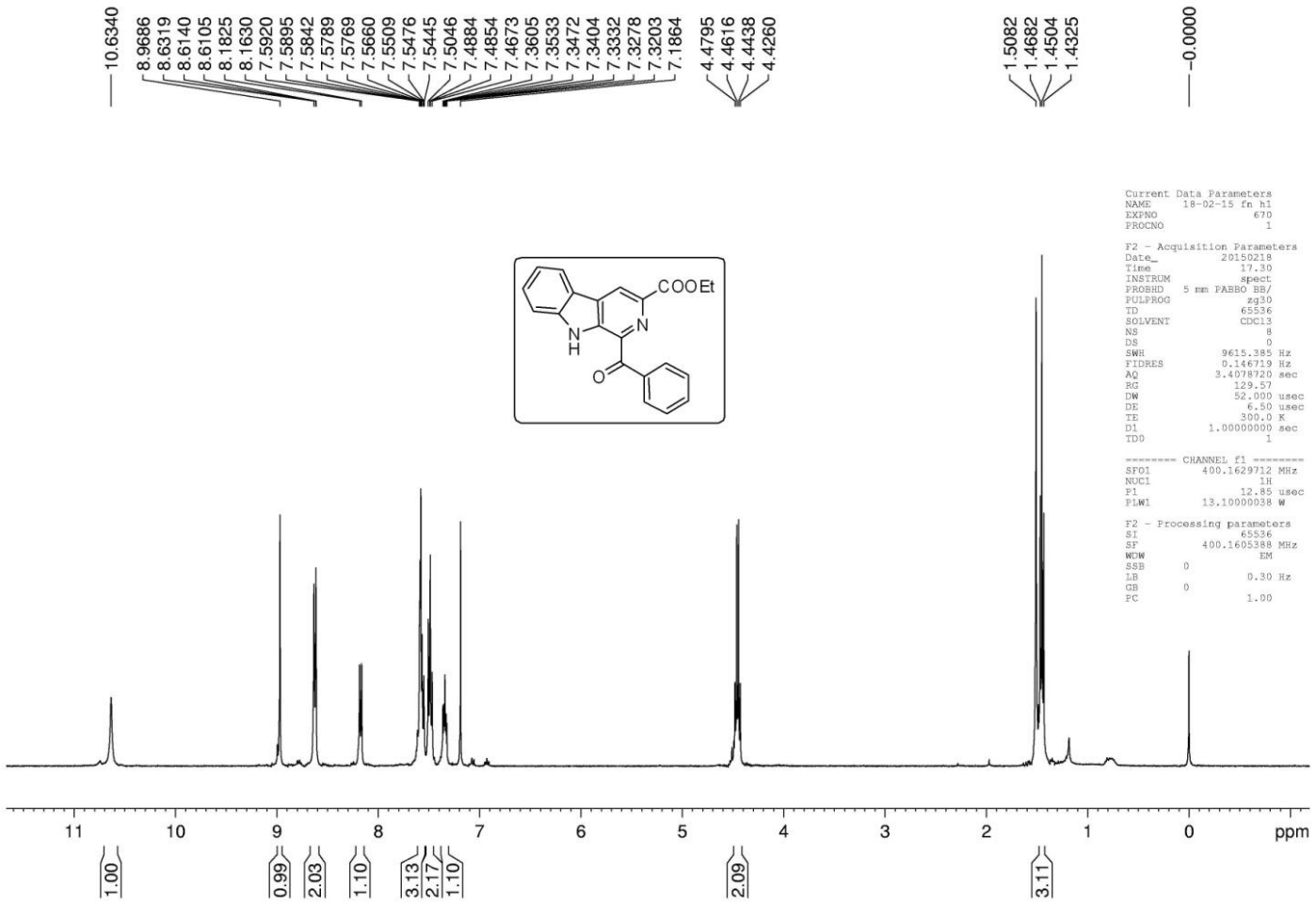

Figure. S-11**:** ^{1}H-NMR spectrum of ethyl 1-benzoyl-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3).**

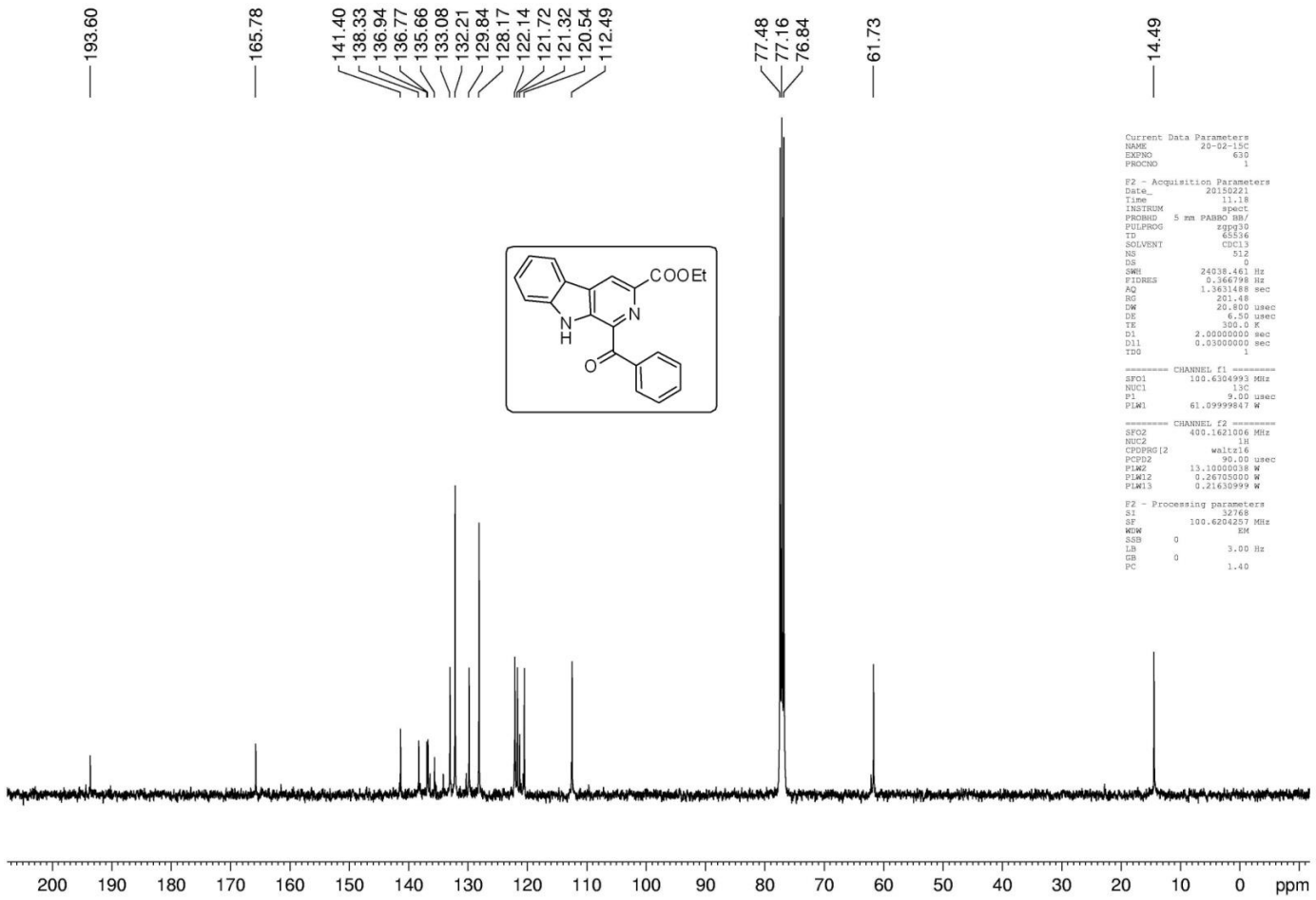

Figure. S-12**:** ^{13}C-NMR spectrum of ethyl 1-benzoyl-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3).**

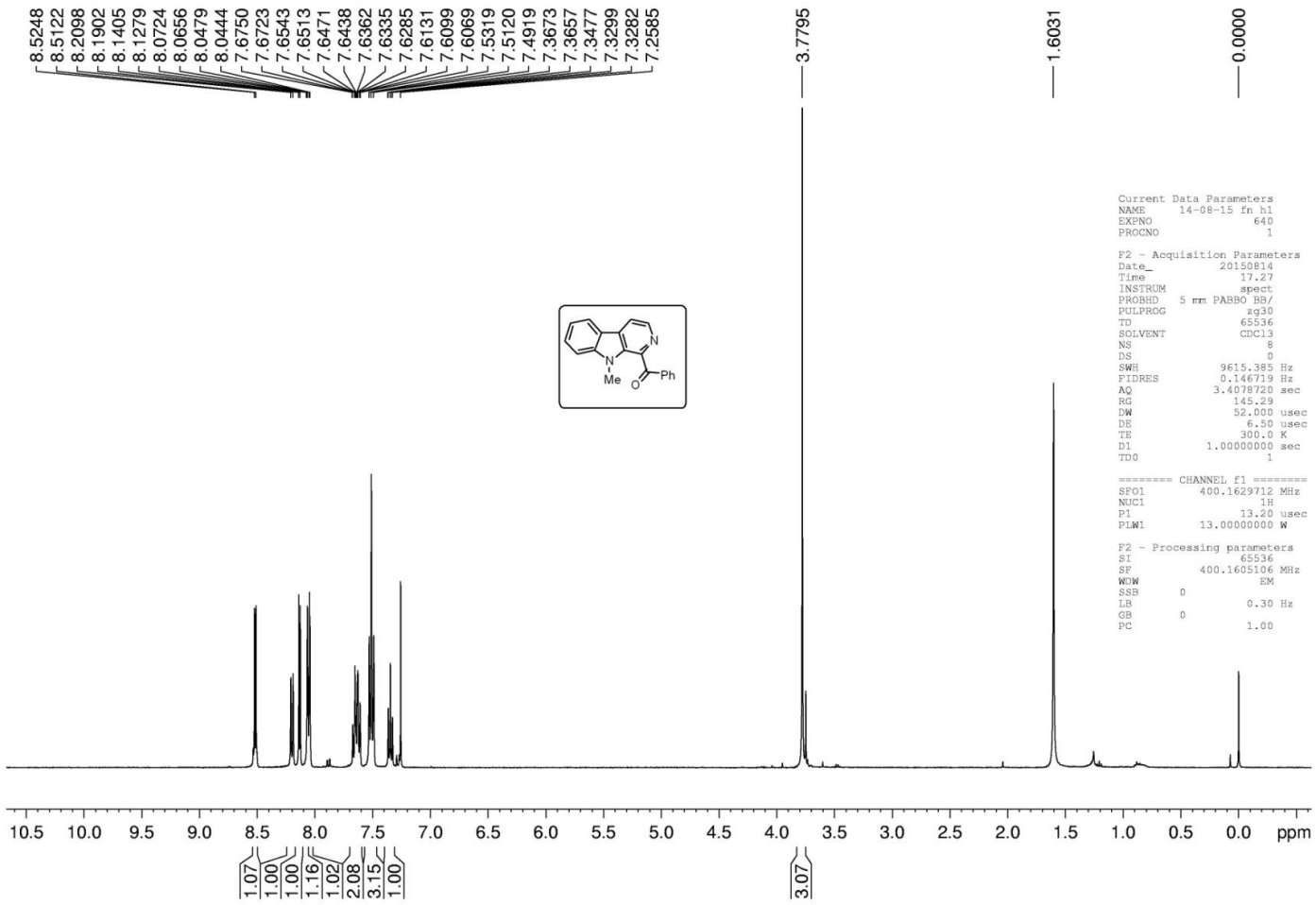

Figure. S-13: ^{1}H-NMR spectrum of (9-Methyl-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone (**9**).

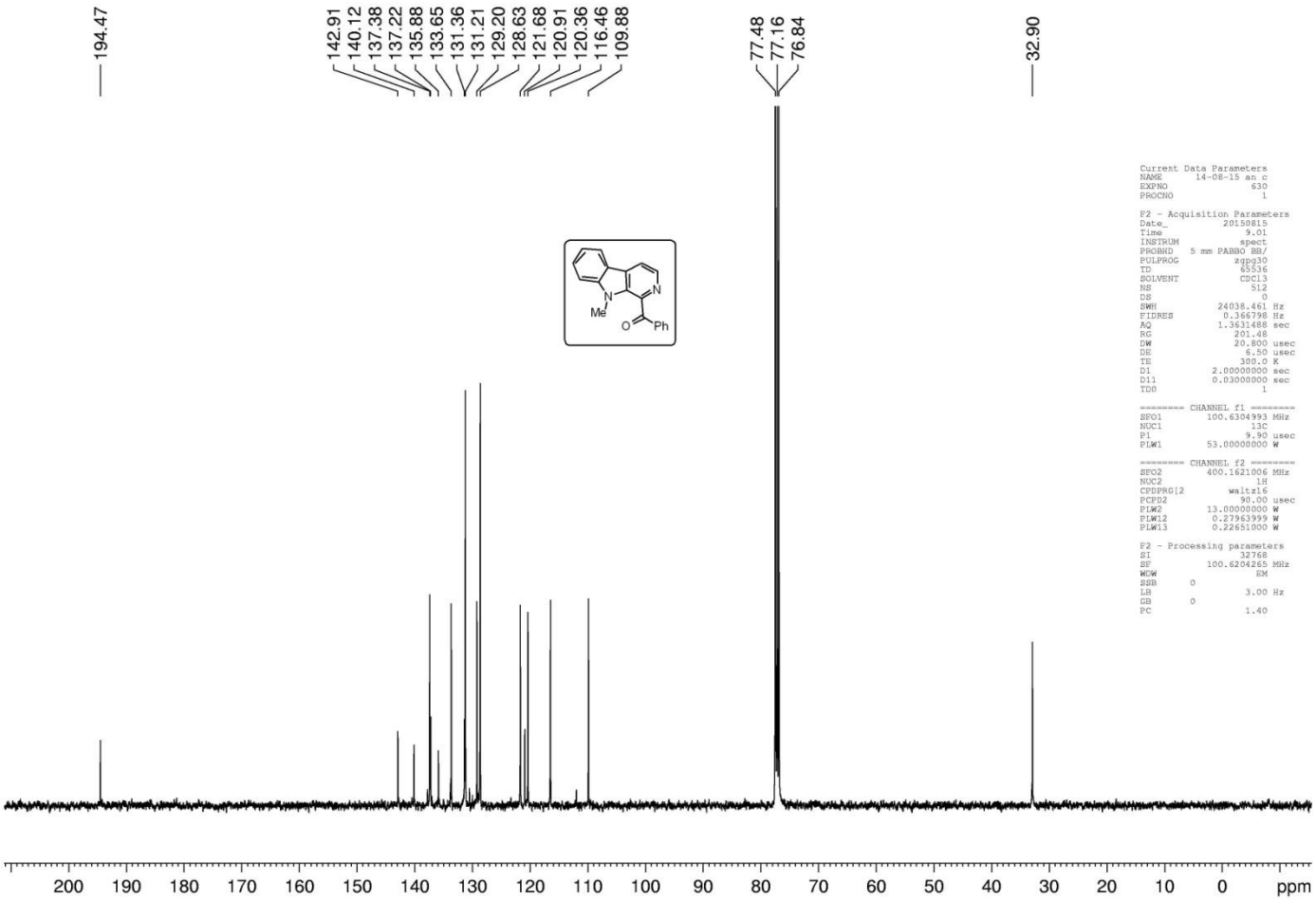

Figure. S-14: ^{13}C-NMR spectrum of (9-Methyl-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone (**9**).

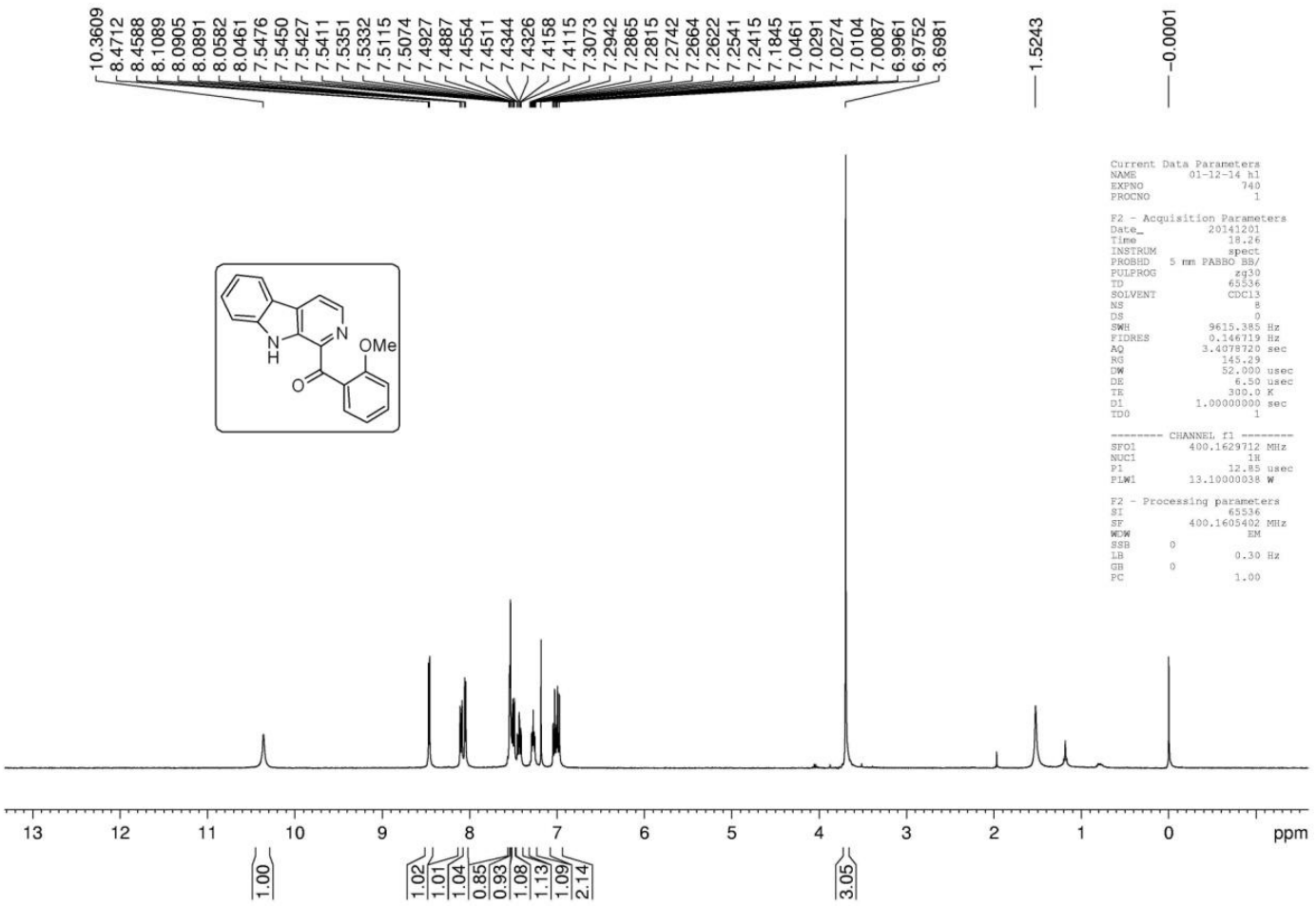

Figure. S-15: ^{1}H-NMR spectrum of (2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (**4aa**).

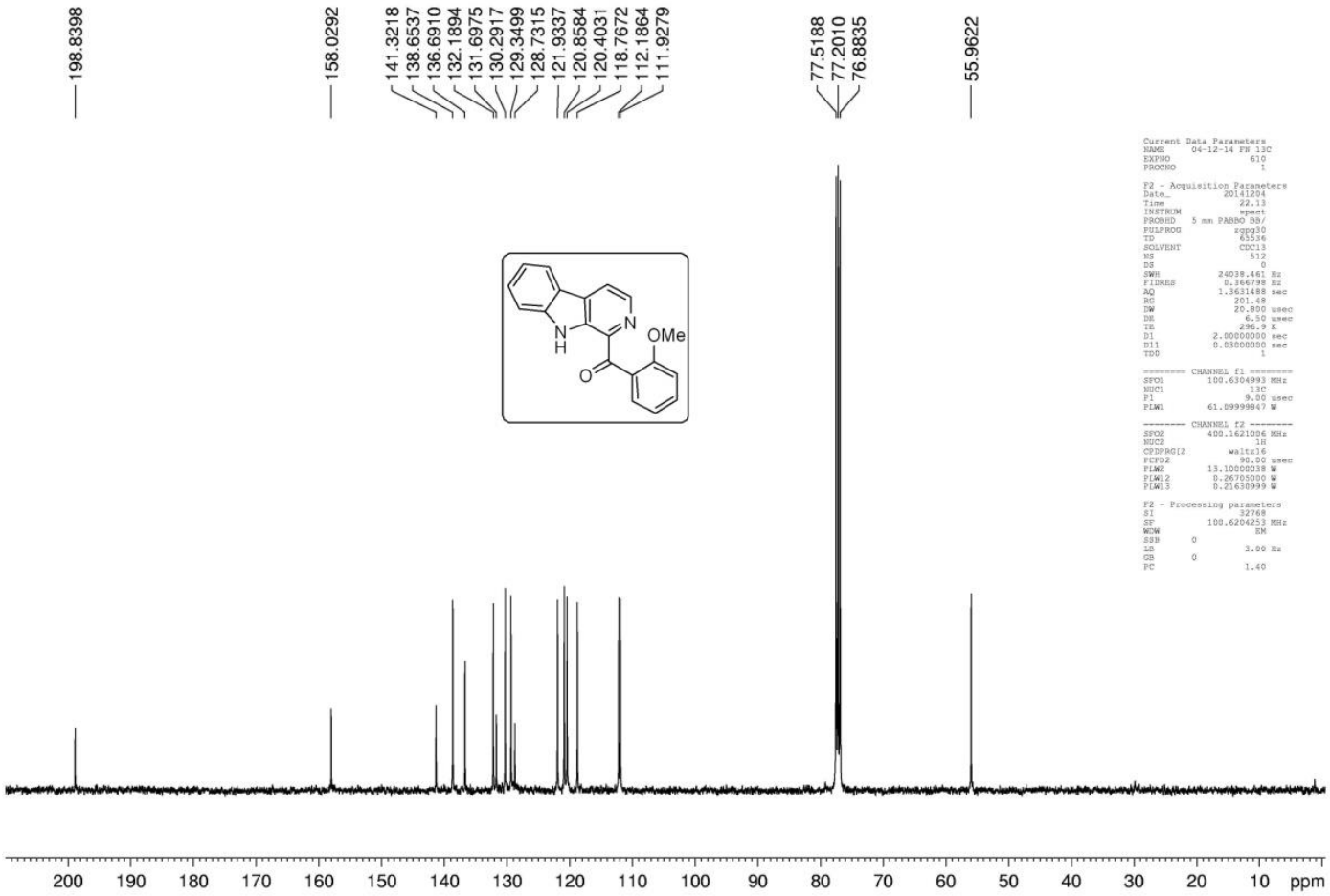

Figure. S-16: ^{13}C-NMR spectrum of (2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone (**4aa**).

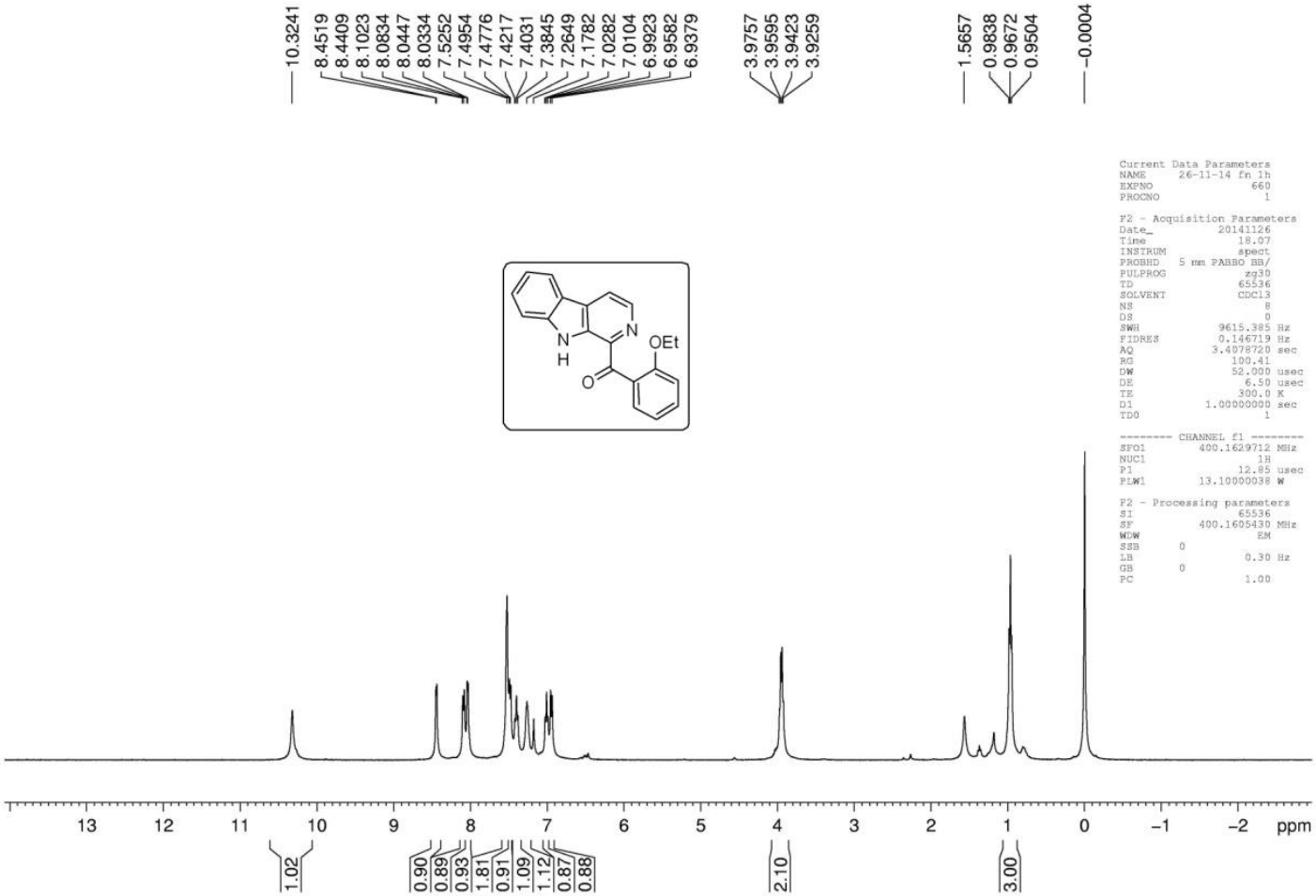

Figure. S-17: ^{1}H-NMR spectrum of (2-ethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ab)**.

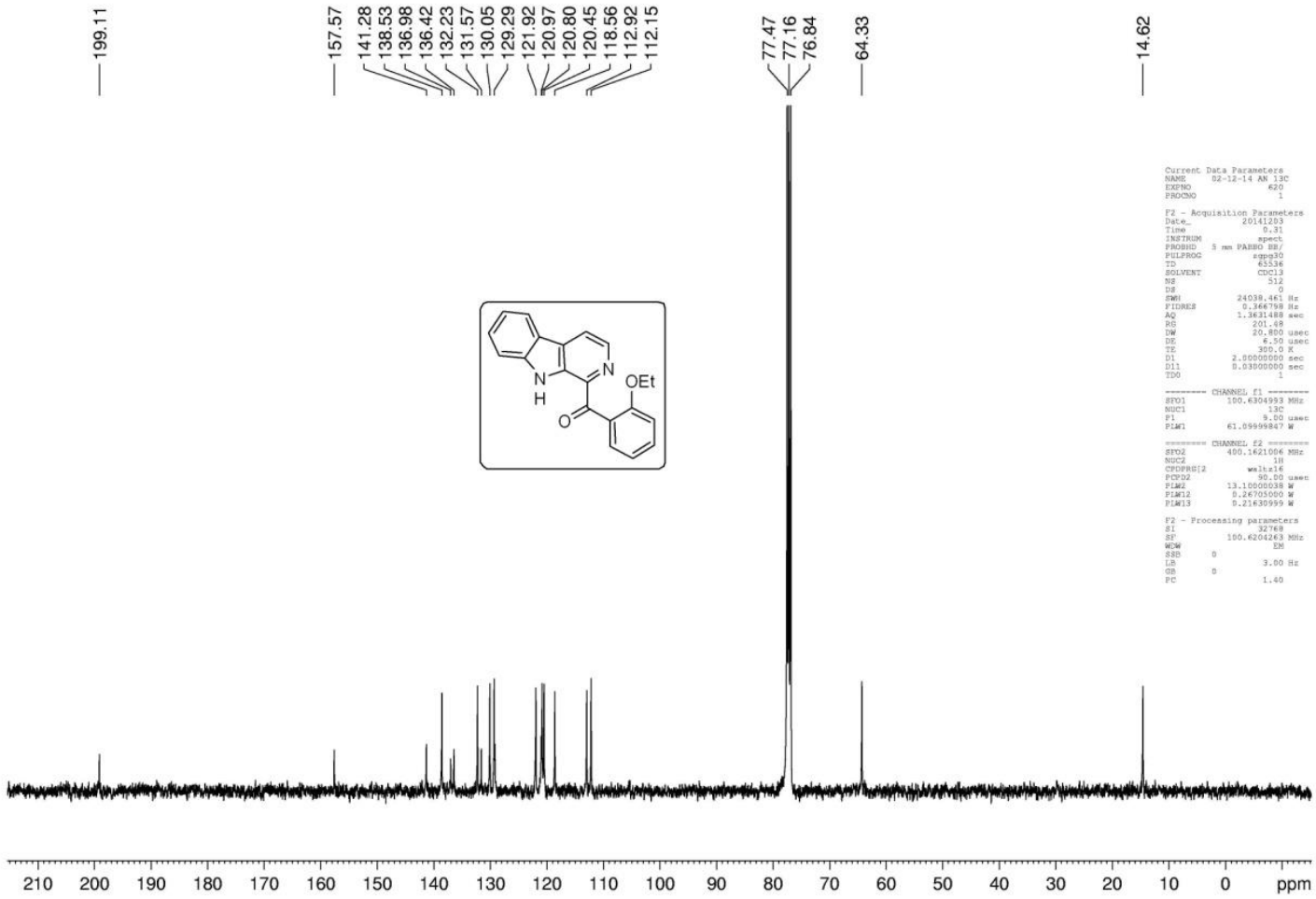

Figure. S-18: ^{13}C-NMR spectrum of (2-ethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ab)**.

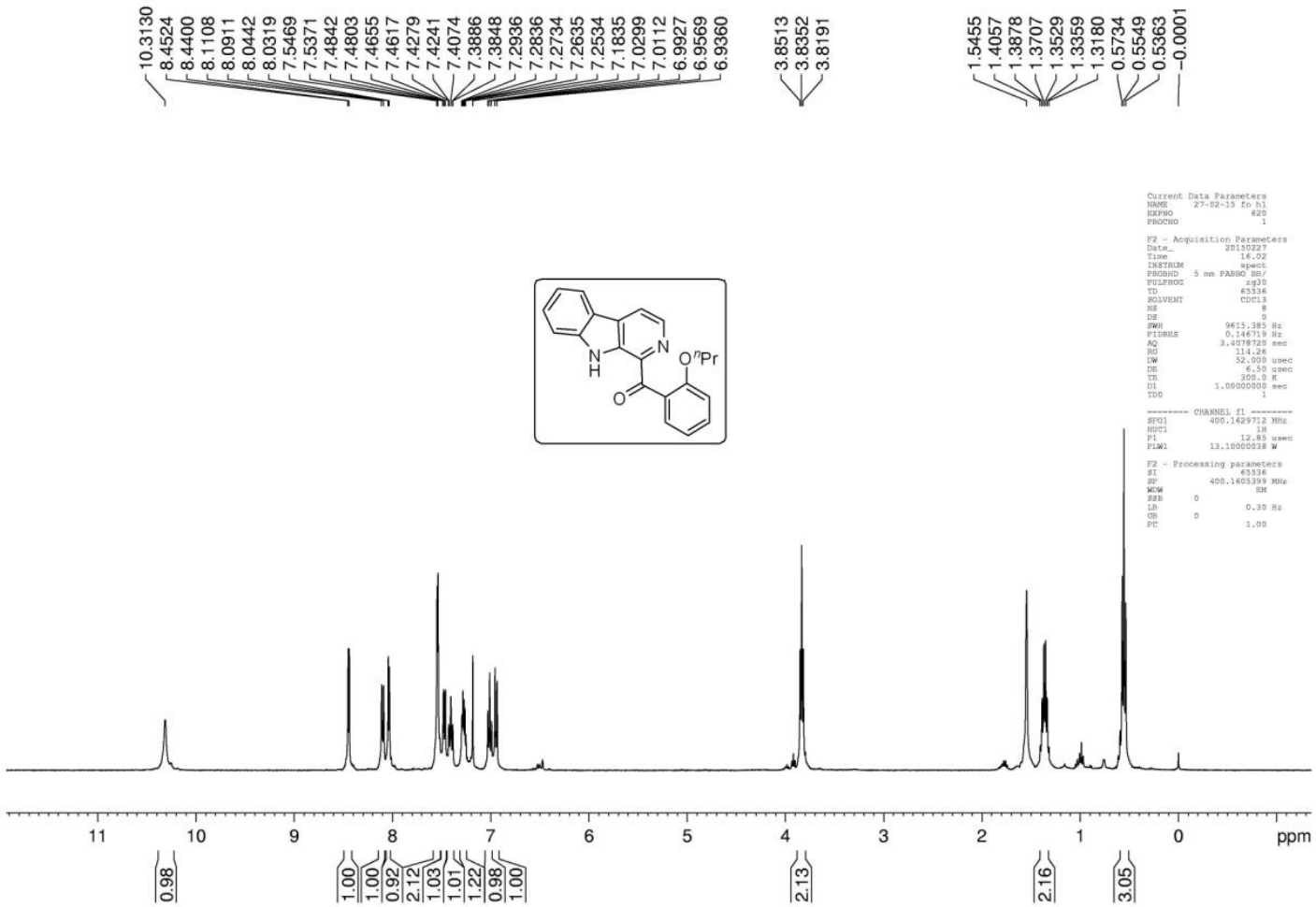

Figure. S-19: ^{1}H-NMR spectrum of (2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ac)**.

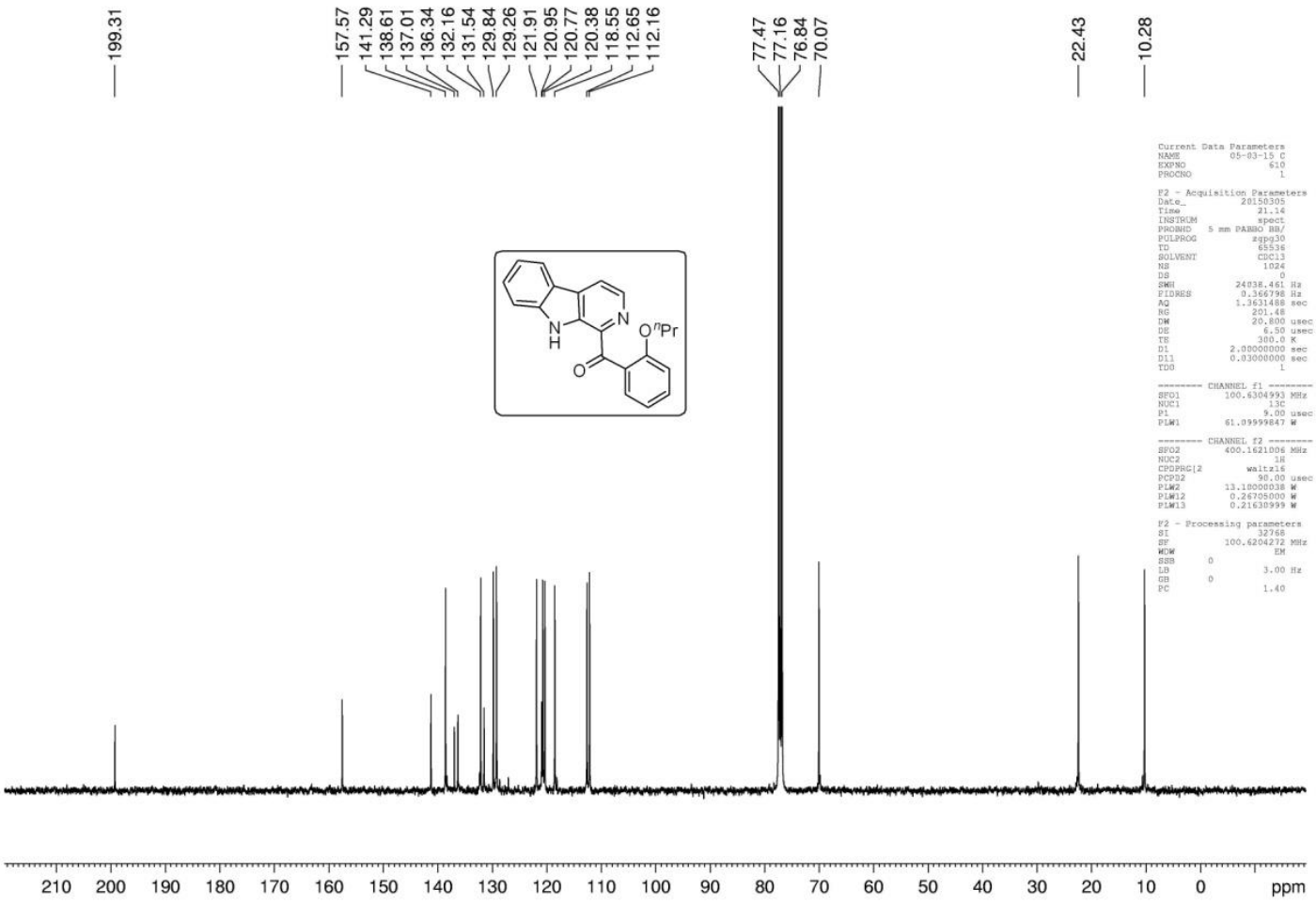

Figure. S-20: ^{13}C-NMR spectrum of (2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ac)**.

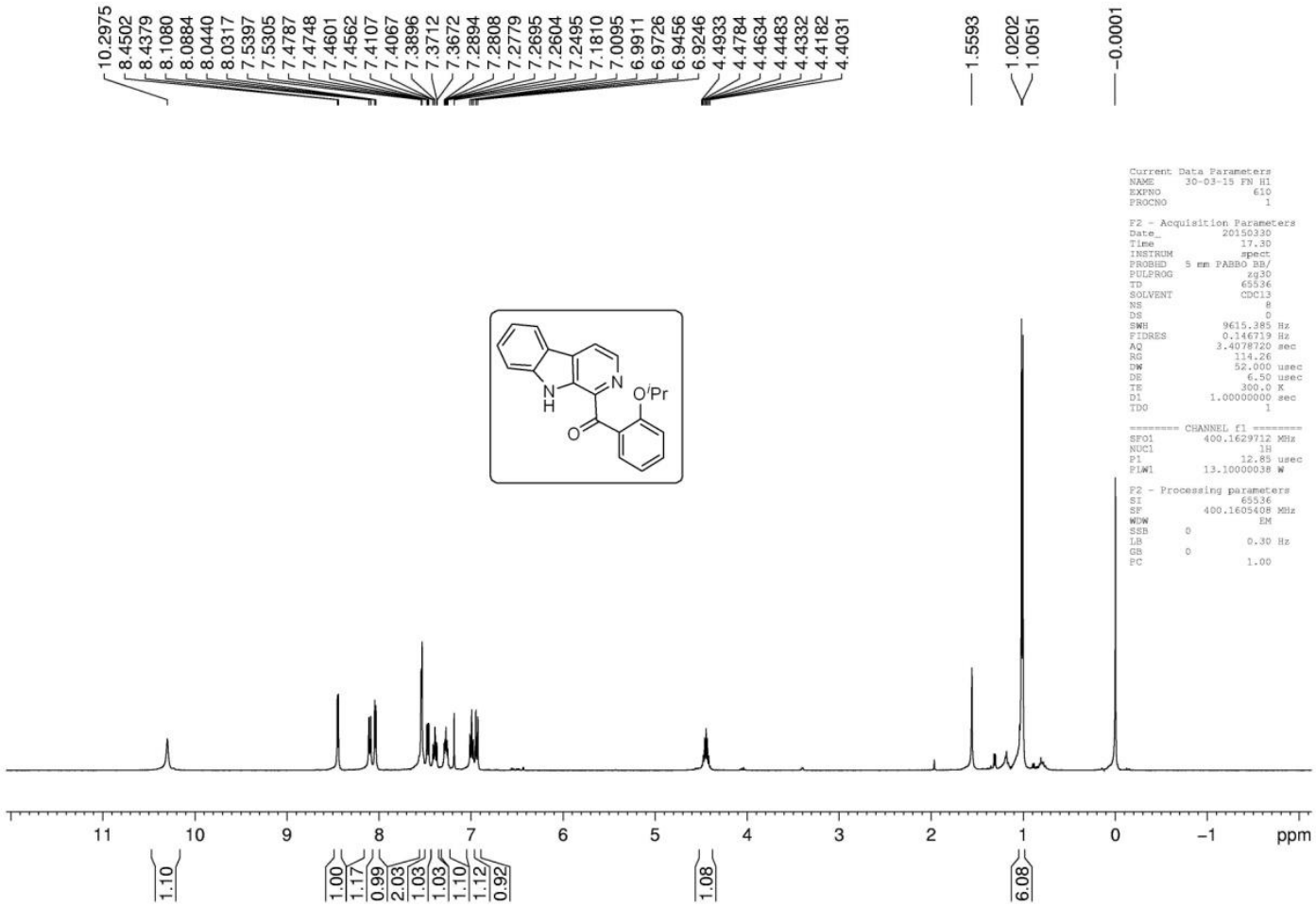

Figure. S-21: ^{1}H-NMR spectrum of (2-isopropoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ad)**.

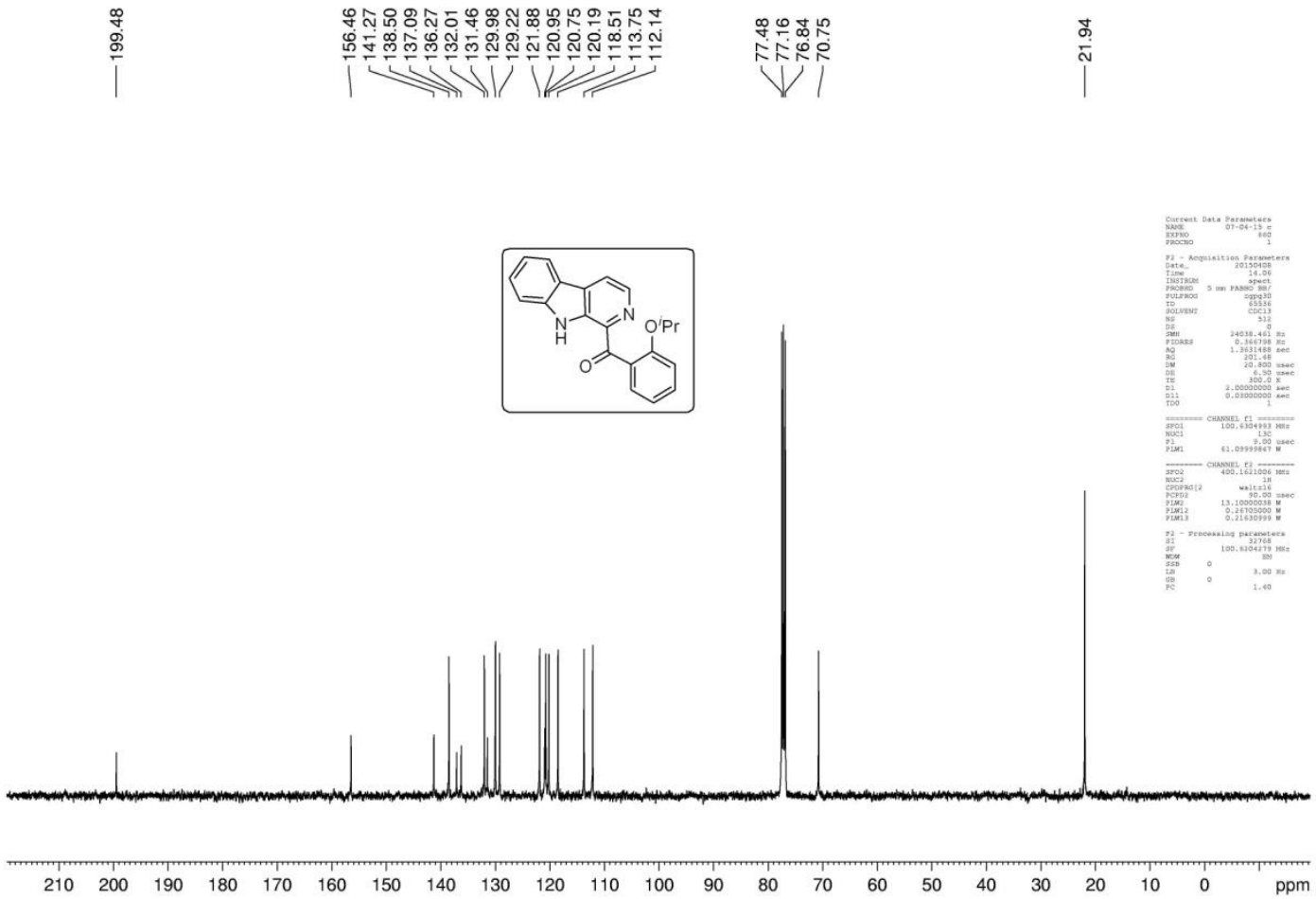

Figure. S-22: ^{13}C-NMR spectrum of (2-isopropoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ad)**.

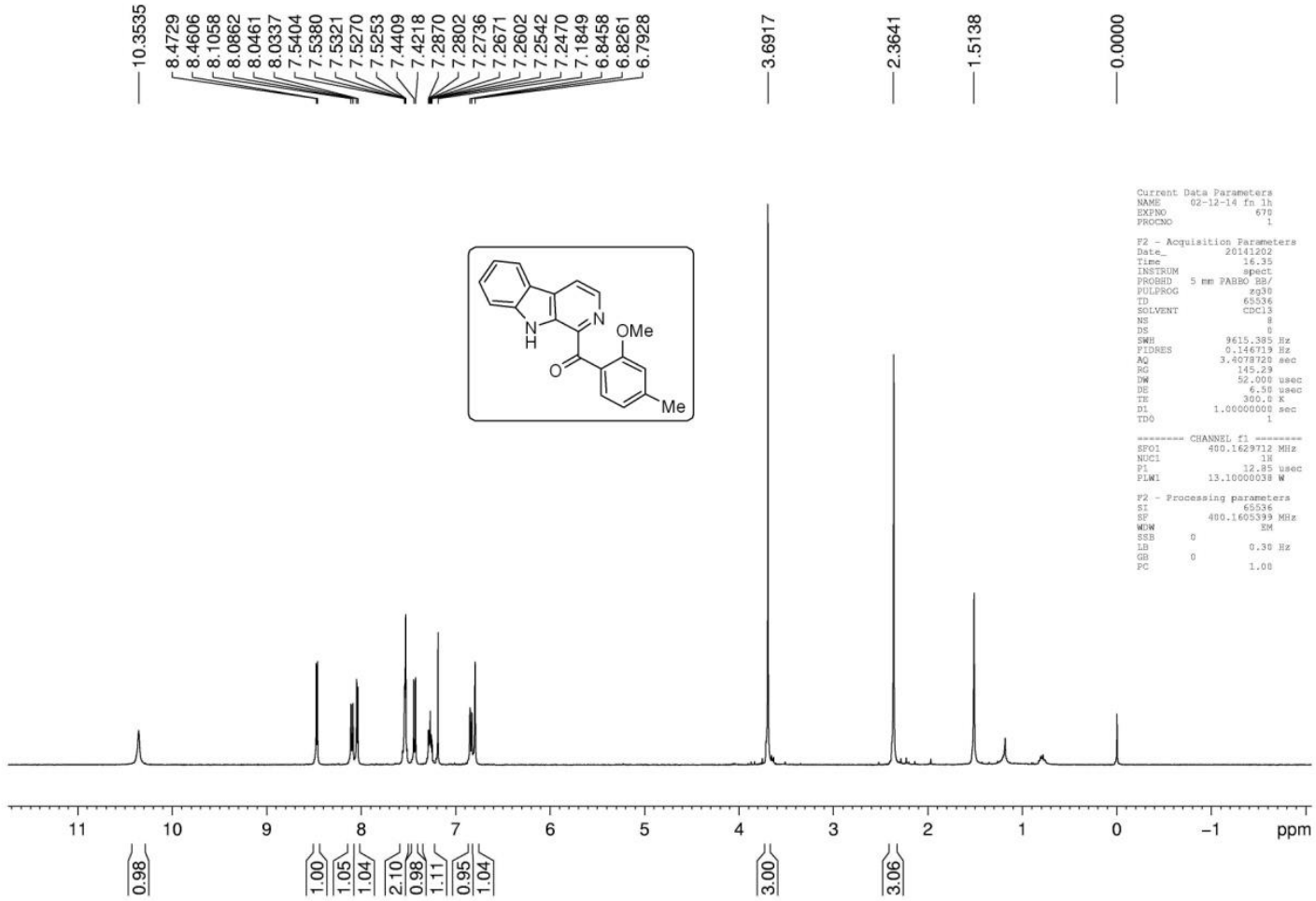

Figure. S-23: ^{1}H-NMR spectrum of (2-methoxy-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ba)**.

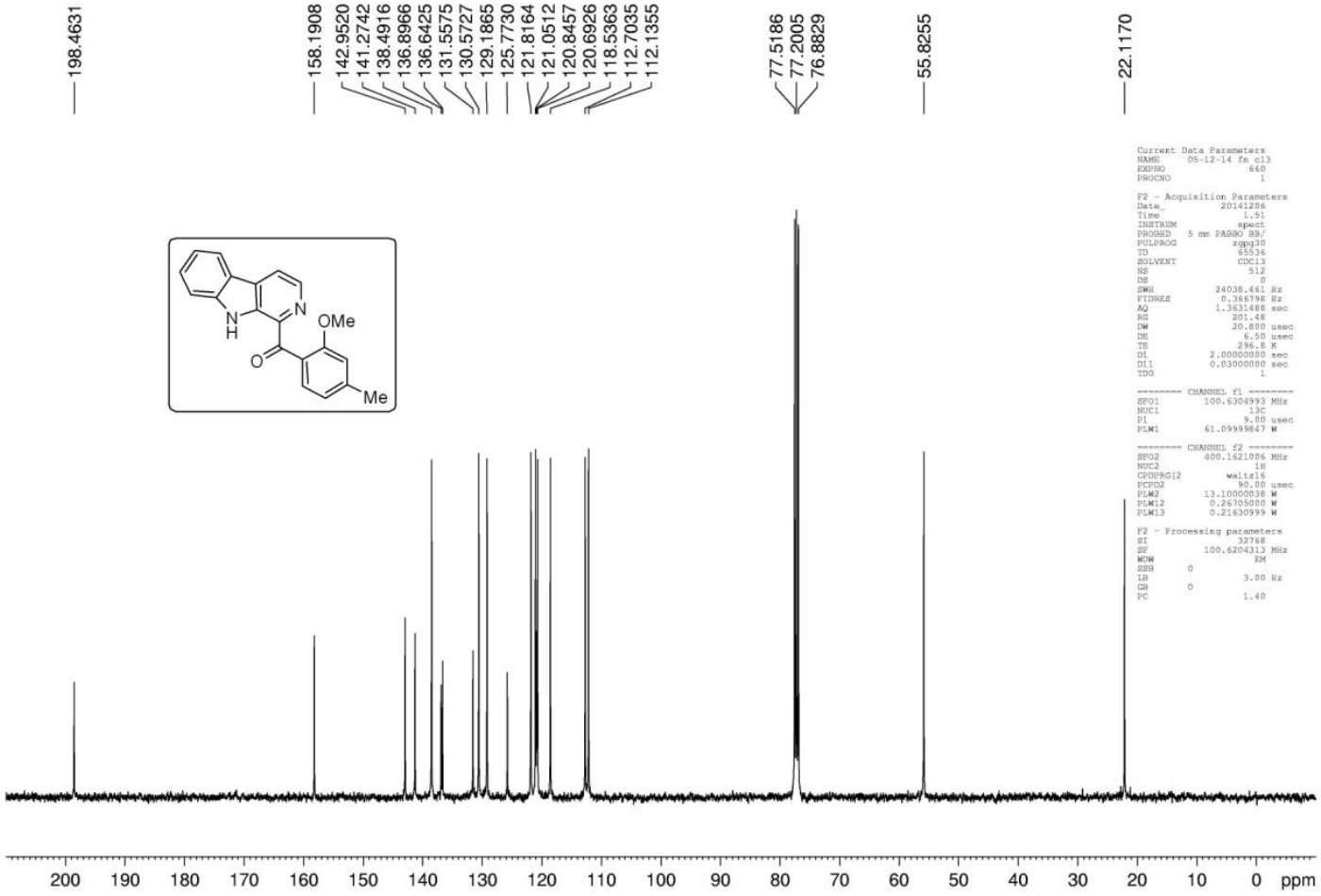

Figure. S-24: ^{13}C-NMR spectrum of (2-methoxy-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ba)**.

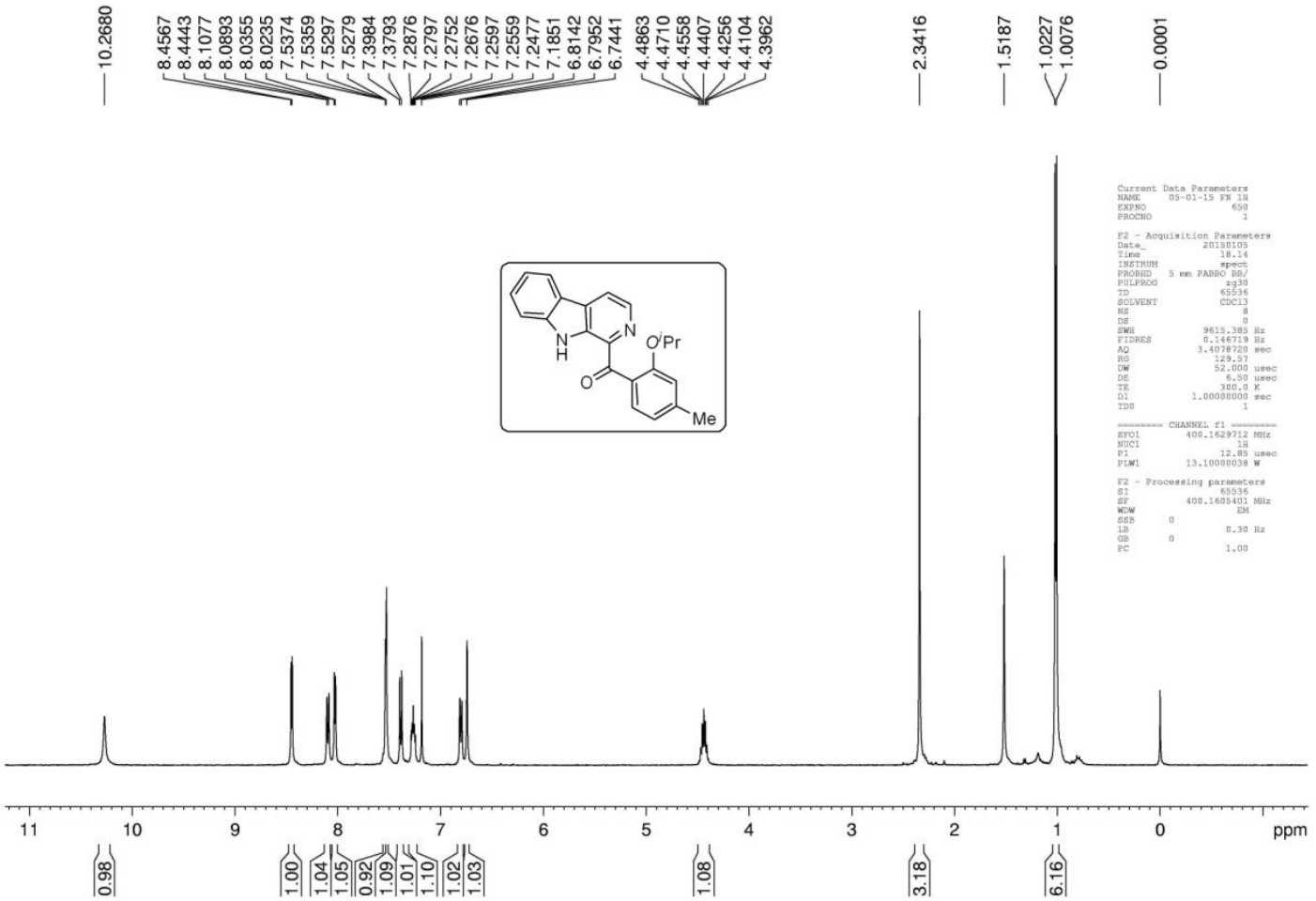

Figure. S-25: ^{1}H-NMR spectrum of (2-isopropoxy-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4bd)**.

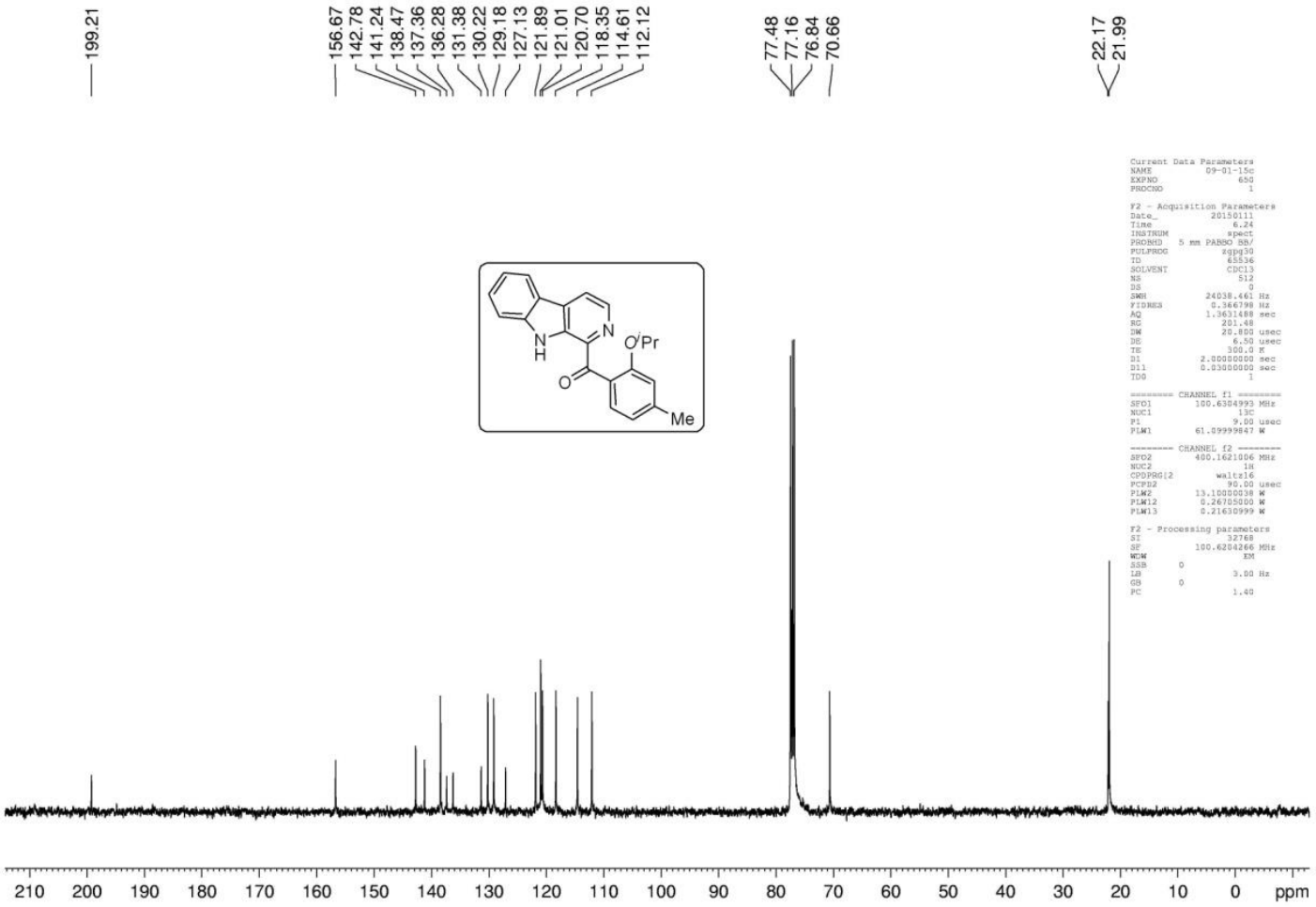

Figure. S-26: ^{13}C-NMR spectrum of (2-isopropoxy-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4bd)**.

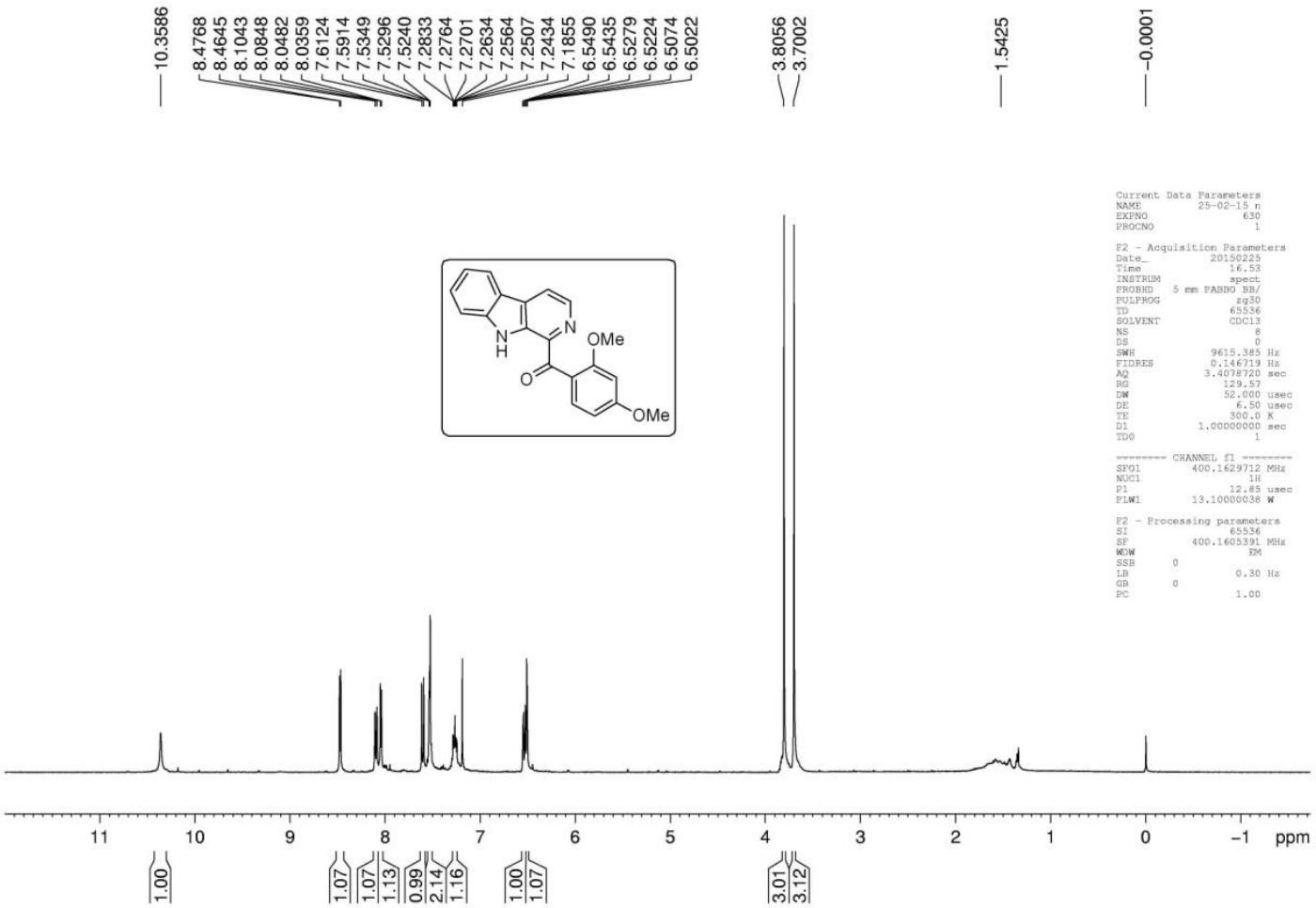

Figure. S-27: ^{1}H-NMR spectrum of (2,4-dimethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ca)**.

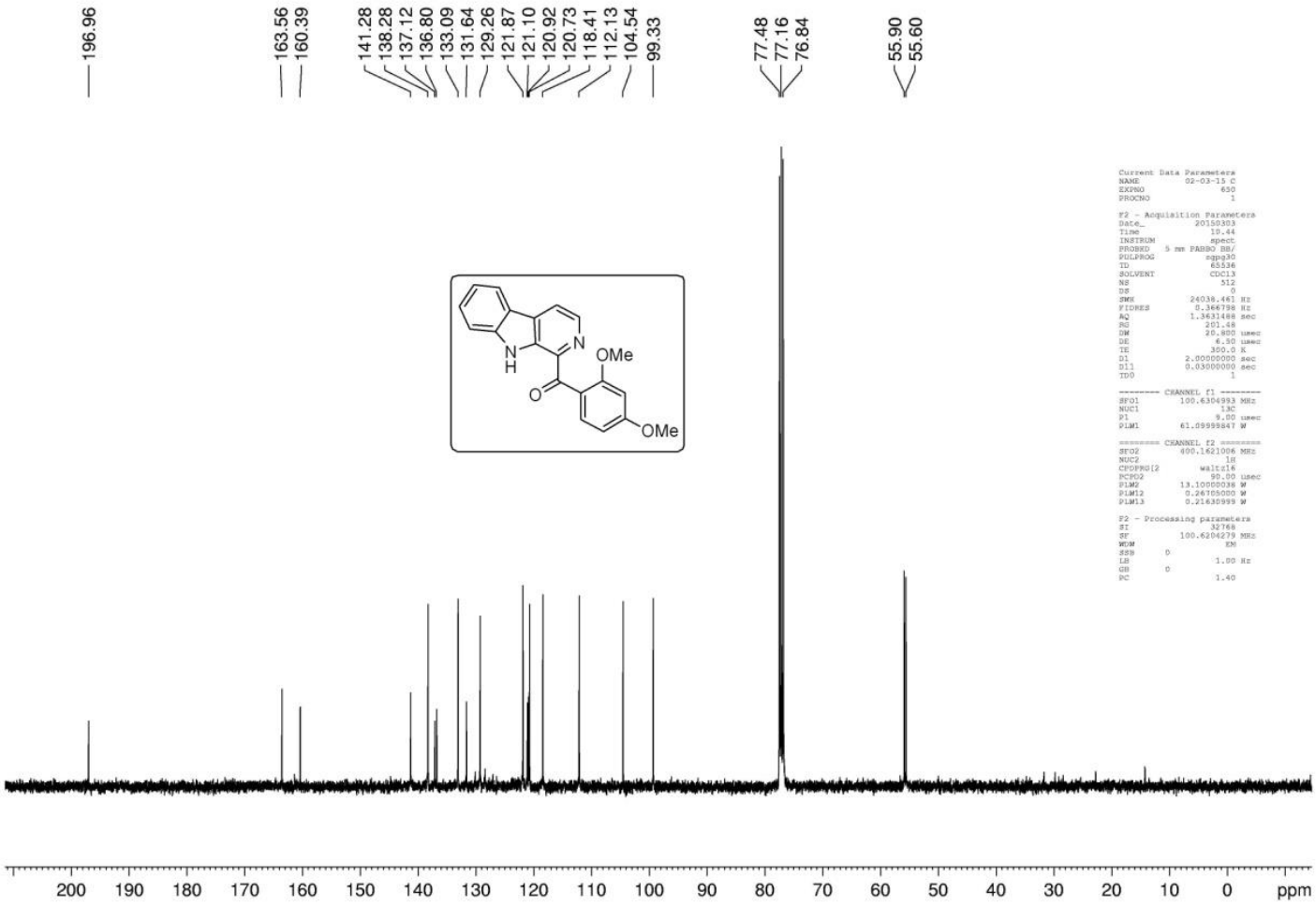

Figure. S-28**:** ^{13}C-NMR spectrum of (2,4-dimethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ca)**.

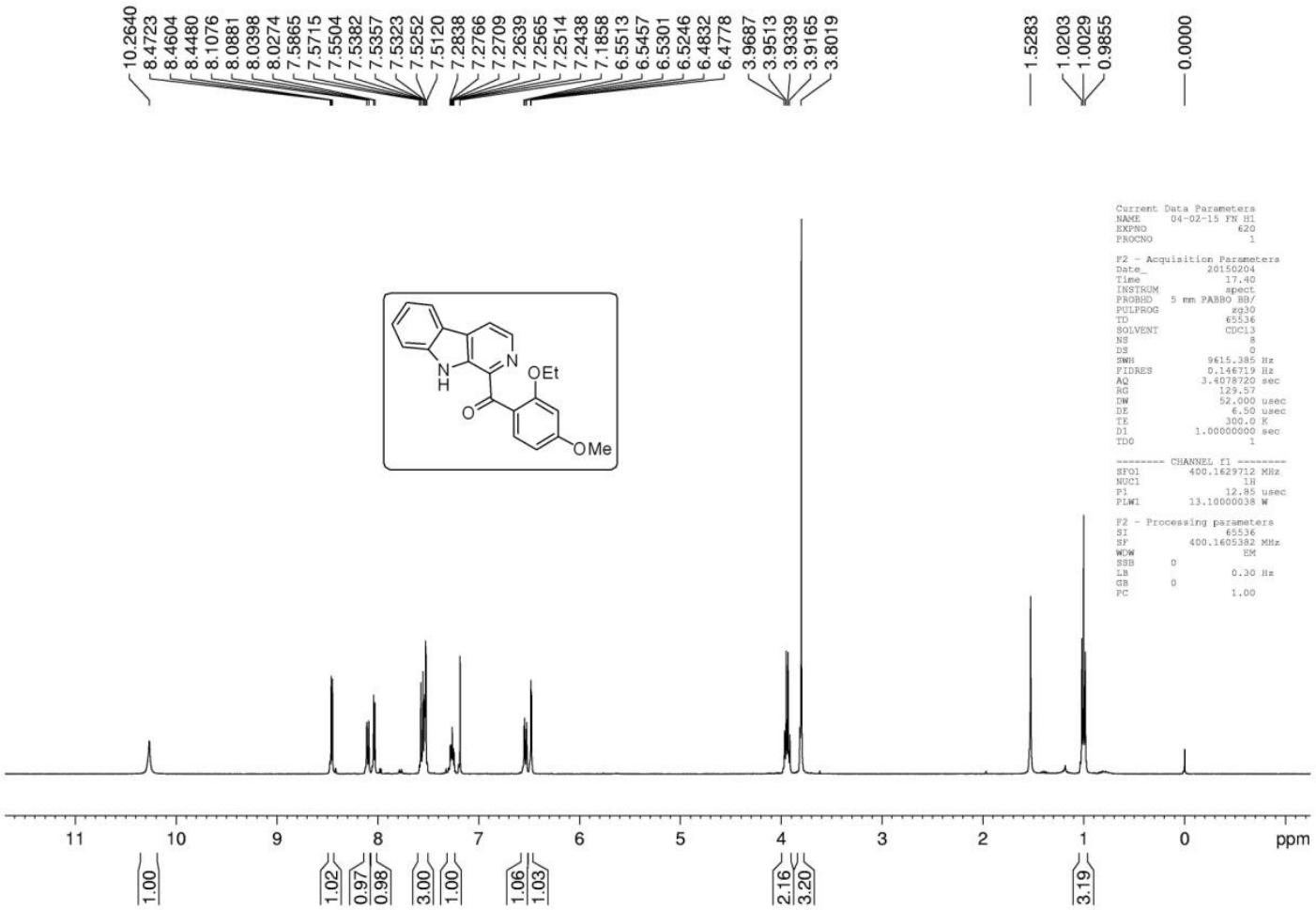

Figure. S-29: ^{1}H-NMR spectrum of (2-ethoxy-4-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4cb)**.

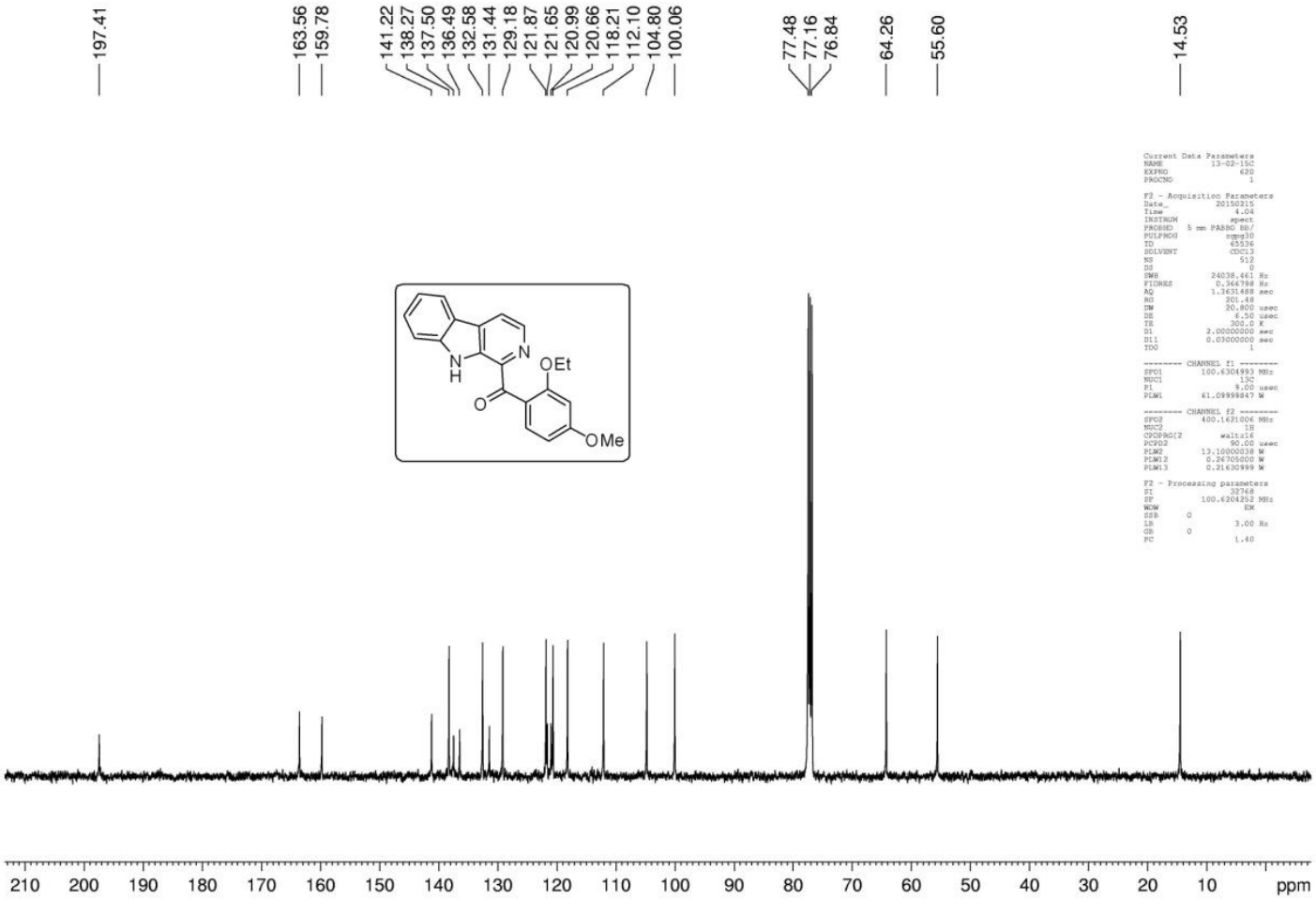

Figure. S-30**:** ^{13}C-NMR spectrum of (2-ethoxy-4-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4cb)**.

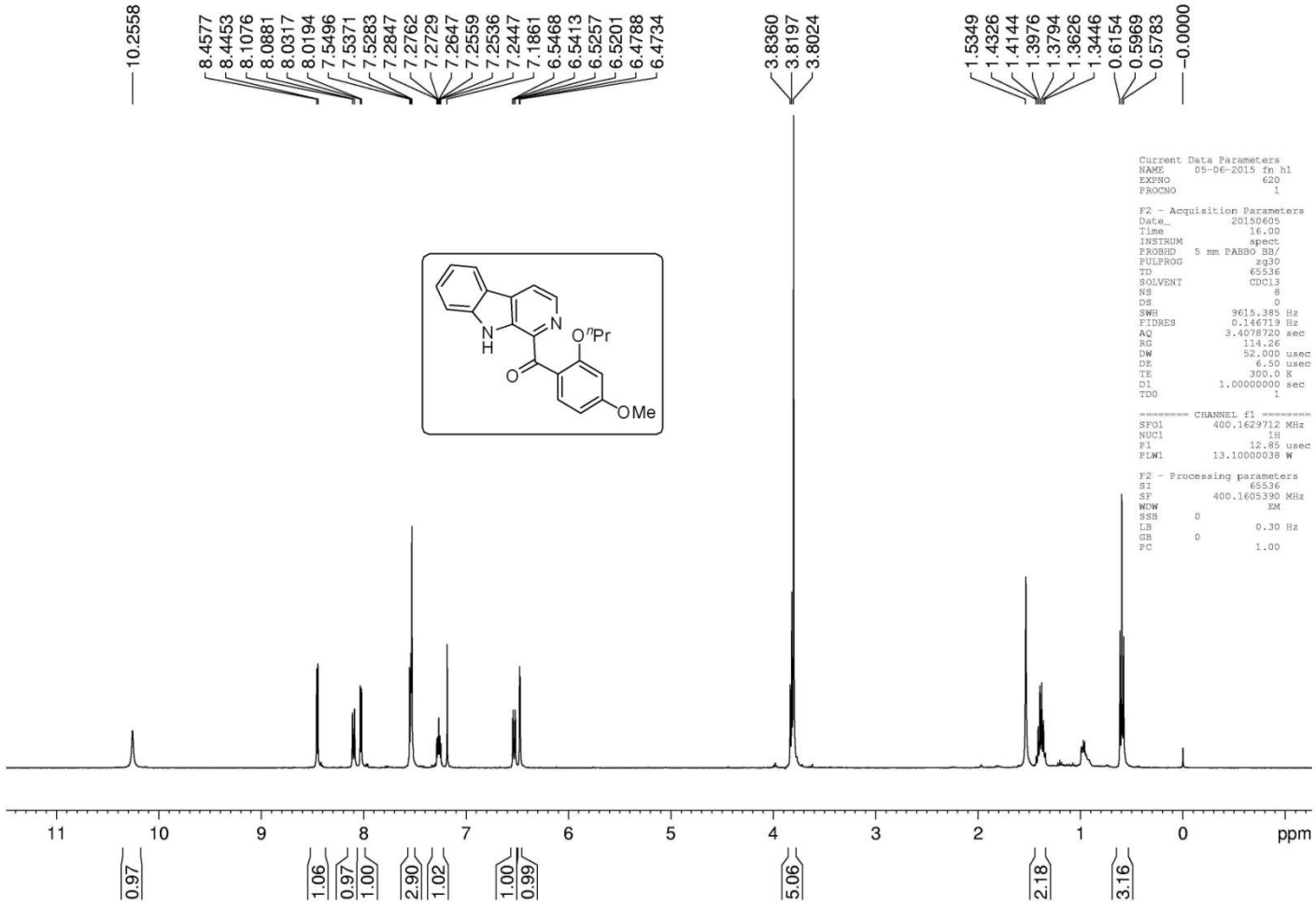

Figure. S-31: ^{1}H-NMR spectrum of (4-methoxy-2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4cc)**.

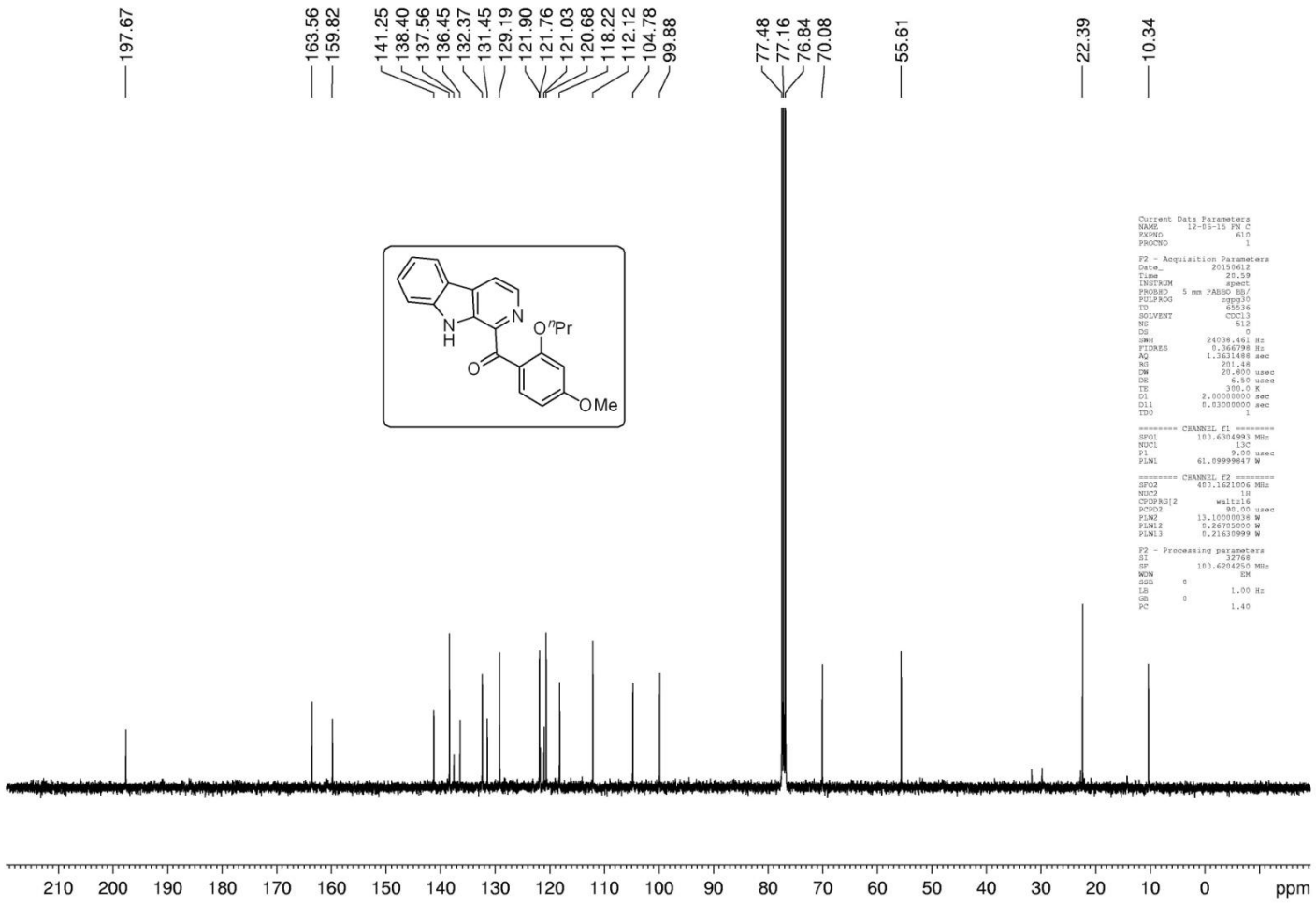

Figure. S-32**:** ^{13}C-NMR spectrum of (4-methoxy-2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4cc)**.

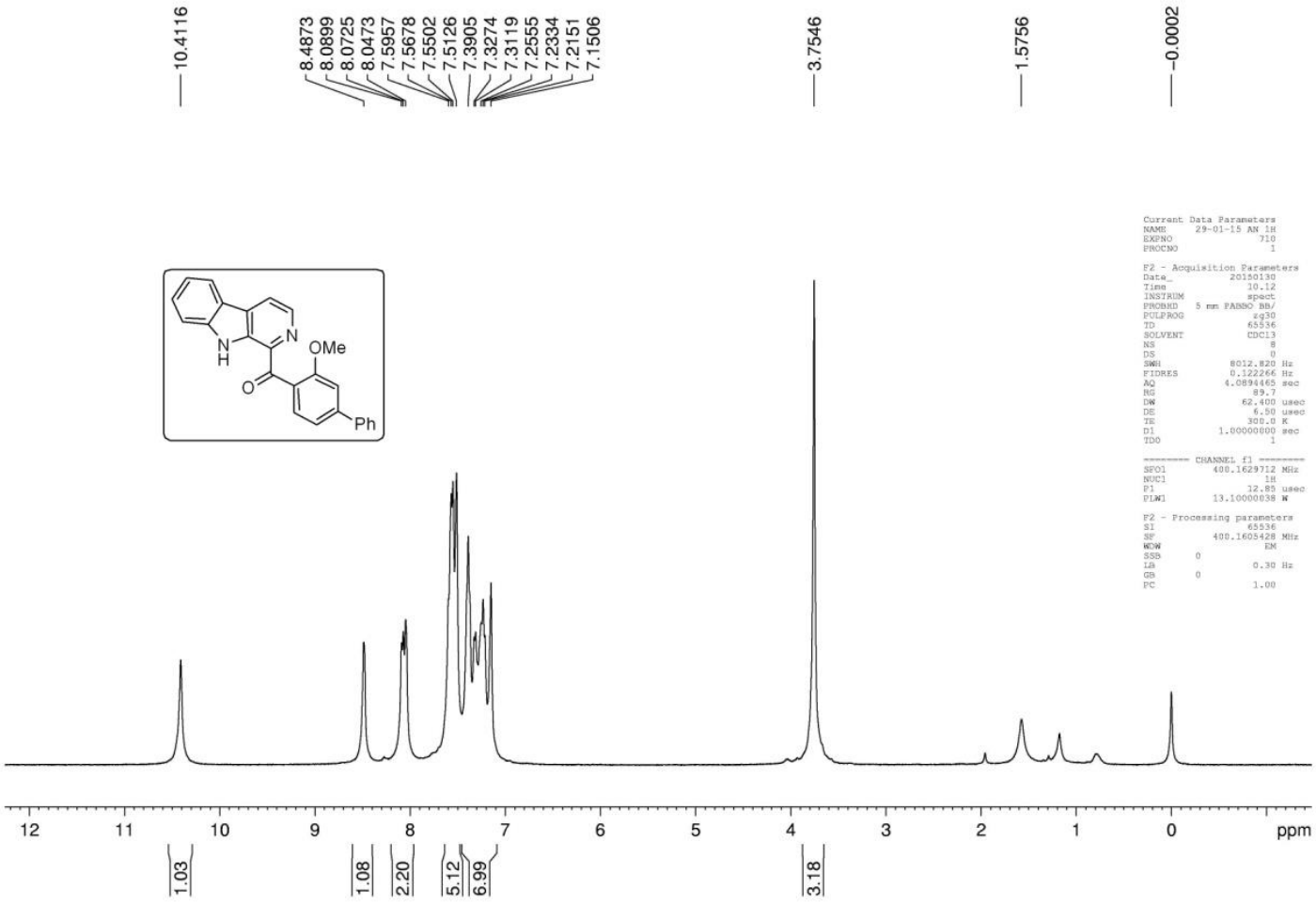

Figure. S-33: ^{1}H-NMR spectrum of (3-methoxy-[1,1'-biphenyl]-4-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4da)**.

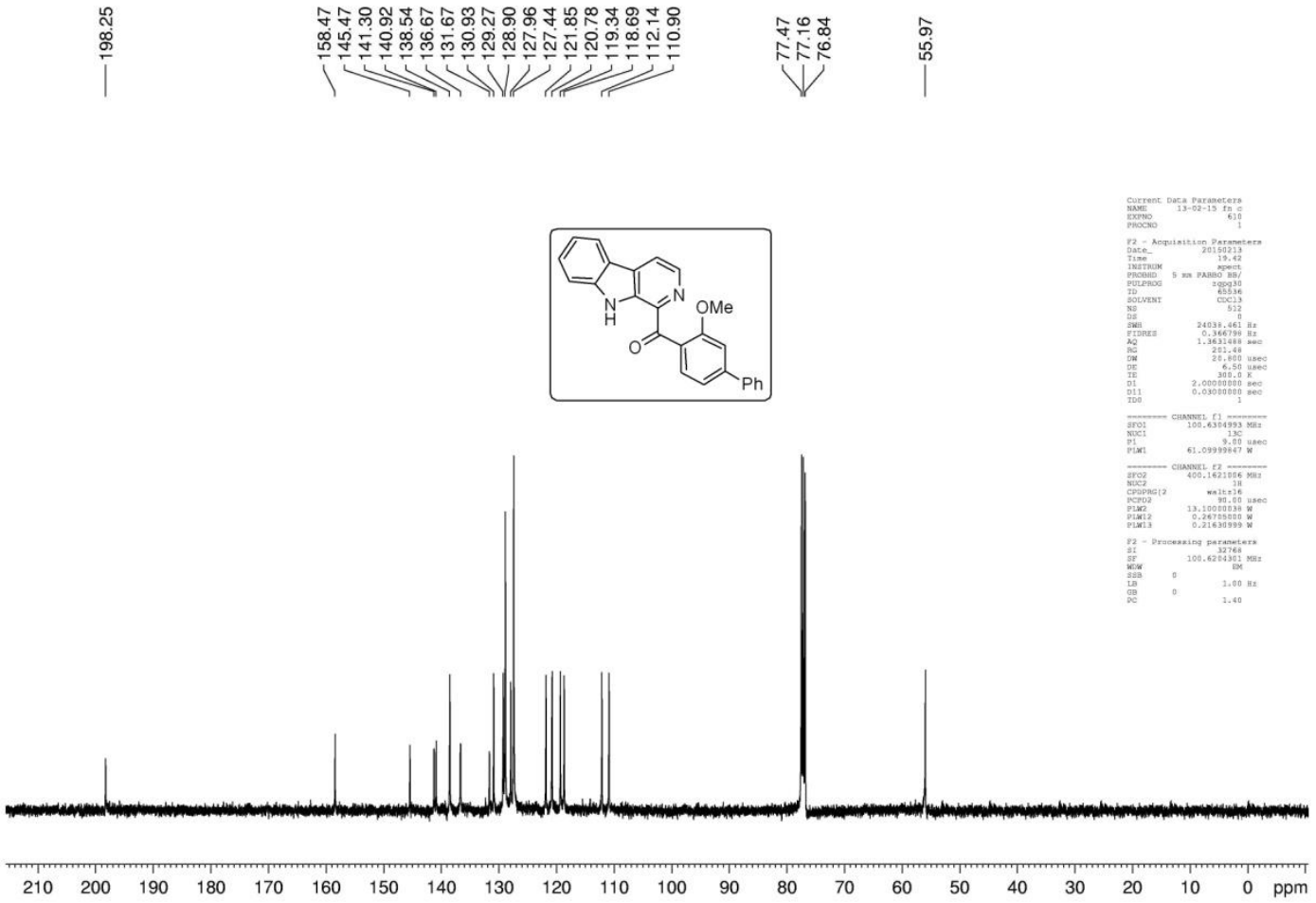

Figure. S-34**:** ^{13}C-NMR spectrum of (3-methoxy-[1,1'-biphenyl]-4-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4da)**.

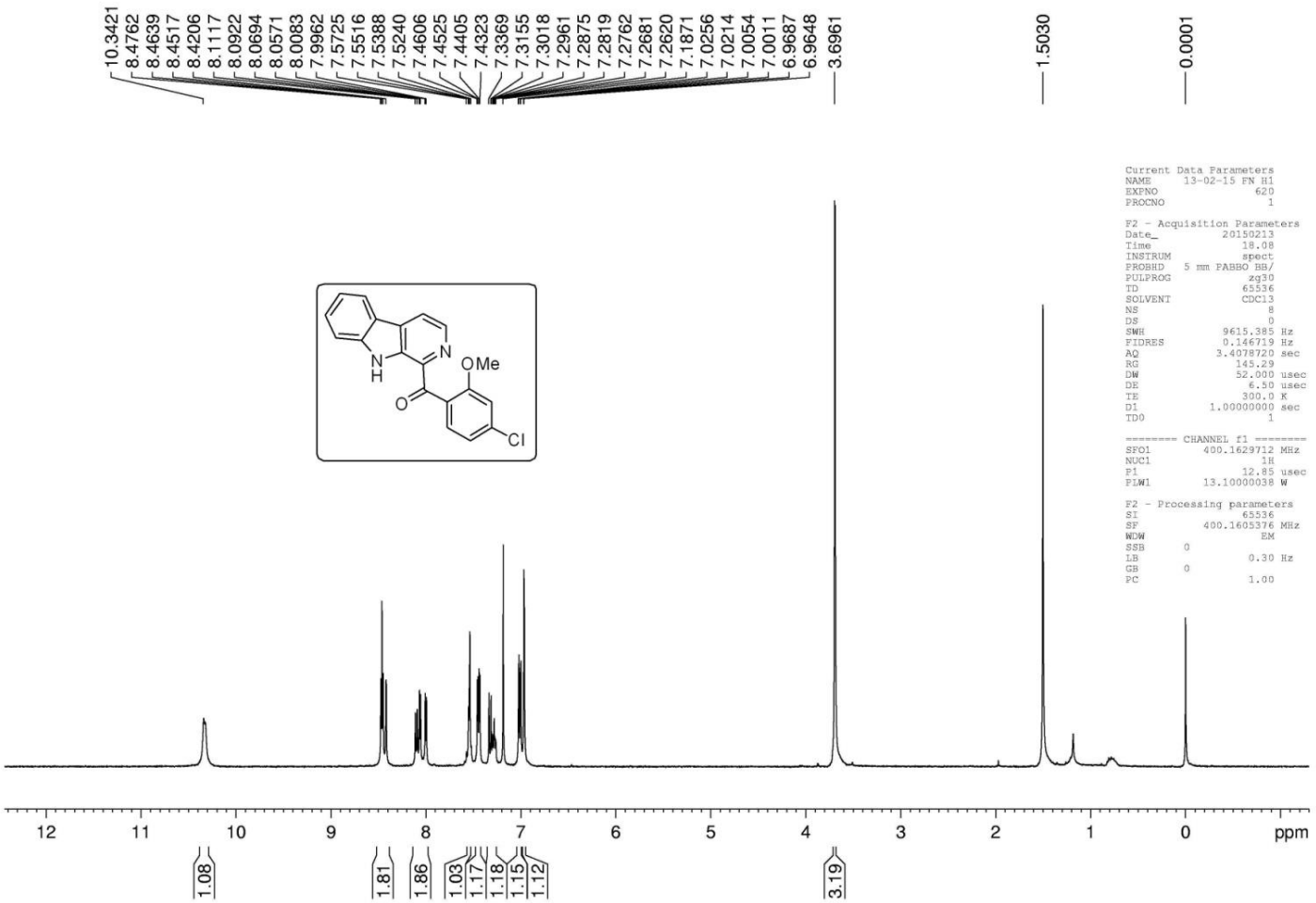

Figure.S-35**:**[1]H-NMR spectrum of (4-chloro-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ea)**.

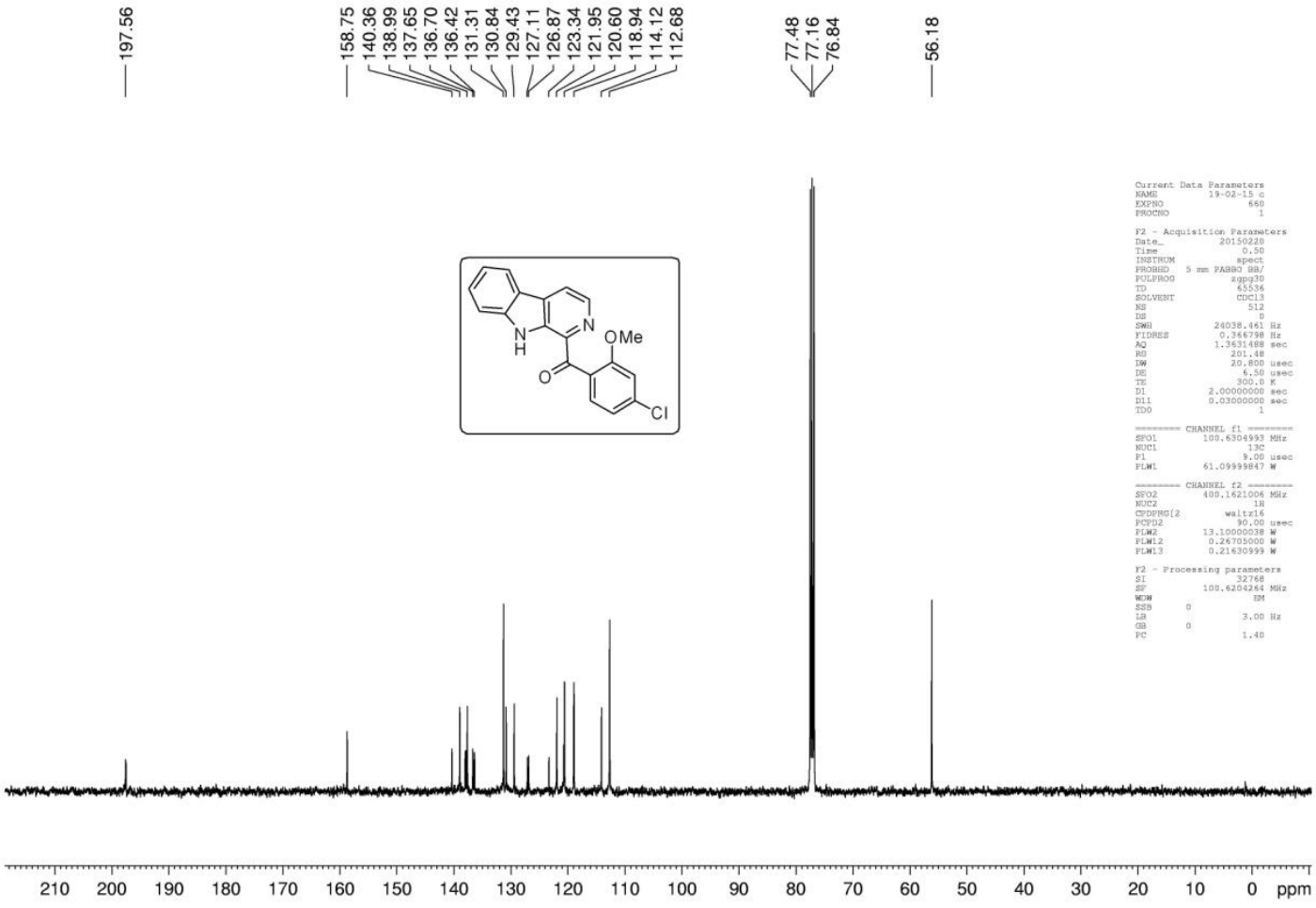

Figure. S-36**:** ^{13}C-NMR spectrum of (4-chloro-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ea)**.

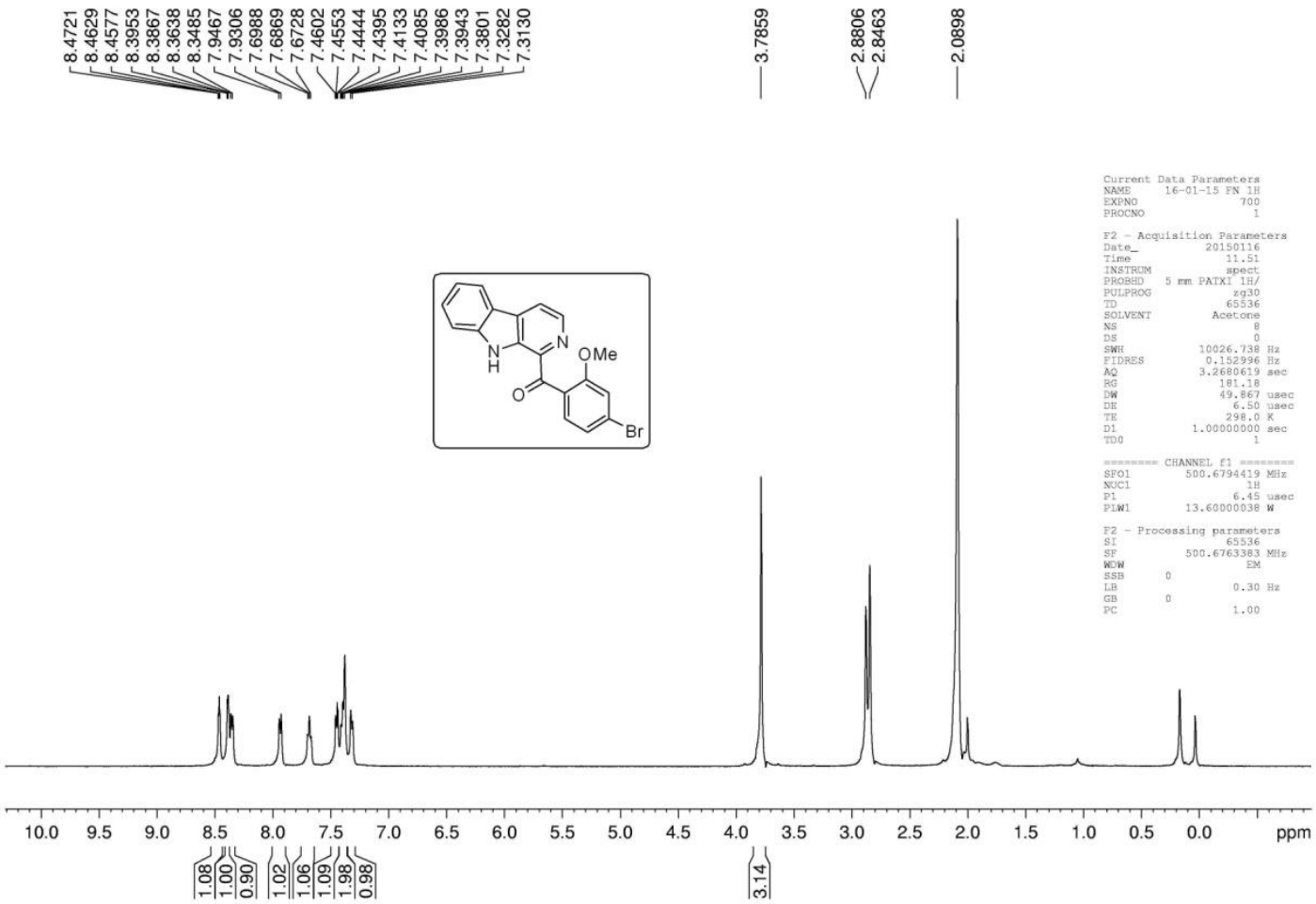

Figure. S-37: ^{1}H-NMR spectrum of (4-bromo-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4fa)**.

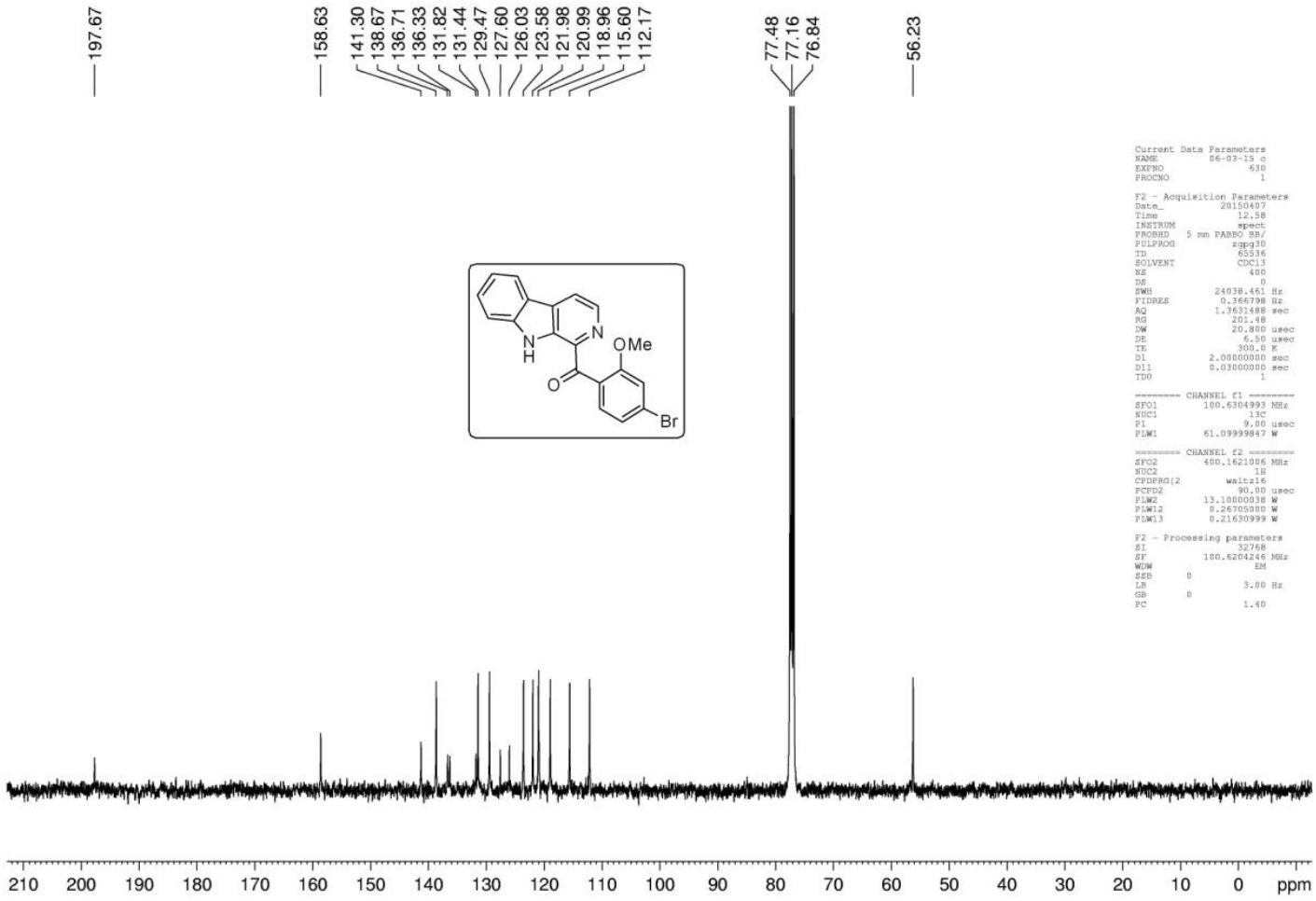

Figure. S-38**:** ^{13}C-NMR spectrum of (4-bromo-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4fa)**.

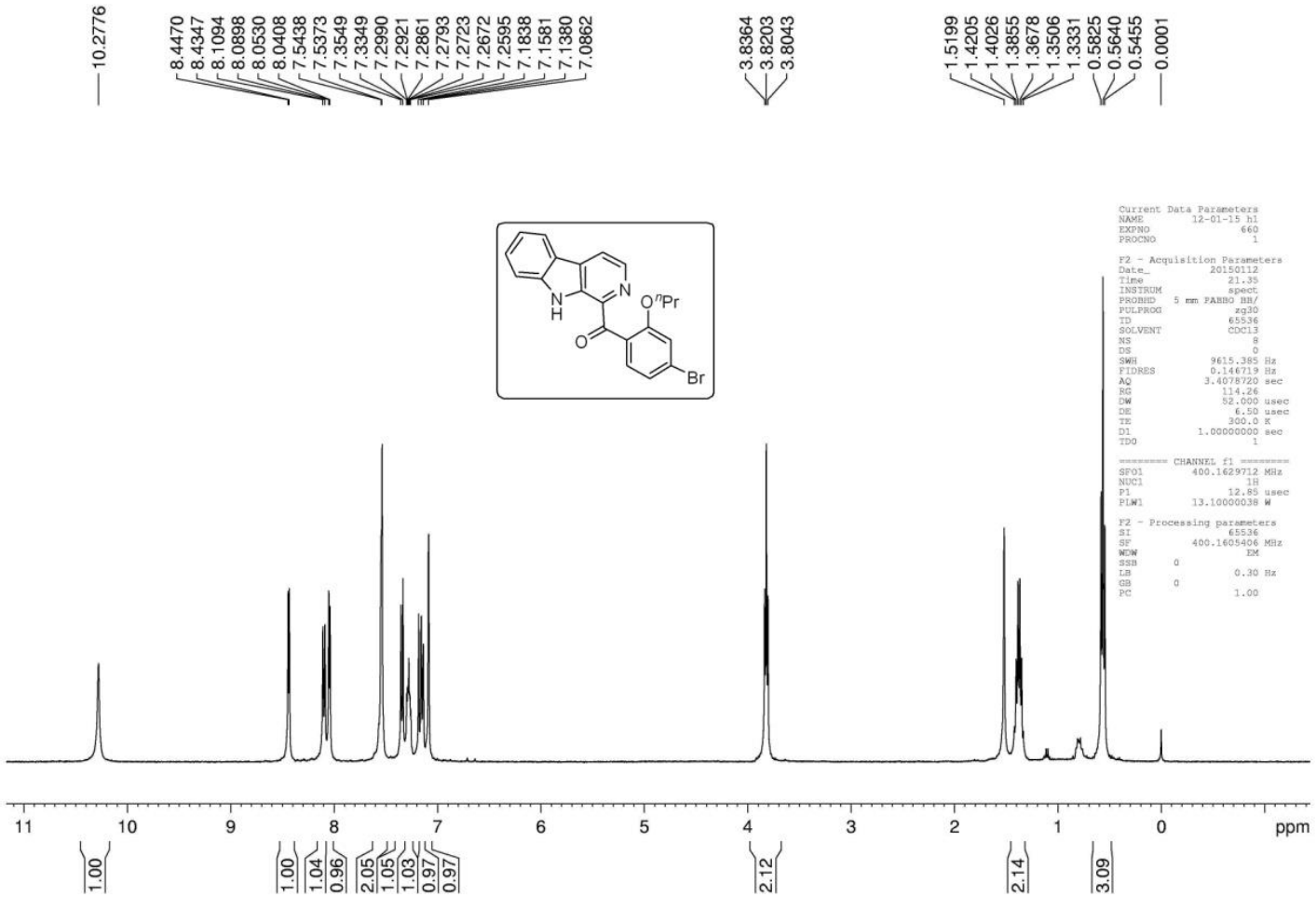

Figure. S-39: ^{1}H-NMR spectrum of (4-bromo-2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4fc)**.

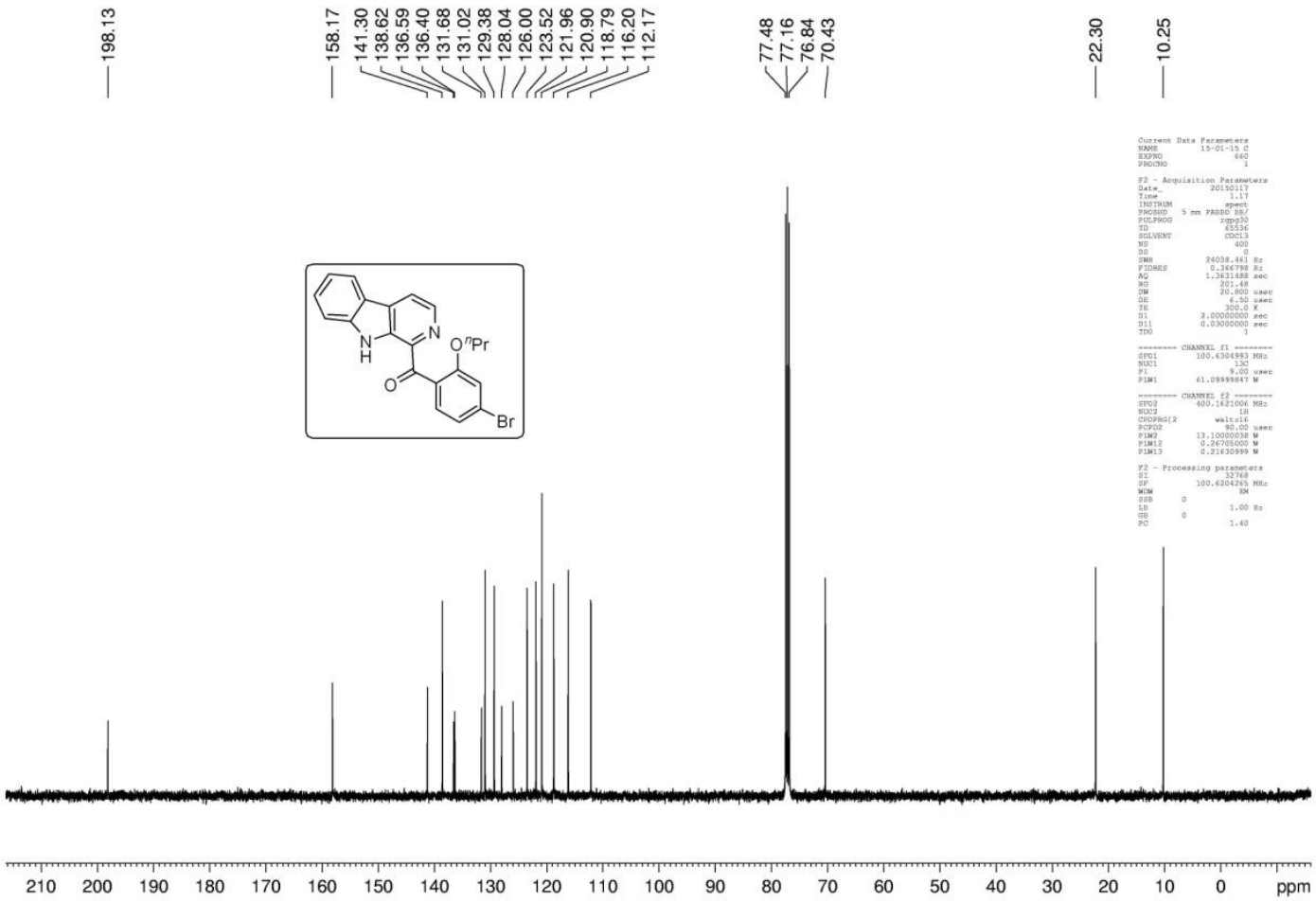

Figure. S-40**:** ^{13}C-NMR spectrum of (4-bromo-2-propoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4fc)**.

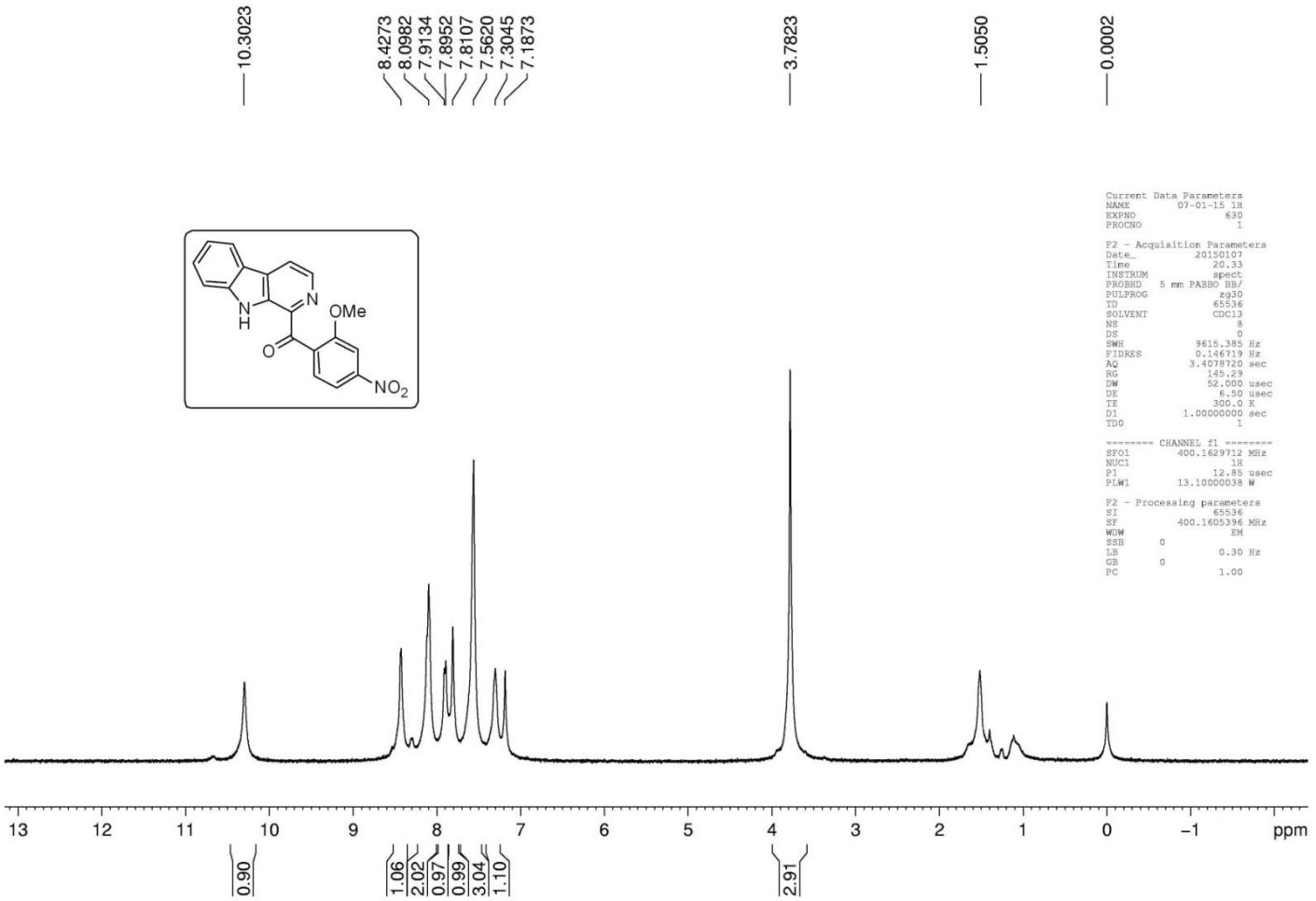

Figure. S-41: ^{1}H-NMR spectrum of (2-methoxy-4-nitrophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ga)**.

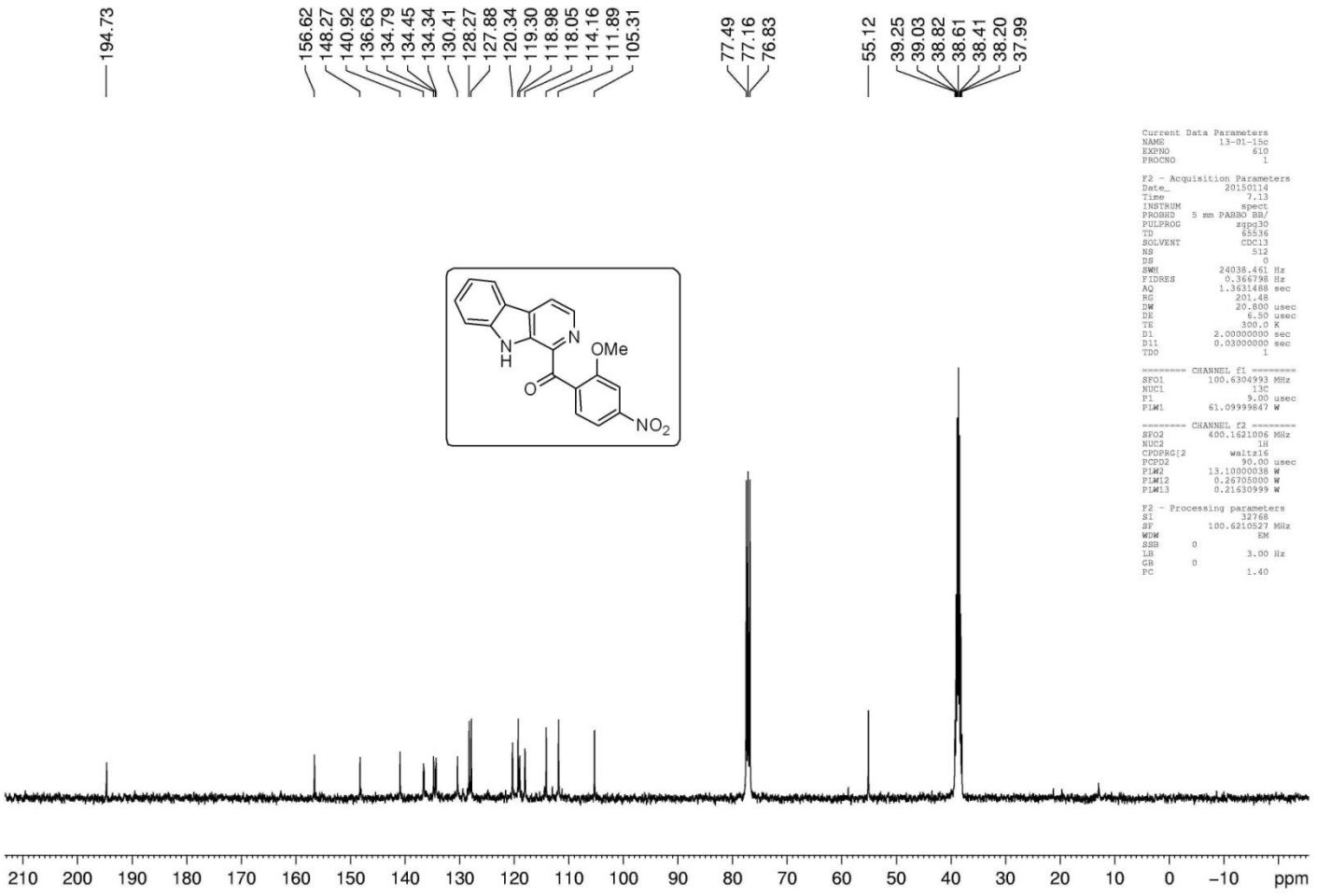

Figure. S-42: ^{13}C -NMR spectrum of (2-methoxy-4-nitrophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ga)**.

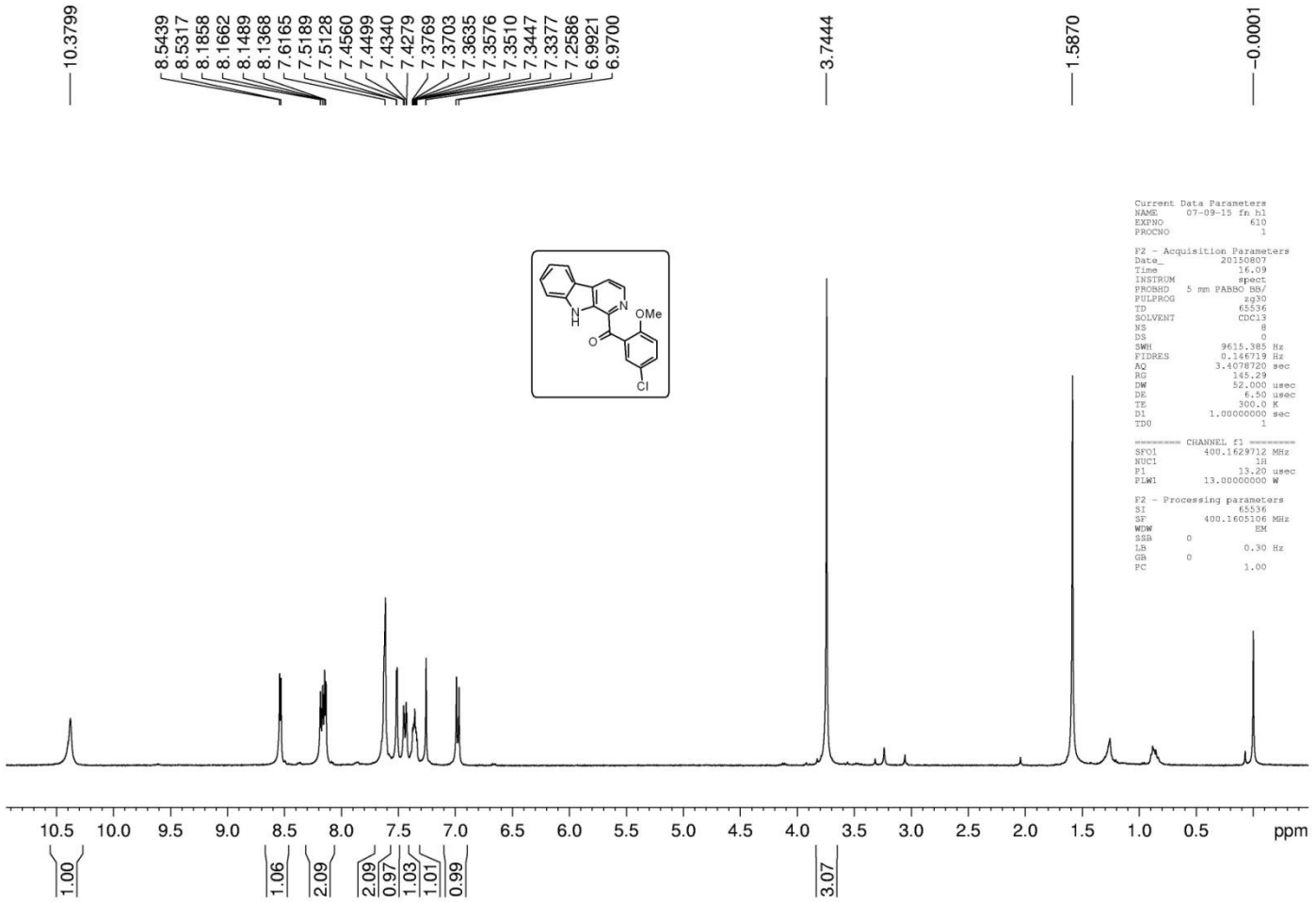

Figure. S-43: [1]H-NMR spectrum of (5-Chloro-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ha)**.

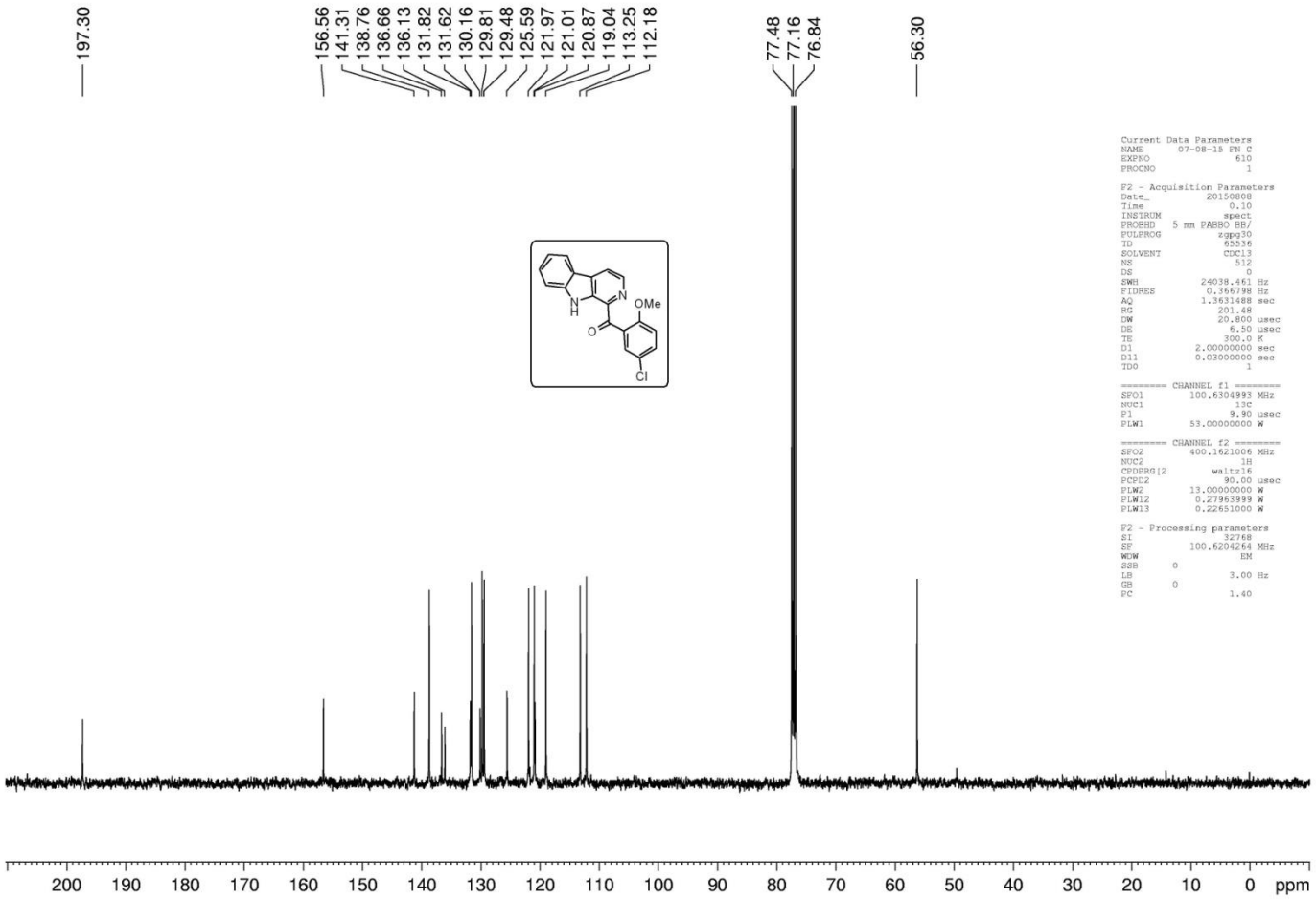

Figure. S-44: ^{13}C -NMR spectrum of (5-Chloro-2-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ha)**.

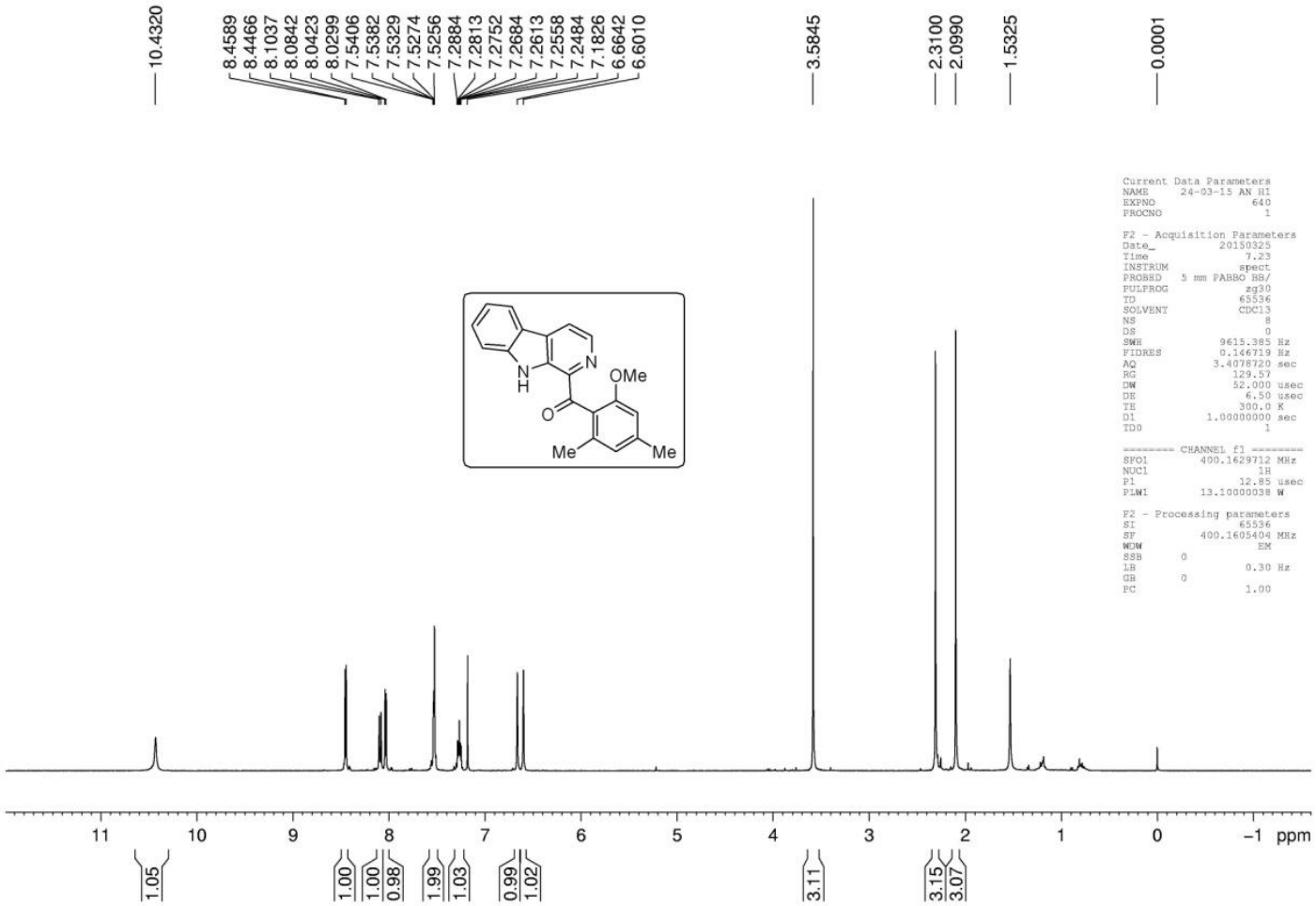

Figure. S-45: ^{1}H-NMR spectrum of (2-methoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ia)**.

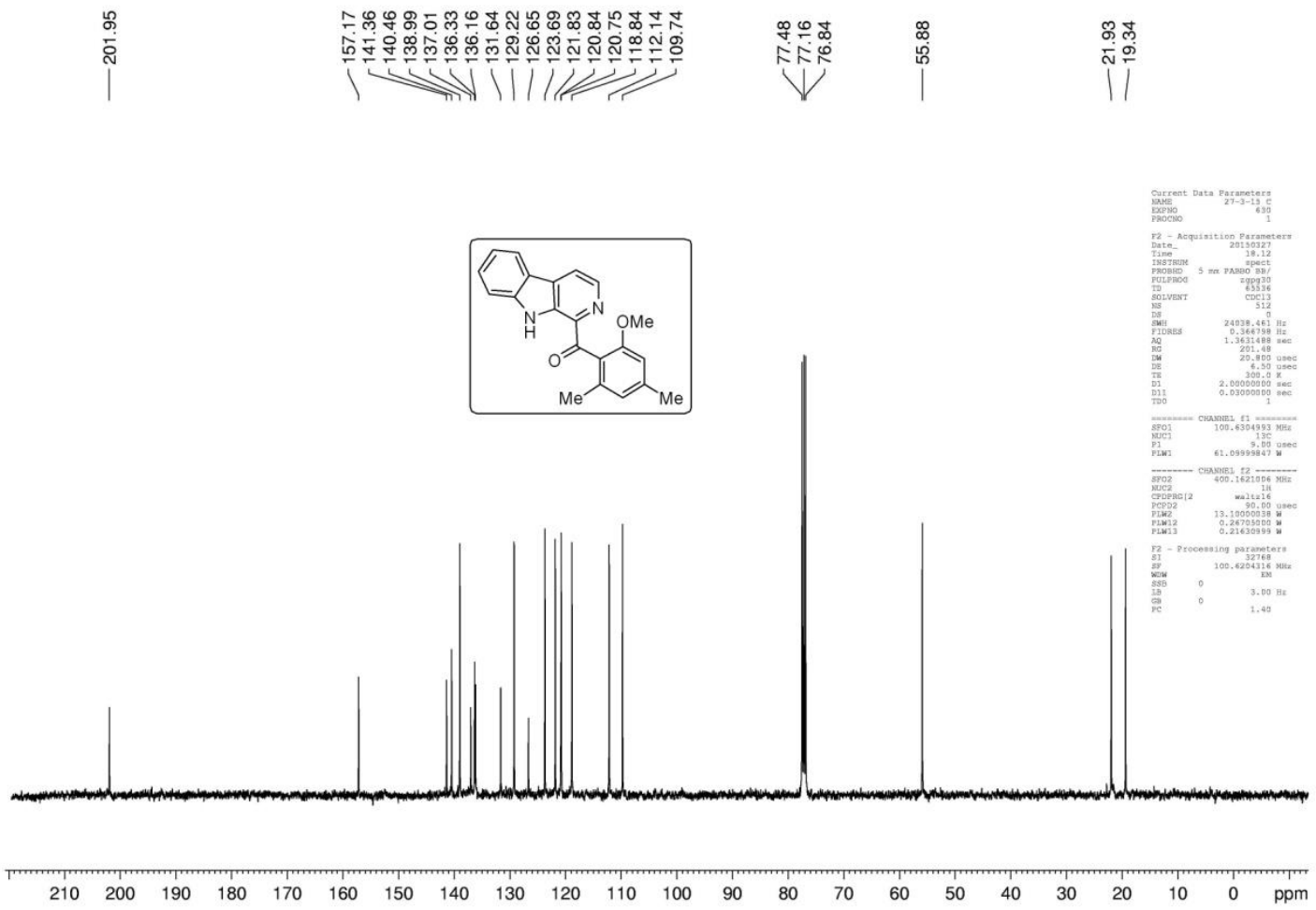

Figure. S-46: ^{13}C -NMR spectrum of (2-methoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ia)**.

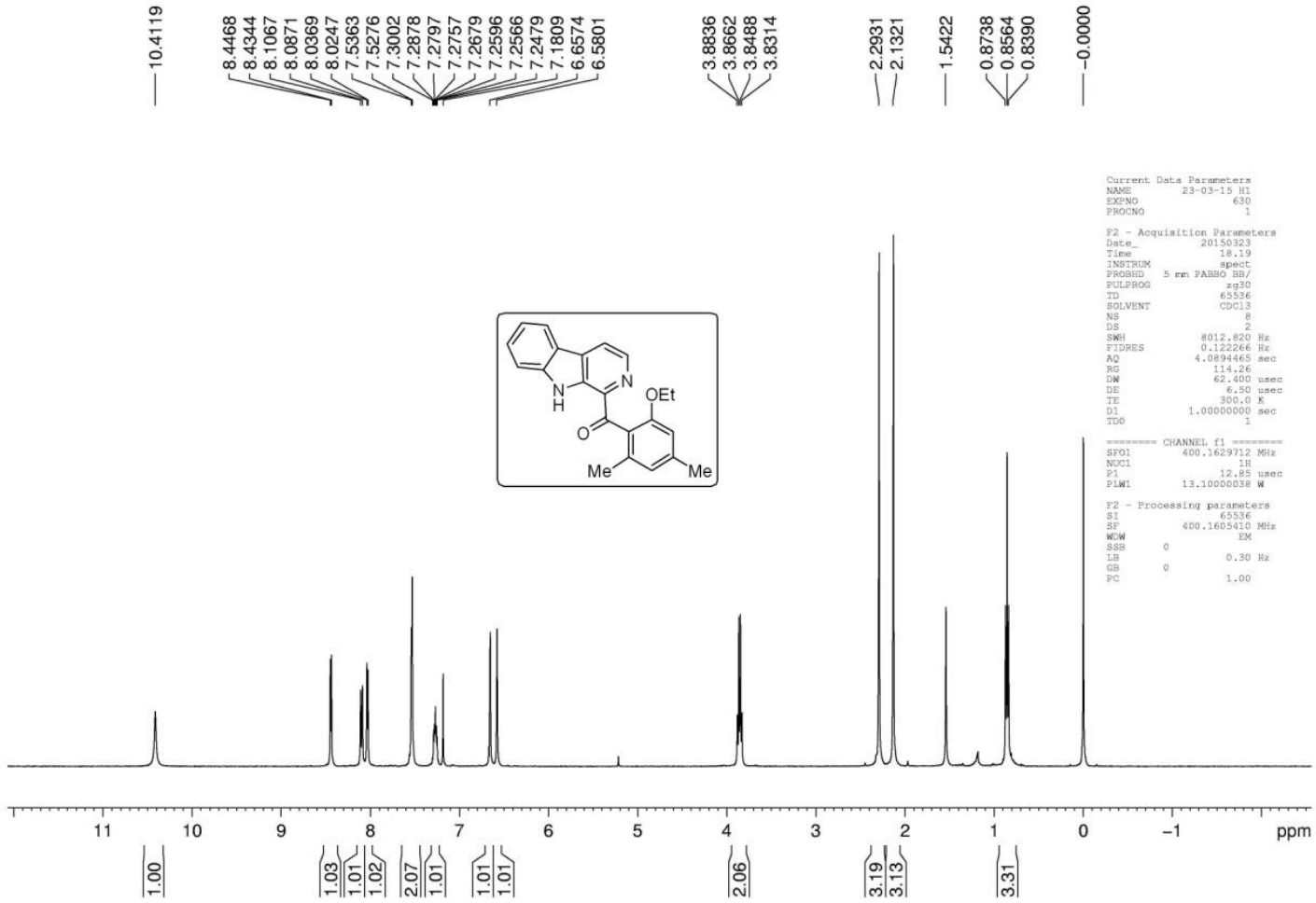

Figure. S-47**:** ^{1}H-NMR spectrum of (2-ethoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ib)**.

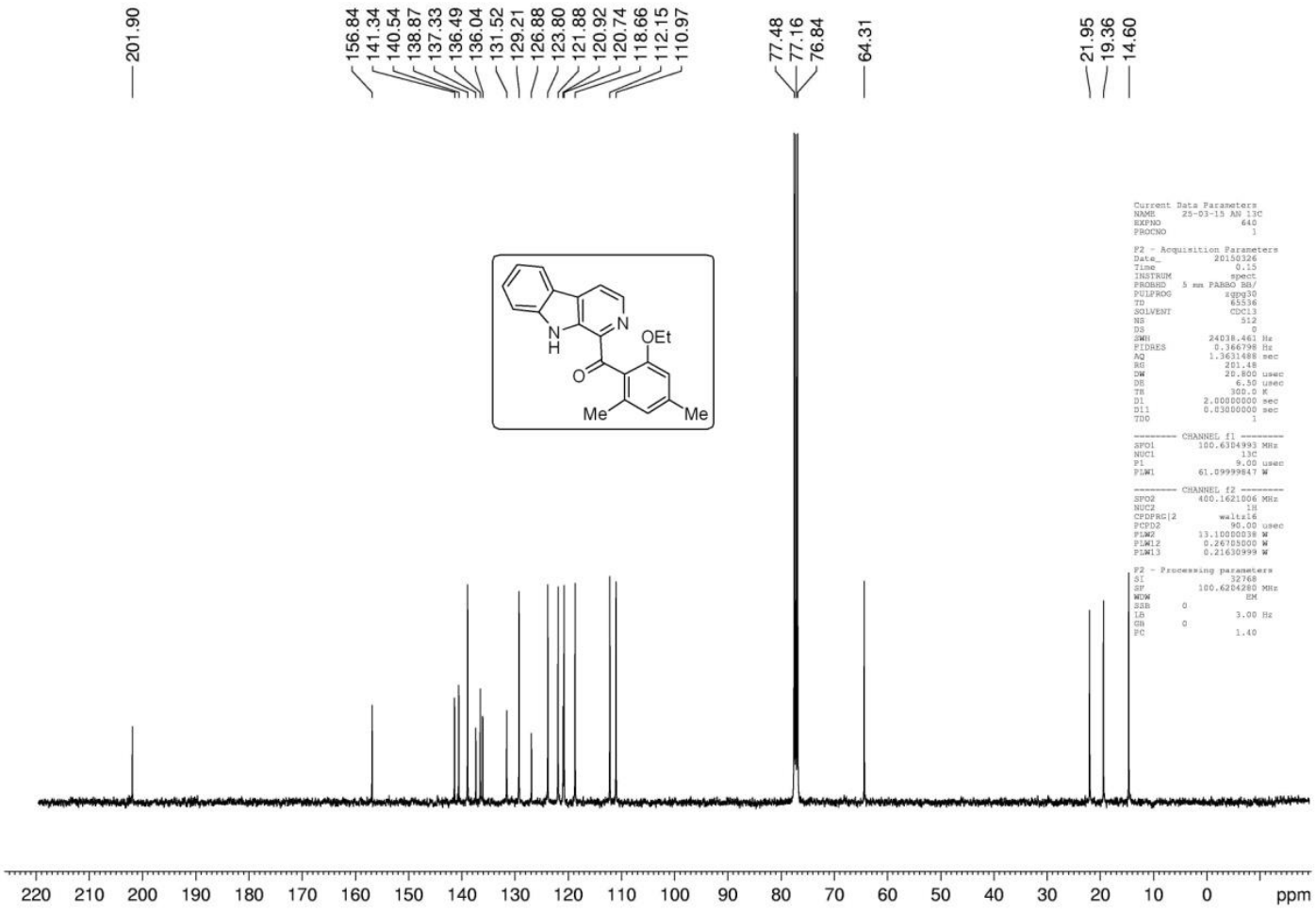

Figure. S-48: ^{13}C -NMR spectrum of (2-ethoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ib)**.

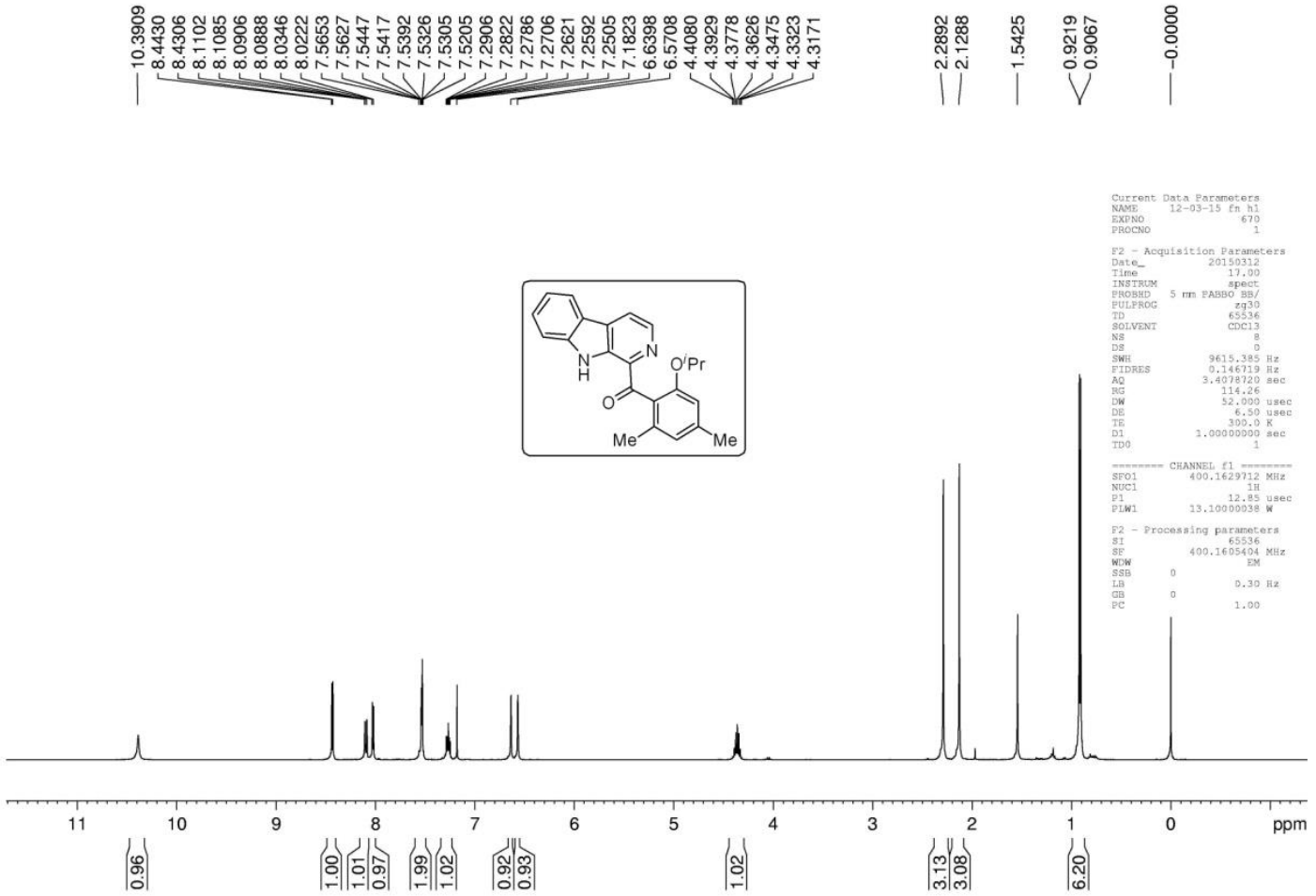

Figure. S-49: ^{1}H-NMR spectrum of (2-isopropoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4id)**.

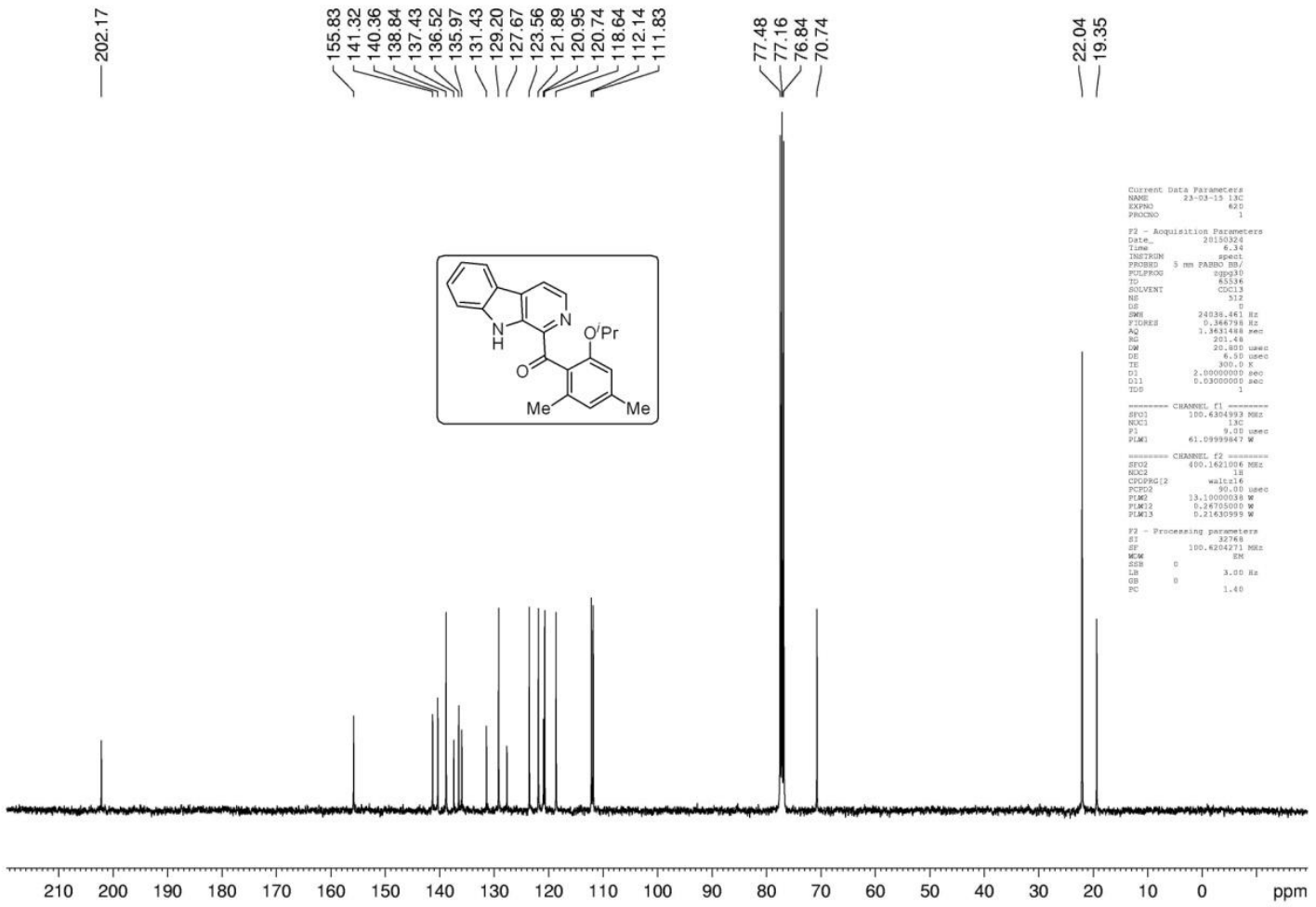

Figure. S-50: ^{13}C -NMR spectrum of (2-isopropoxy-4,6-dimethylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4id)**.

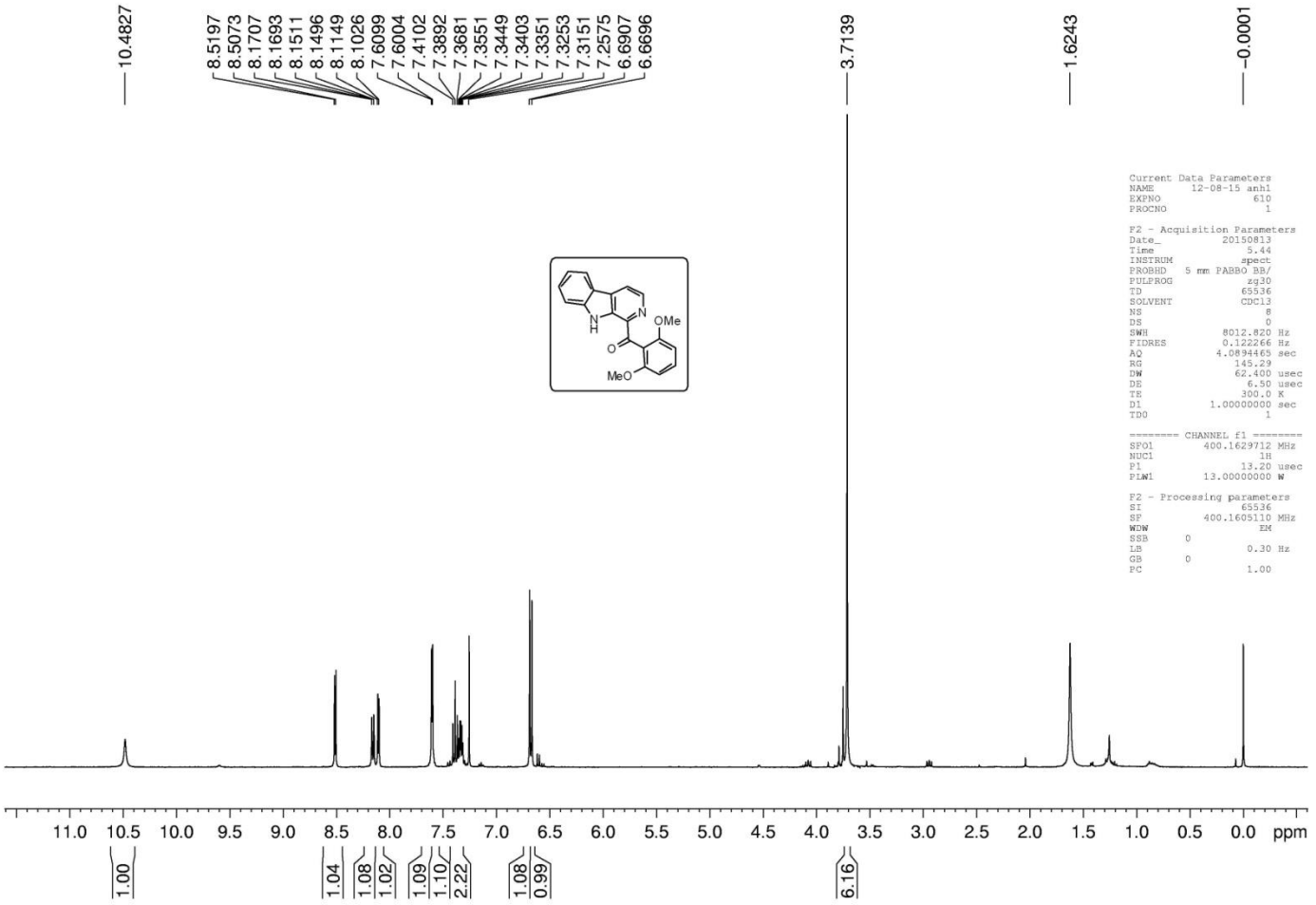

Figure. S-51: ^{1}H-NMR spectrum of (2,6-Dimethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ja)**.

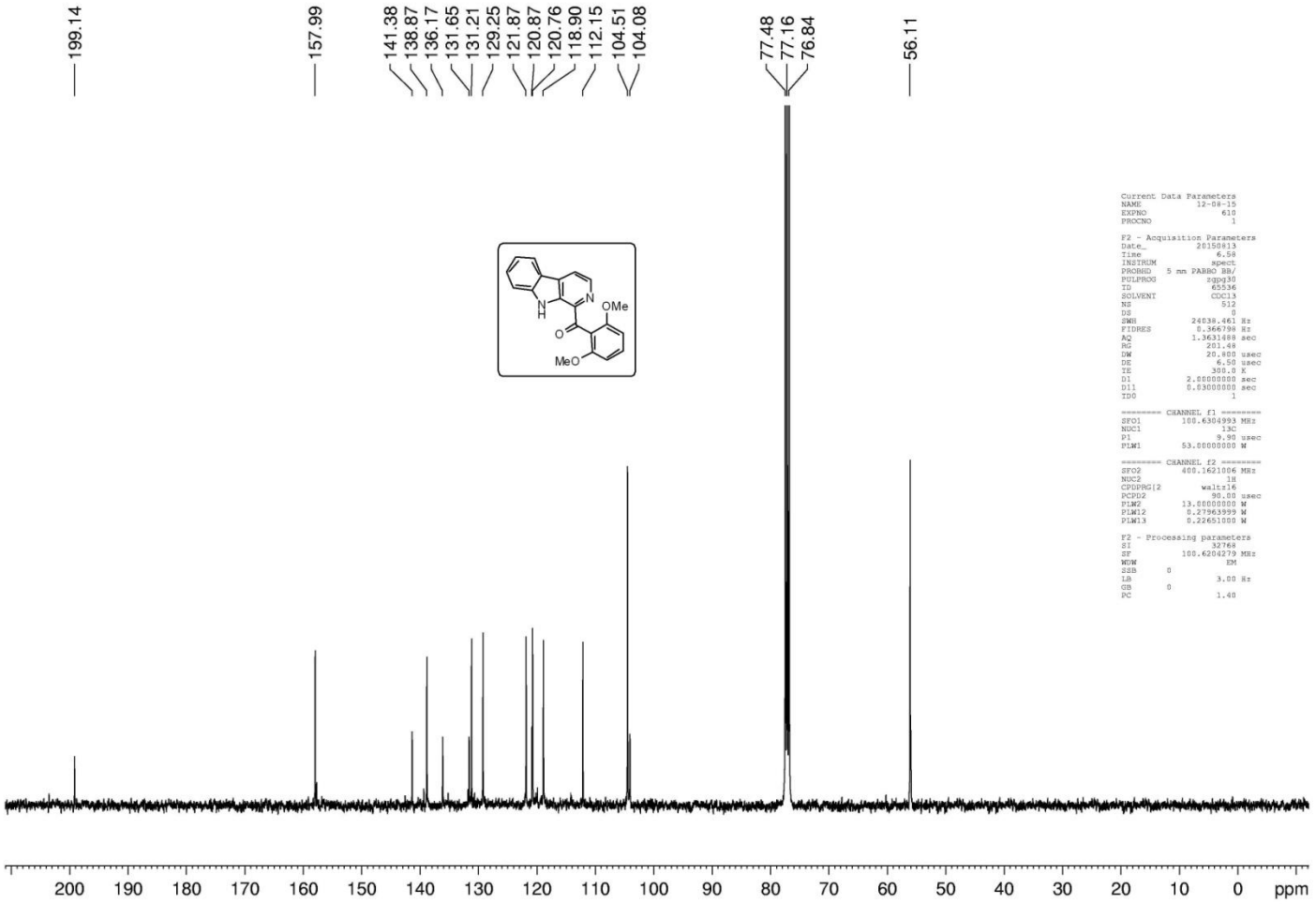

Figure. S-52: ^{13}C -NMR spectrum of (2,6-Dimethoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4ja)**.

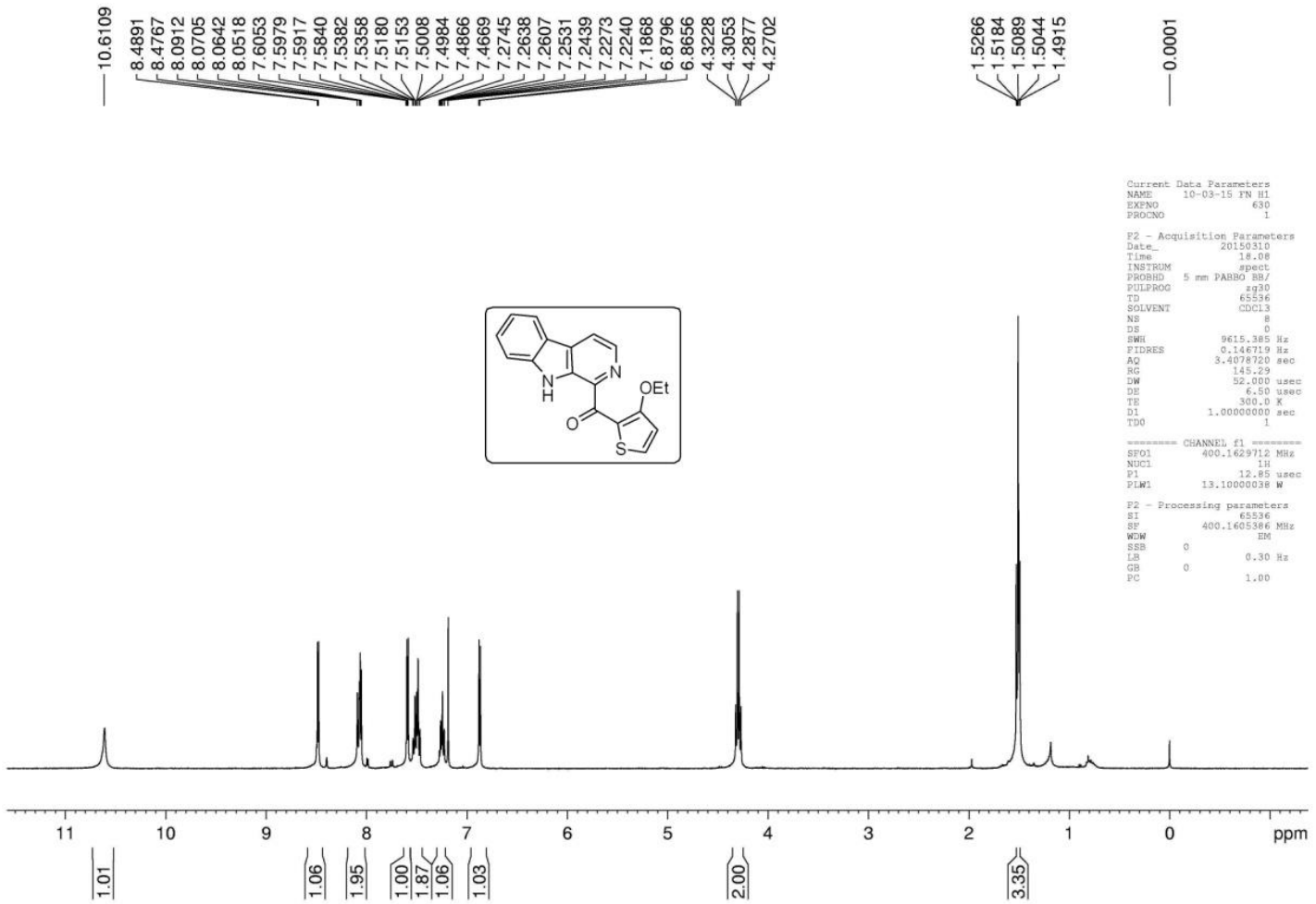

Figure. S-53: ^{1}H-NMR spectrum of (3-ethoxythiophen-2-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4kb)**.

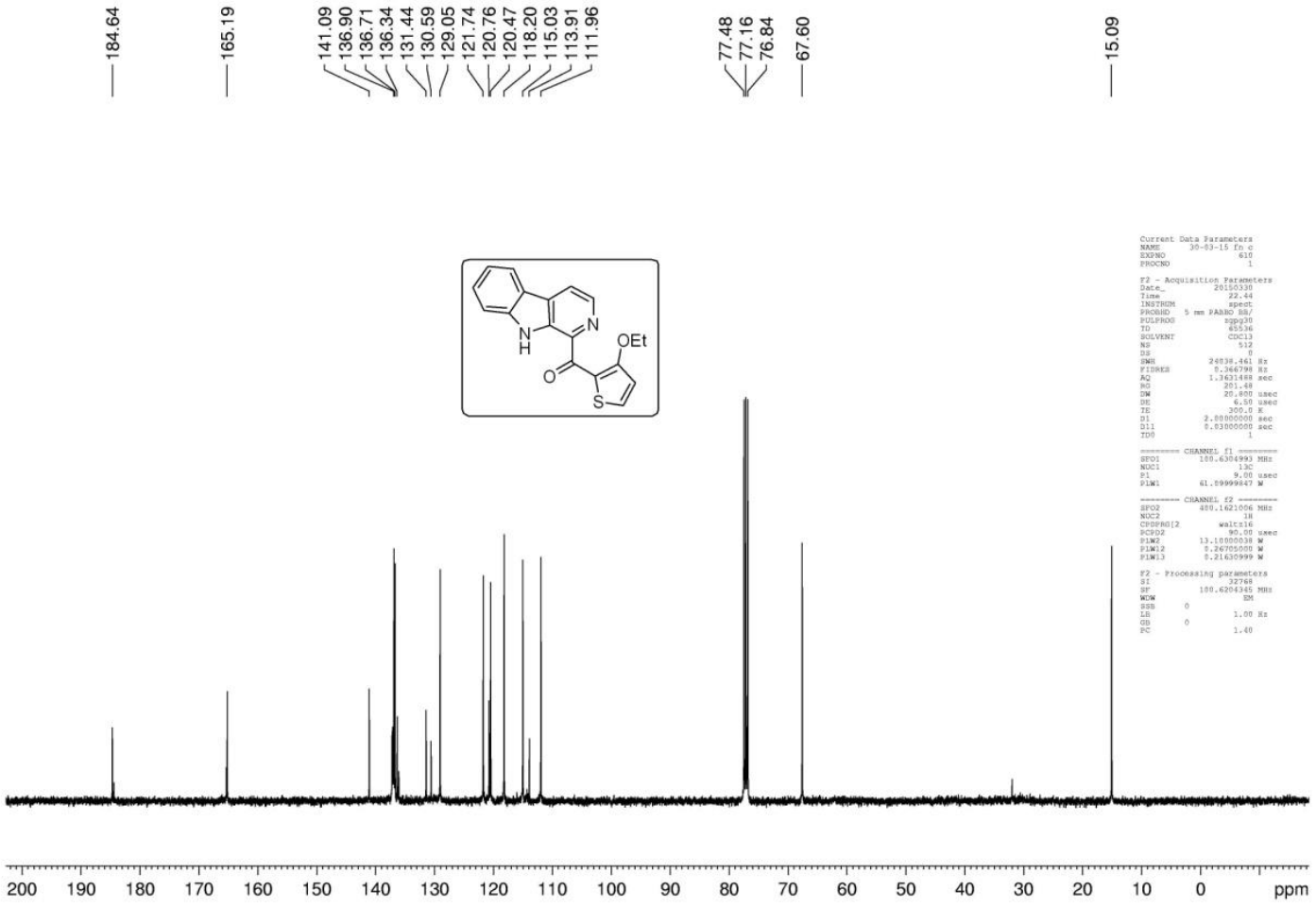

Figure. S-54: ^{13}C -NMR spectrum of (3-ethoxythiophen-2-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4kb)**.

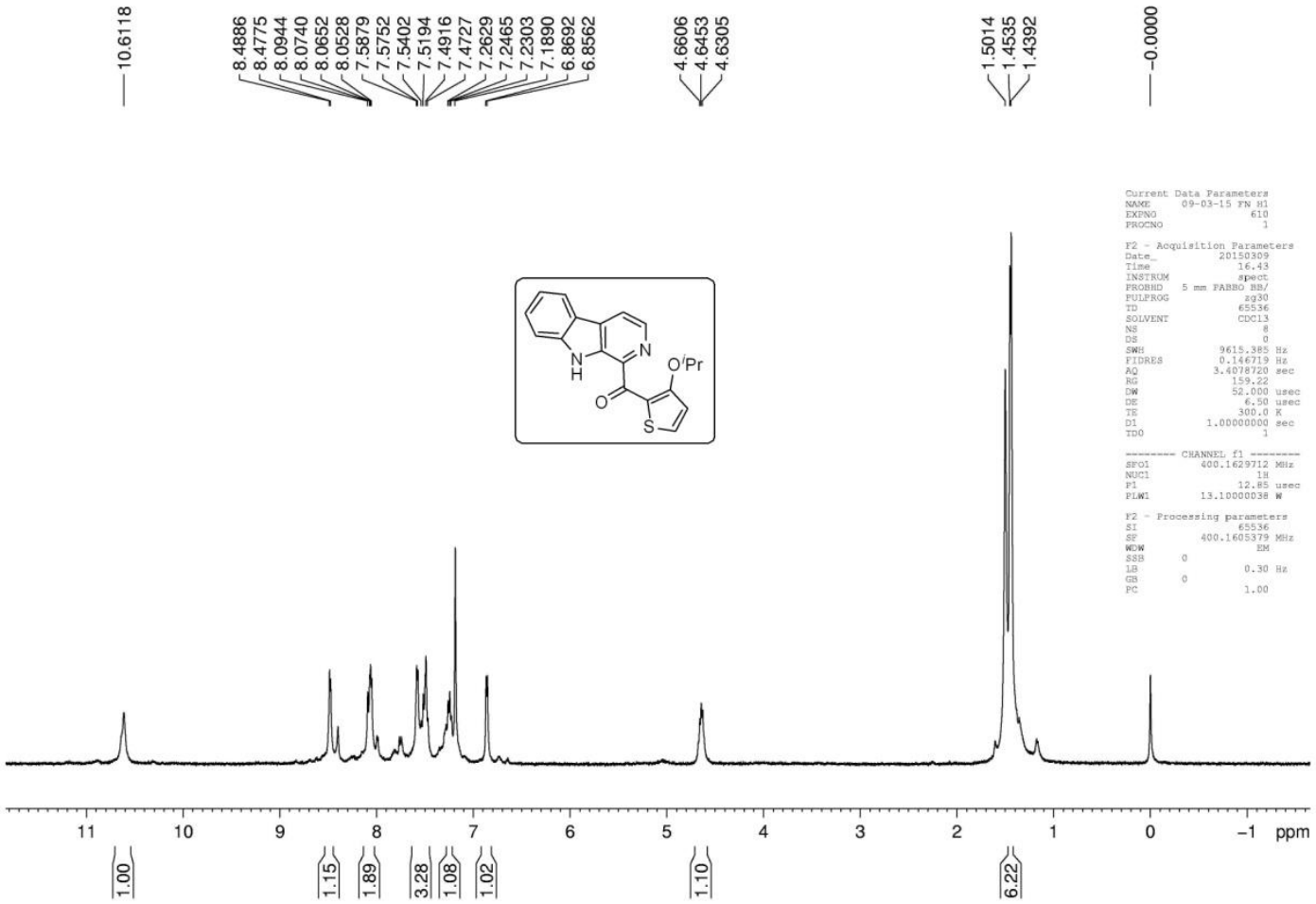

Figure. S-55: ^{1}H-NMR spectrum of (3-isopropoxythiophen-2-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4kd)**.

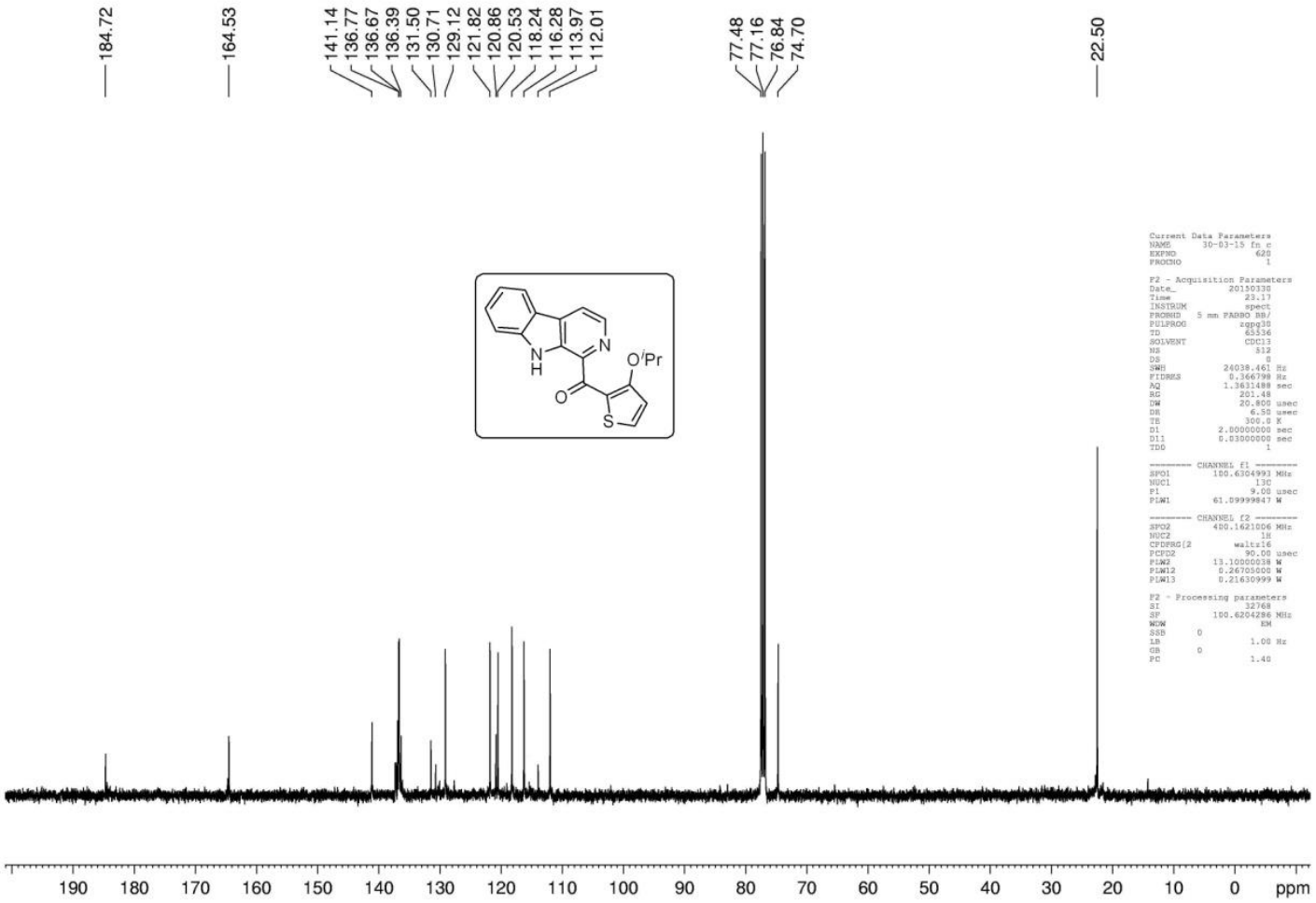

Figure. S-56: ^{13}C -NMR spectrum of (3-isopropoxythiophen-2-yl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(4kd)**.

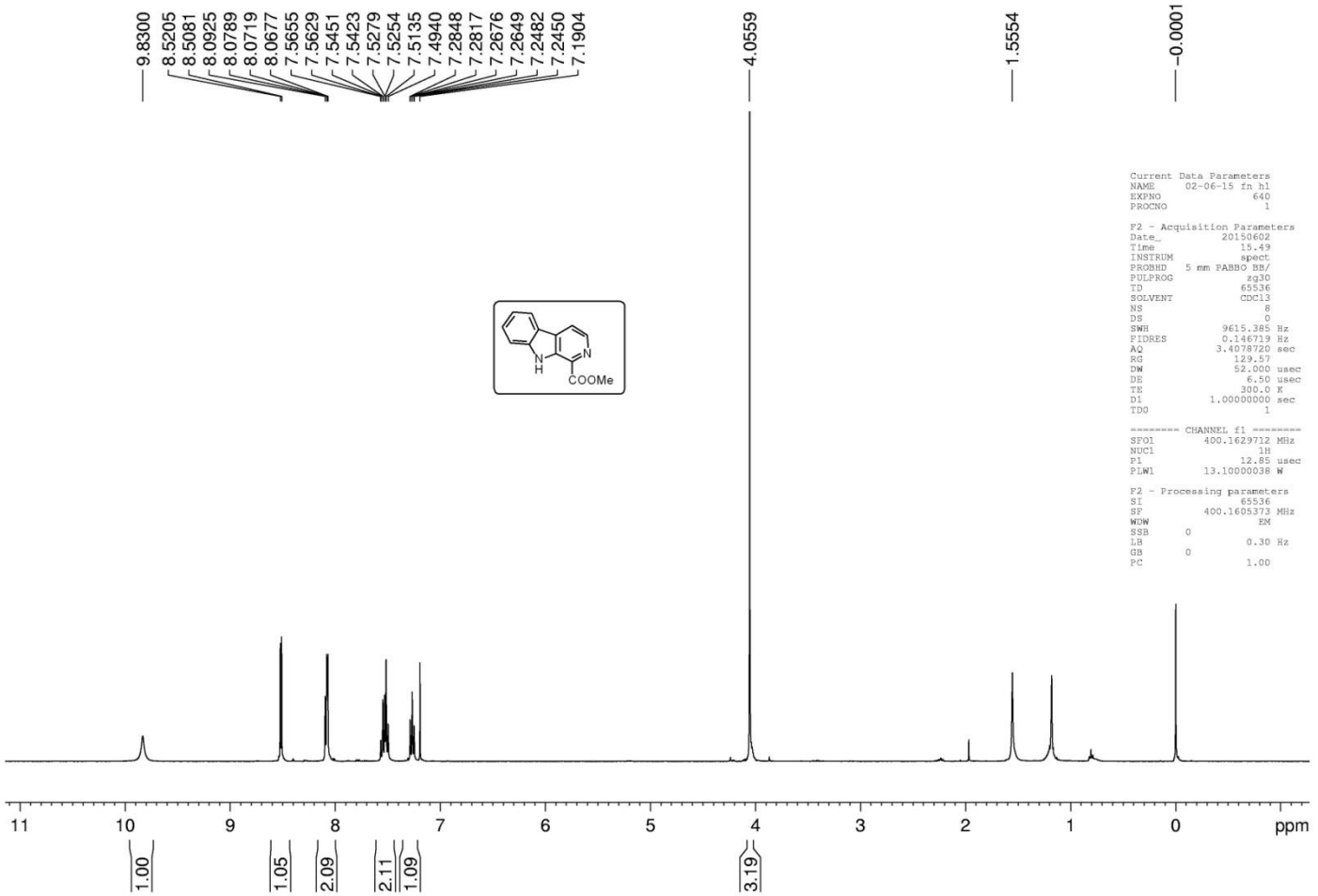

Figure. S-57: ^{1}H-NMR spectrum of methyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate **(7)**.

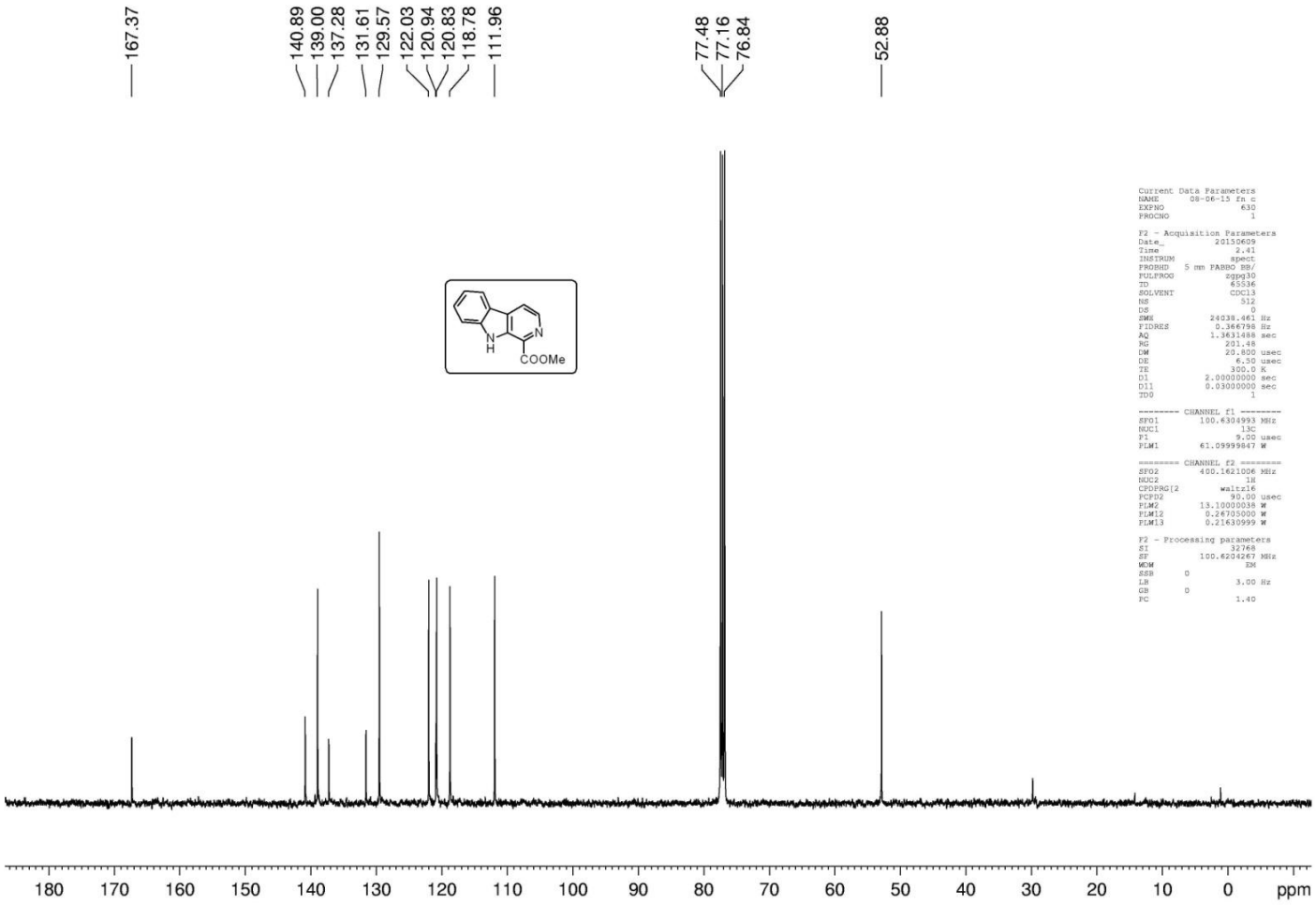

Figure. S-58: ^{13}C -NMR spectrum of methyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate **(7)**.

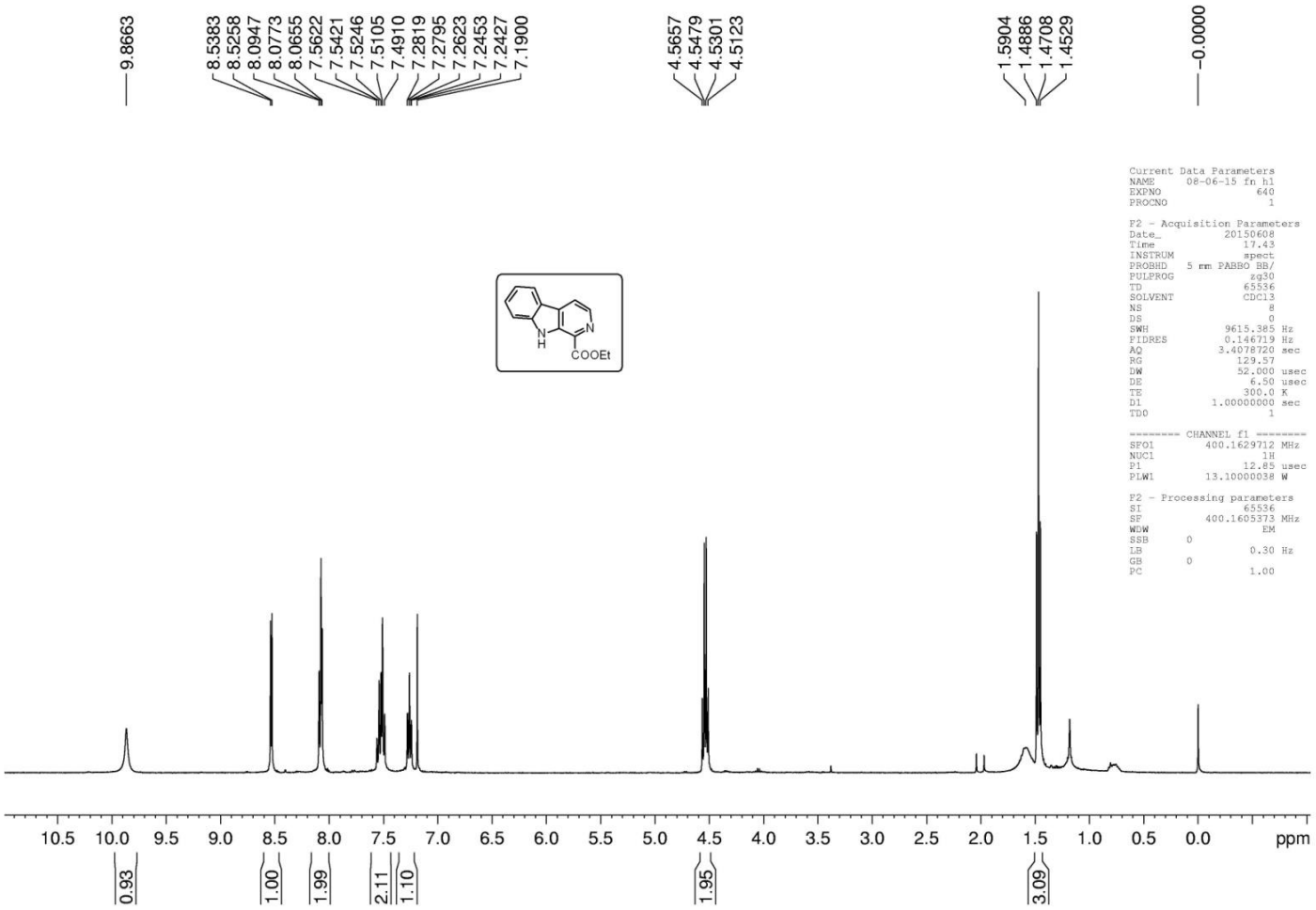

Figure. S-59: ^{1}H-NMR spectrum of ethyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate **(8)**.

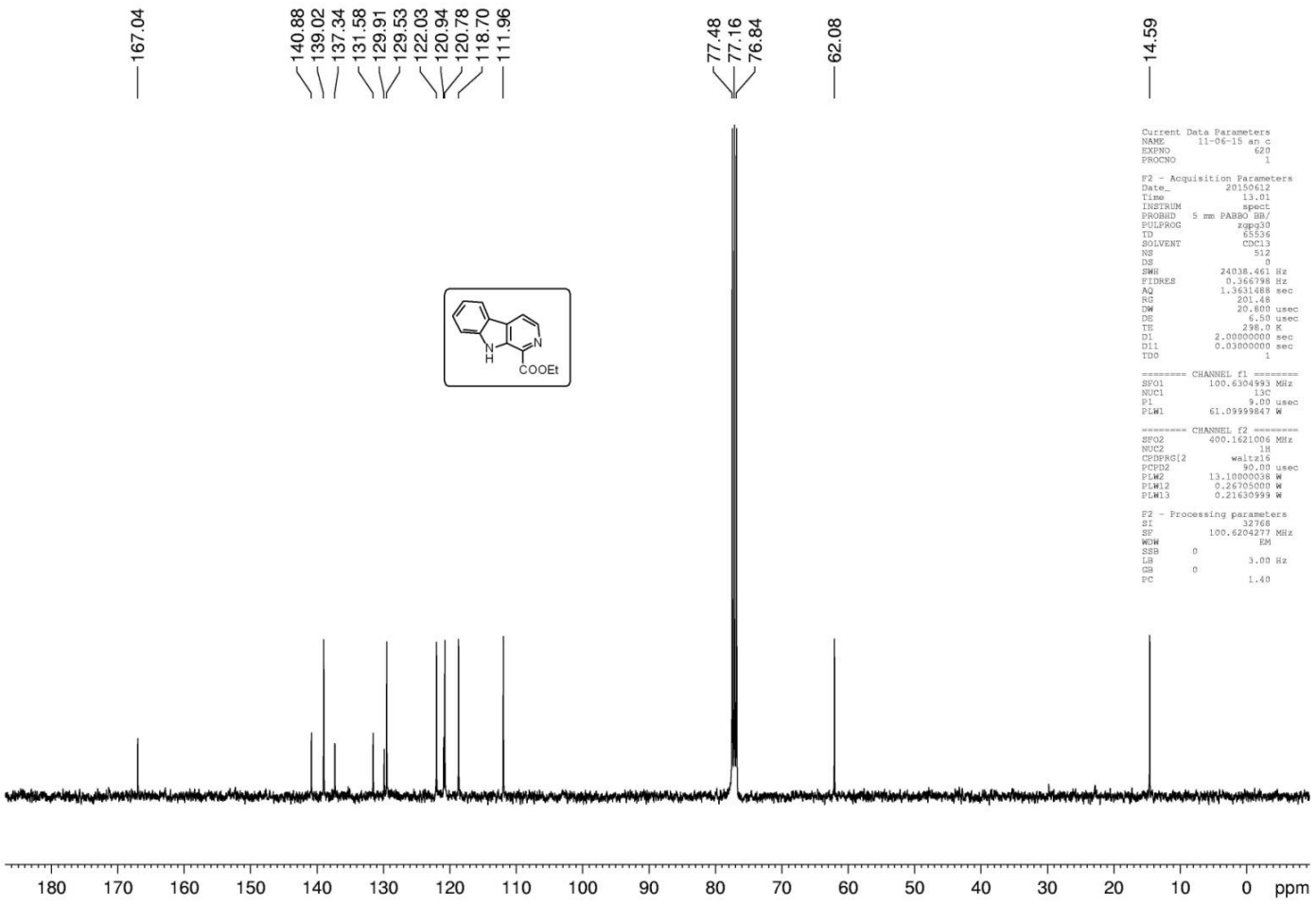

Figure. S-60: ^{13}C -NMR spectrum of ethyl 9*H*-pyrido[3,4-*b*]indole-1-carboxylate **(8)**.

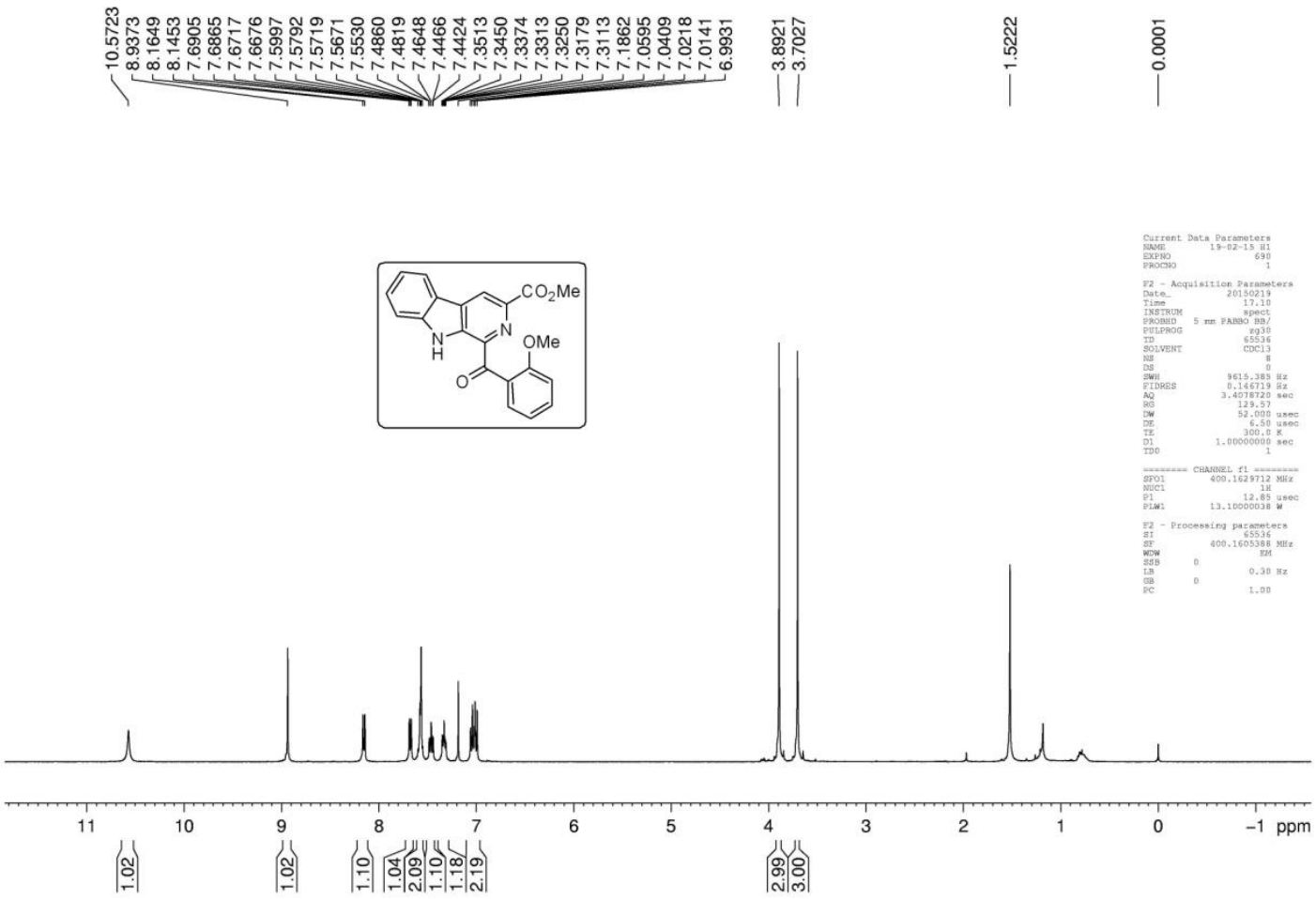

Figure. S-61: ^{1}H-NMR spectrum of methyl 1-(2-methoxybenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(5)**.

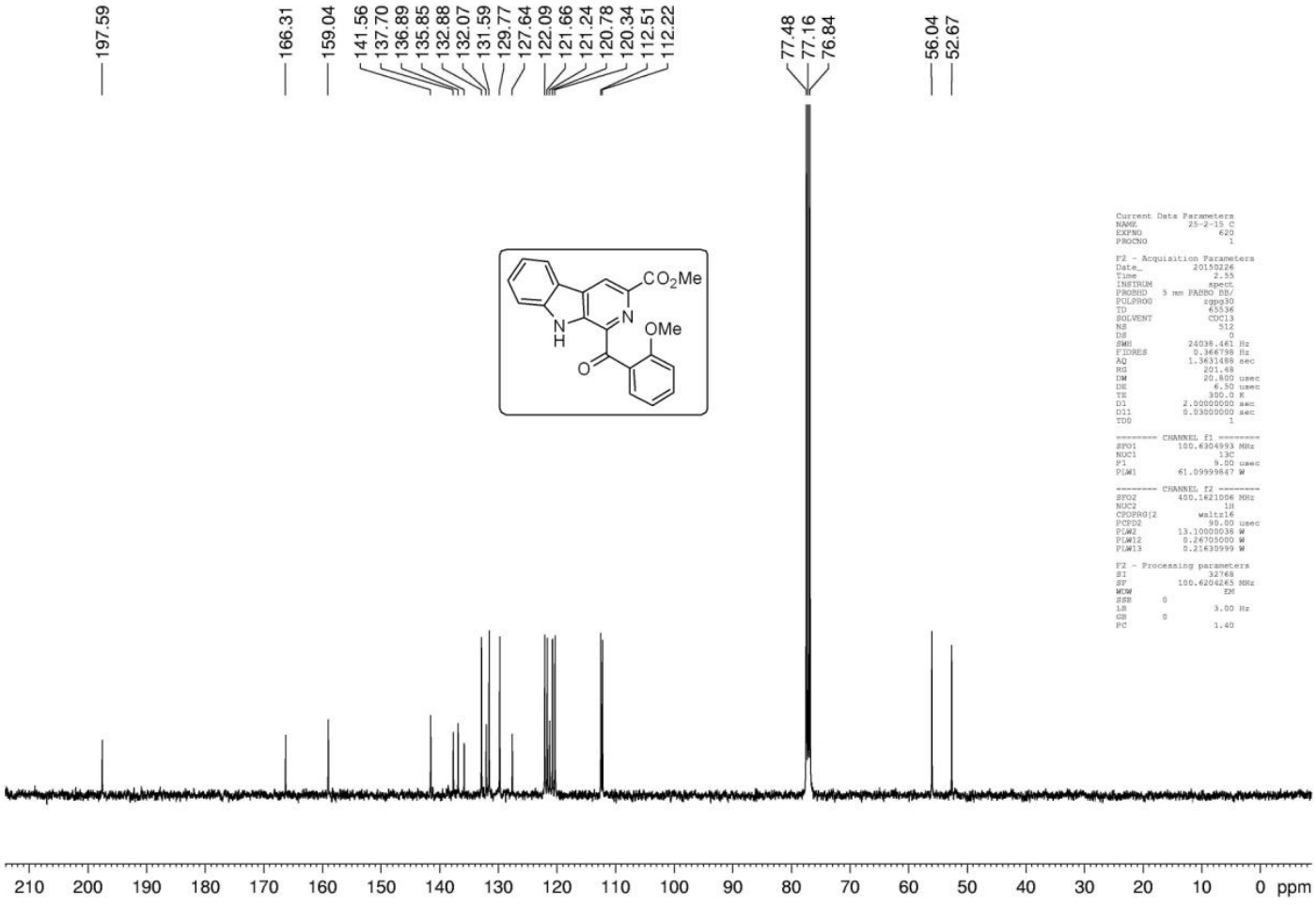

Figure. S-62: ^{13}C -NMR spectrum of methyl 1-(2-methoxybenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(5)**.

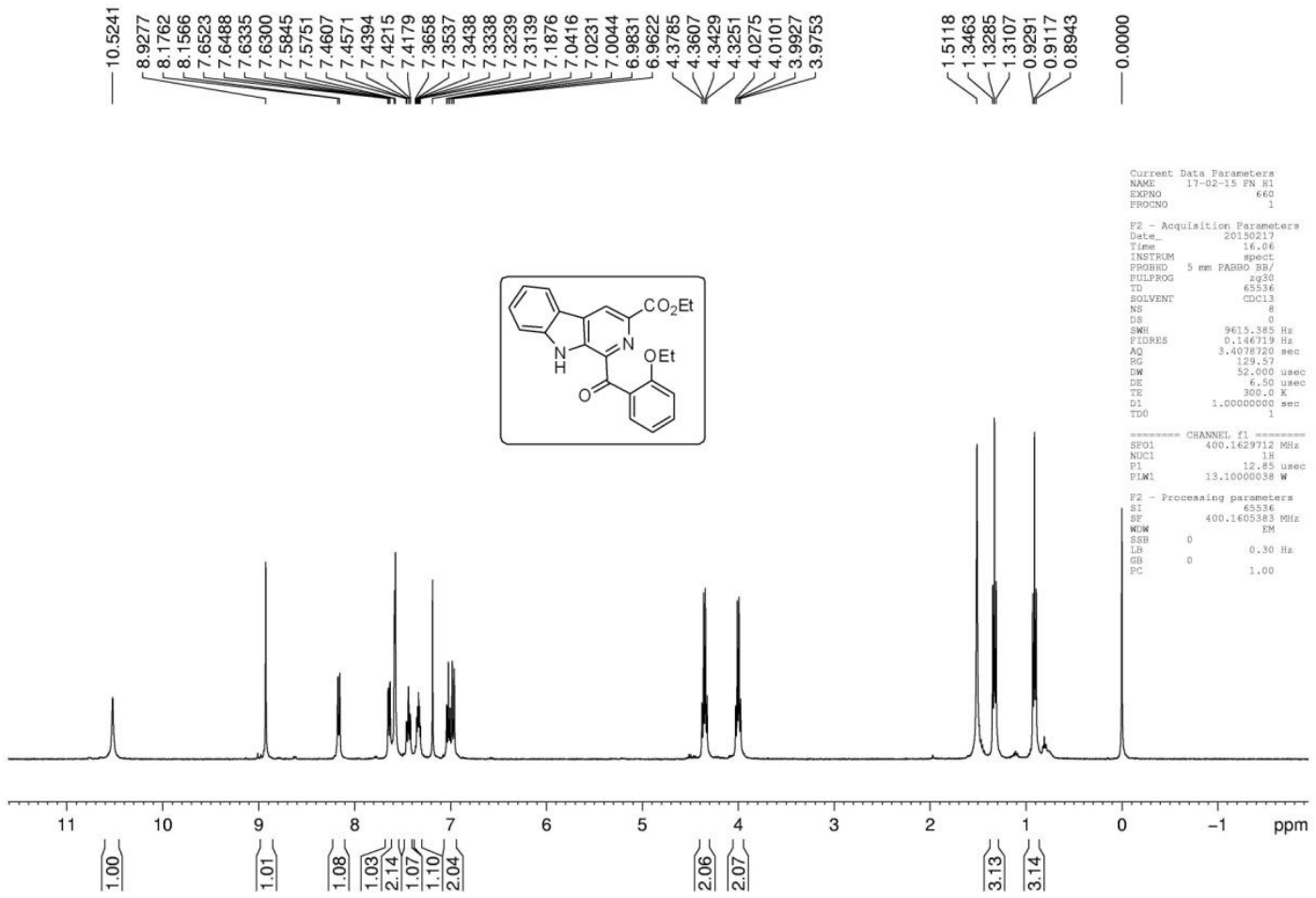

Figure. S-63: ^{1}H-NMR spectrum of ethyl 1-(2-ethoxybenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(6)**.

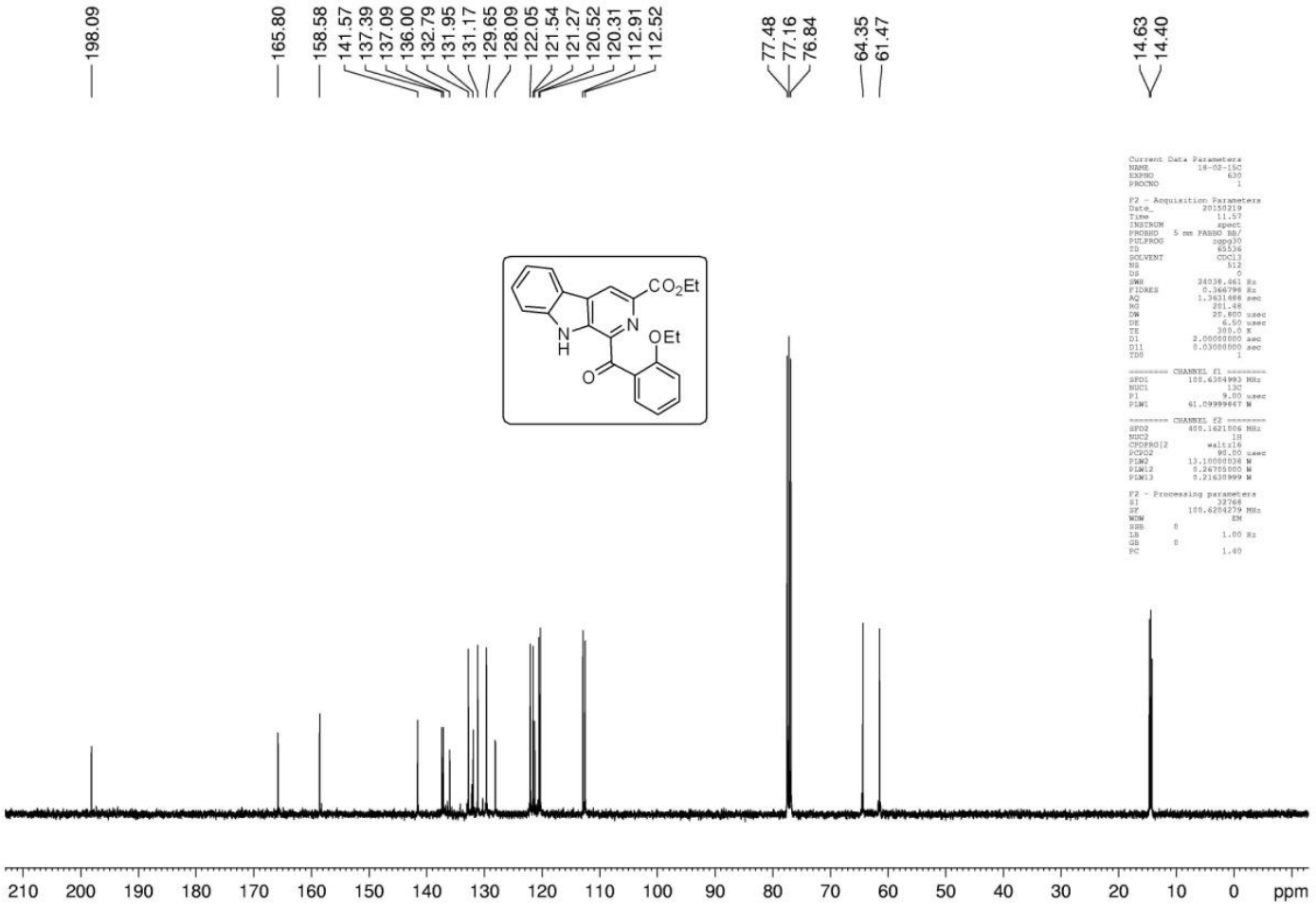

Figure. S-64: ^{13}C -NMR spectrum of ethyl 1-(2-ethoxybenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(6)**.

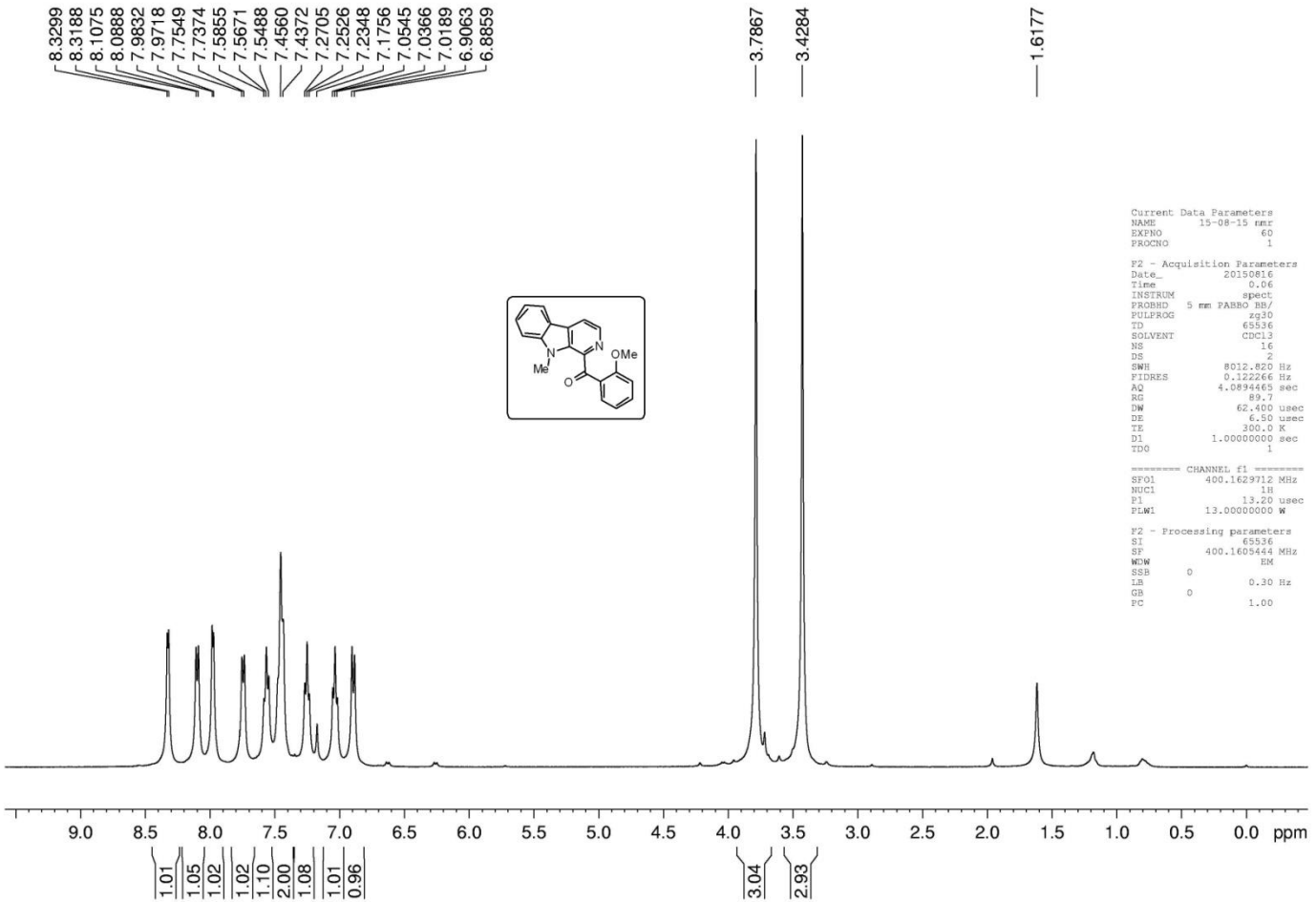

Figure. S-65: ^{1}H-NMR spectrum of (2-Methoxyphenyl)(9-methyl-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(10)**.

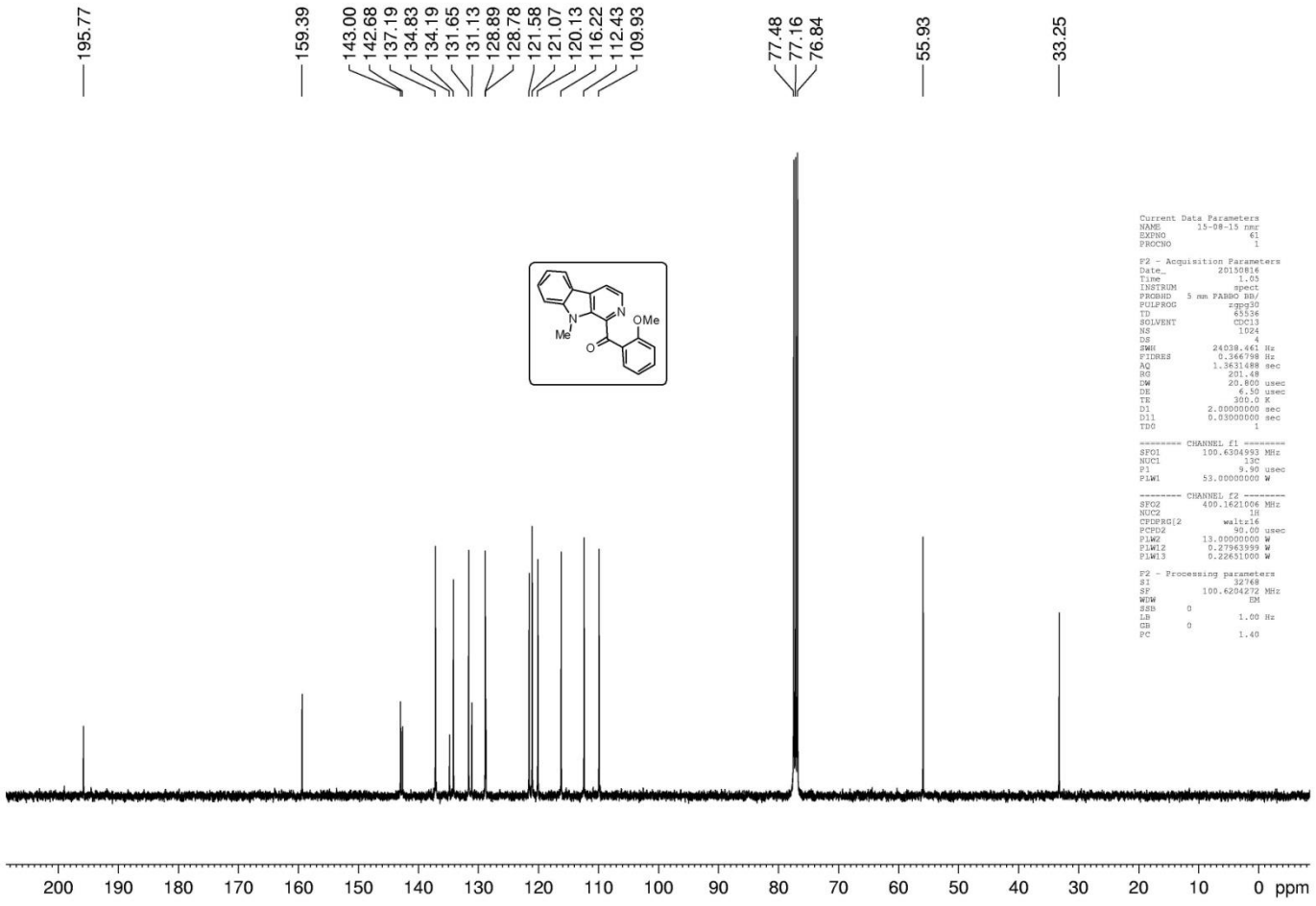

Figure. S-66: ^{13}C -NMR spectrum of (2-Methoxyphenyl)(9-methyl-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(10)**.

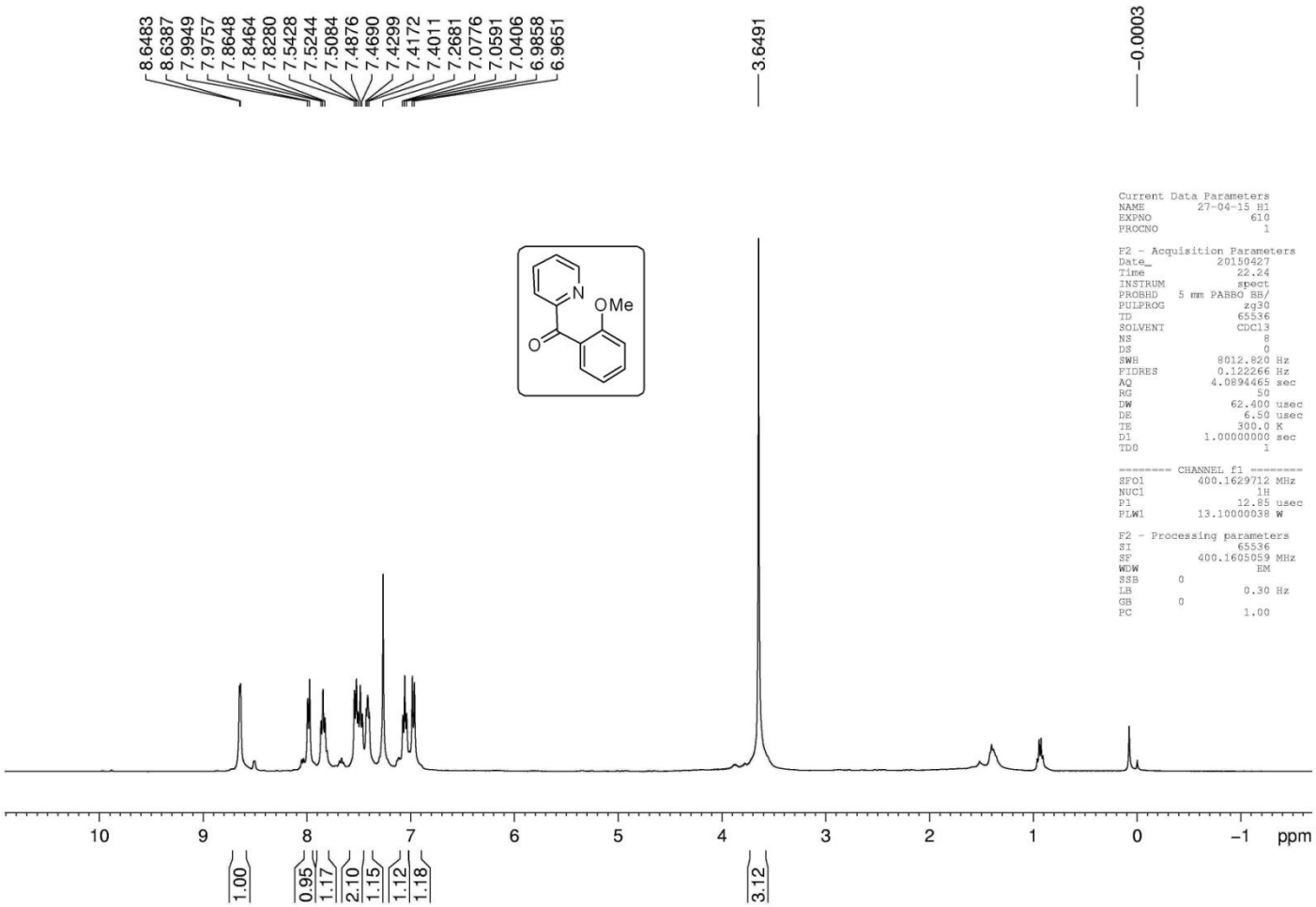

Figure. S-67: ^{1}H-NMR spectrum of (2-methoxyphenyl)(pyridin-2-yl)methanone **(14)**.

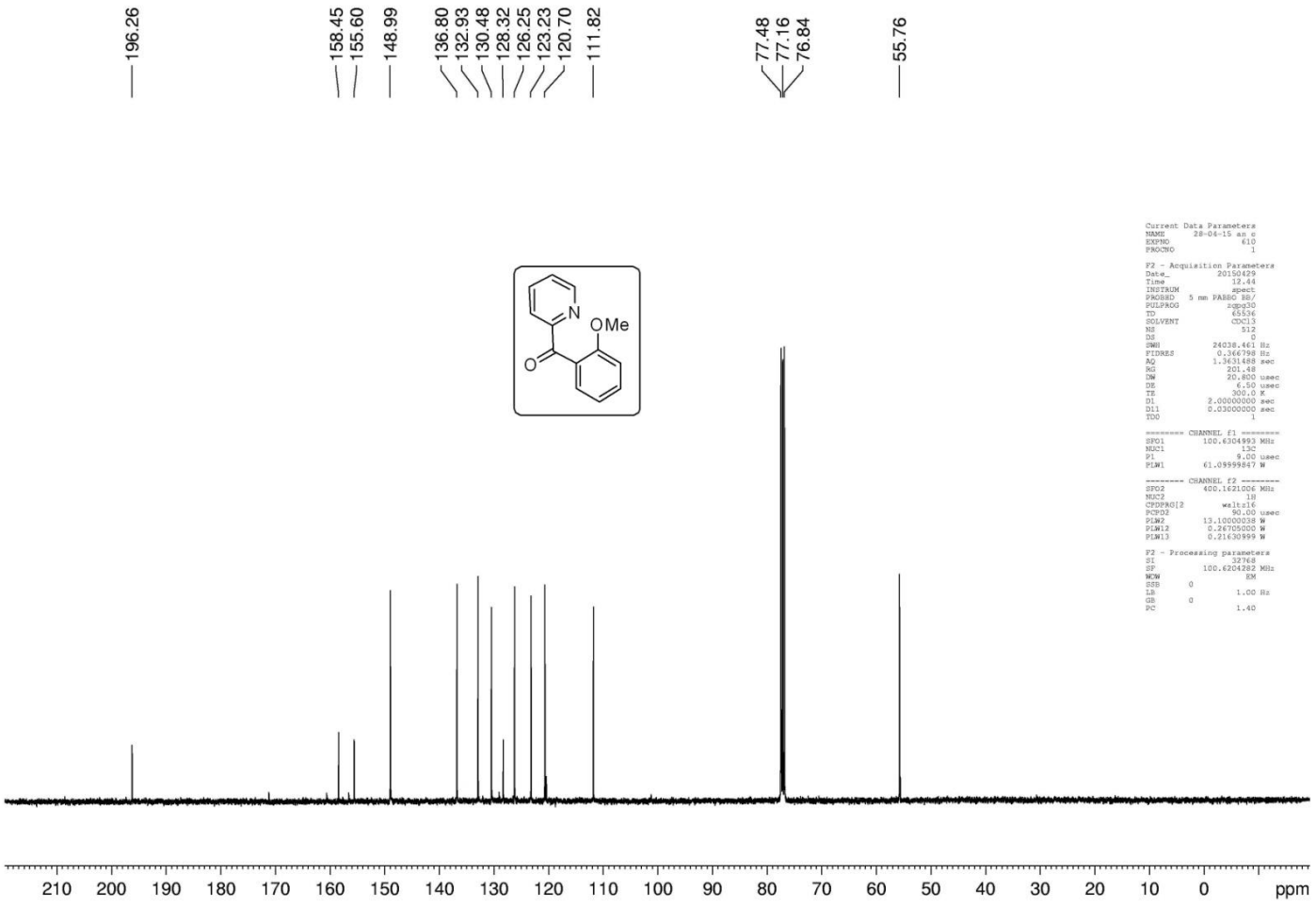

Figure. S-68: ^{13}C -NMR spectrum of (2-methoxyphenyl)(pyridin-2-yl)methanone **(14)**.

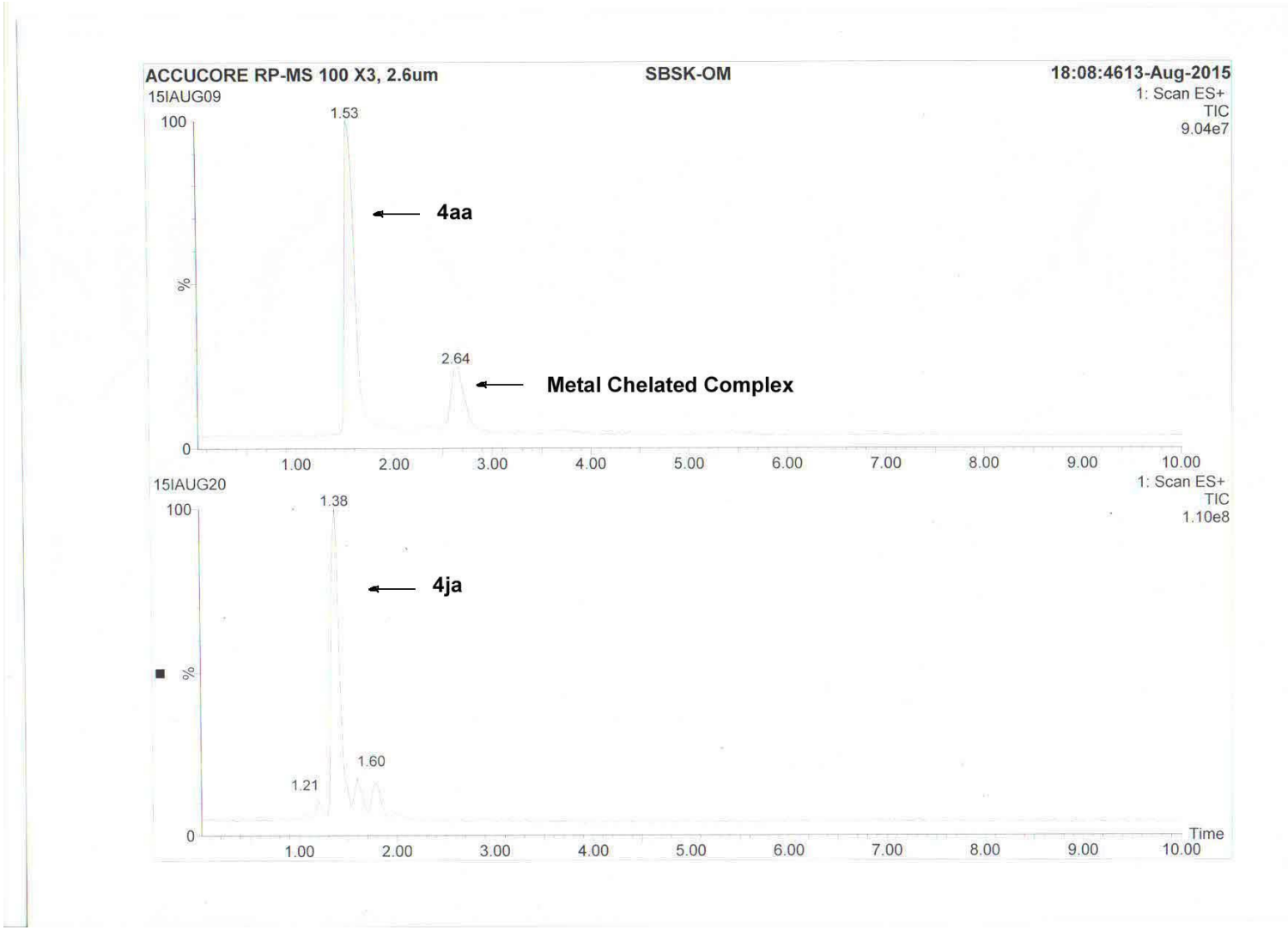

Figure. S-67: The LCMS chromatograms a) the LC chromatogram of the crude **4aa** does not contain corresponding peak for **4ja**; b) the LC chromatogram for pure **4ja**