Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting information

***for***

## β-Carboline-directed decarboxylative acylation of *ortho*-C(sp2)-H of aryl ring of aryl (β-carbolin-1-yl) methanones with α-ketoacids under Palladium catalysis

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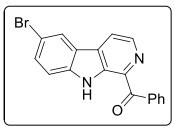
**Contents:**

## 1. General information:

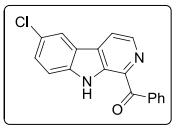
All reactions were monitored by thin layer chromatography (TLC). TLC was performed on pre-coated silica gel plates. After elution, plate was visualized under UV illumination at 254 nm. The melting points were recorded on a hot stage apparatus using silicone oil and are uncorrected. IR spectra were recorded 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 $\delta$). 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.[1]

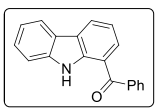
**(6-Bromo-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone (1m)**. A yellow solid, mp 106-108 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ (ppm) = 7.42-7.49 (m, 3H), 7.55 (t, *J* = 6.9 Hz, 1H), 7.62-7.64 (m, 1H), 8.05 (d, *J* = 4.8 Hz, 1H), 8.23-8.26 (m, 3H), 8.56 (d, *J* = 4.9 Hz, 1H), 10.44 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ (ppm) = 113.7, 118.7, 122.7, 124.7, 128.2, 130.7, 131.4, 132.2, 132.7, 136.7, 137.4, 137.5, 138.4, 139.7, 195.5. MS (ESI+) m/z = 351.1. ESI-HRMS calculated for $C_{18}H_{11}BrN_2O$ $[MH]^+$: 351.0133, found: 351.0135.




**(6-Chloro-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone (1n)**. A yellow solid, mp 124-126 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ (ppm) = 7.45-7.54 (m, 5H), 8.04 (d, *J* = 8.6 Hz, 2H), 8.25 (d, *J* = 7.5 Hz, 2H), 8.55 (d, *J* = 4.3 Hz, 1H), 10.42 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ (ppm) = 113.2, 118.7, 121.6, 122.2, 126.5, 128.2, 129.6, 130.9, 131.4, 132.7, 136.8, 137.5, 137.8, 138.4, 139.4, 195.5. MS (ESI+) m/z = 307.1. ESI-HRMS calculated for $C_{18}H_{11}ClN_2O$ $[MH]^+$: 307.0638, found: 307.0636.




**(9*H*-carbazol-1-yl)(phenyl)methanone (4)**[2]. A pale yellow solid, mp 154-156 $^{o}$C. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ (ppm) = 7.15-7.19 (m, 1H), 7.23 (t, *J* = 7.3 Hz, 1H), 7.40-7.55 (m, 5H), 7.73 (d, *J* = 7.6 Hz, 3H), 8.05 (d, *J* = 7.8 Hz, 1H), 8.25 (d, *J* = 7.5 Hz, 1H), 10.47 (s, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ (ppm) = 111.5, 118.1, 118.6, 120.3, 120.5, 122.4, 125.2, 126.1, 126.8, 128.4, 129.5, 130.9, 131.6, 139.2, 140.1, 140.4, 198.2. MS (ESI+) m/z = 272.1.



**References:**


1. (a) Y. P Zhu, M. C Liu, Q Cai, F. C Jia and A. X. Wu, *Chem. Eur. J*., 2013, **19**, 10132. (b) N. Battini, A. K. Padala, N. Mupparapu, R. A. Vishwakarma and Q. N. Ahmed, *RSC Adv*., 2014, **4**, 26258.
2. A. R. Katritzky, G. W. Rewcastle and L. M. V. de Miguel, *J. Org.* Chem., 1988, **53**, 794.

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

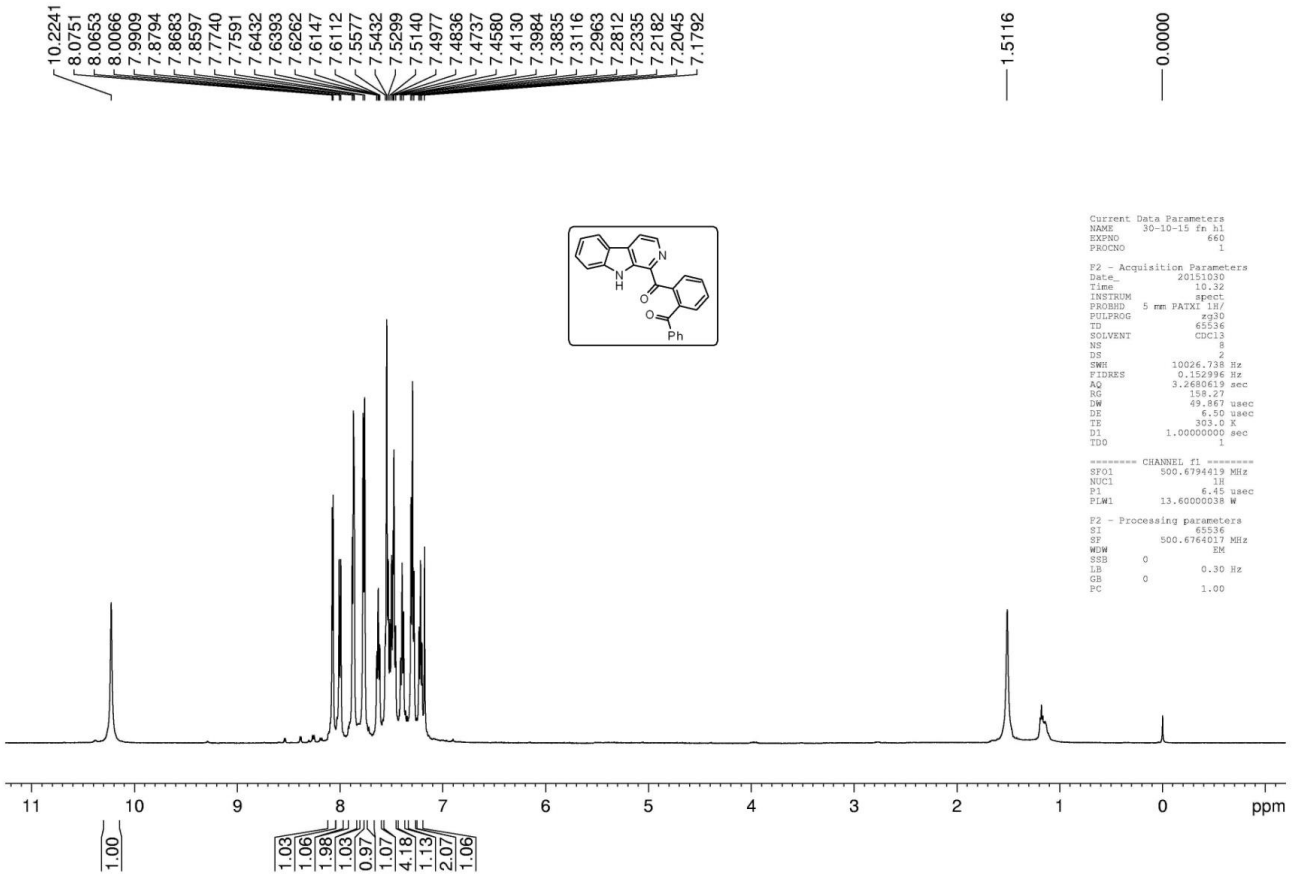



**Figure.** S-1**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(phenyl)methanone **(3aa).**

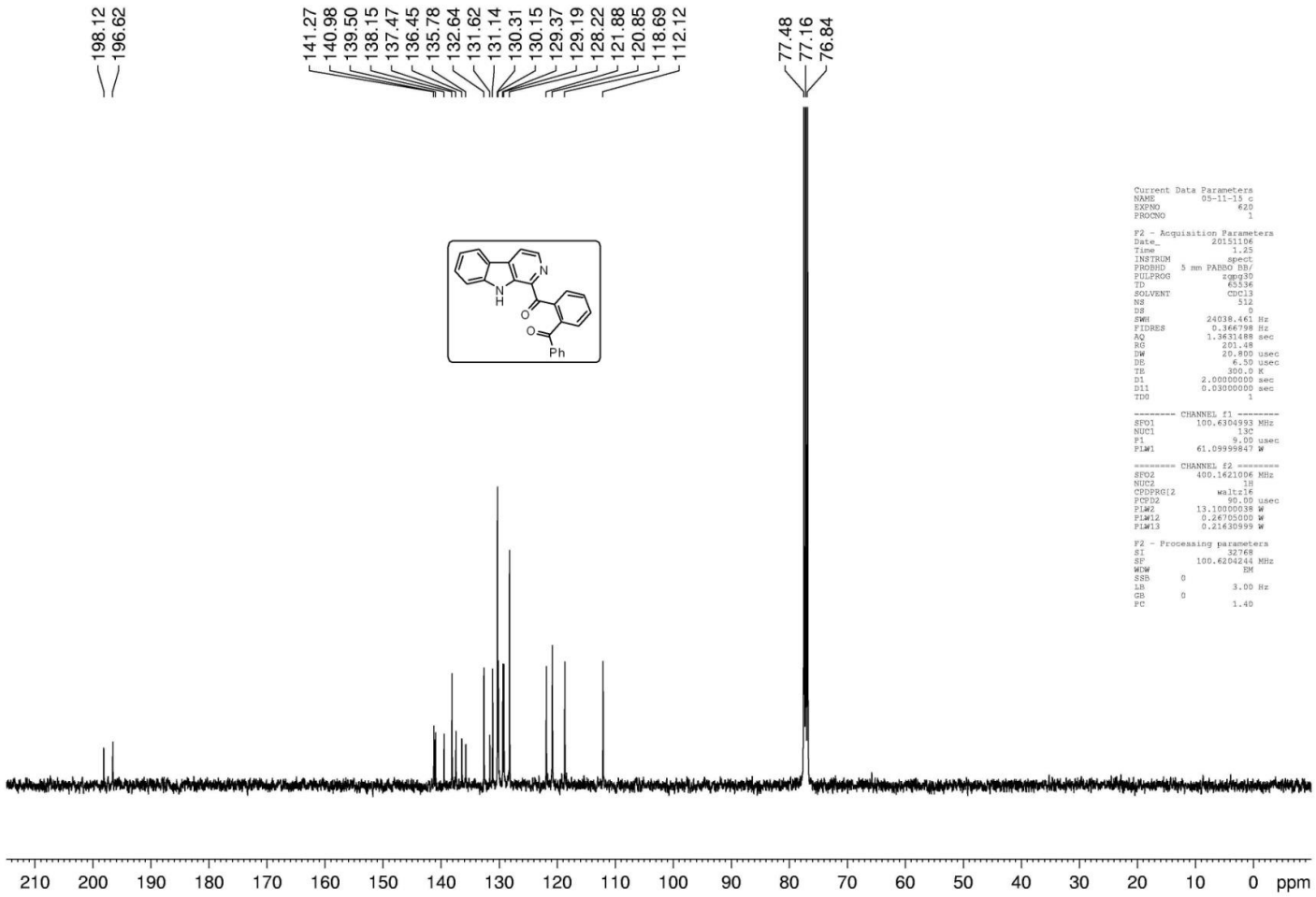



**Figure.** S-2**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(phenyl)methanone **(3aa).**

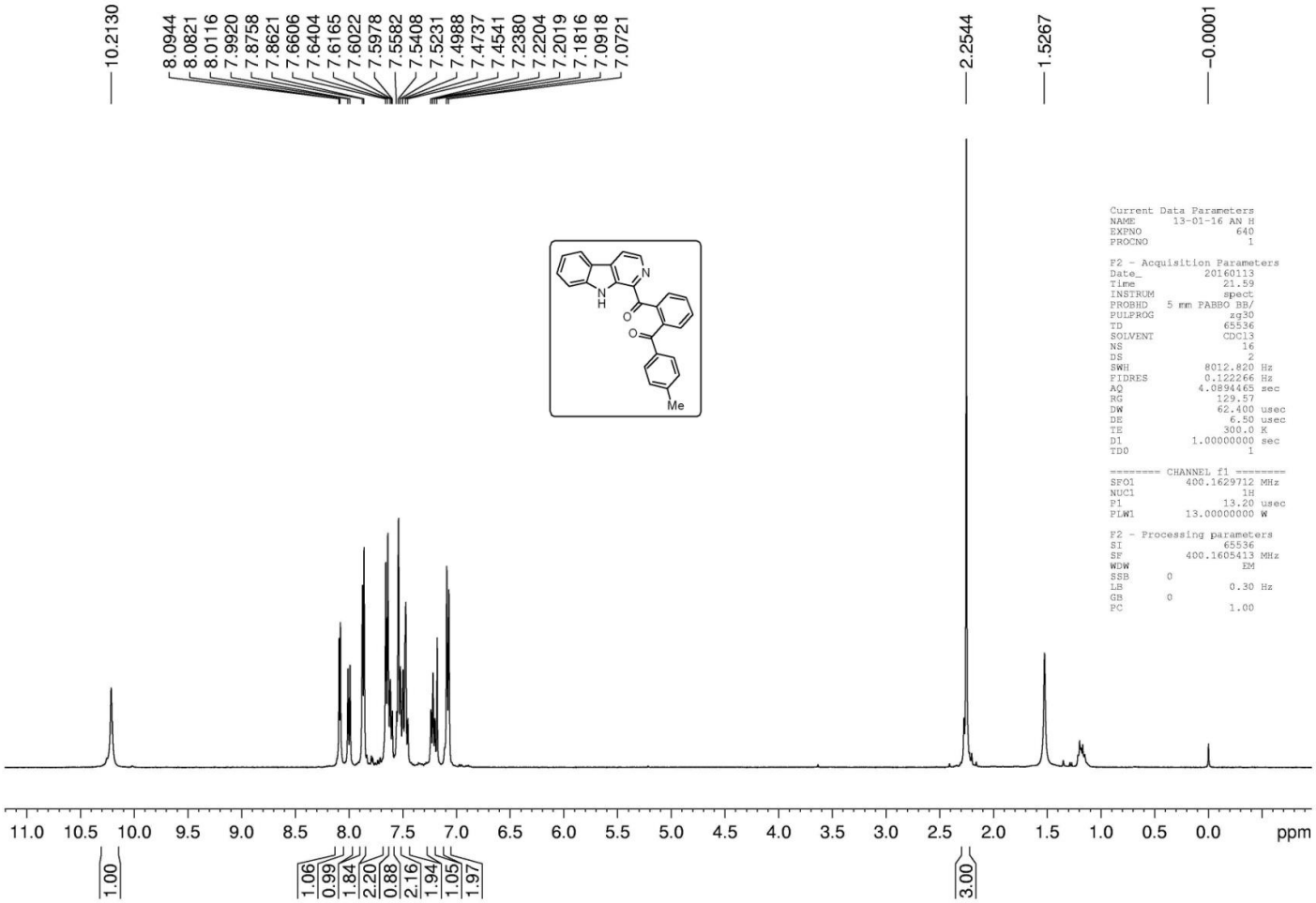



**Figure.** S-3**:** [1]H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(p-tolyl)methanone **(3ab).**

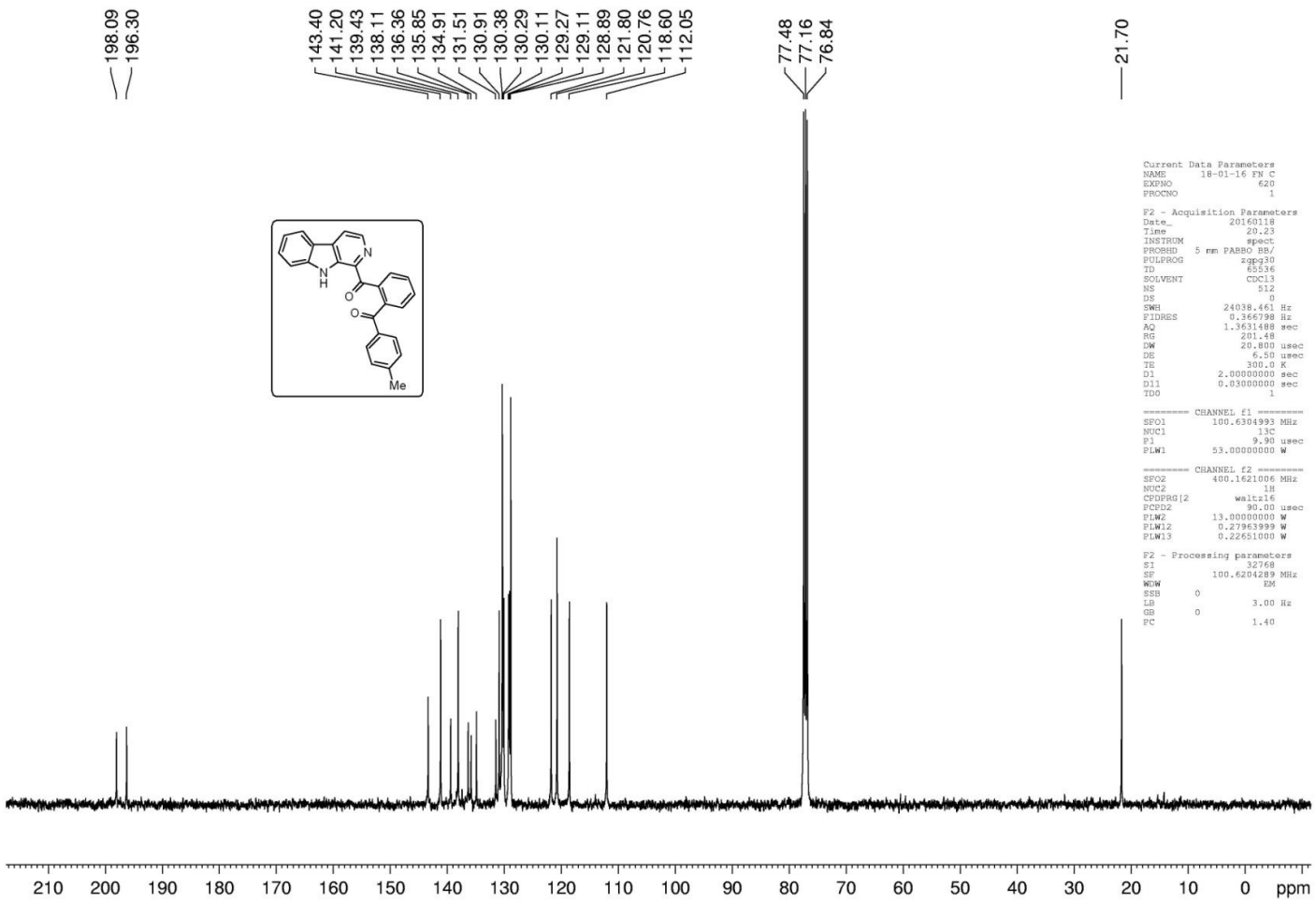



**Figure.** S-4**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(p-tolyl)methanone **(3ab).**

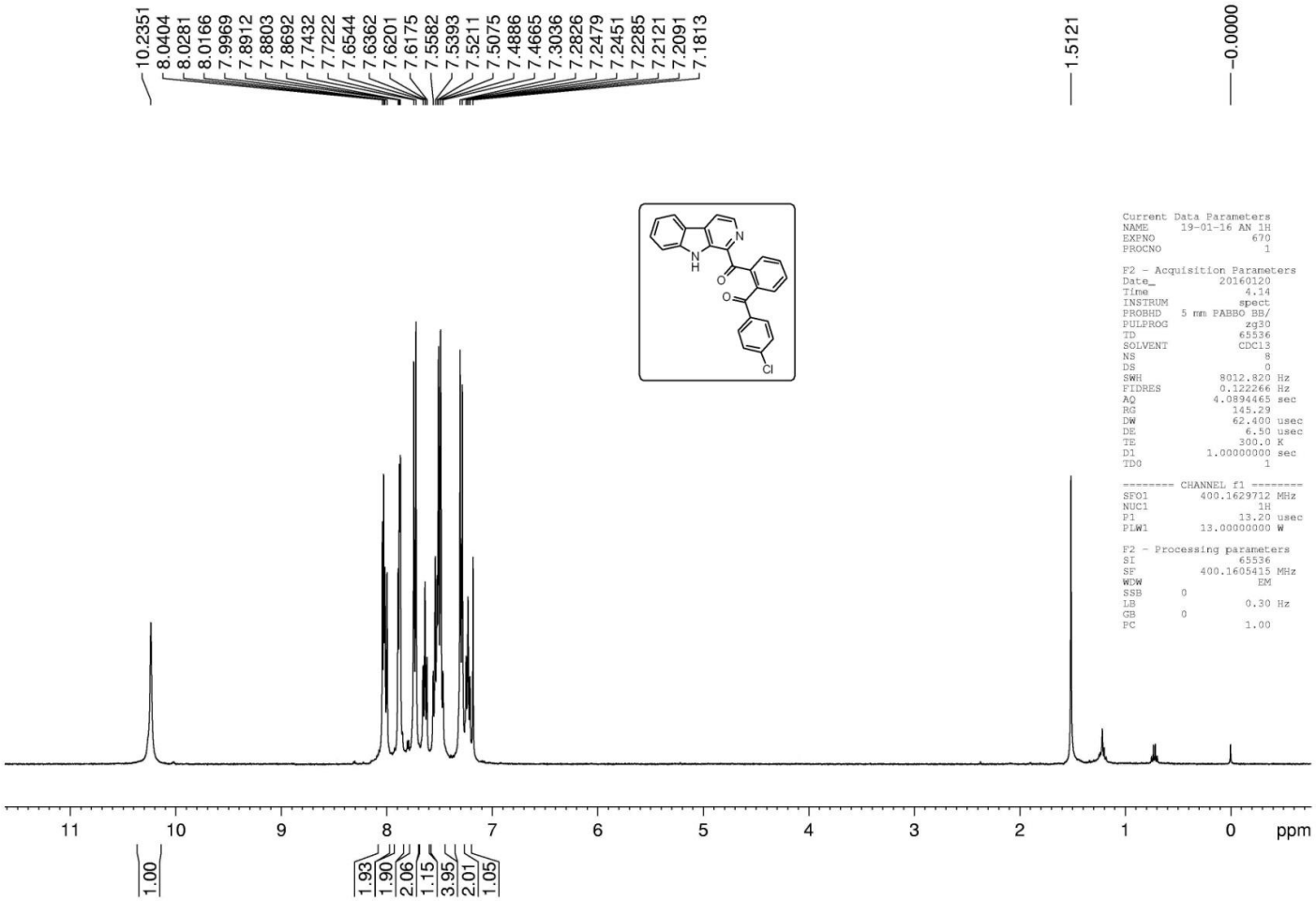



**Figure.** S-5**:** [1]H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(4-chlorophenyl)methanone **(3ac)**.

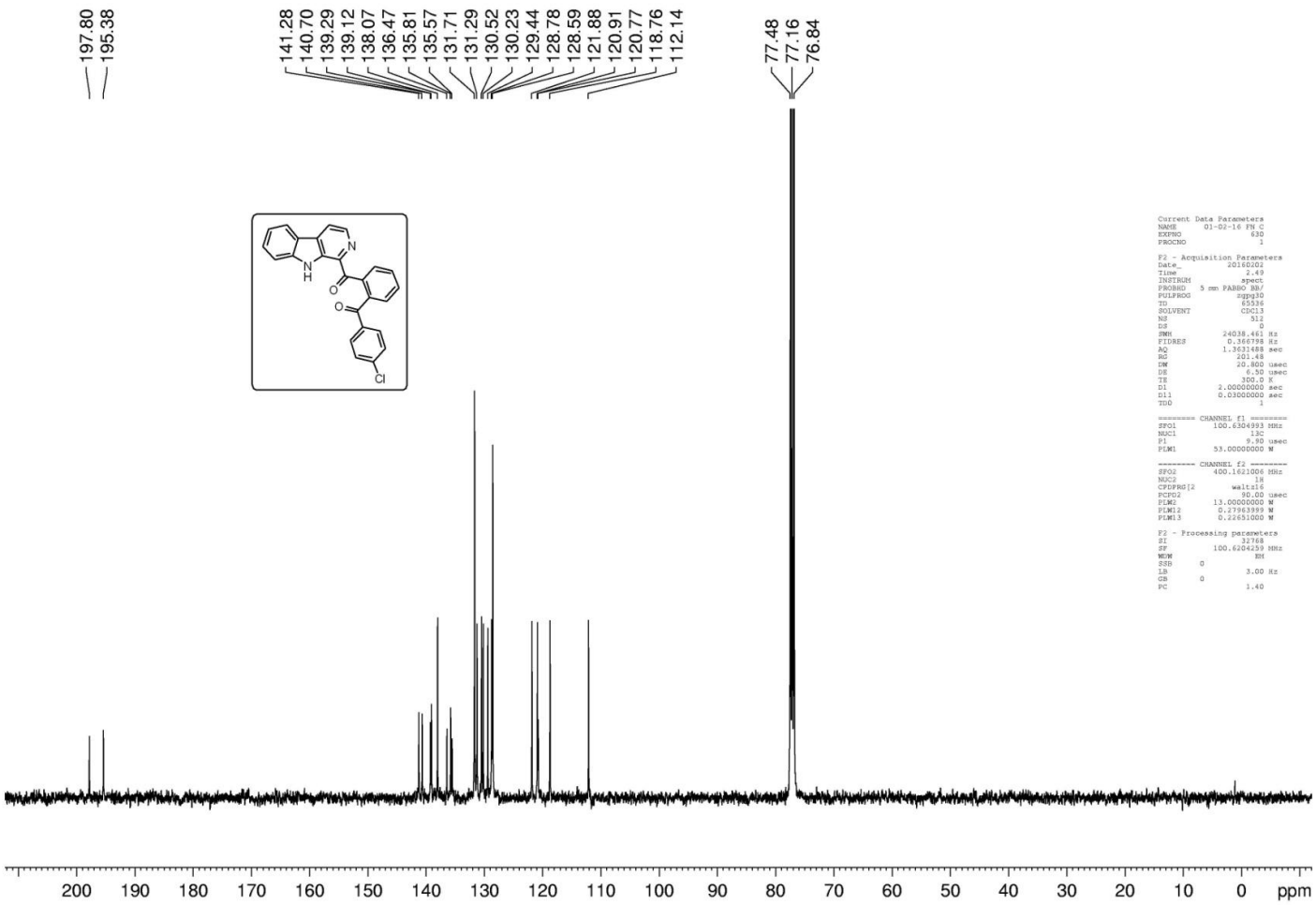



**Figure.** S-6**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(4-chlorophenyl)methanone **(3ac)**.

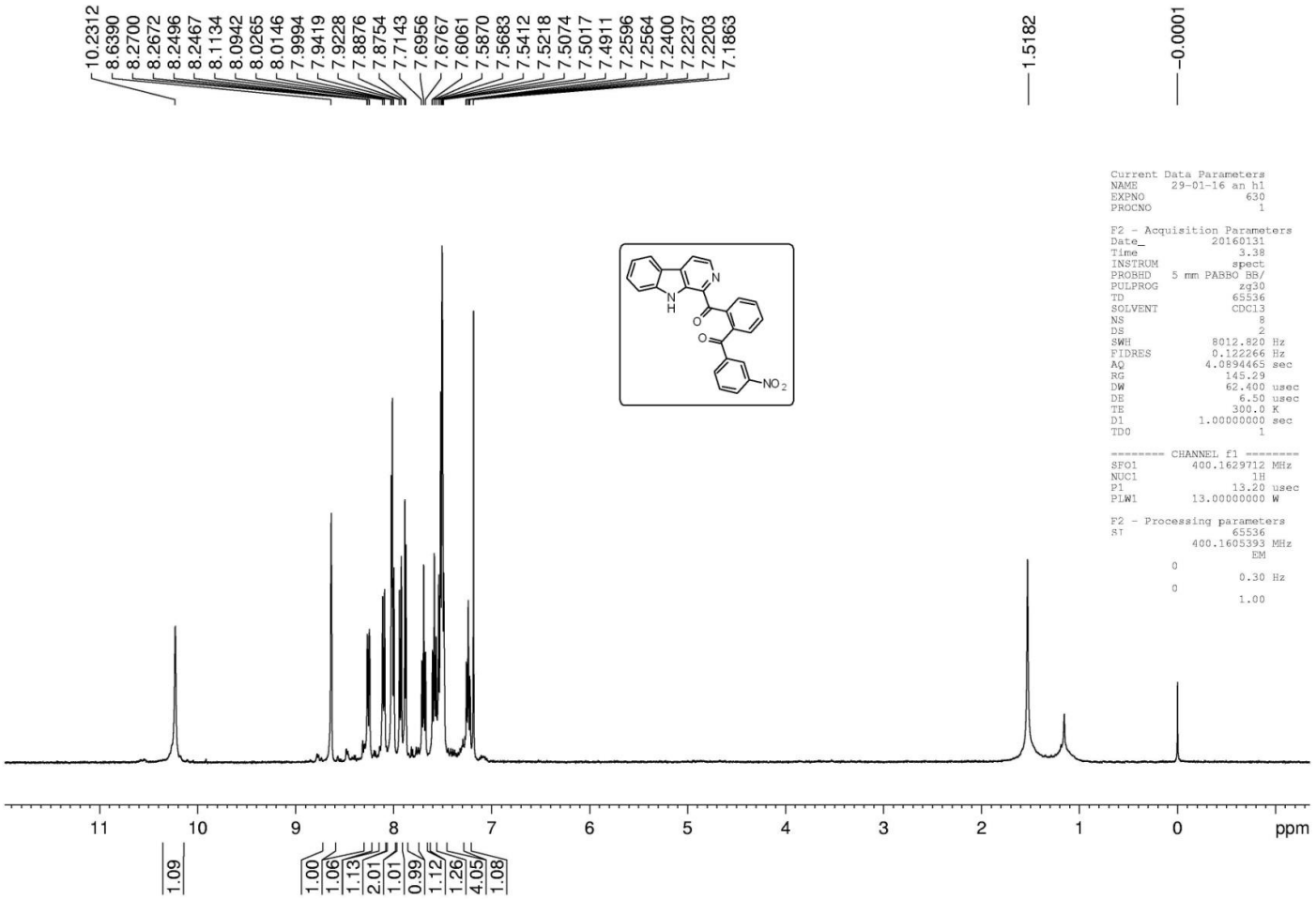



**Figure.** S-7**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(3-nitrophenyl)methanone **(3ad)**.

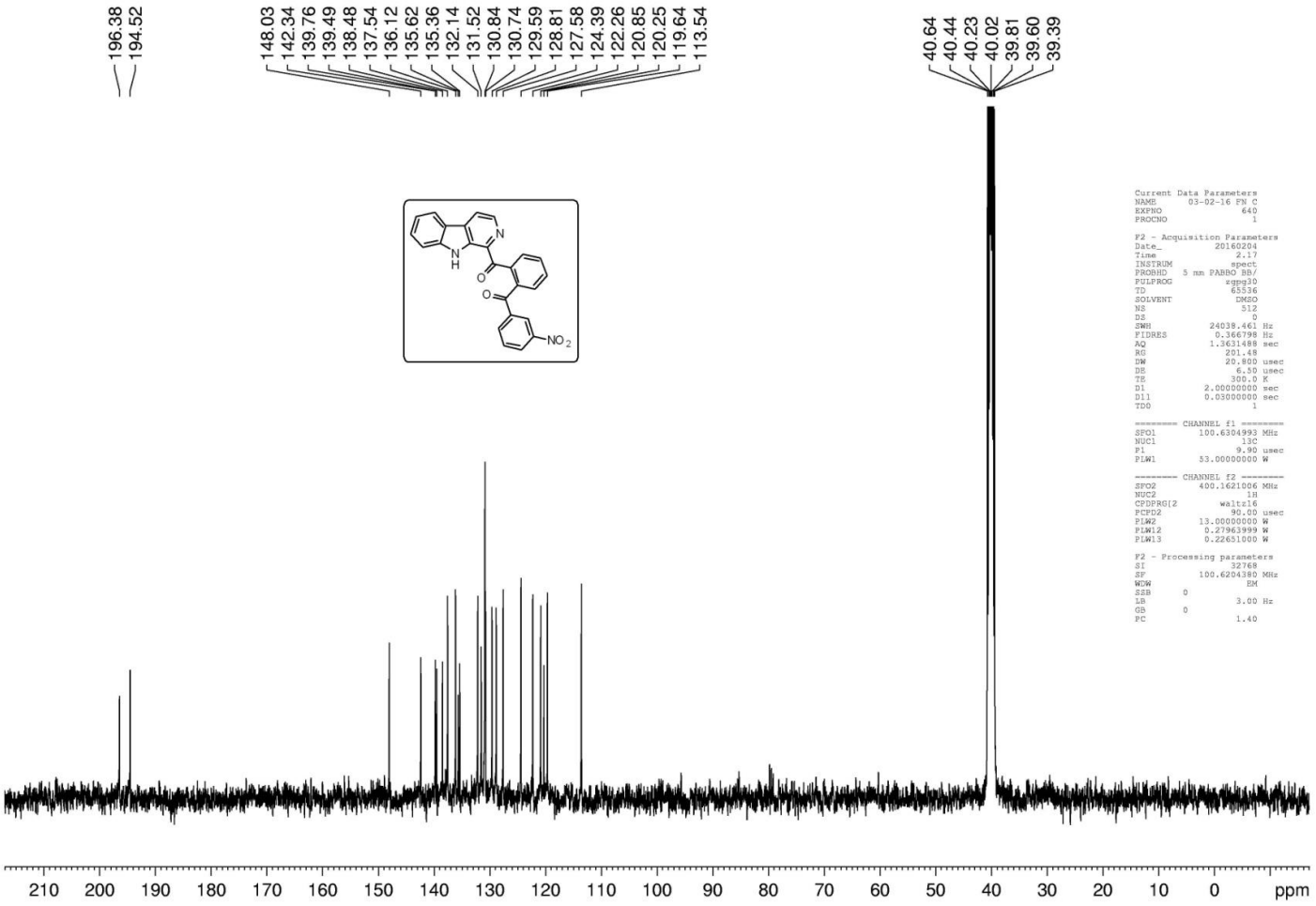



**Figure.** S-8**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(3-nitrophenyl)methanone **(3ad)**.

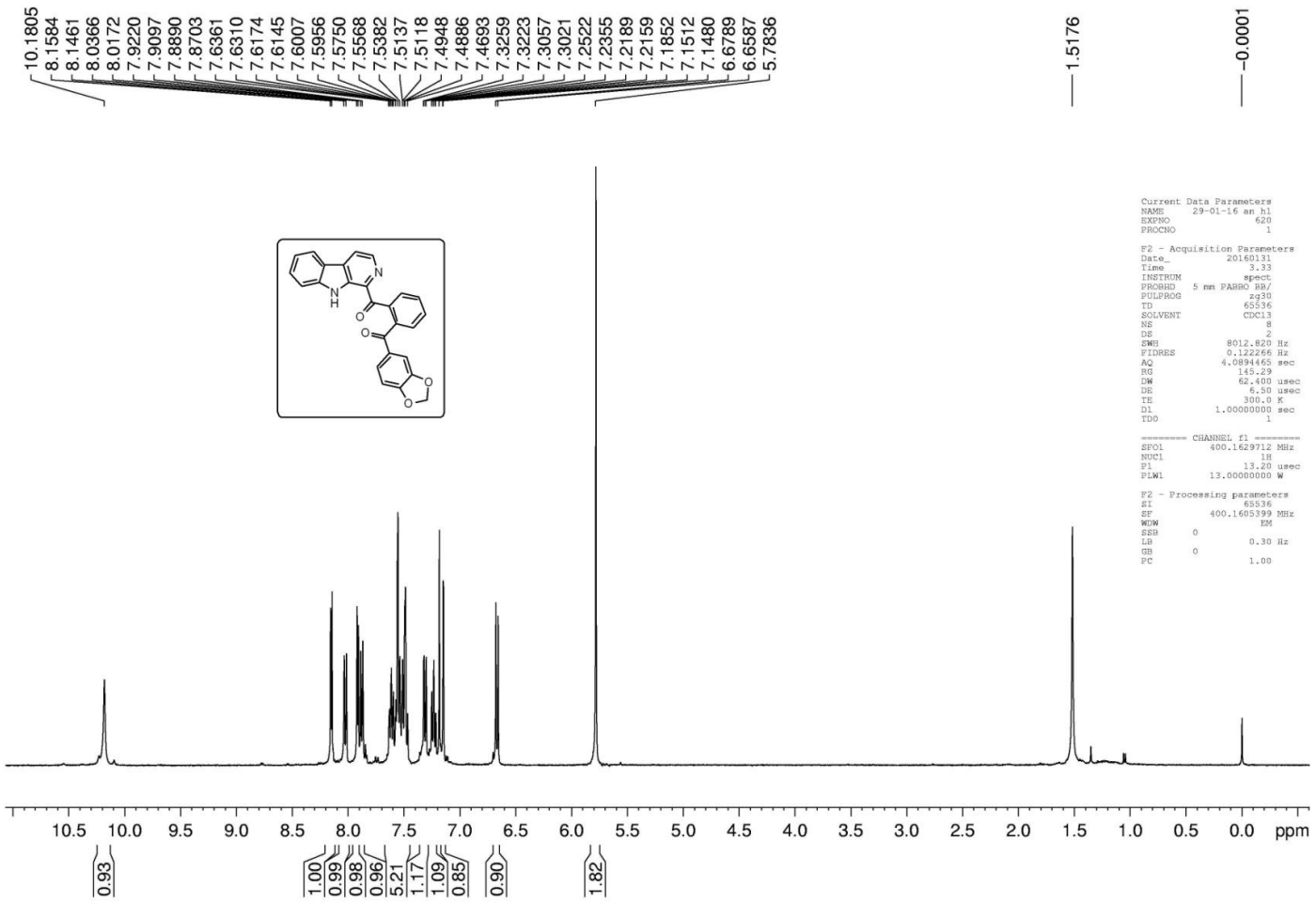



**Figure.** S-9**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(benzo[d][1,3]dioxol-5-yl)methanone **(3ae)**.

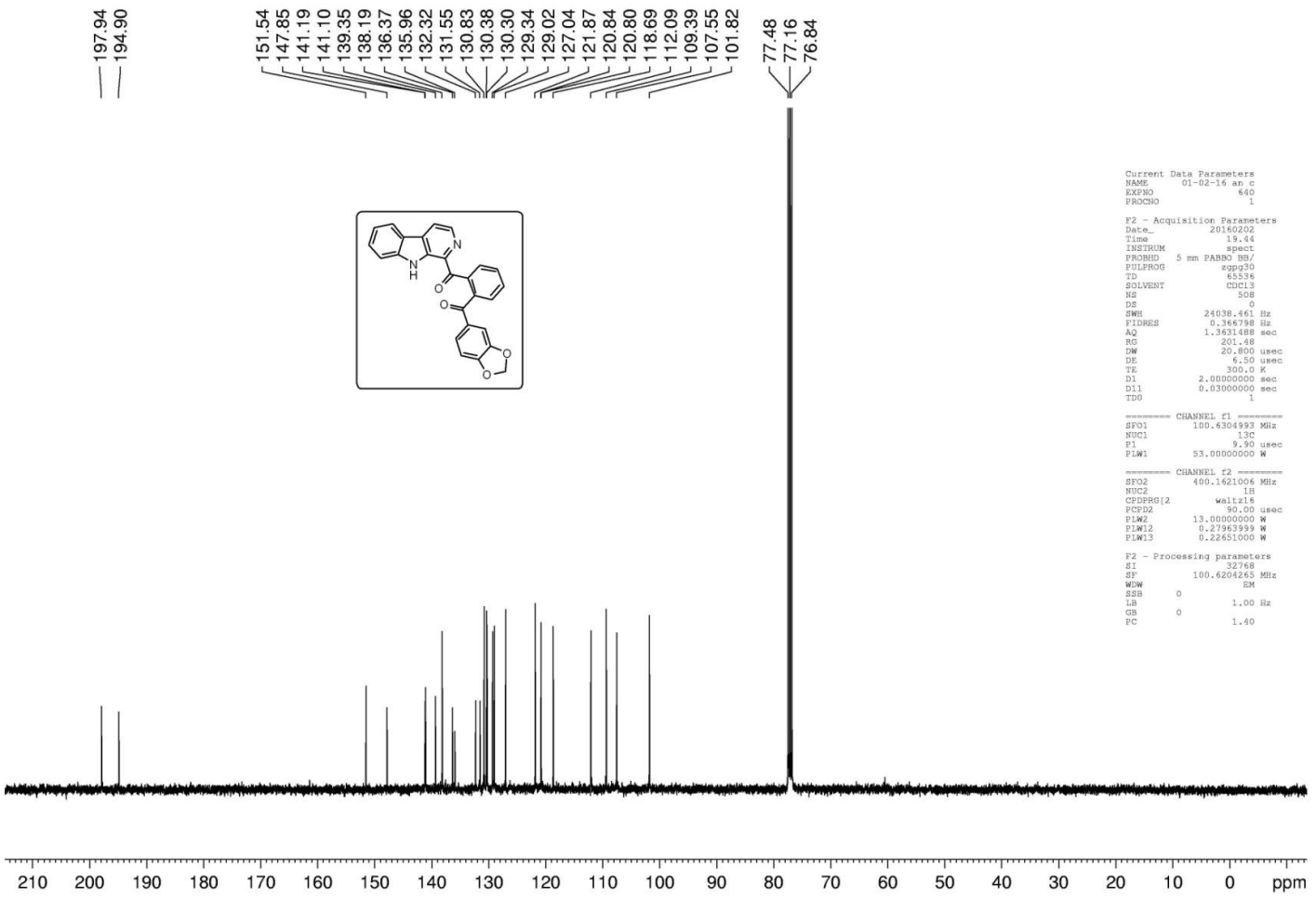



**Figure.** S-10**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(benzo[d][1,3]dioxol-5-yl)methanone **(3ae)**.

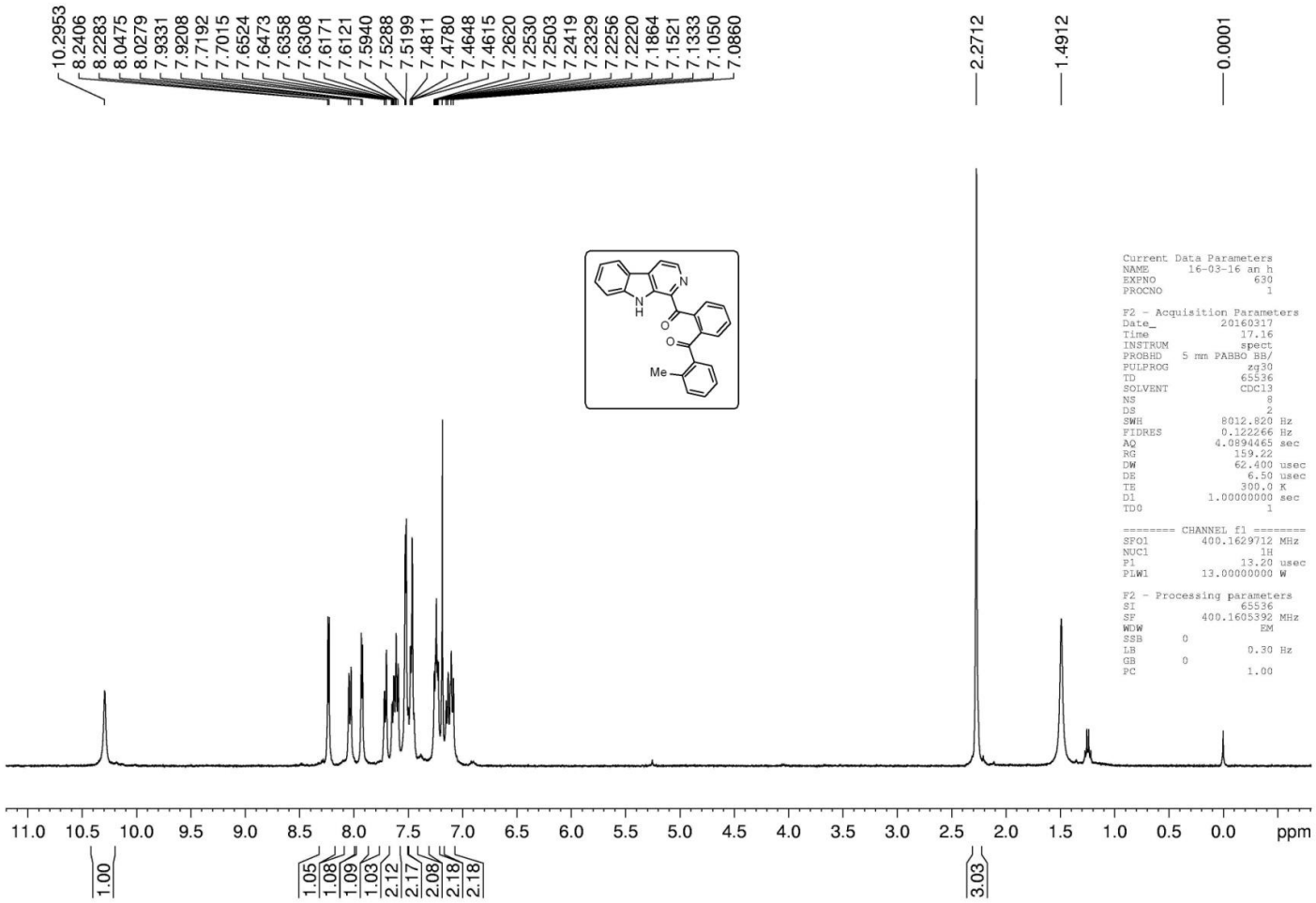



**Figure.** S-11**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(o-tolyl)methanone **(3af)**.

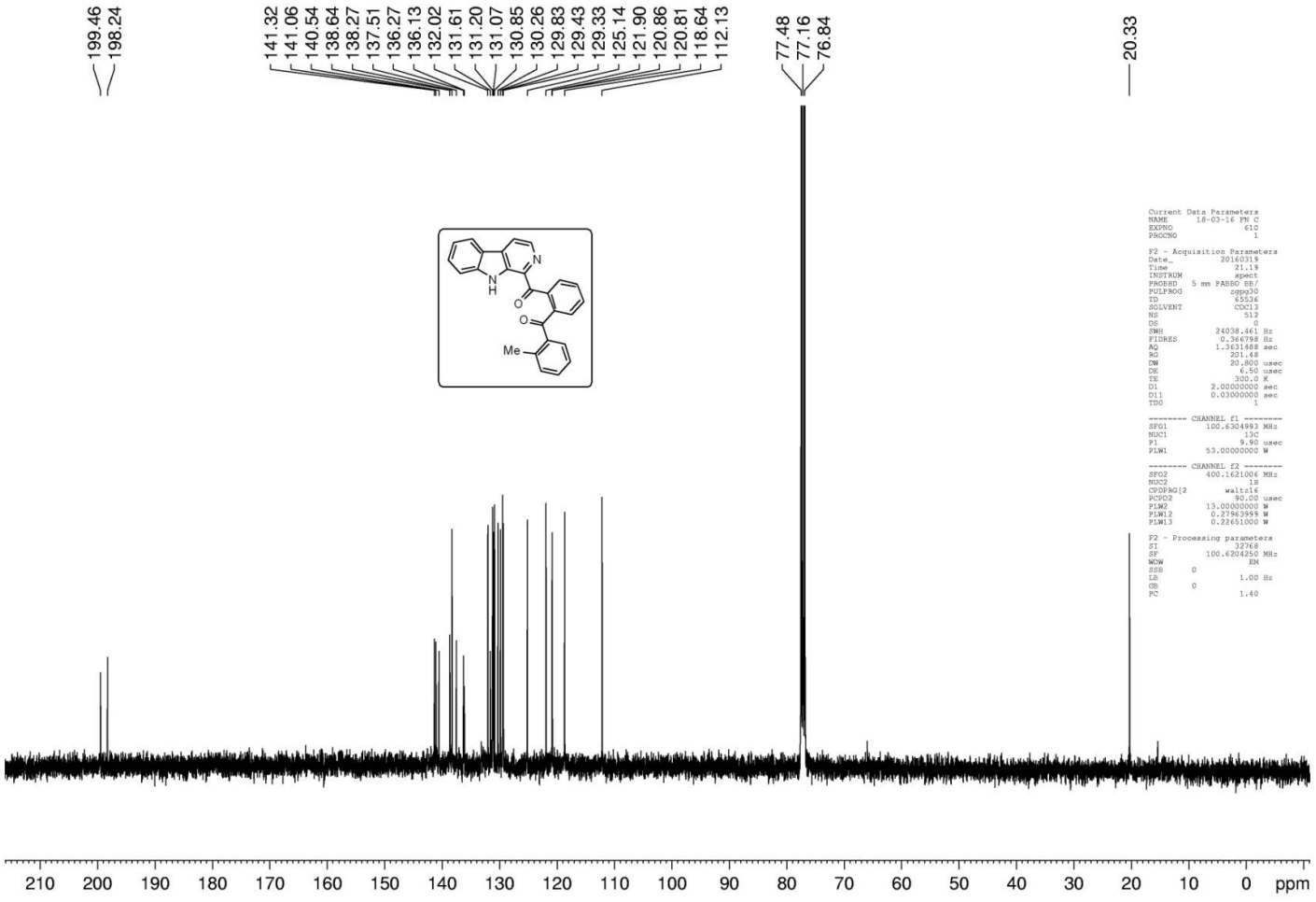



**Figure.** S-12**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(o-tolyl)methanone **(3af)**.

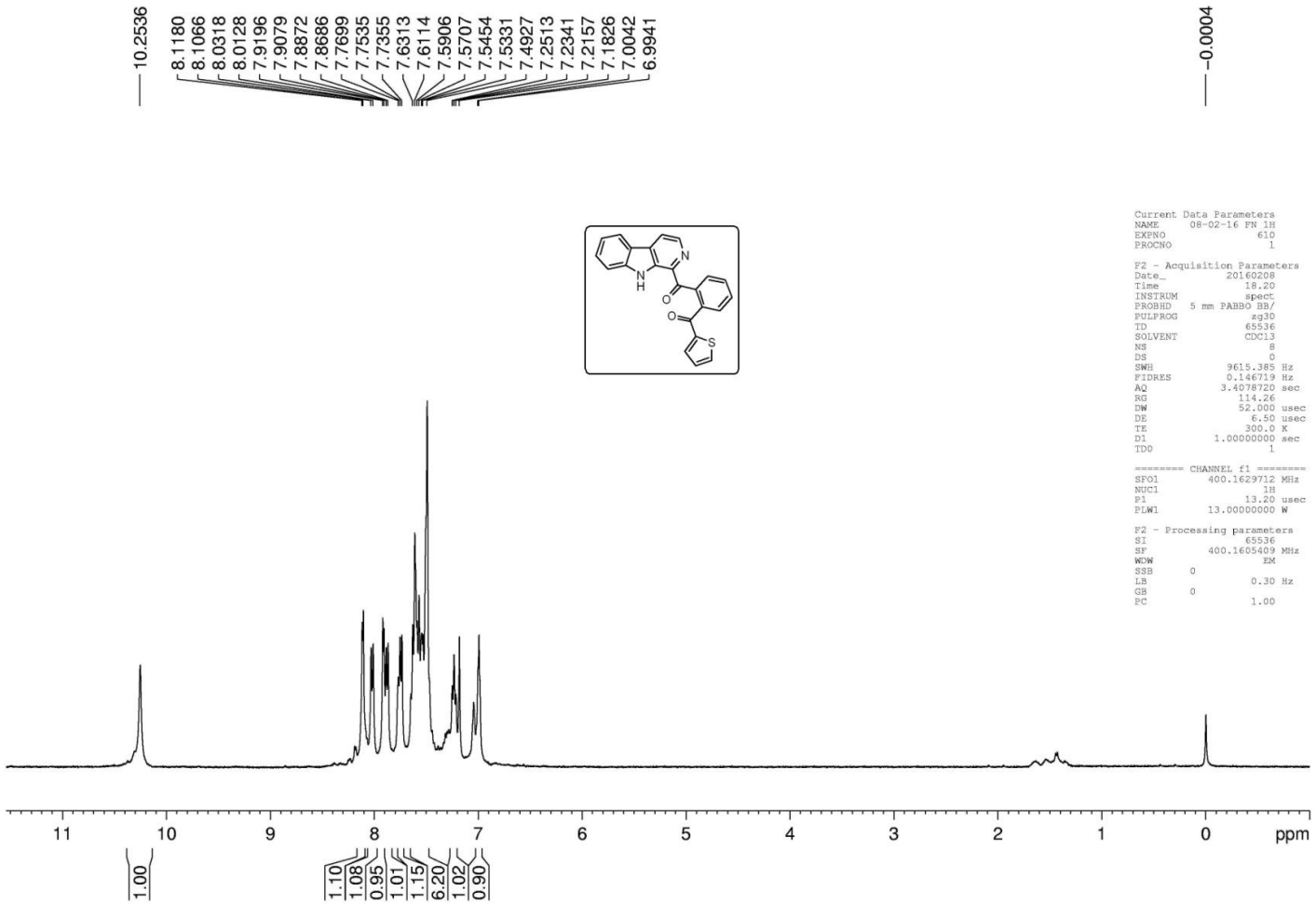



**Figure.** S-13**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(thiophen-2-yl)methanone **(3ag)**.

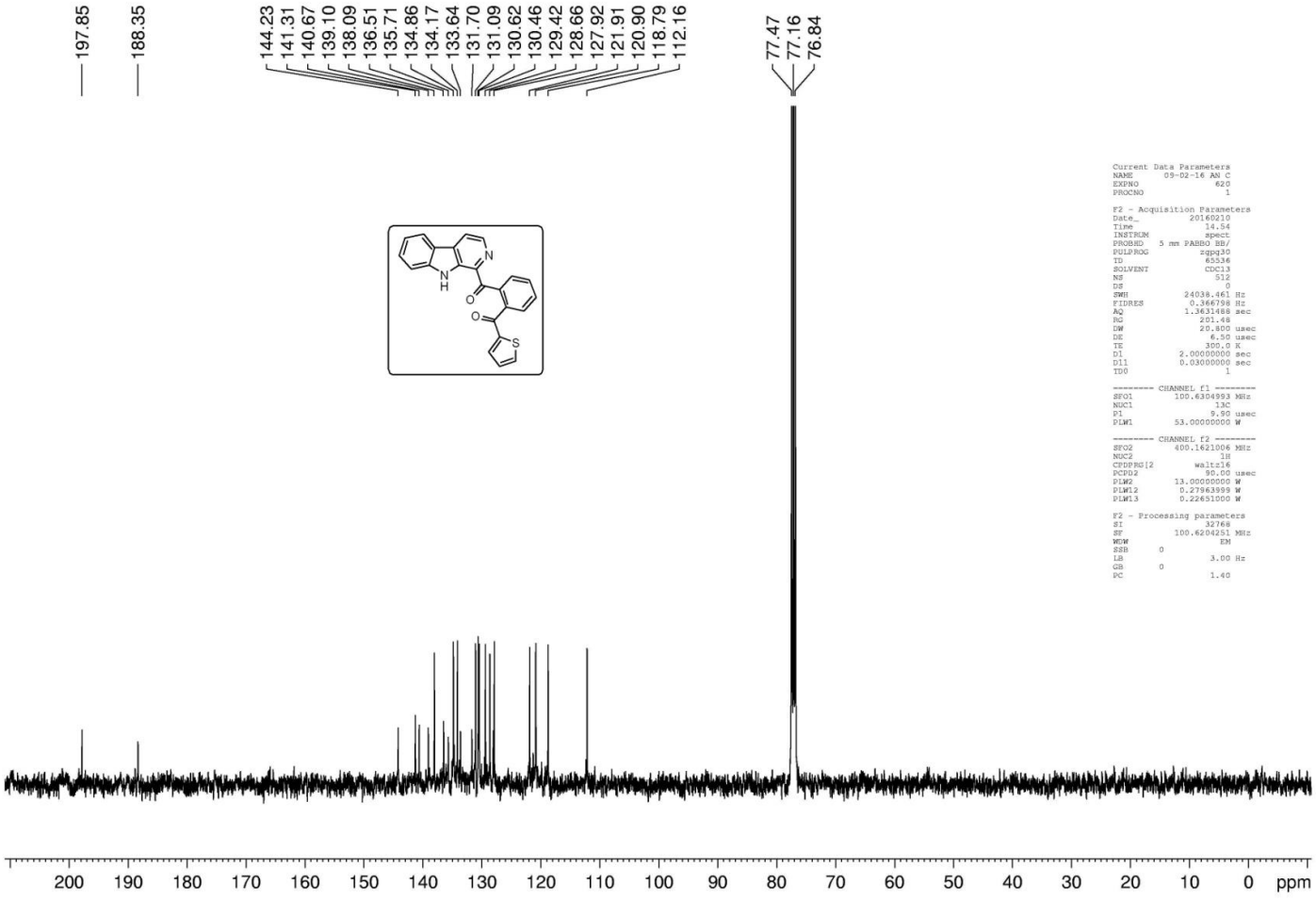



**Figure.** S-14**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)phenyl)(thiophen-2-yl)methanone **(3ag)**.

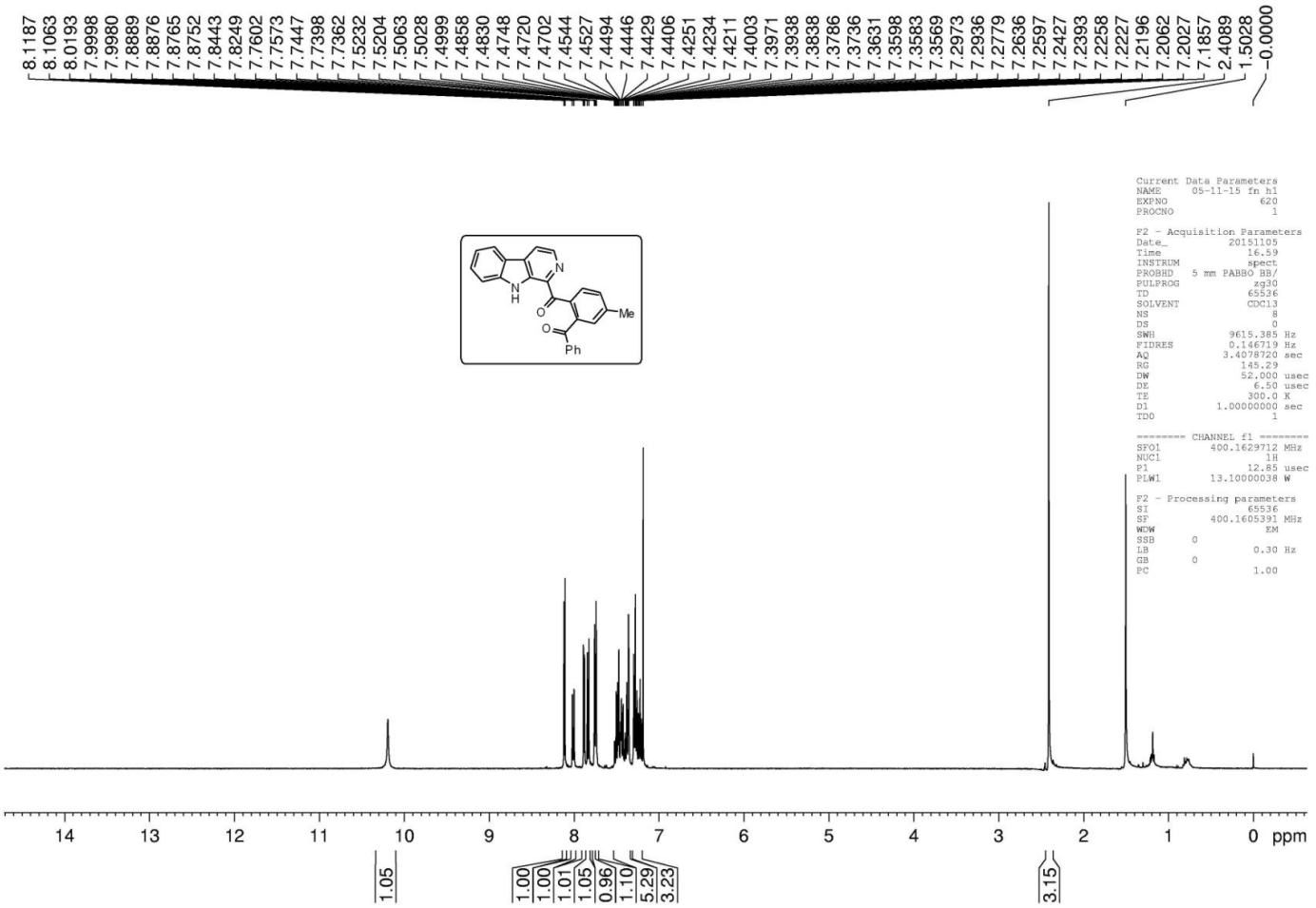



**Figure.** S-15**:** $^{1}$H-NMR spectrum of (2-Benzoyl-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ba)**.

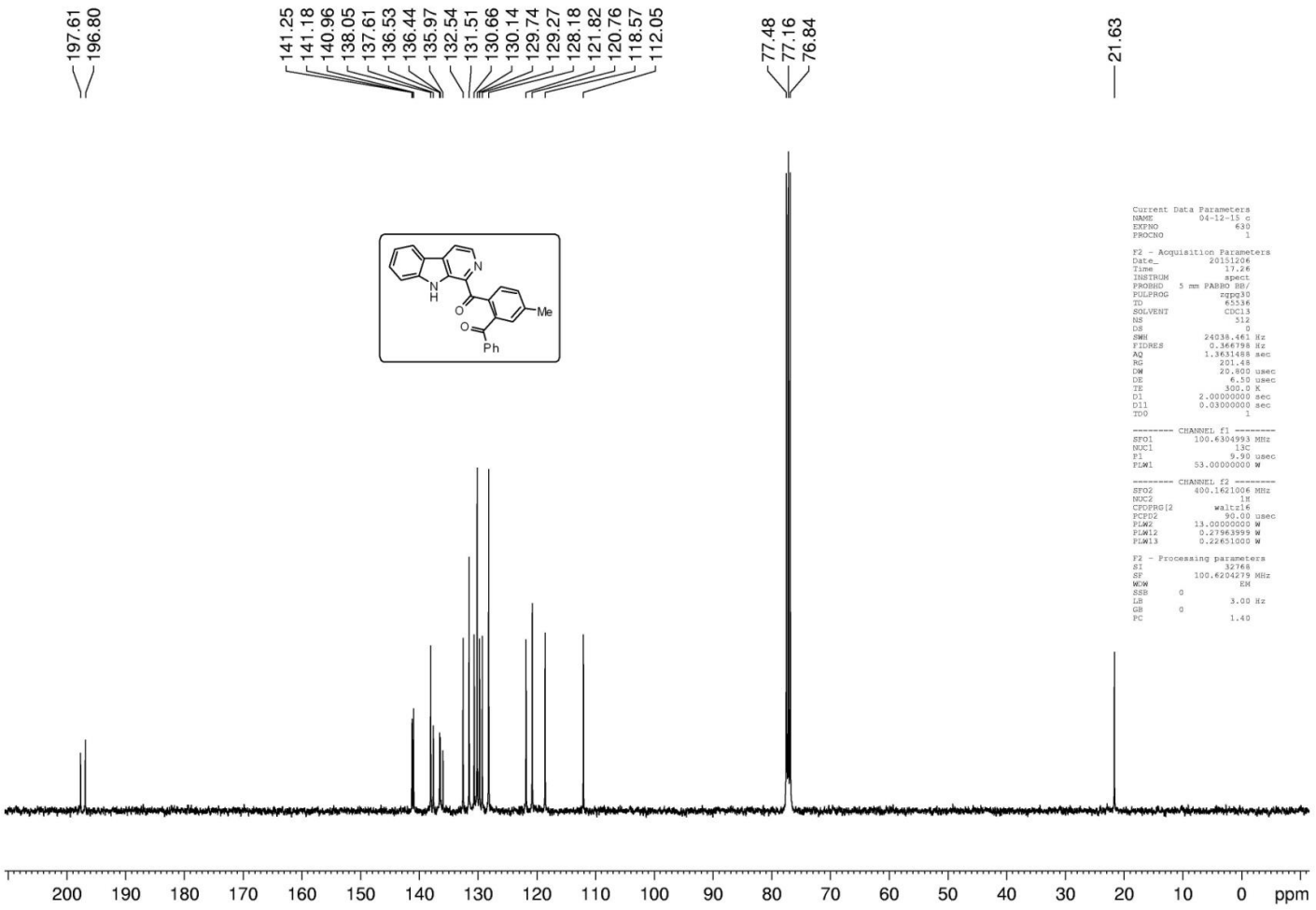



**Figure.** S-16**:** $^{13}$C-NMR spectrum of (2-Benzoyl-4-methylphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ba)**.

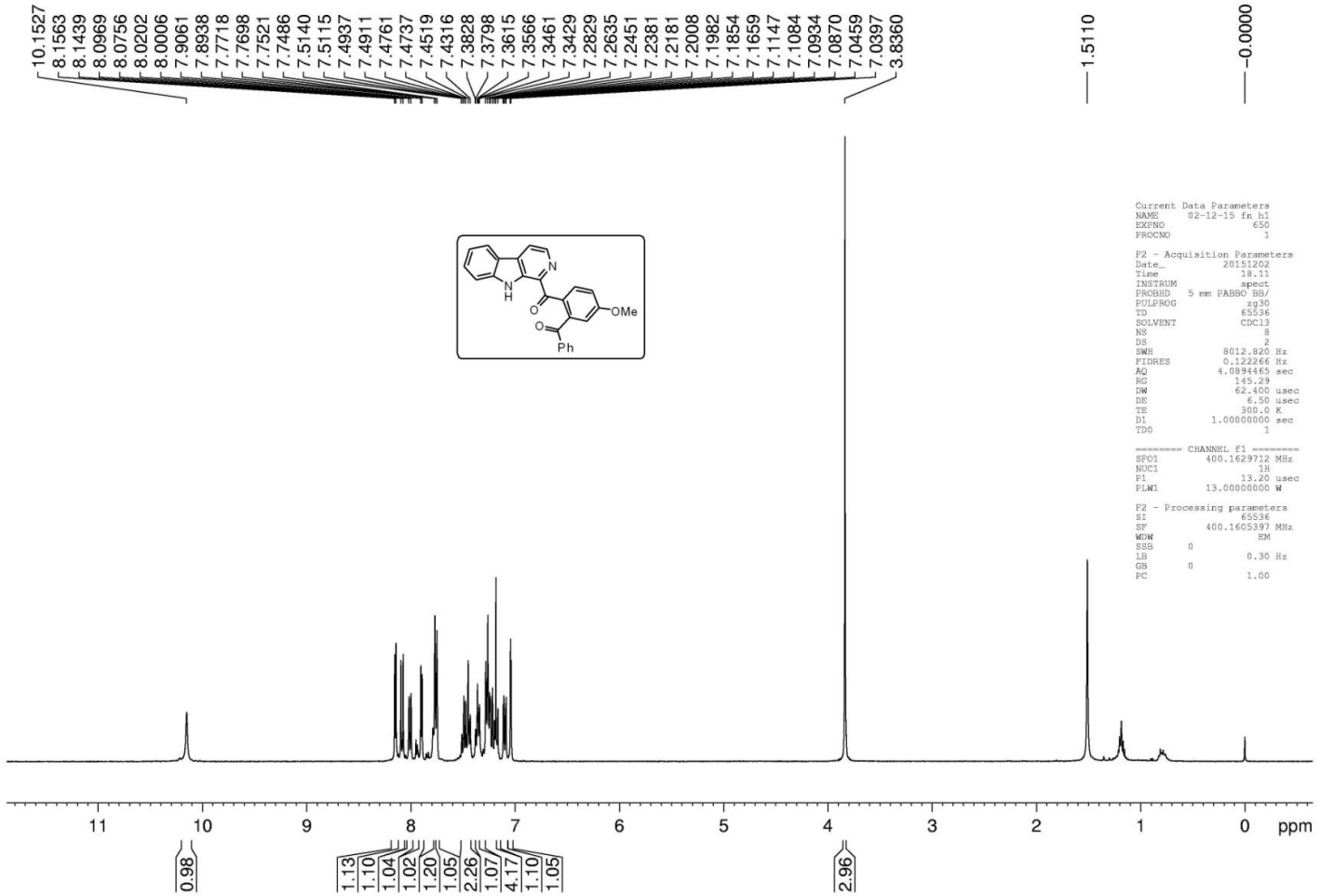



**Figure.** S-17**:** $^{1}$H-NMR spectrum of (2-Benzoyl-4-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ca).**

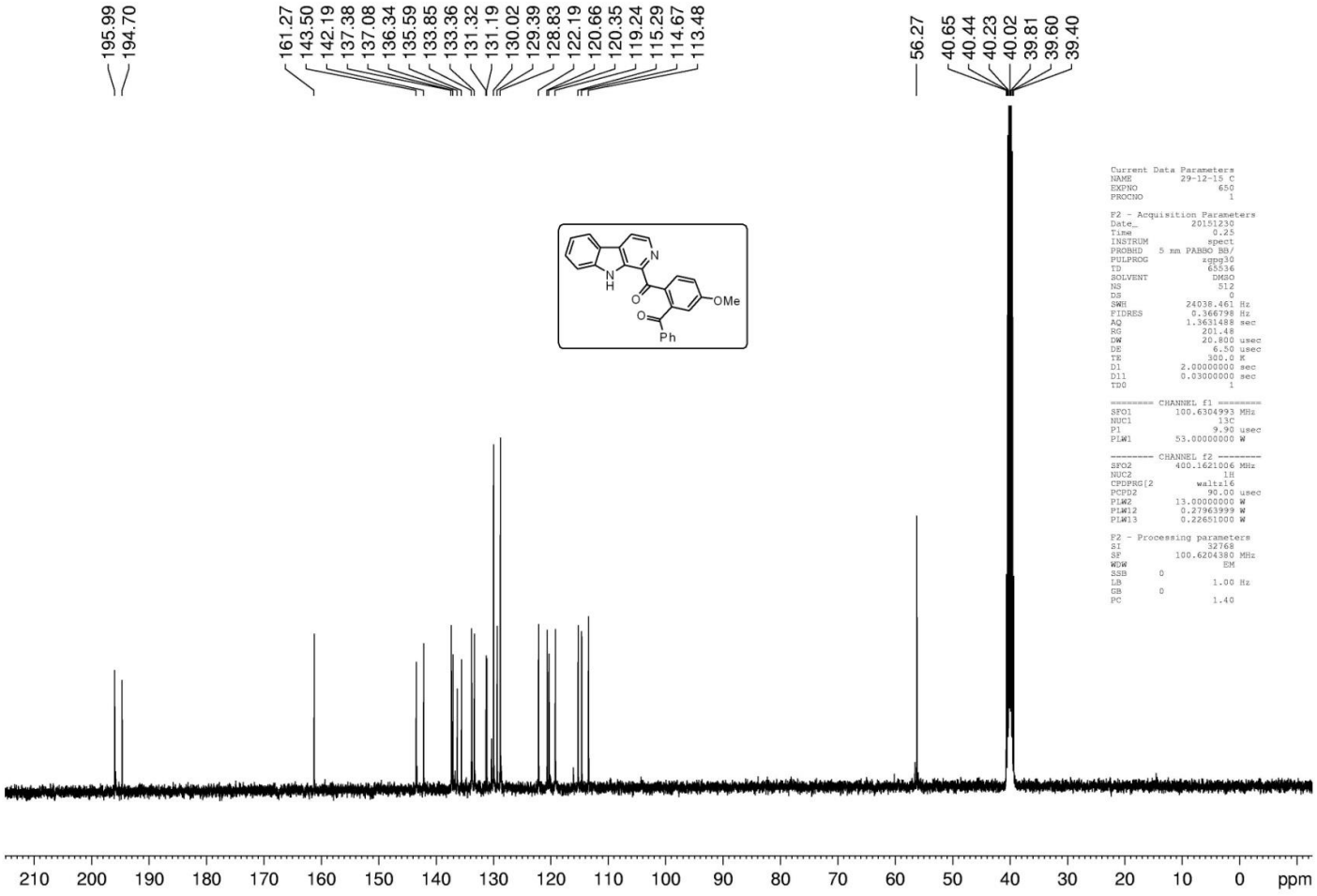



**Figure.** S-18**:** $^{13}$C-NMR spectrum of (2-Benzoyl-4-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ca).**

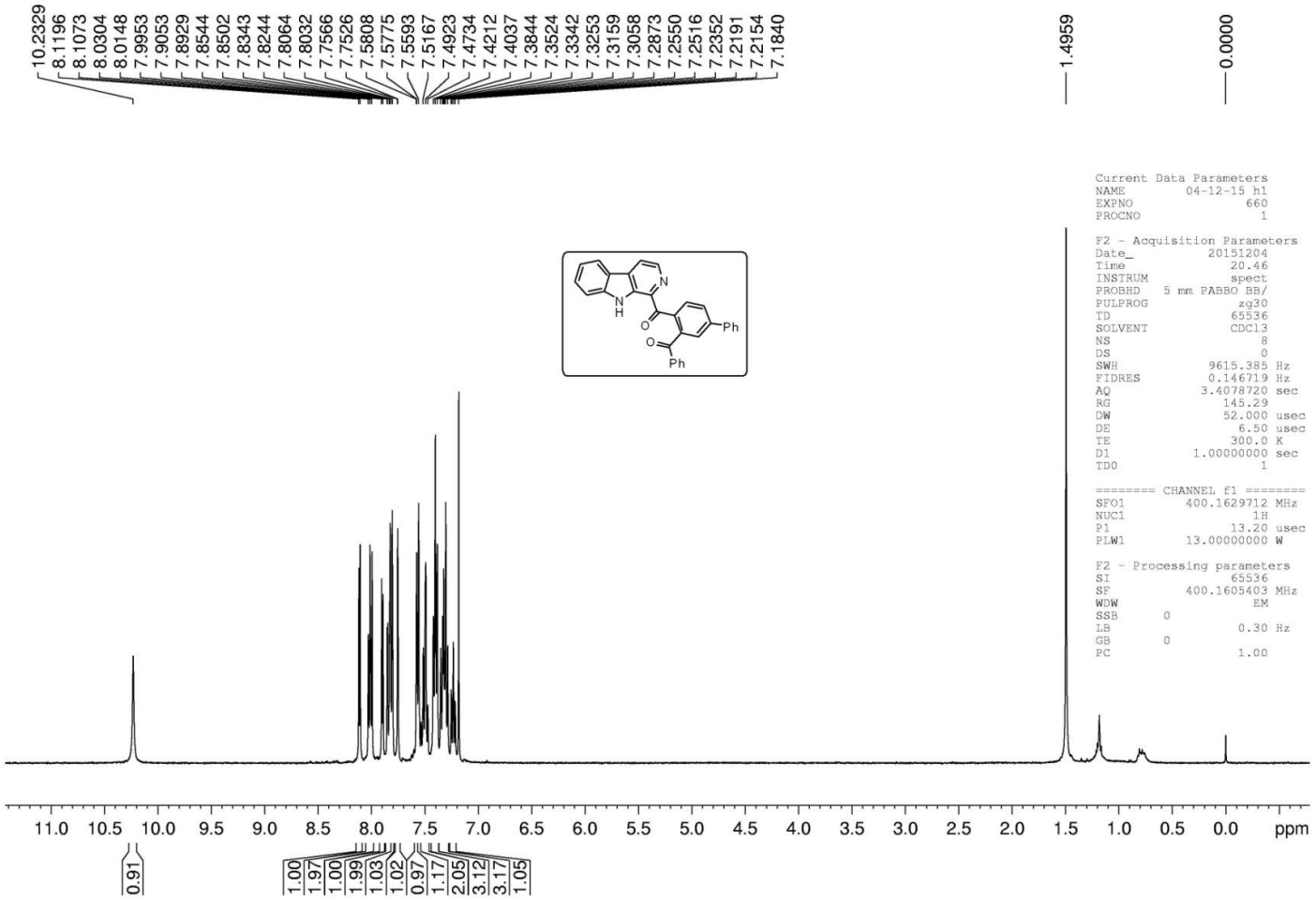



**Figure.** S-19**:** $^{1}$H-NMR spectrum of (4-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)-[1,1'-biphenyl]-3-yl)(phenyl)methanone **(3da)**.

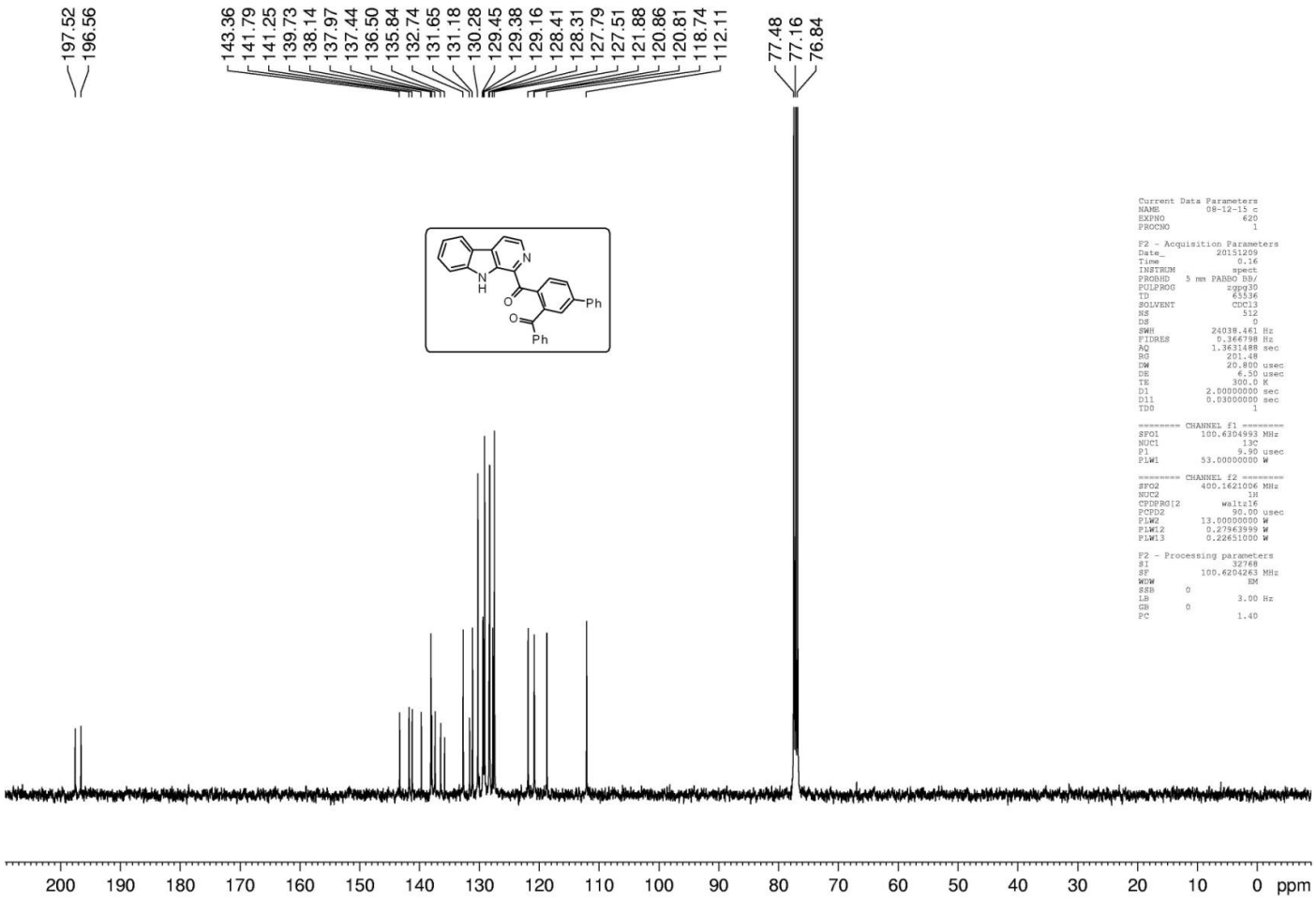



**Figure.** S-20**:** $^{13}$C-NMR spectrum of (4-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)-[1,1'-biphenyl]-3-yl)(phenyl)methanone **(3da)**.

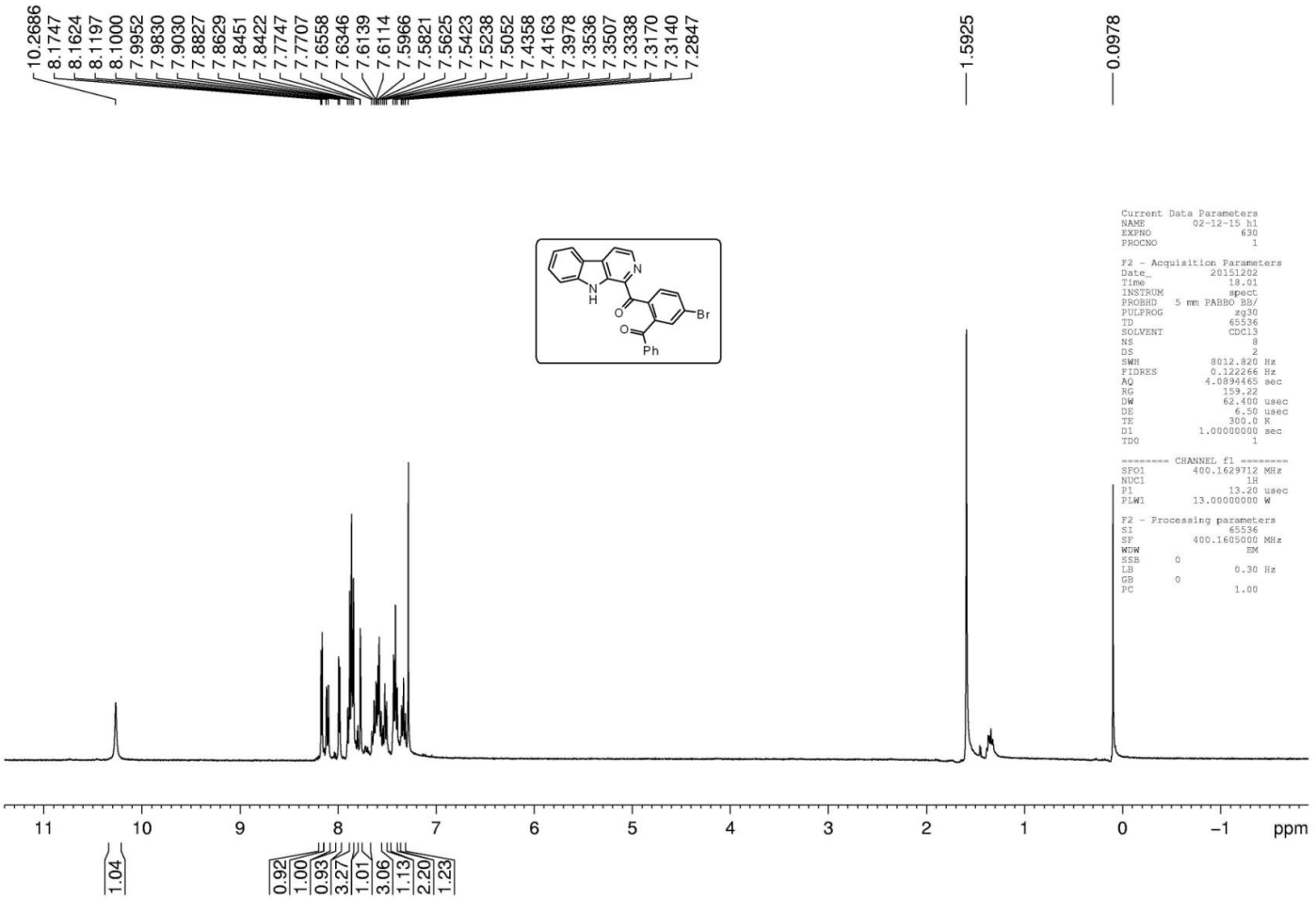



**Figure.** S-21**:** $^{1}$H-NMR spectrum of (2-Benzoyl-4-bromophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ea)**.

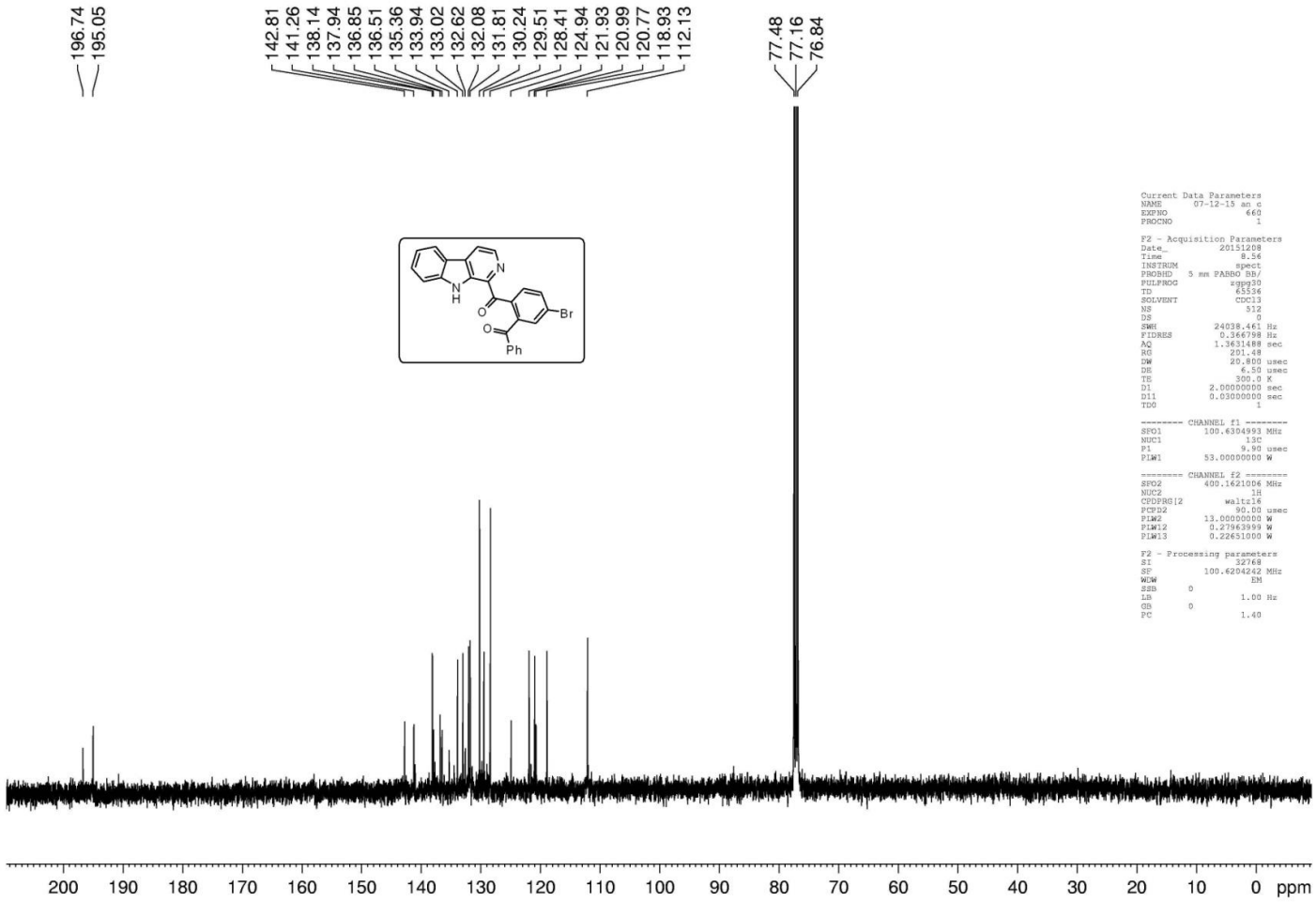



**Figure.** S-22**:** $^{13}$C-NMR spectrum of (2-Benzoyl-4-bromophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ea)**.

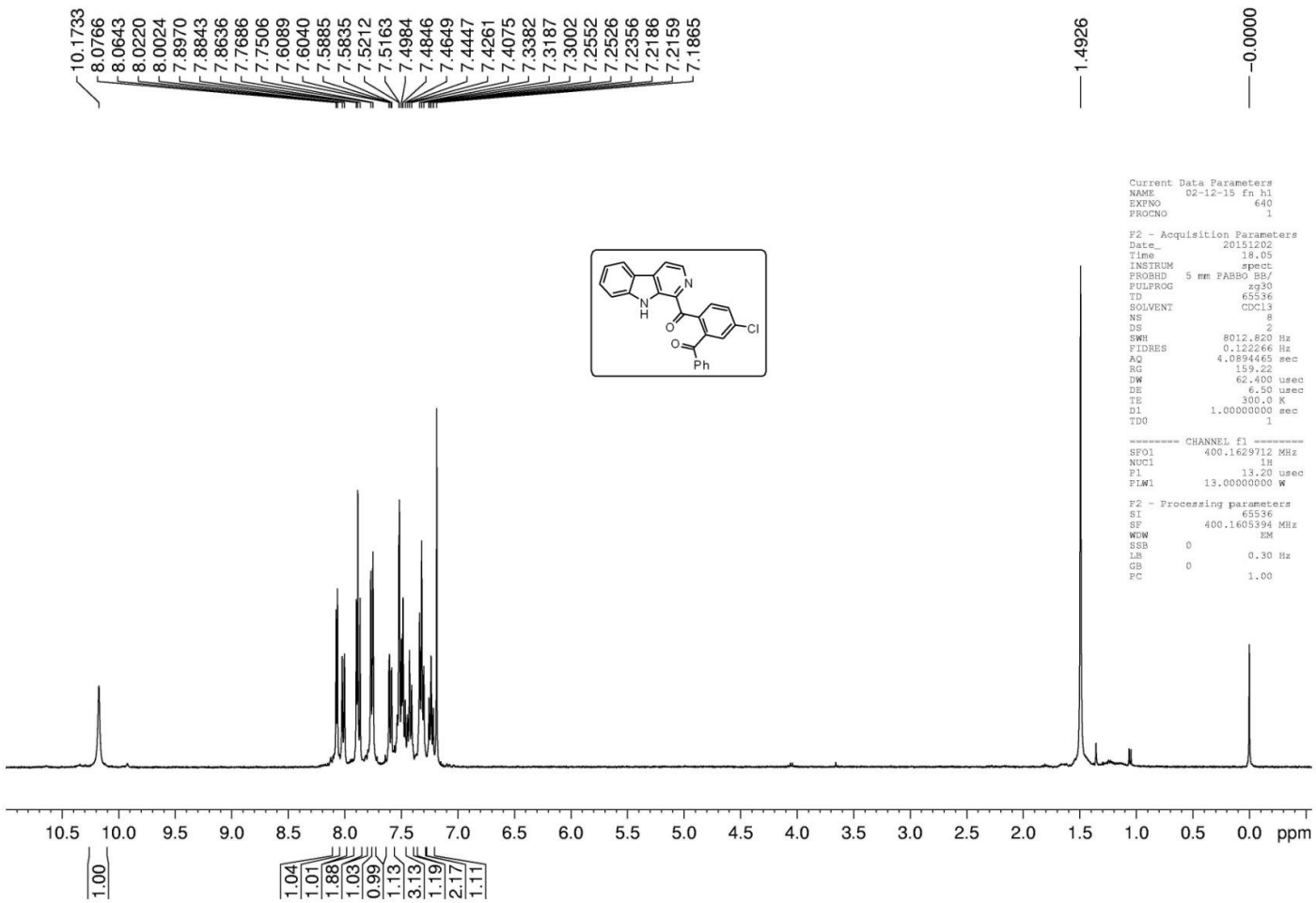



**Figure.** S-23**:** $^{1}$H-NMR spectrum of (2-Benzoyl-4-chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3fa)**.

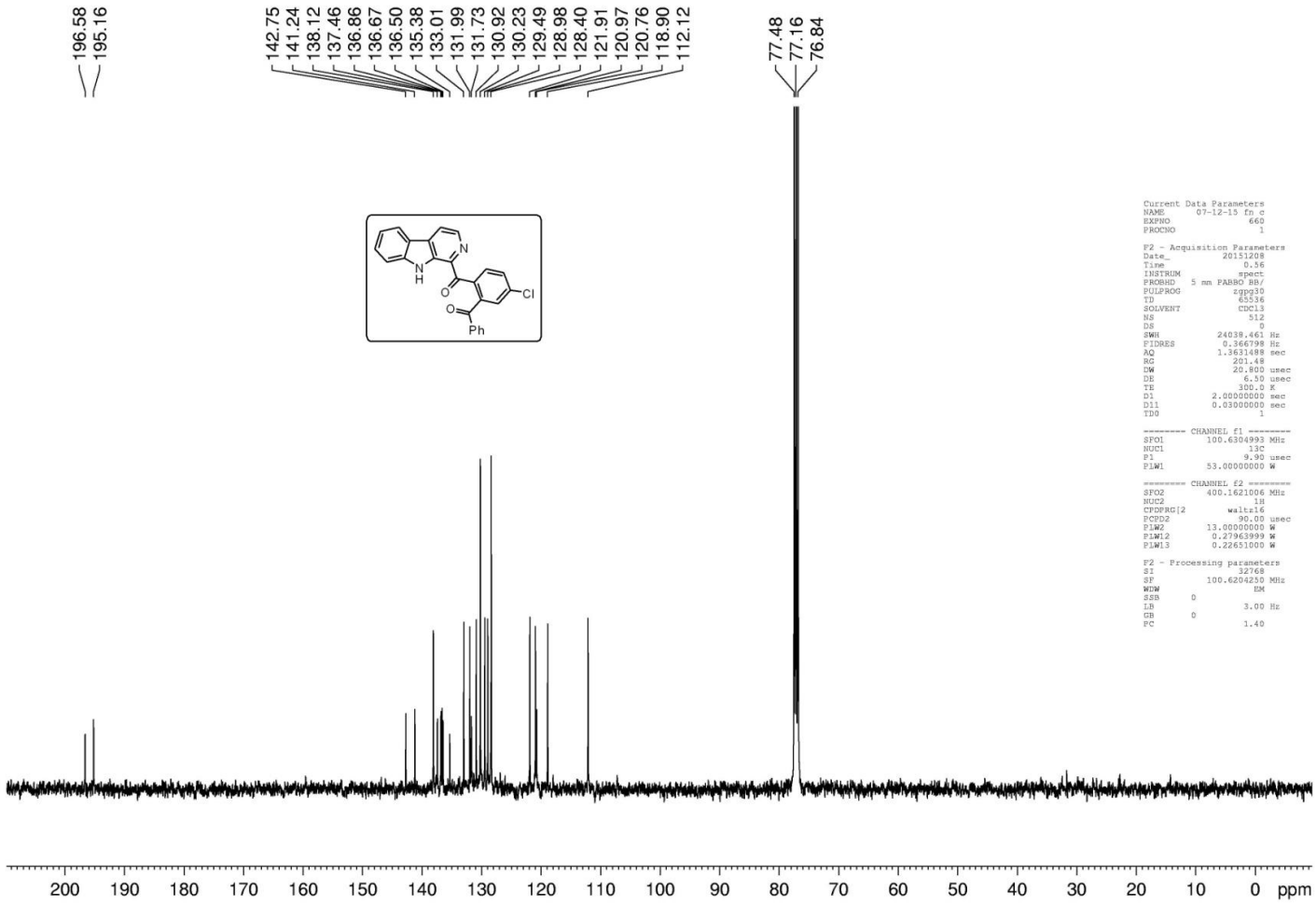



**Figure**. S-24**:** $^{13}$C-NMR spectrum of (2-Benzoyl-4-chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3fa)**.

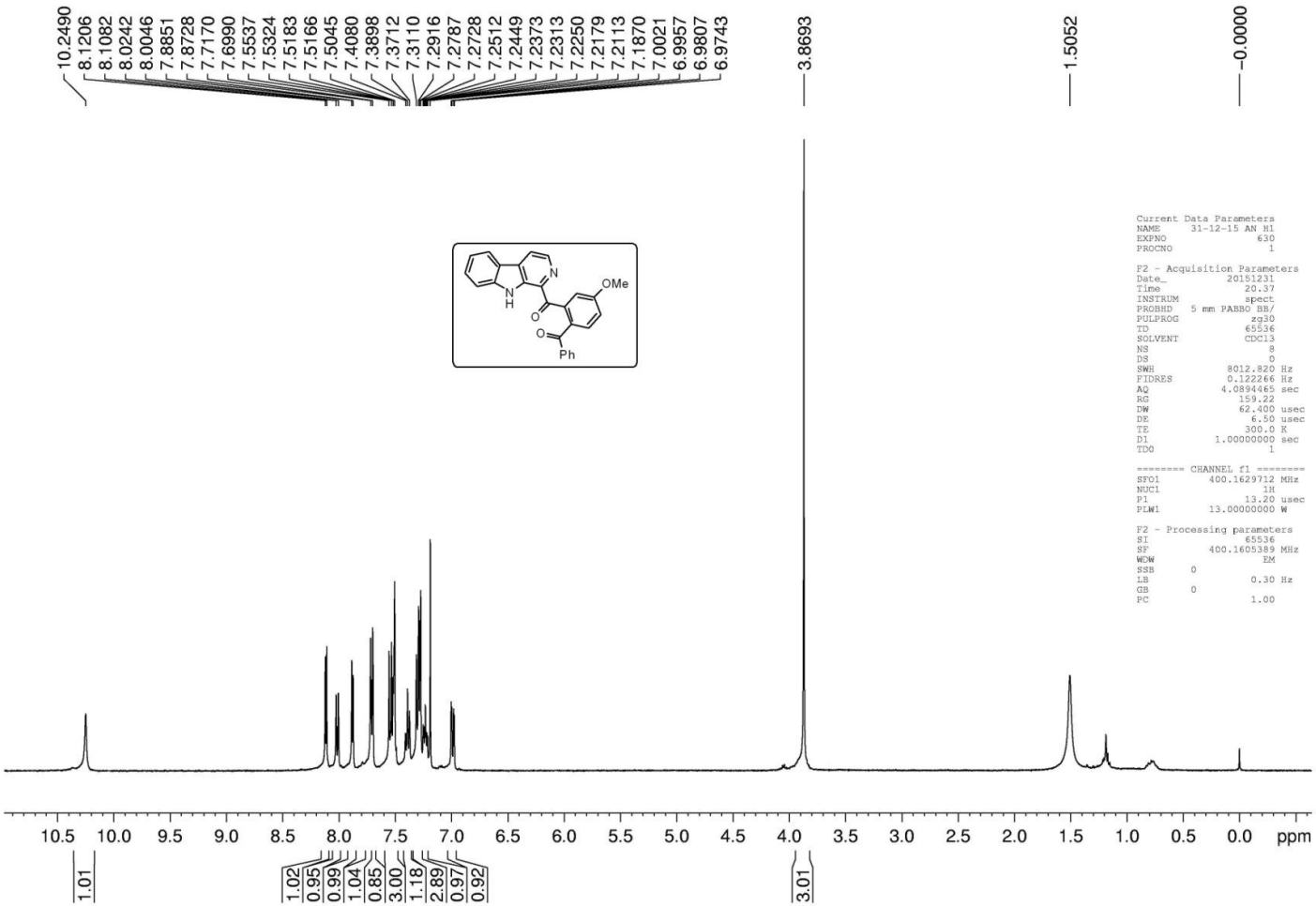



**Figure.** S-25**:** $^{1}$H-NMR spectrum of (2-Benzoyl-5-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ga)**.

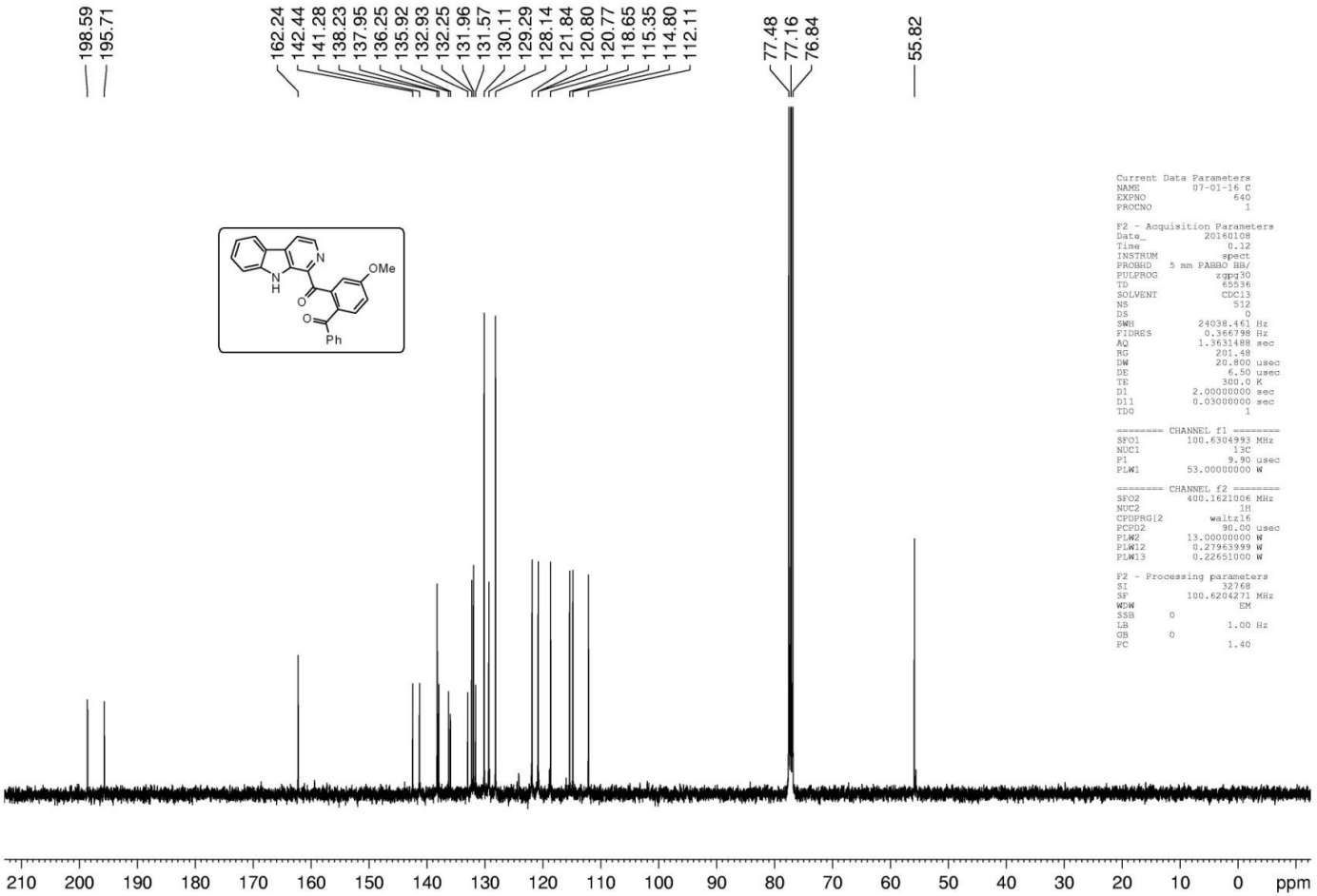



**Figure.** S-26**:** $^{13}$C-NMR spectrum of (2-Benzoyl-5-methoxyphenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ga)**.

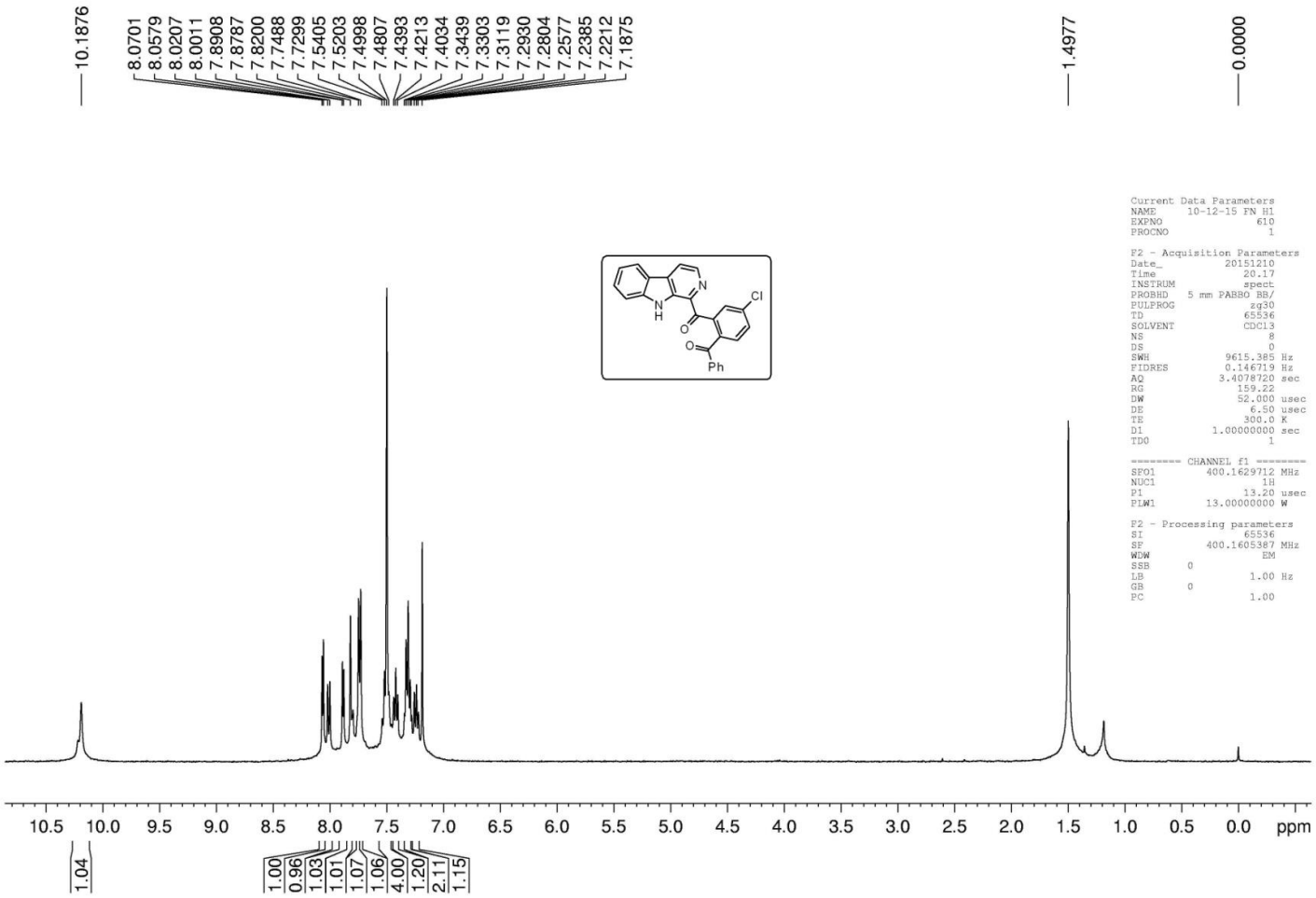



**Figure.** S-27**:** $^{1}$H-NMR spectrum of (2-Benzoyl-5-chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ha)**.

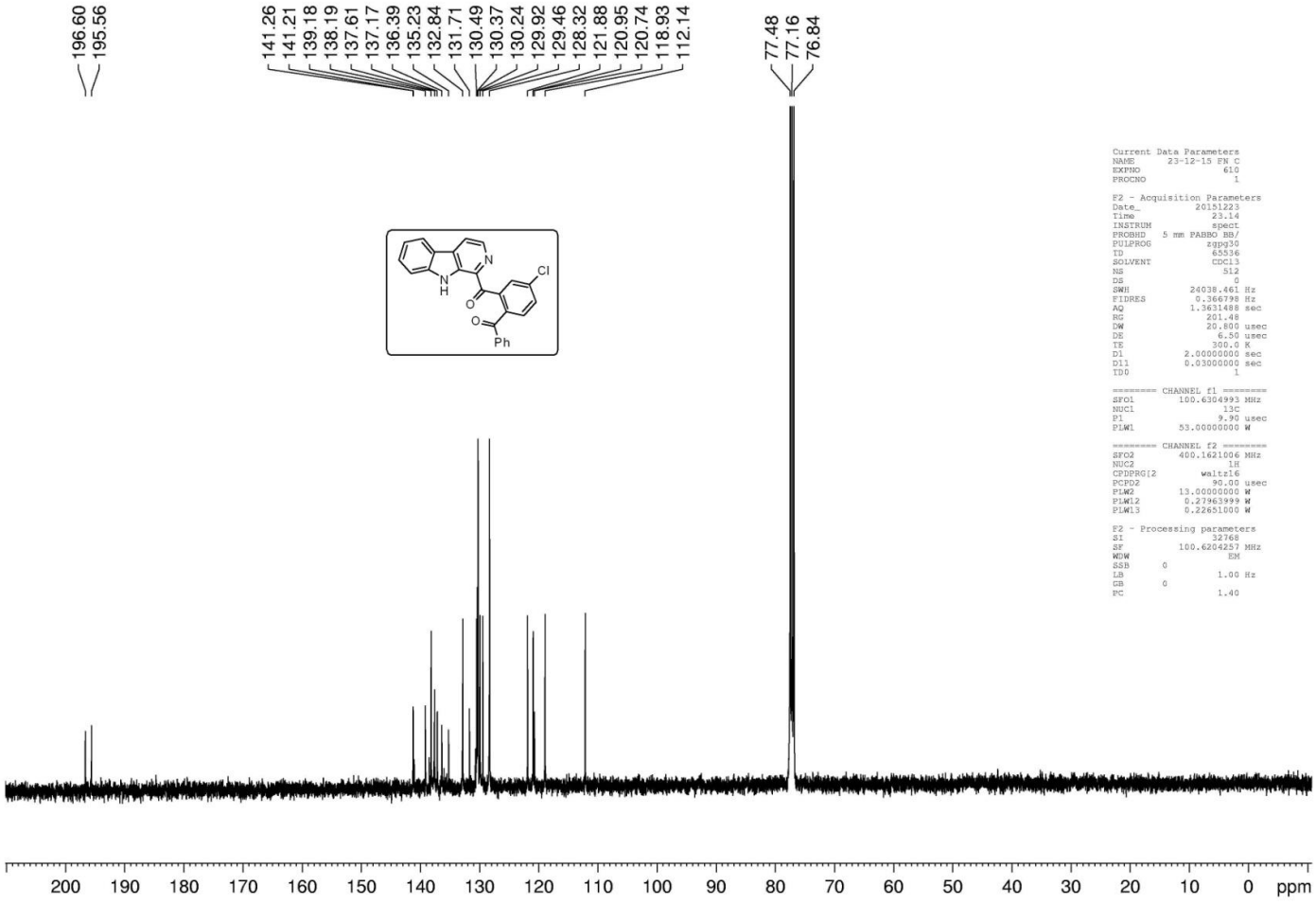



**Figure.** S-28**:** $^{13}$C-NMR spectrum of (2-Benzoyl-5-chlorophenyl)(9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ha)**.

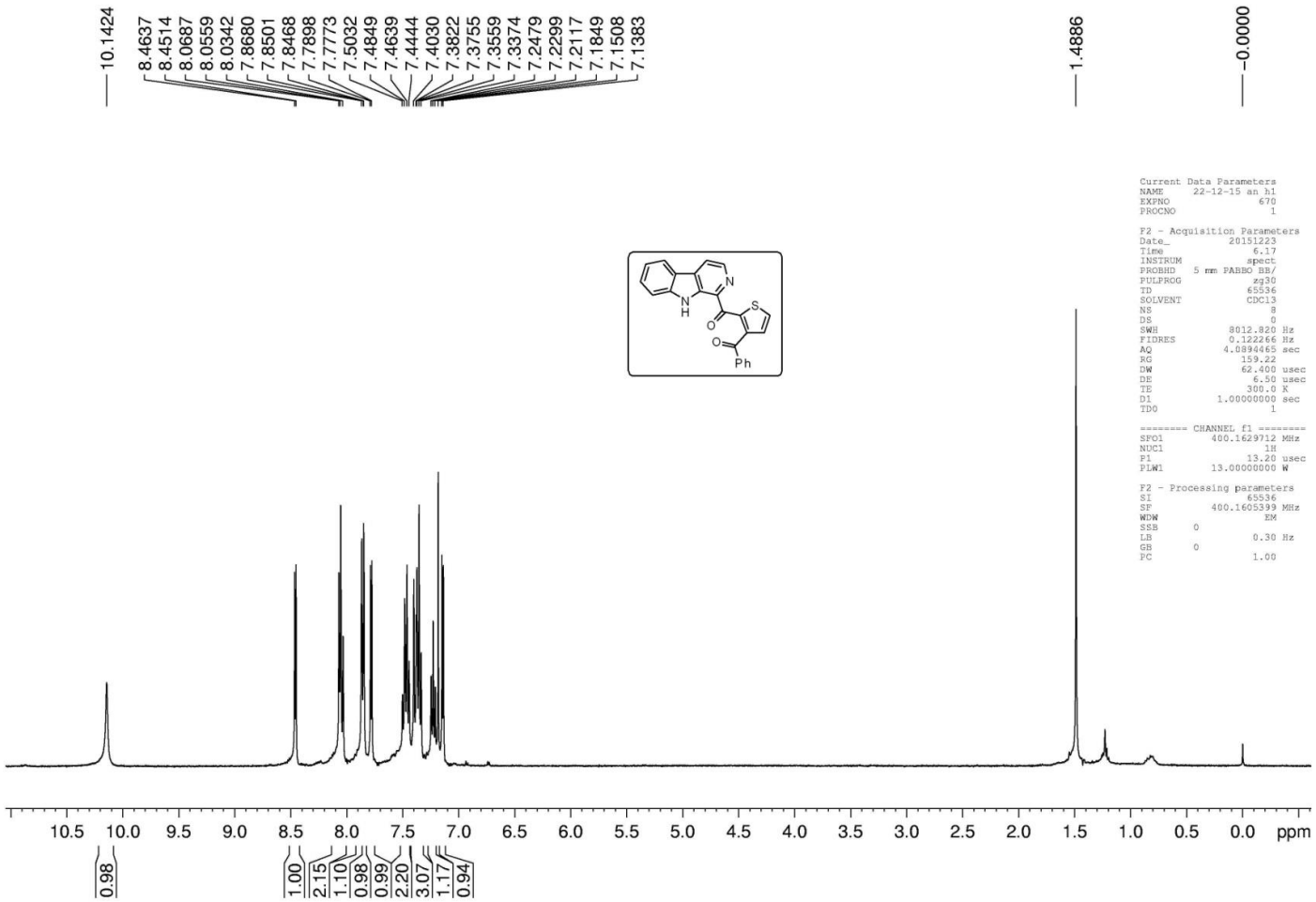



**Figure.** S-29**:** $^{1}$H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)thiophen-3-yl)(phenyl)methanone **(3ka)**.

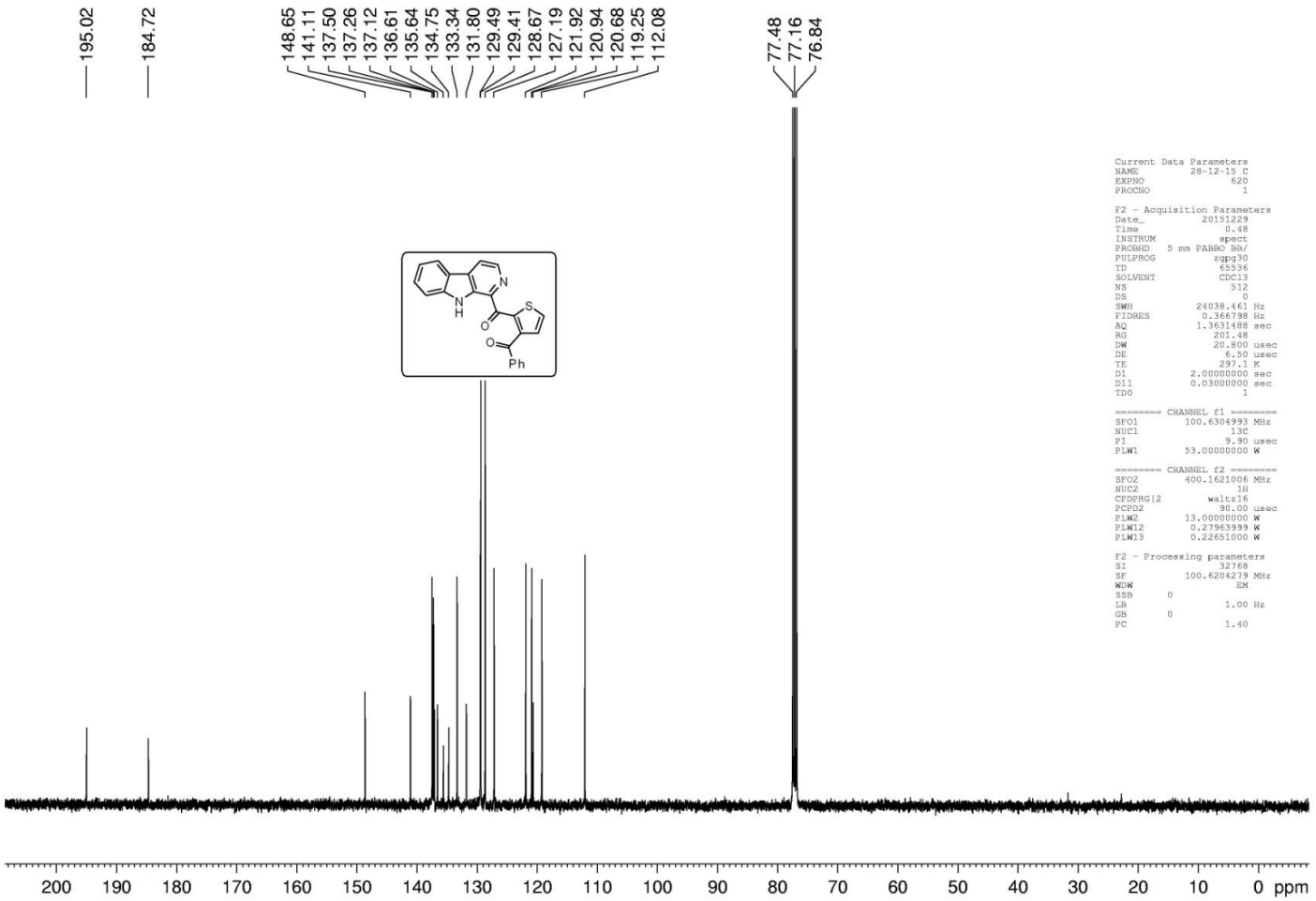



**Figure.** S-30**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)thiophen-3-yl)(phenyl)methanone **(3ka)**.

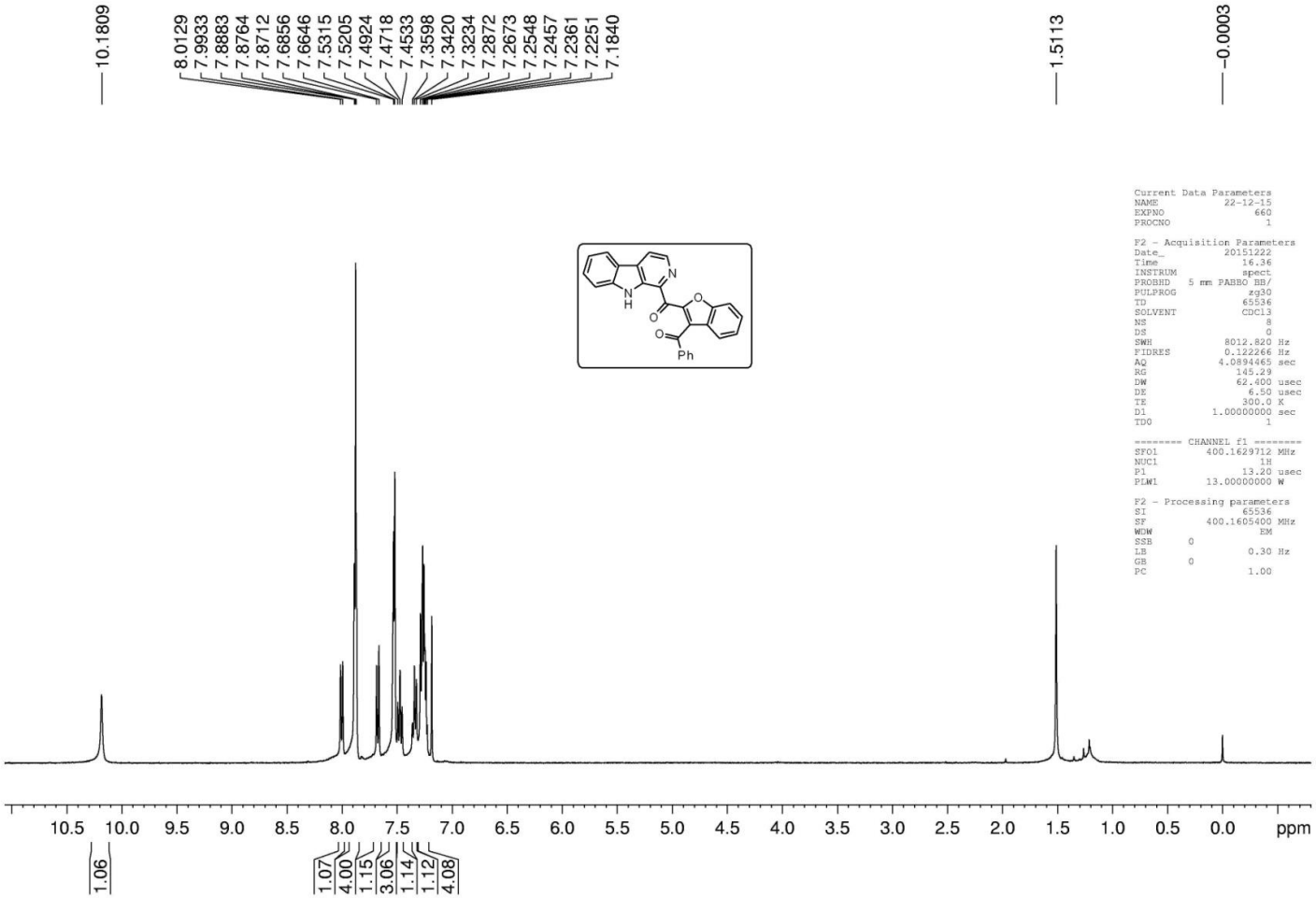



**Figure.** S-31**:** [1]H-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)benzofuran-3-yl)(phenyl)methanone **(3la)**.

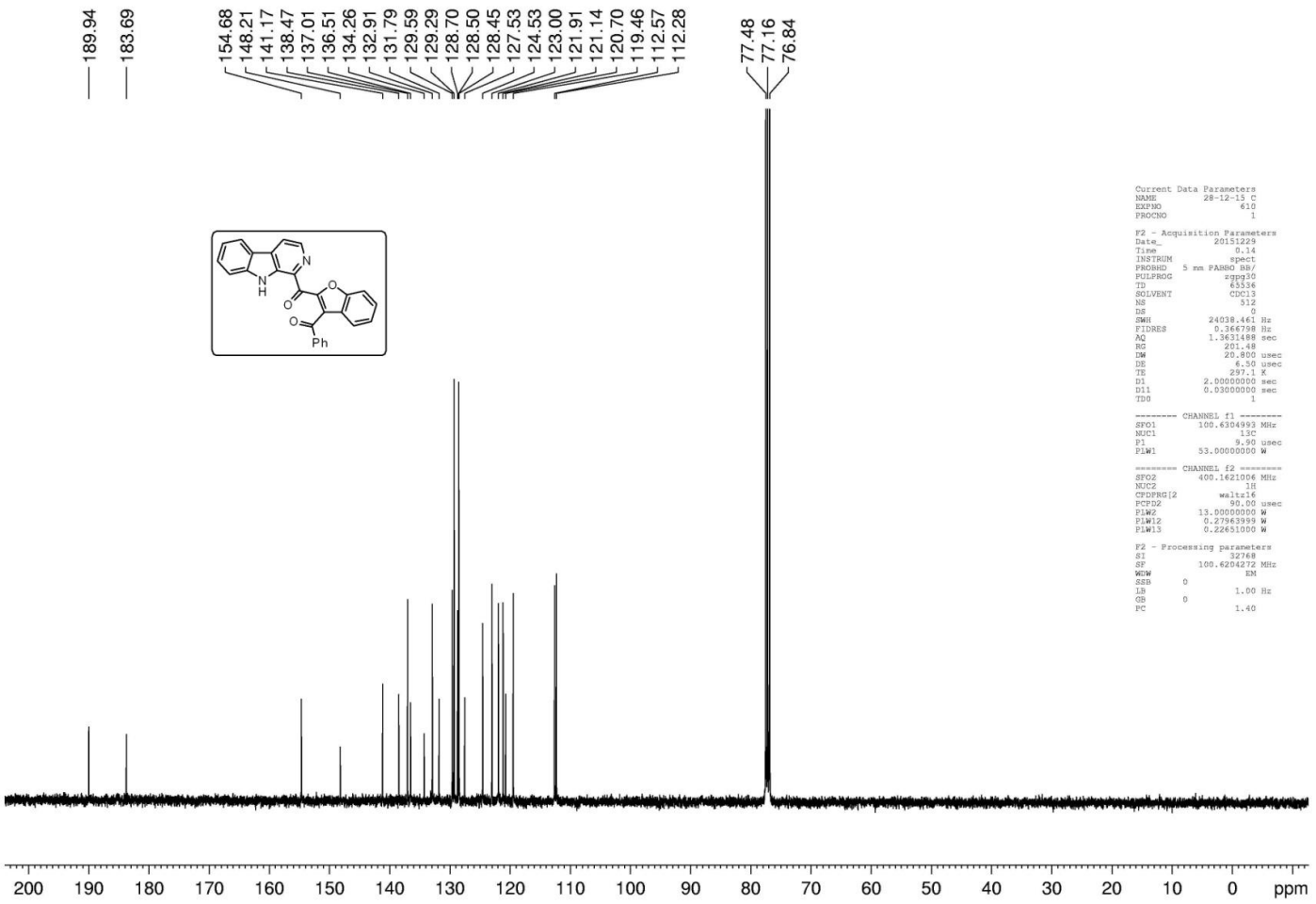



**Figure.** S-32**:** $^{13}$C-NMR spectrum of (2-(9*H*-pyrido[3,4-*b*]indole-1-carbonyl)benzofuran-3-yl)(phenyl)methanone **(3la)**.

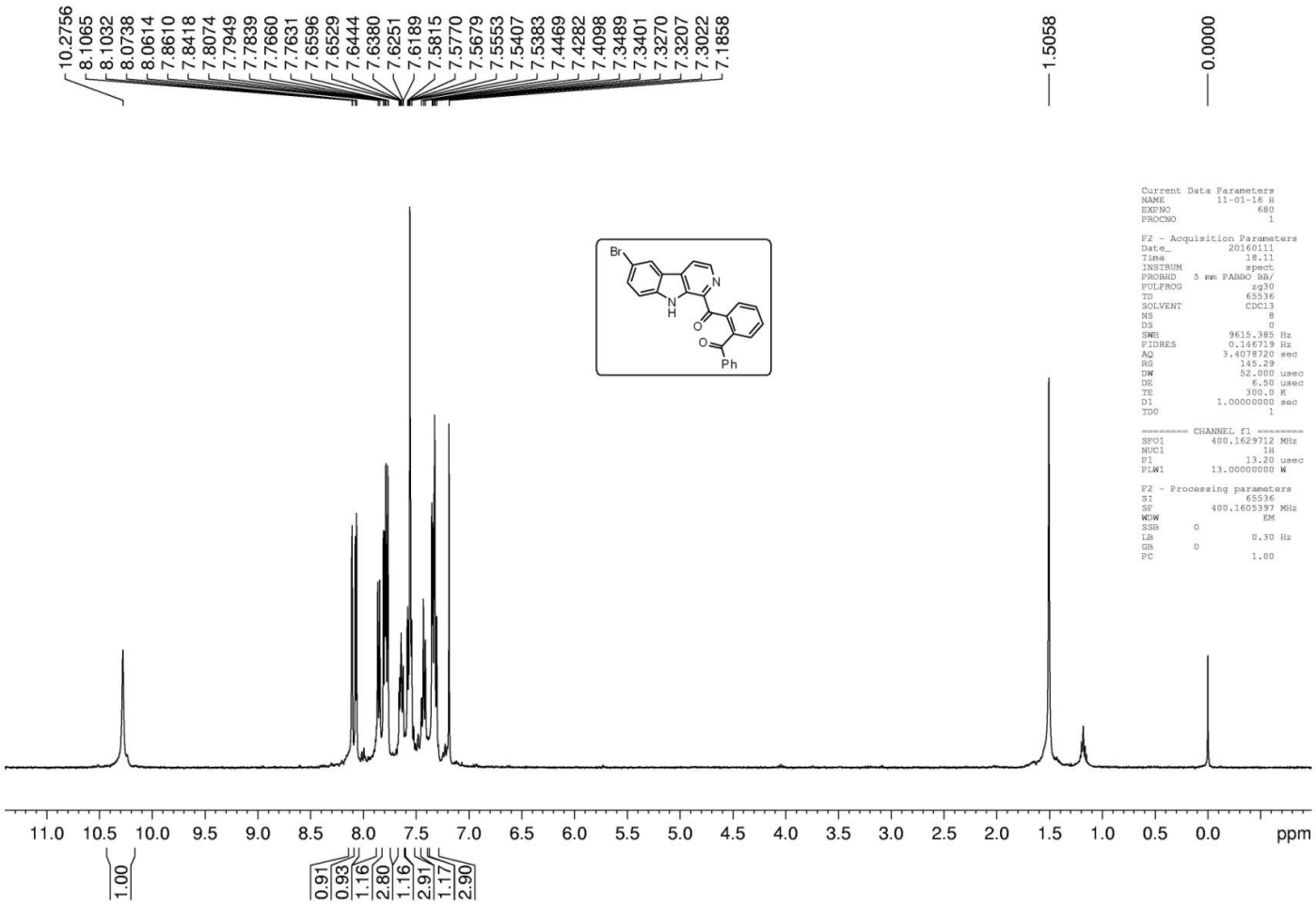



**Figure.** S-33**:** $^{1}$H-NMR spectrum of (2-Benzoylphenyl)(6-bromo-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ma)**.

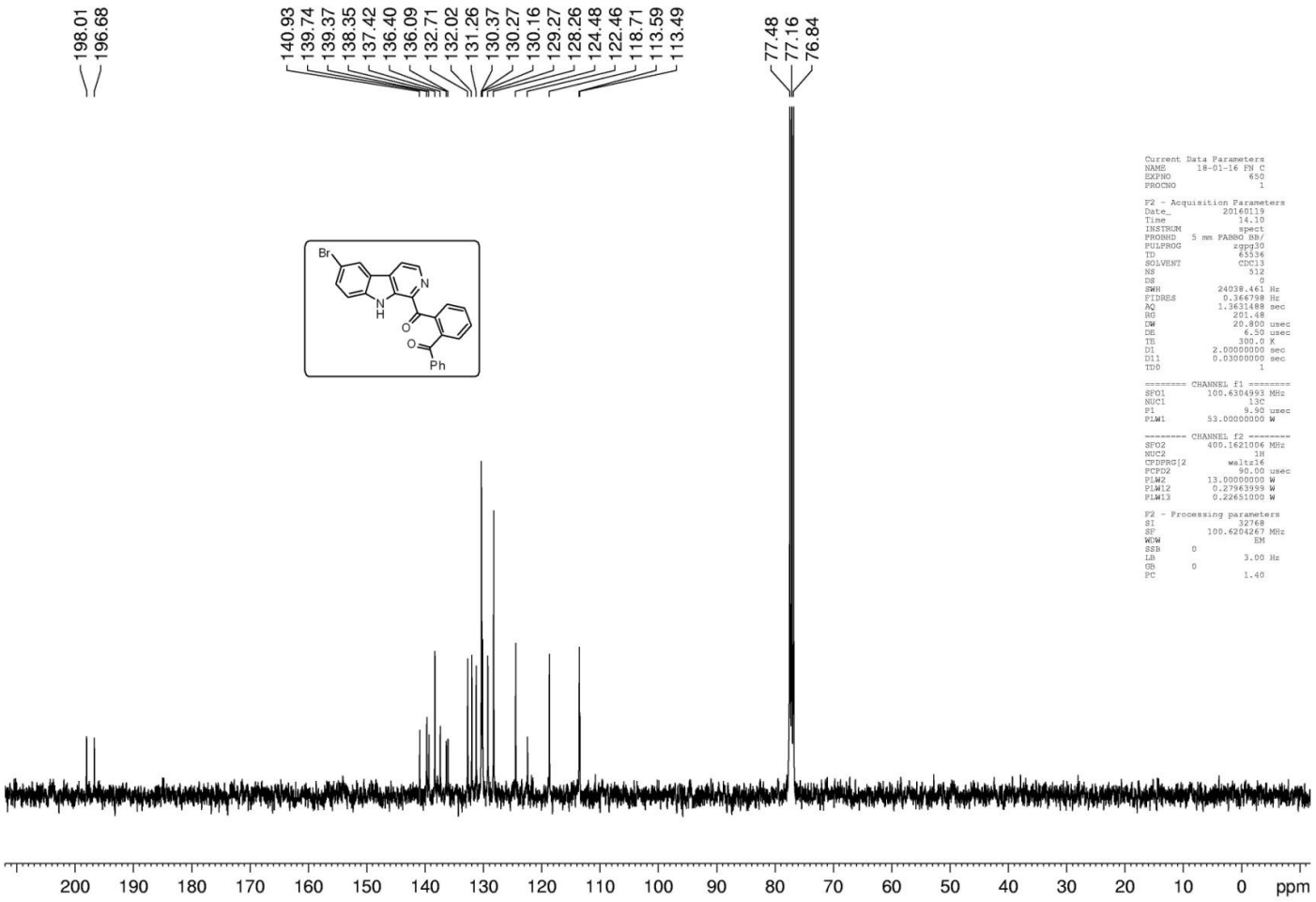



**Figure.** S-34**:** $^{13}$C-NMR spectrum of (2-Benzoylphenyl)(6-bromo-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3ma)**.

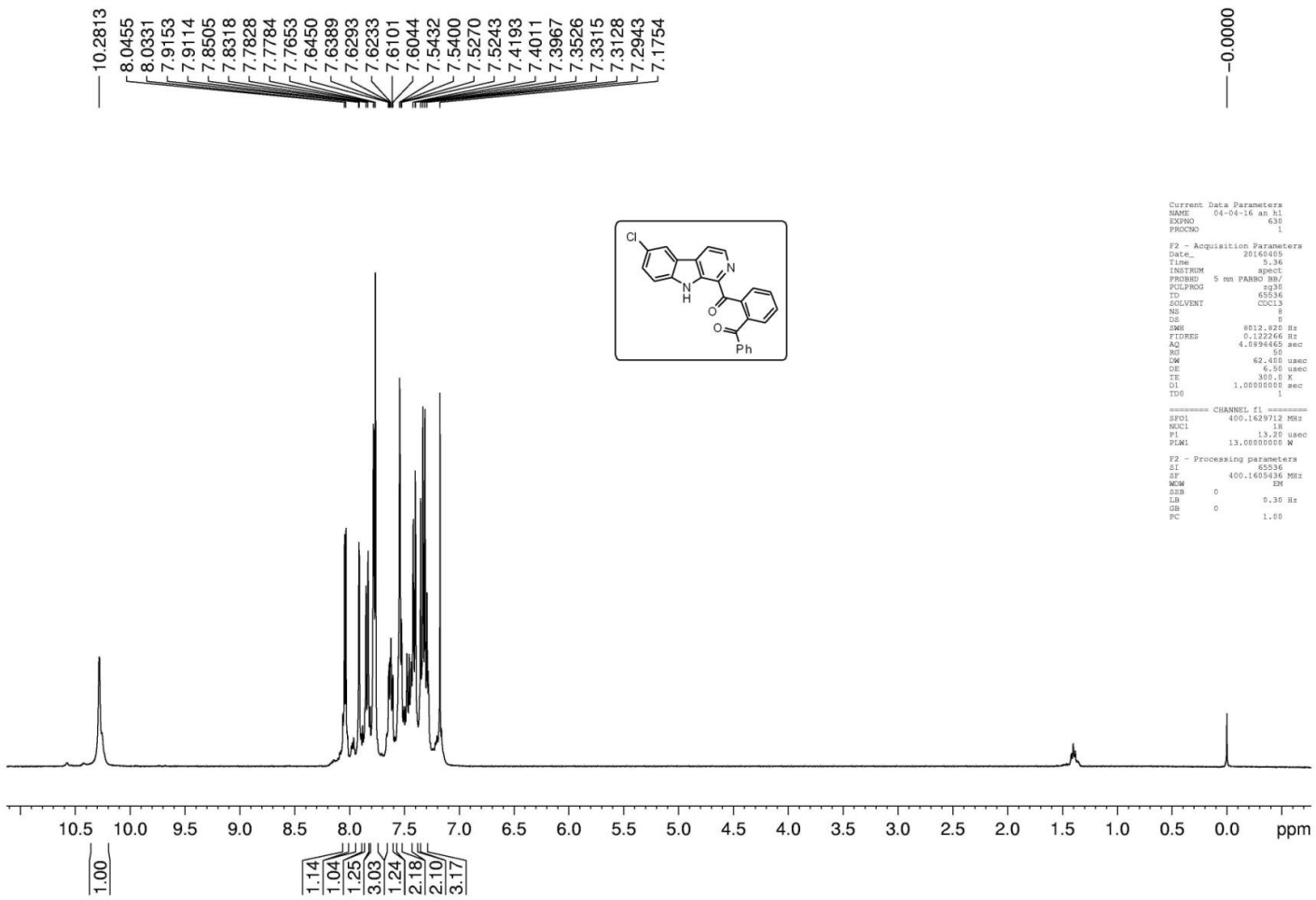



**Figure.** S-35**:** $^{1}$H-NMR spectrum of (2-Benzoylphenyl)(6-chloro-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3na)**.

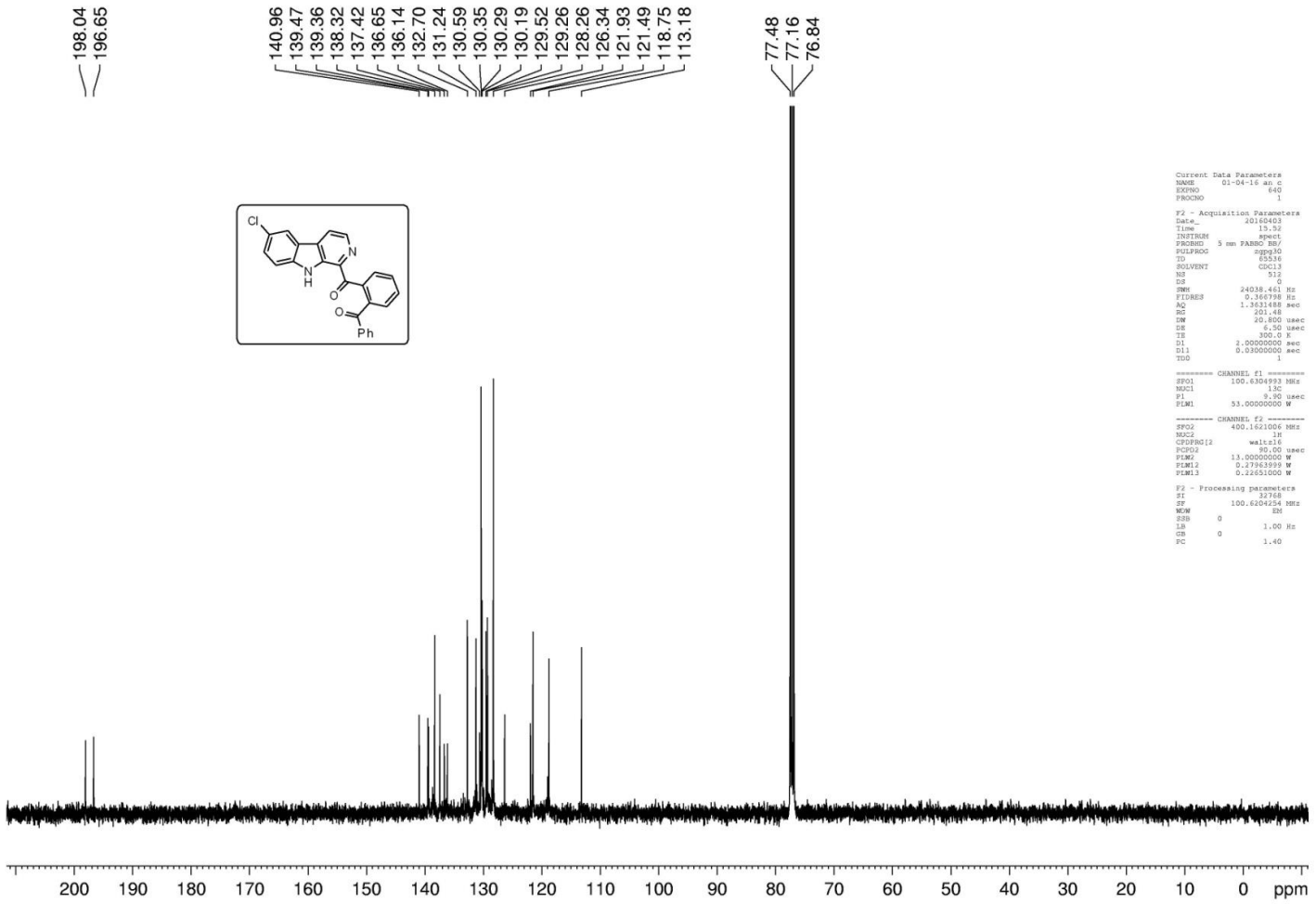



**Figure.** S-36**:** $^{13}$C-NMR spectrum of (2-Benzoylphenyl)(6-chloro-9*H*-pyrido[3,4-*b*]indol-1-yl)methanone **(3na)**.

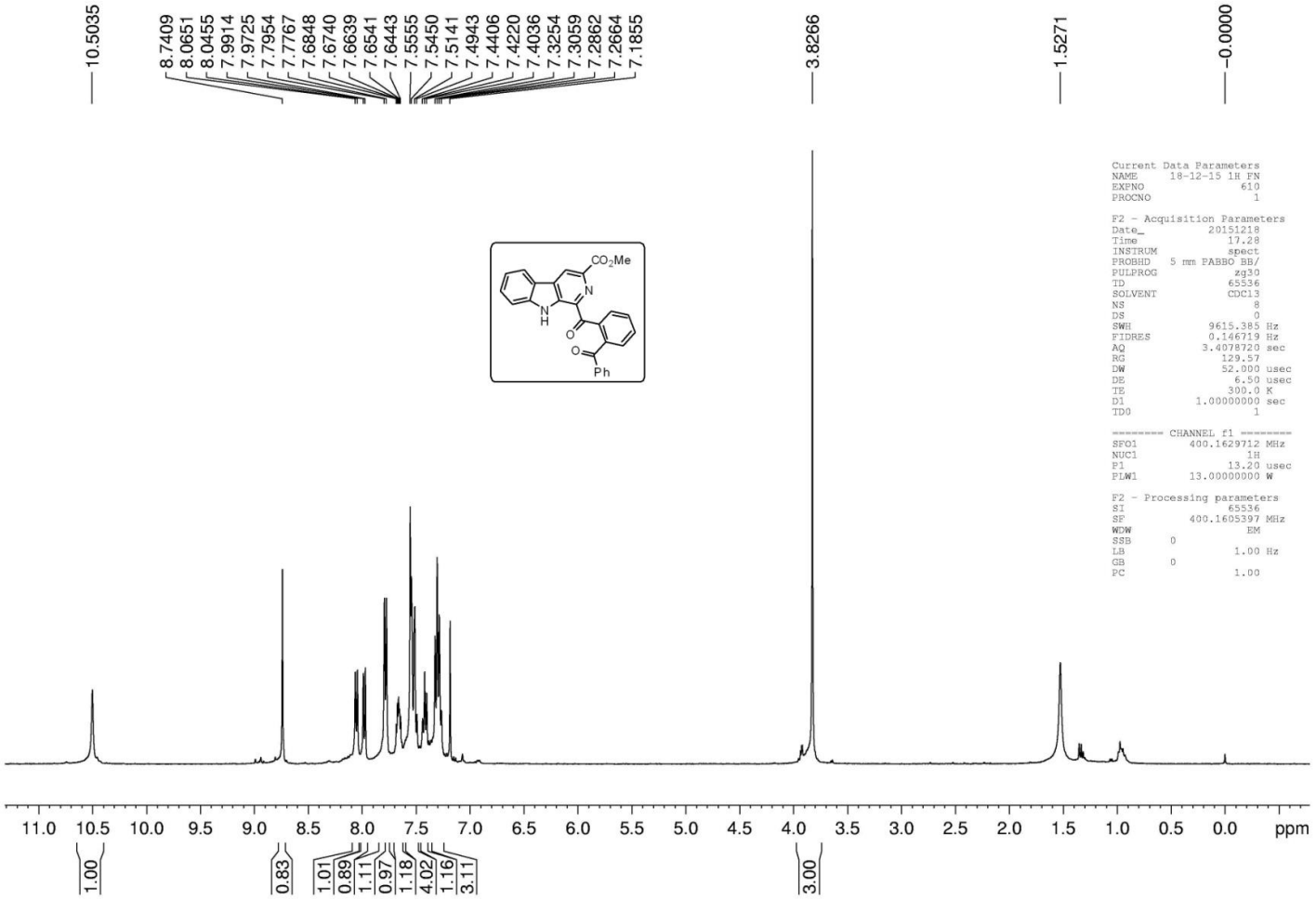



**Figure.** S-37**:** $^{1}$H-NMR spectrum of Methyl 1-(2-benzoylbenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3oa)**.

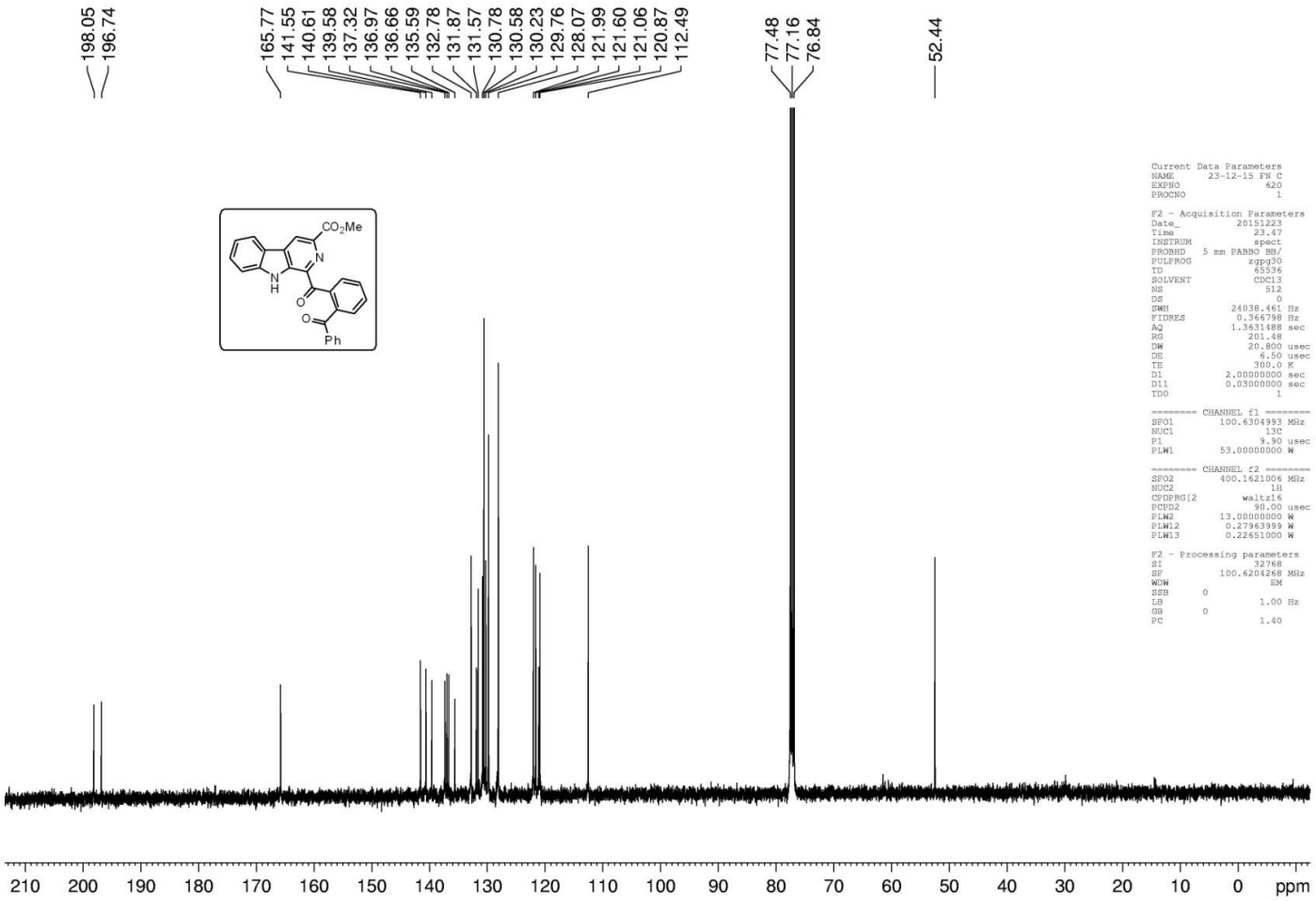



**Figure.** S-38**:** $^{13}$C-NMR spectrum of Methyl 1-(2-benzoylbenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3oa)**.

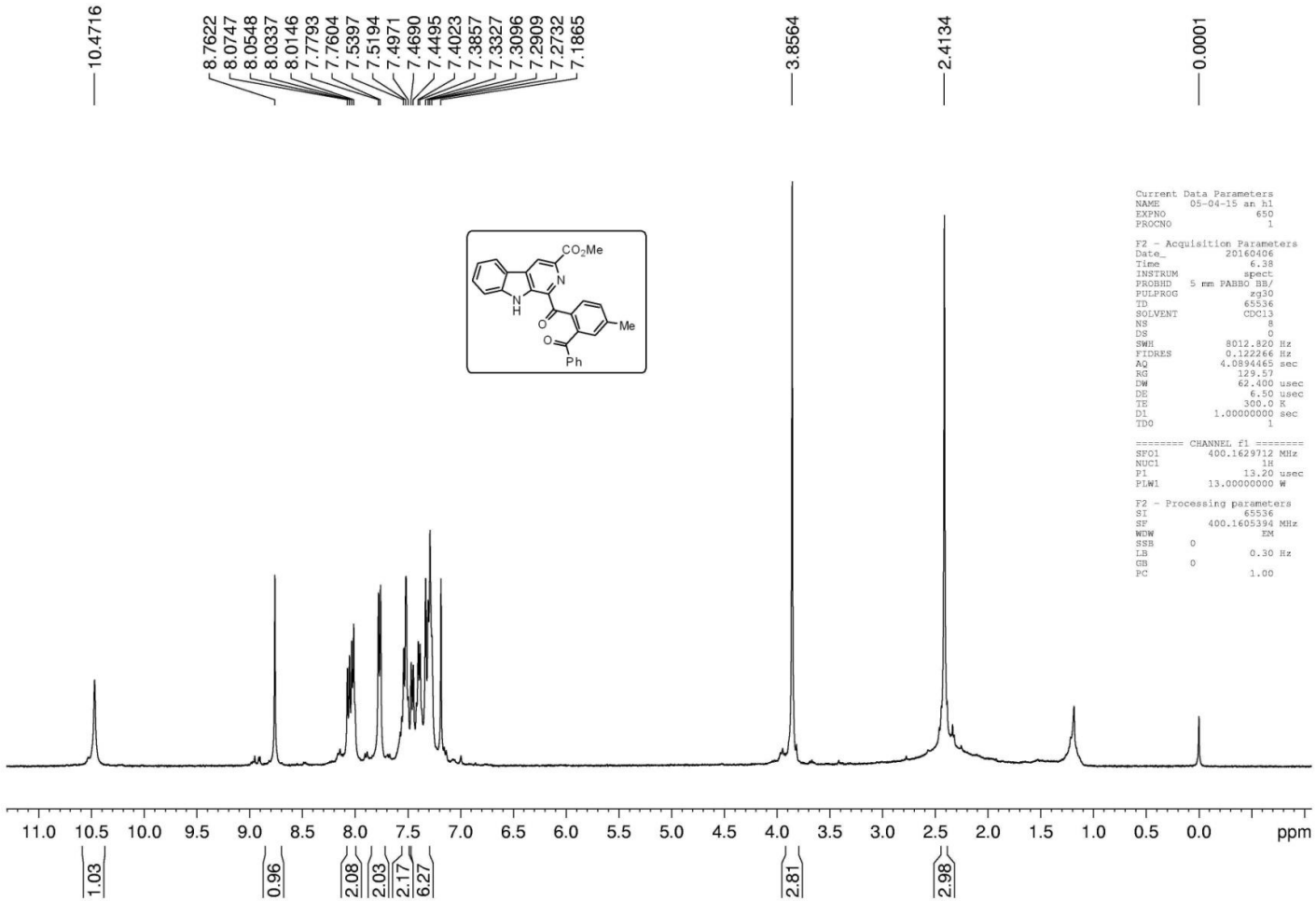



**Figure.** S-39**:** $^{1}$H-NMR spectrum of Methyl 1-(2-benzoyl-4-methylbenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3pa)**.

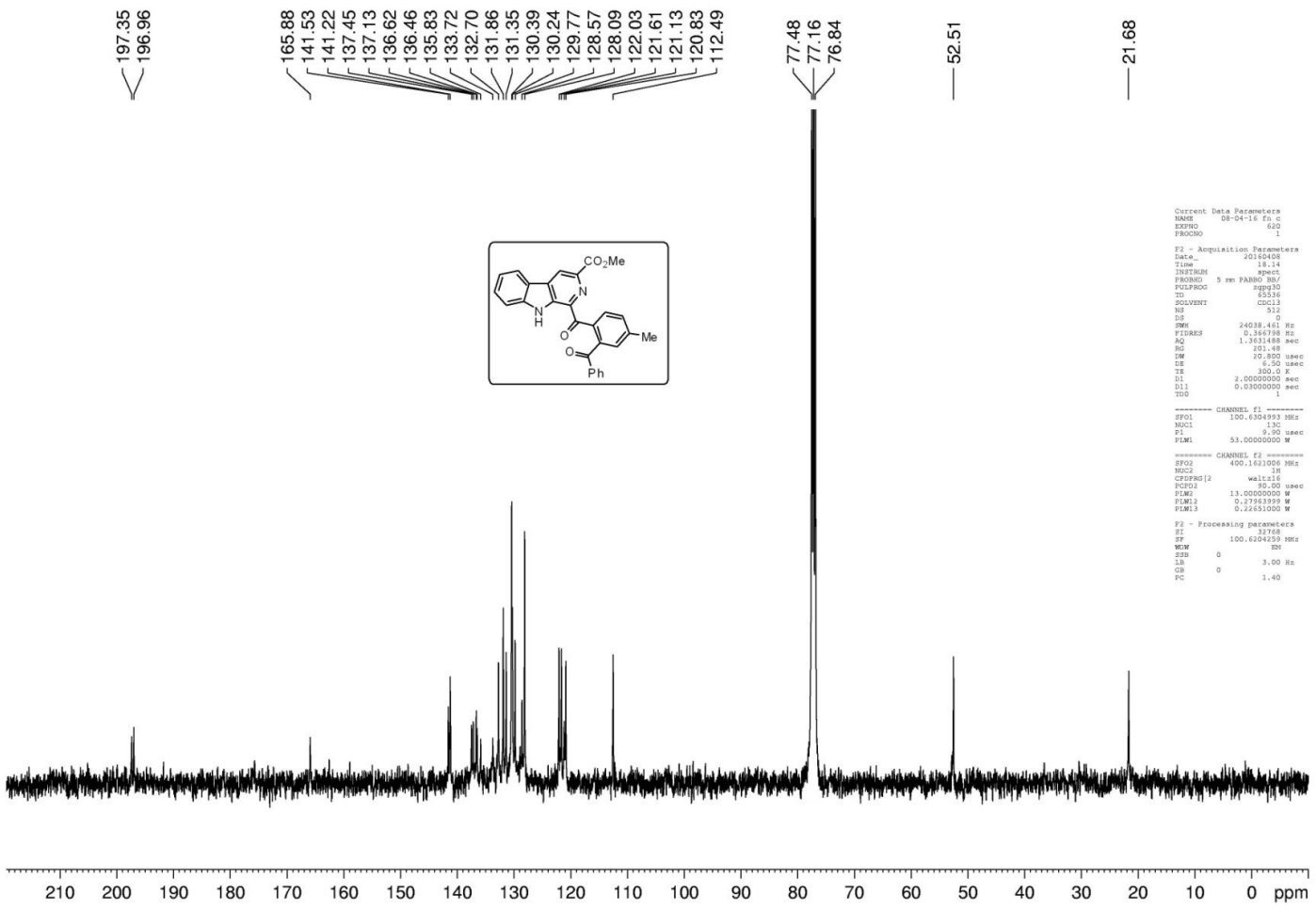



**Figure.** S-40**:** $^{13}$C-NMR spectrum of Methyl 1-(2-benzoyl-4-methylbenzoyl)-9*H*-pyrido[3,4-*b*]indole-3-carboxylate **(3pa)**.

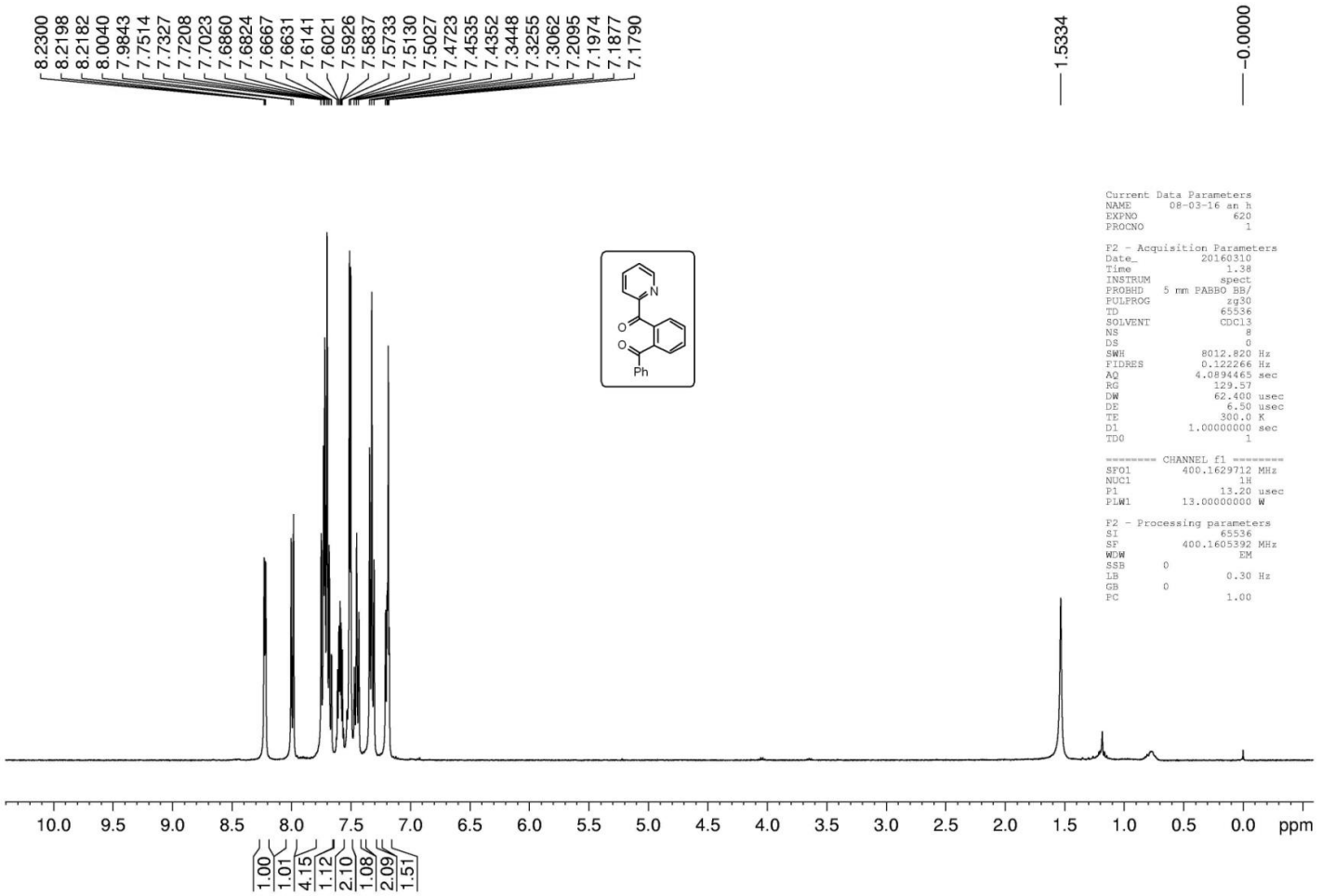



**Figure.** S-41: $^{1}$H-NMR spectrum of (2-Benzoylphenyl)(pyridin-2-yl)methanone **(3qa).**

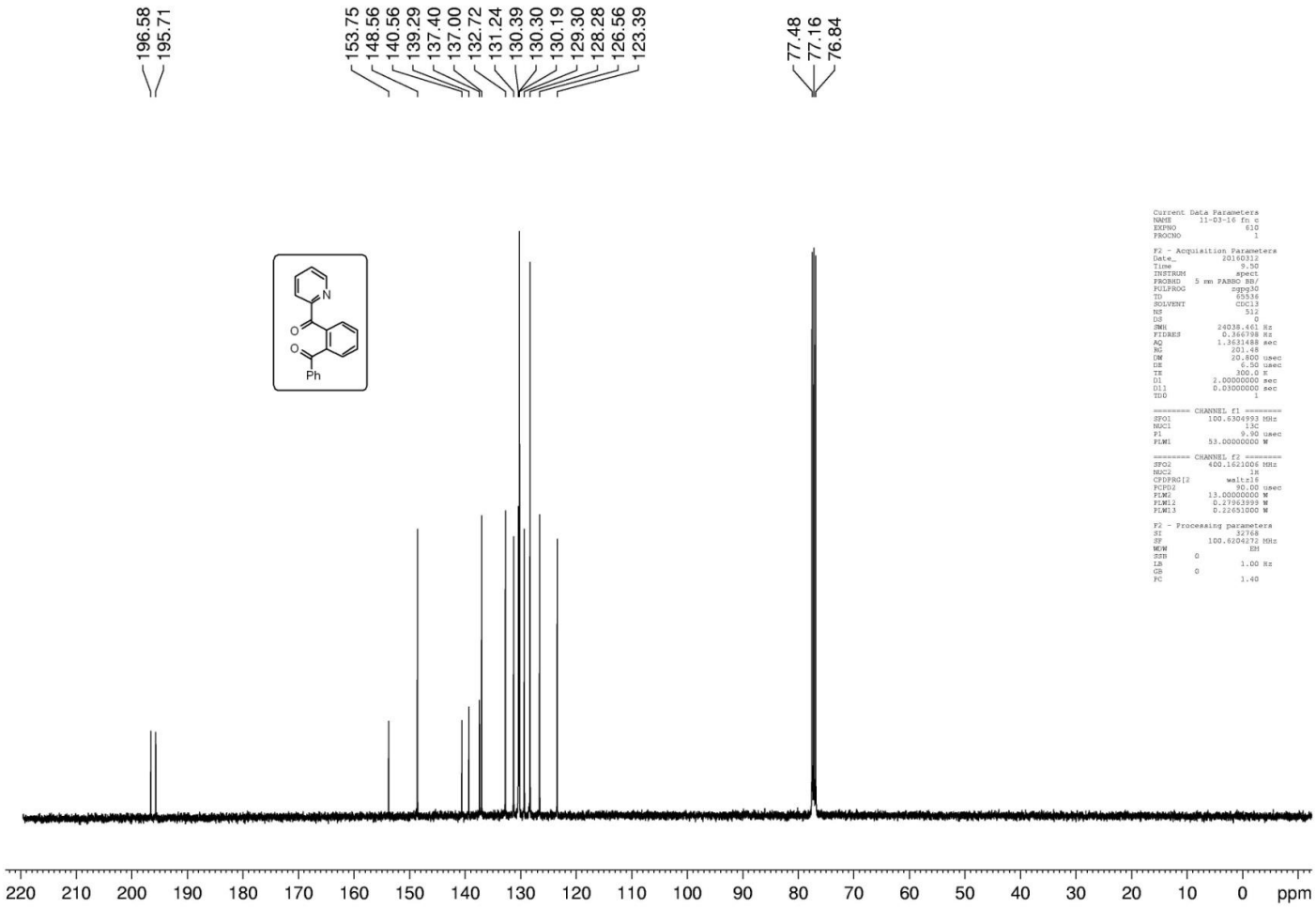



**Figure.** S-42**:** $^{13}$C-NMR spectrum of (2-Benzoylphenyl)(pyridin-2-yl)methanone **(3qa).**

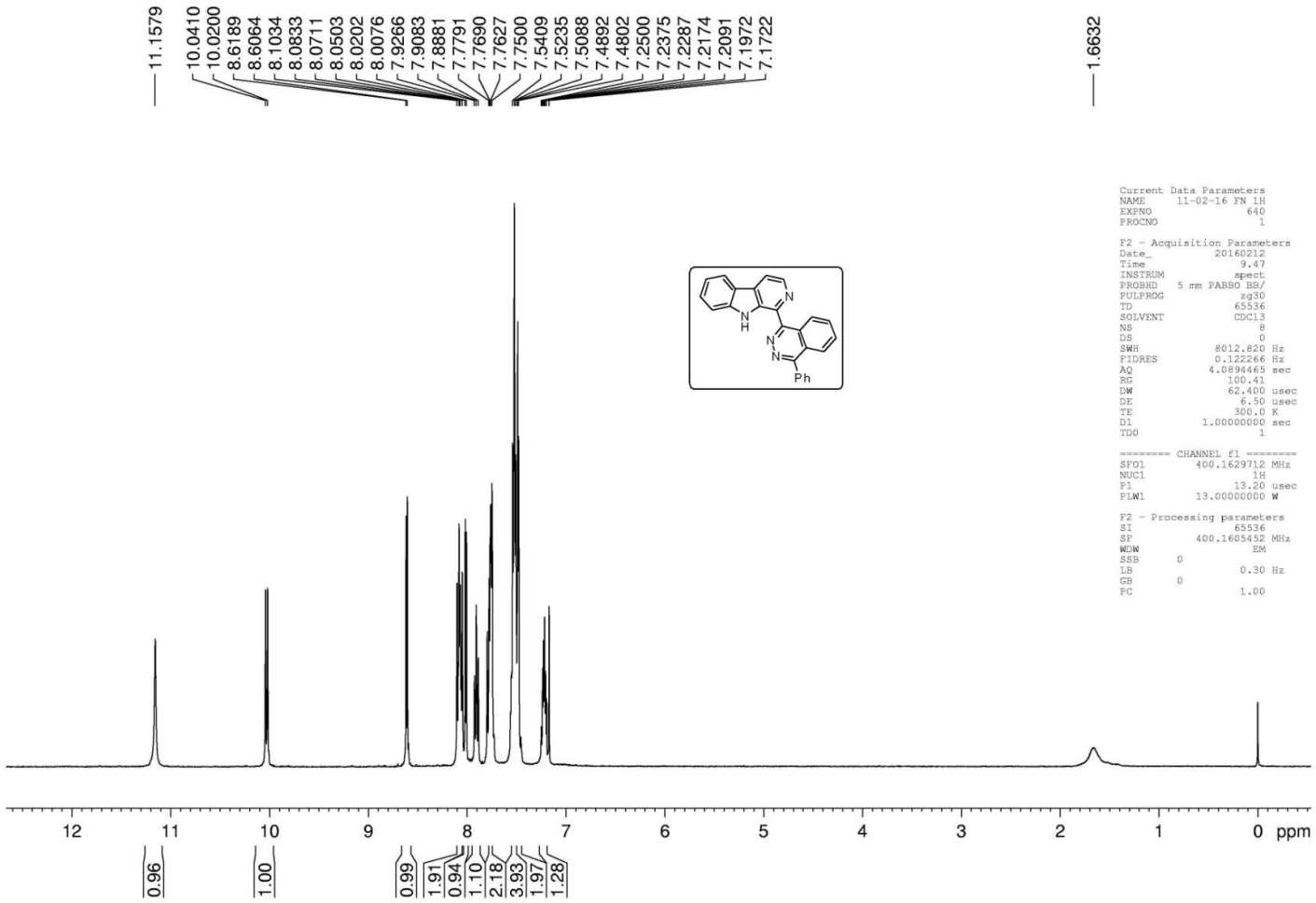



**Figure.** S-43**:** $^{1}$H-NMR spectrum of (1-(4-Phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5aa)**.

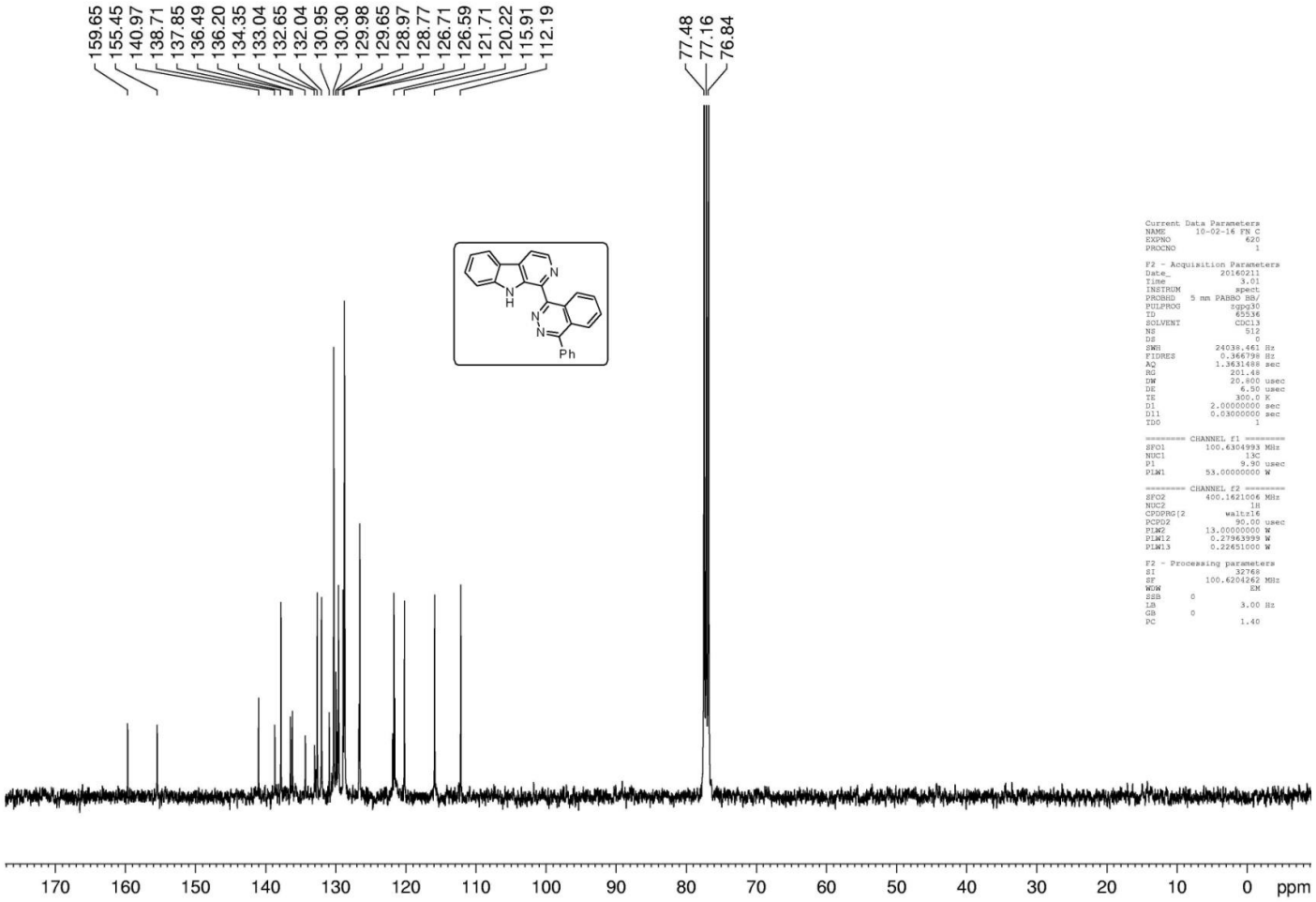



**Figure.** S-44**:** $^{13}$C-NMR spectrum of (1-(4-Phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5aa)**.

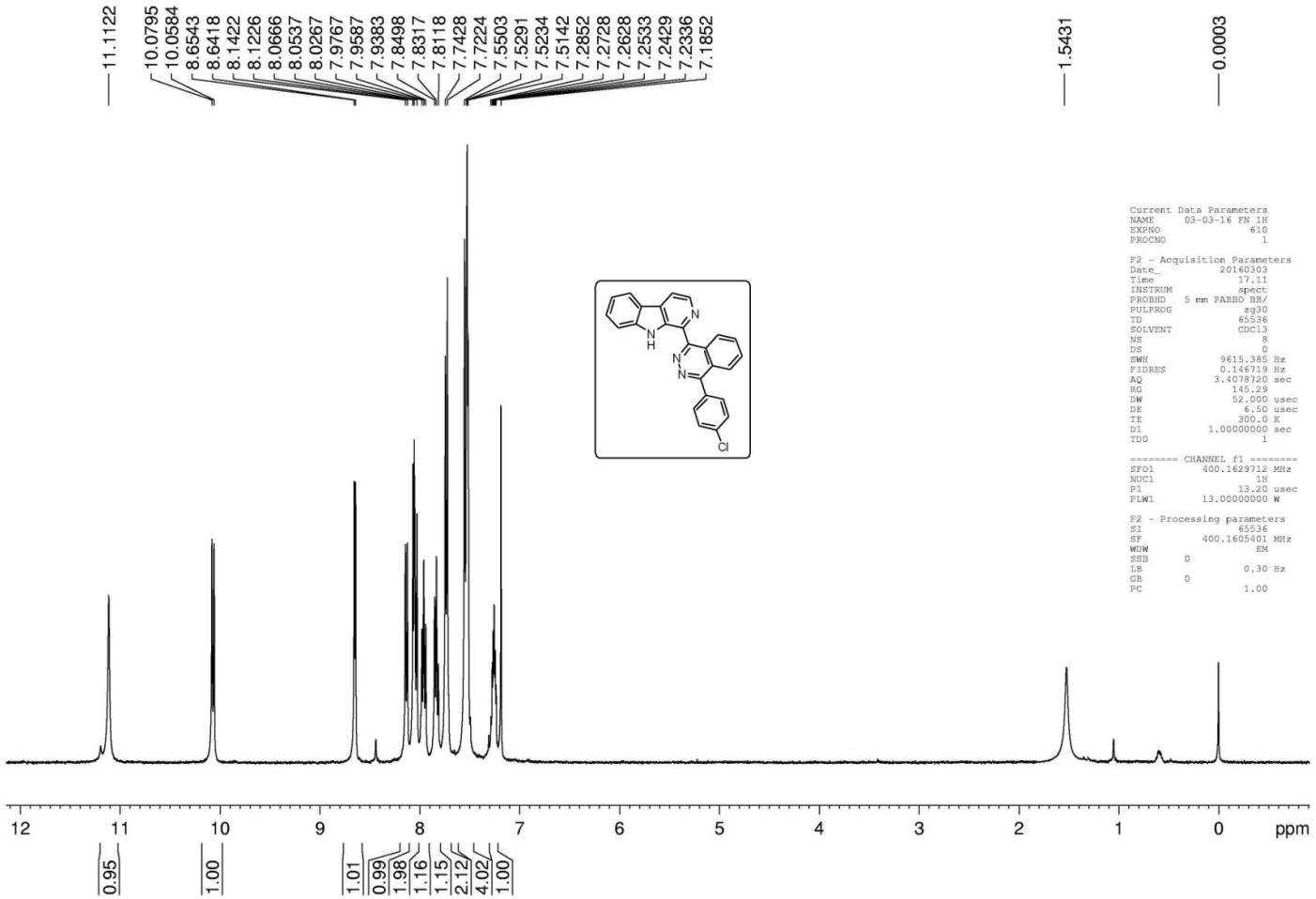



**Figure.** S-45**:** $^{1}$H-NMR spectrum of 1-(4-(4-Chlorophenyl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ac)**.

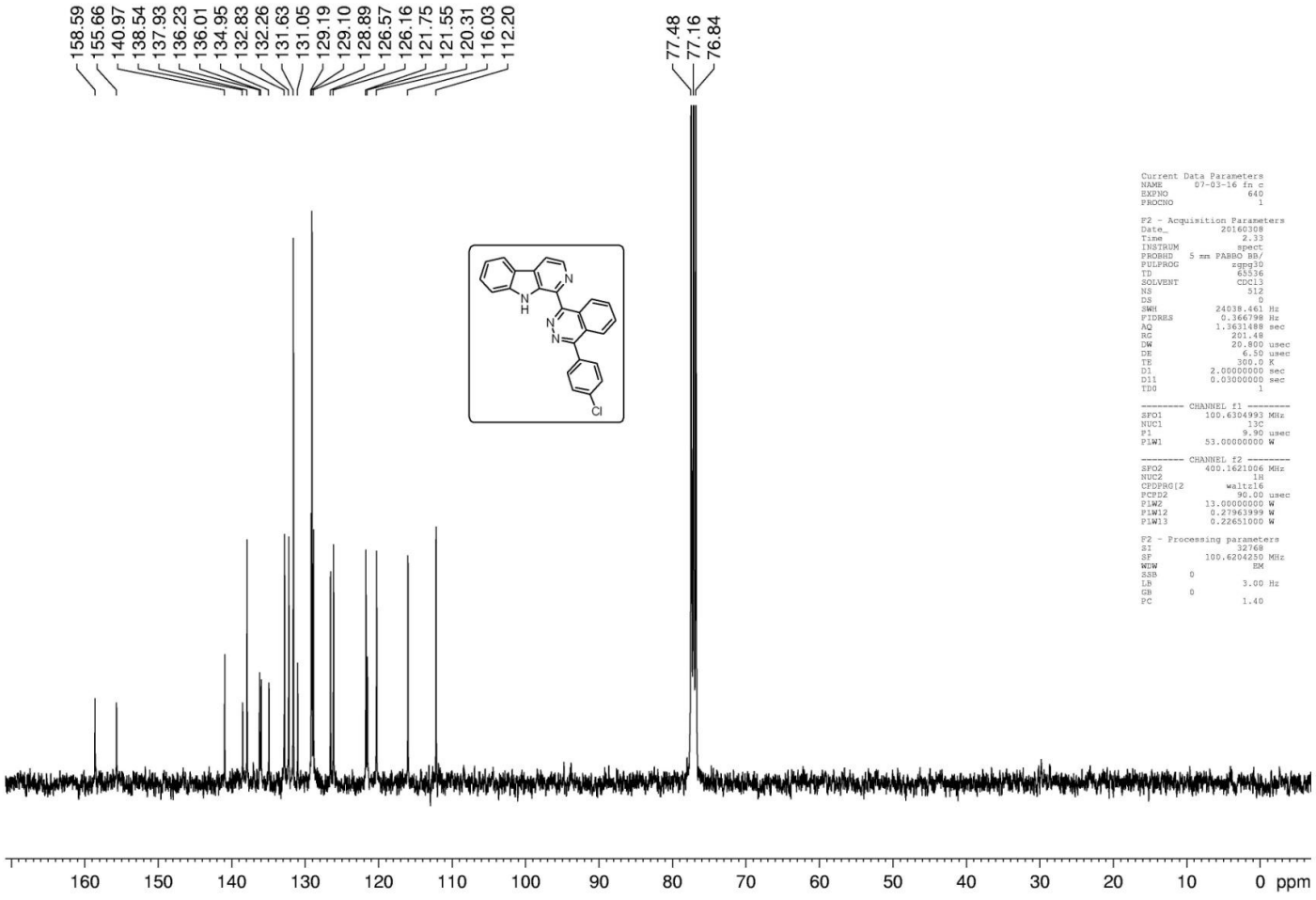



**Figure.** S-46**:** $^{13}$C-NMR spectrum of 1-(4-(4-Chlorophenyl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ac)**.

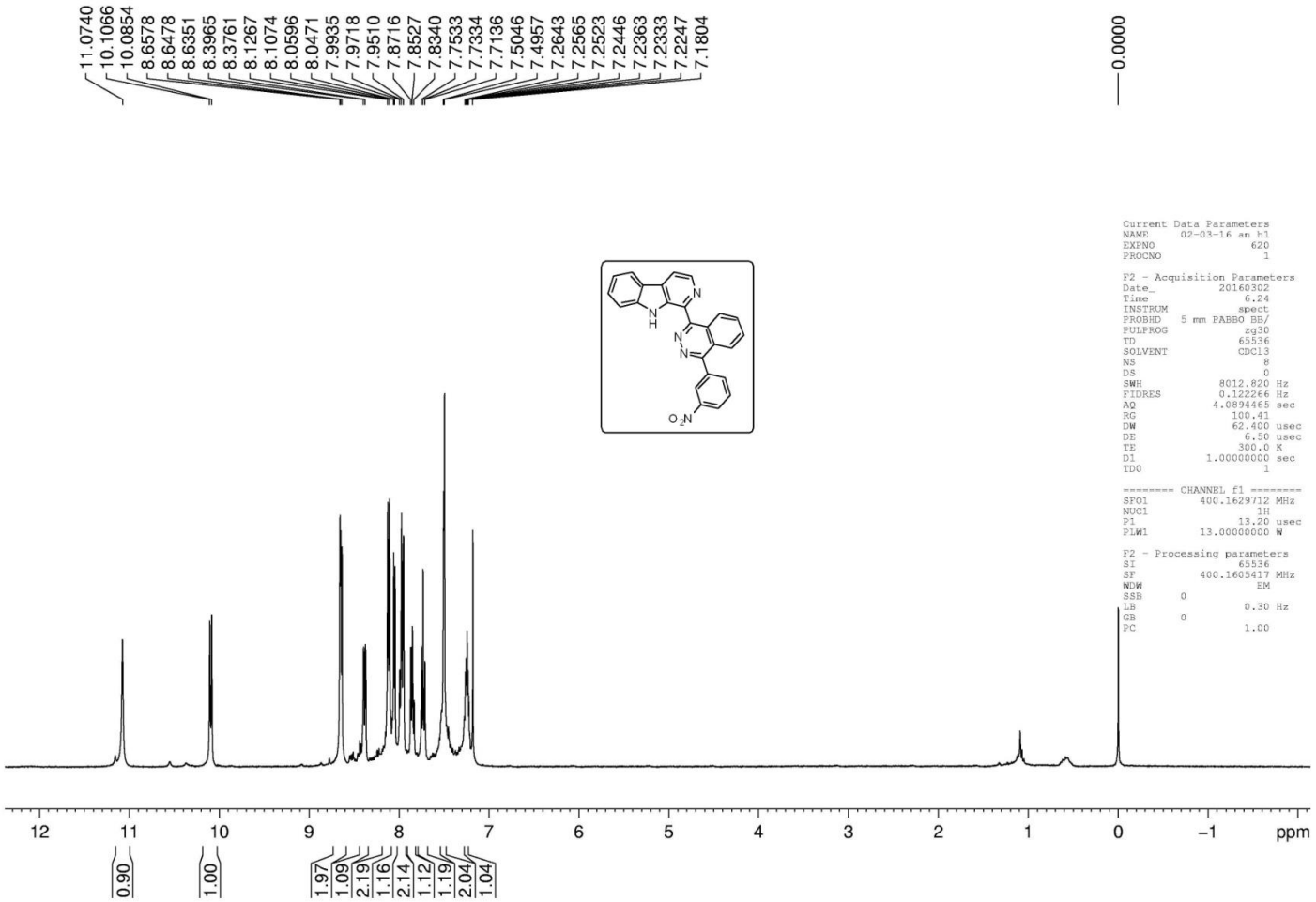



**Figure.** S-47**:** $^{1}$H-NMR spectrum of 1-(4-(3-Nitrophenyl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ad)**.

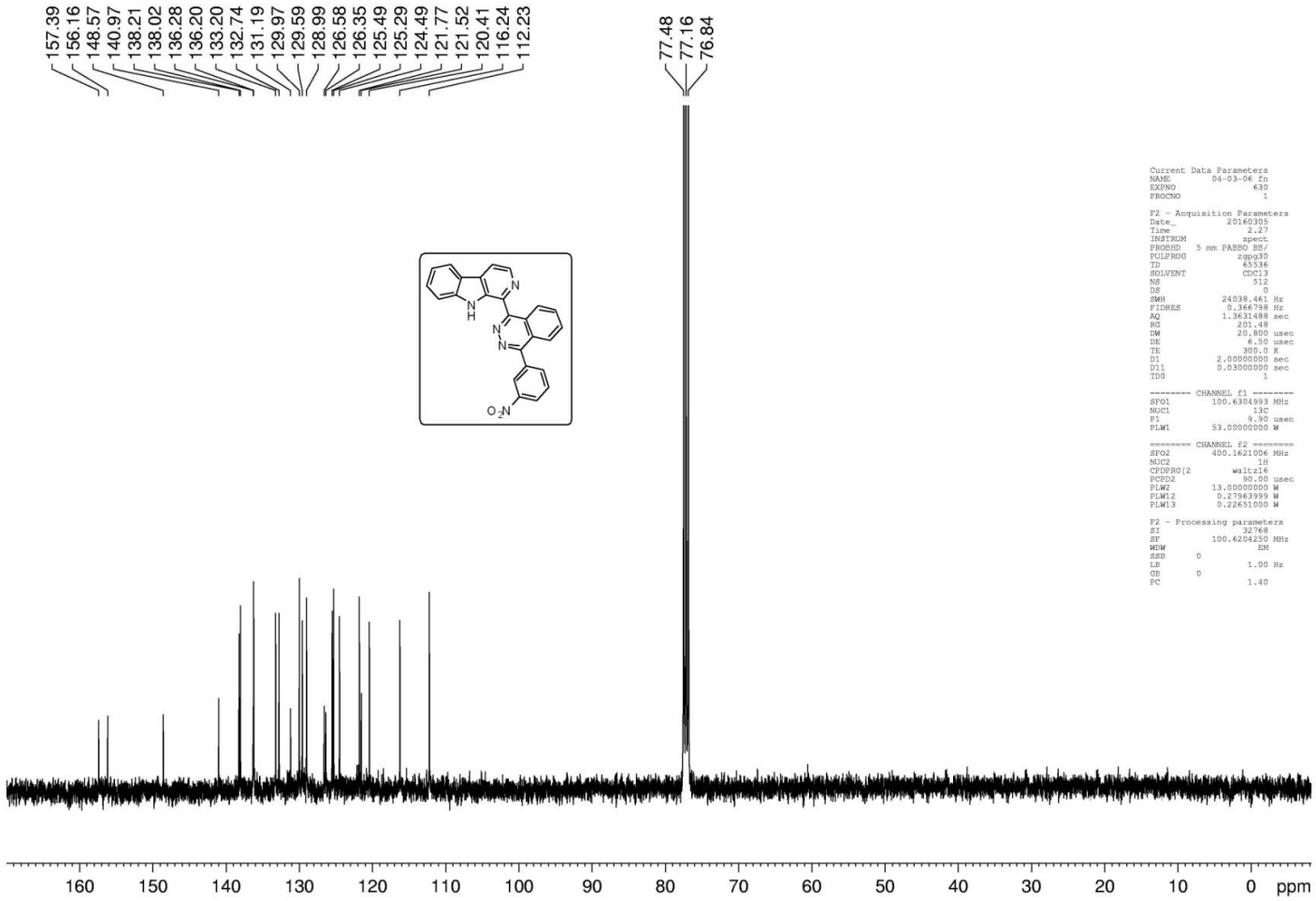



**Figure.** S-48**:** $^{13}$C-NMR spectrum of 1-(4-(3-Nitrophenyl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ad)**.

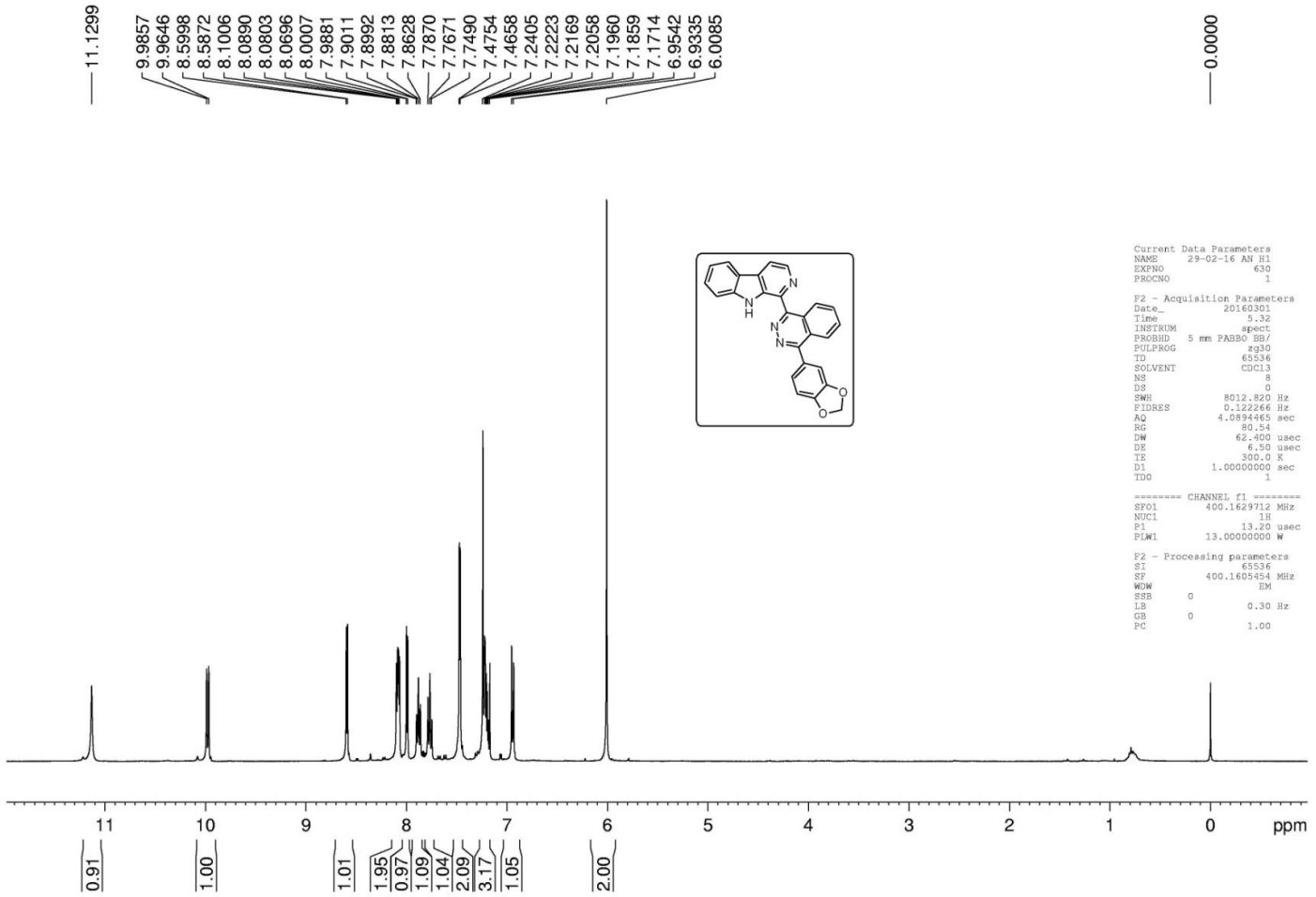



**Figure.** S-49**:** $^{1}$H-NMR spectrum of 1-(4-(Benzo[*d*][1,3]dioxol-5-yl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ae)**.

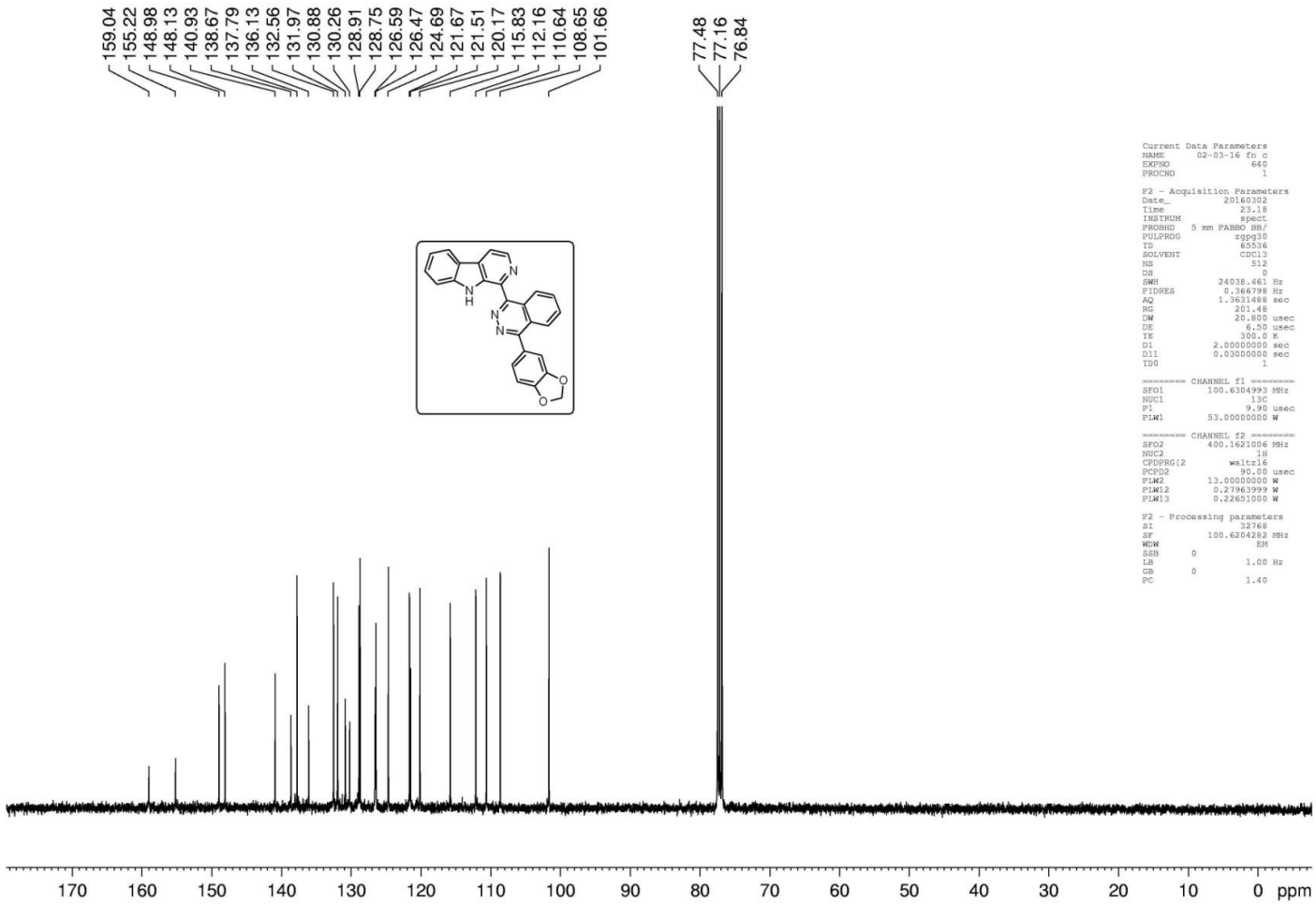



**Figure.** S-50**:** $^{13}$C-NMR spectrum of 1-(4-(Benzo[*d*][1,3]dioxol-5-yl)phthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ae)**.

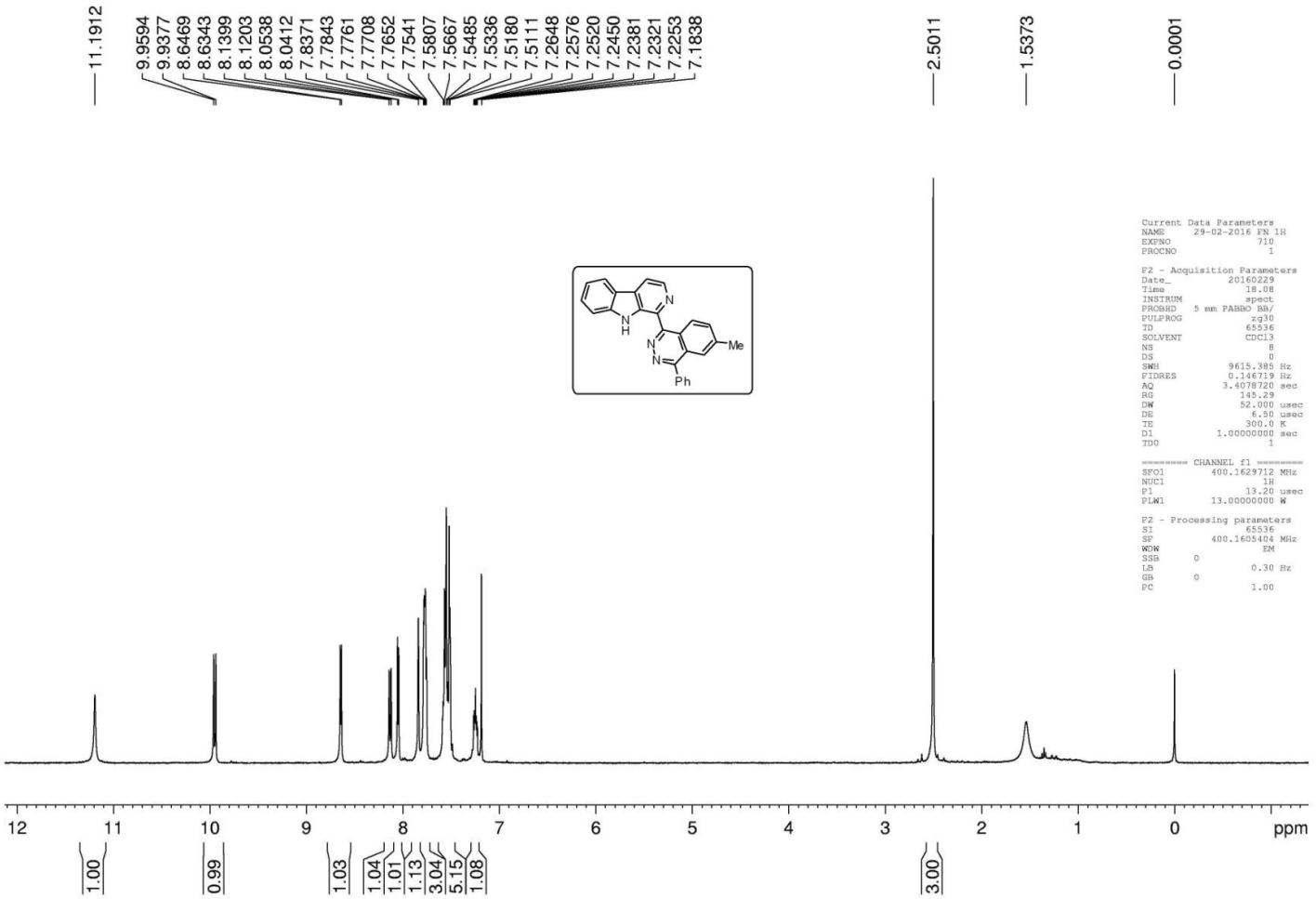



**Figure.** S-51**:** $^{1}$H-NMR spectrum of 1-(6-Methyl-4-phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ba)**.

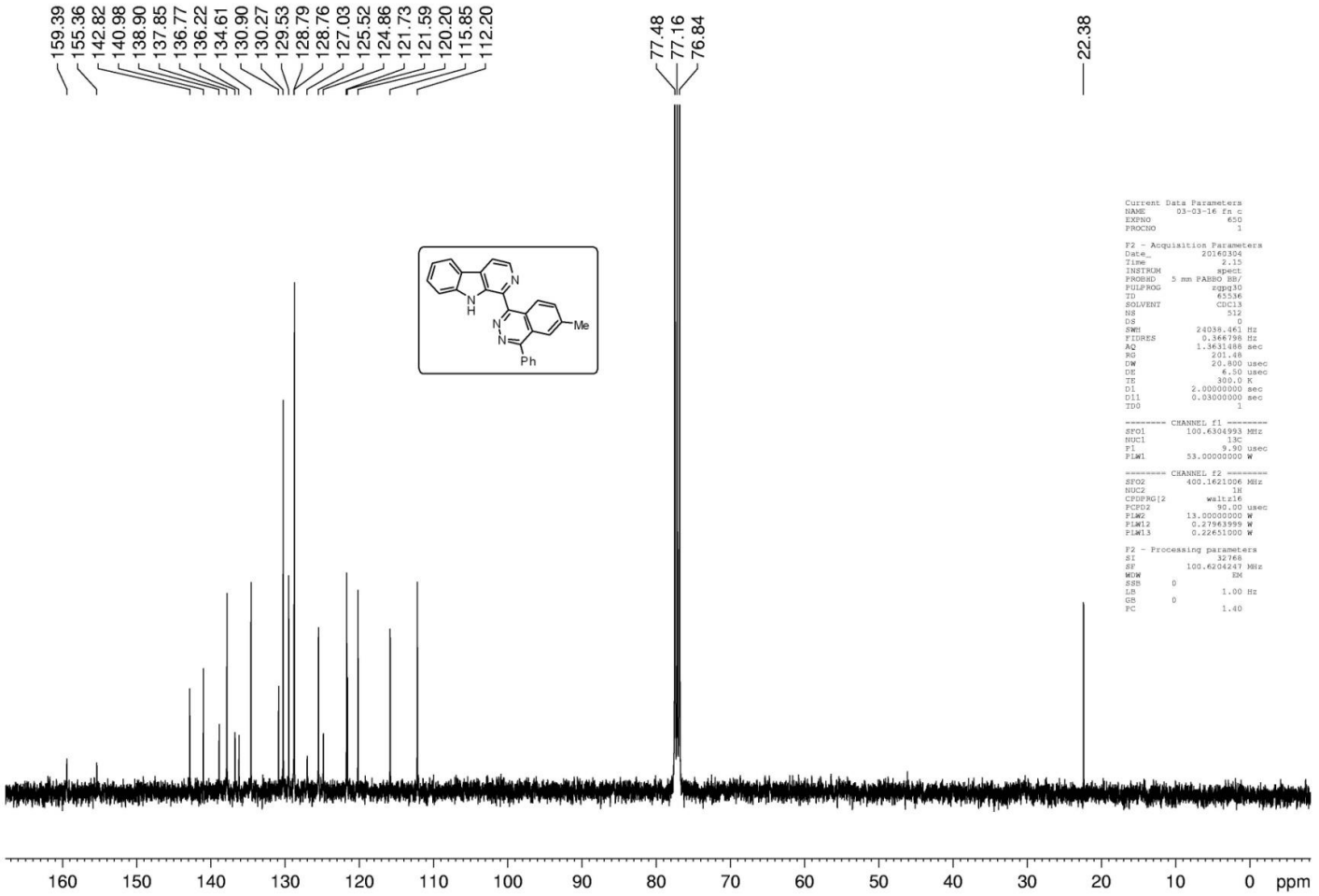



**Figure.** S-52**:** $^{13}$C-NMR spectrum of 1-(6-Methyl-4-phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ba)**.

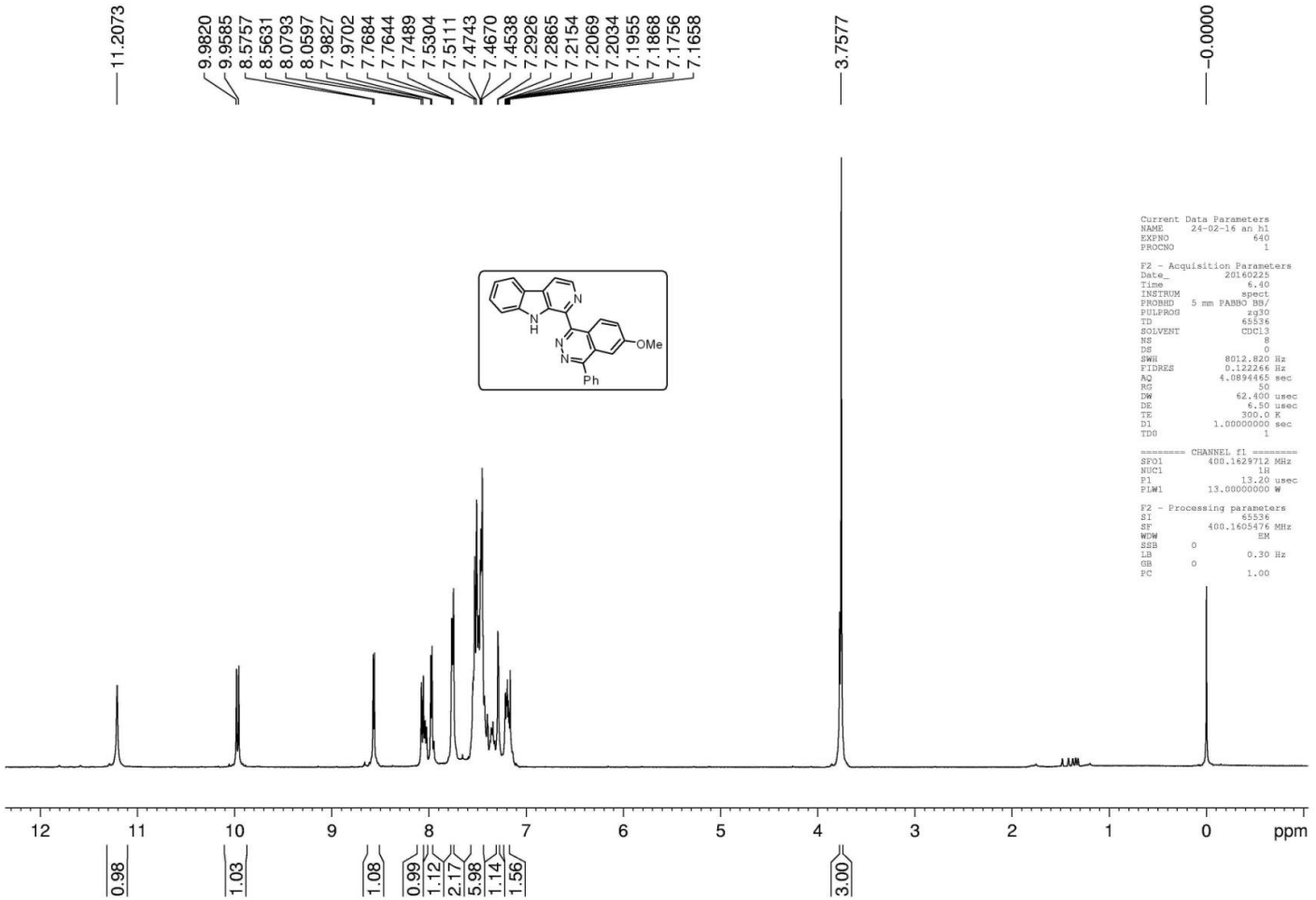



**Figure.** S-53**:** $^{1}$H-NMR spectrum of 1-(6-Methoxy-4-phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ca)**.

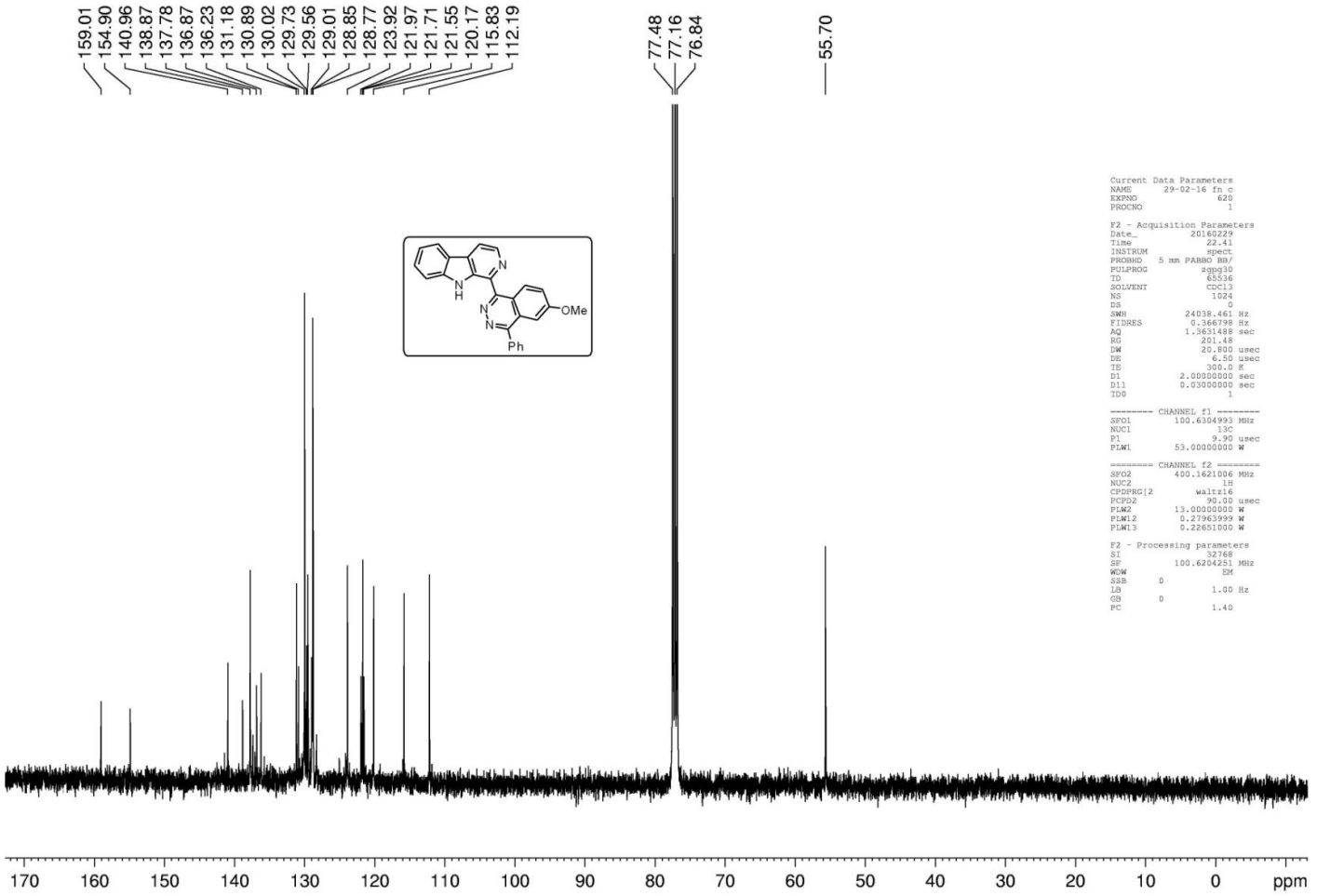



**Figure.** S-54**:** $^{13}$C-NMR spectrum of 1-(6-Methoxy-4-phenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5ca)**.

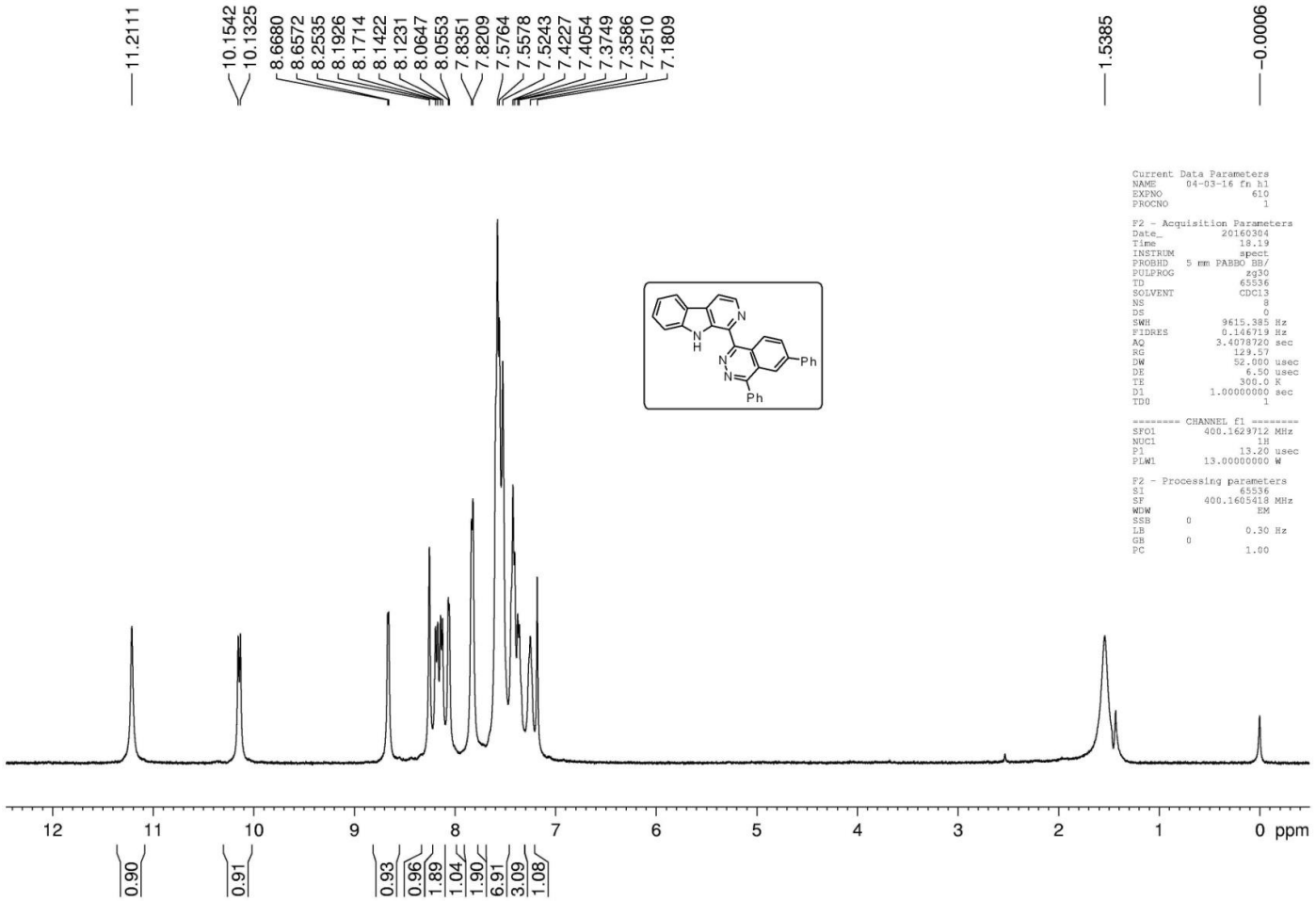



**Figure.** S-55**:** $^{1}$H-NMR spectrum of 1-(4,6-Diphenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5da)**.

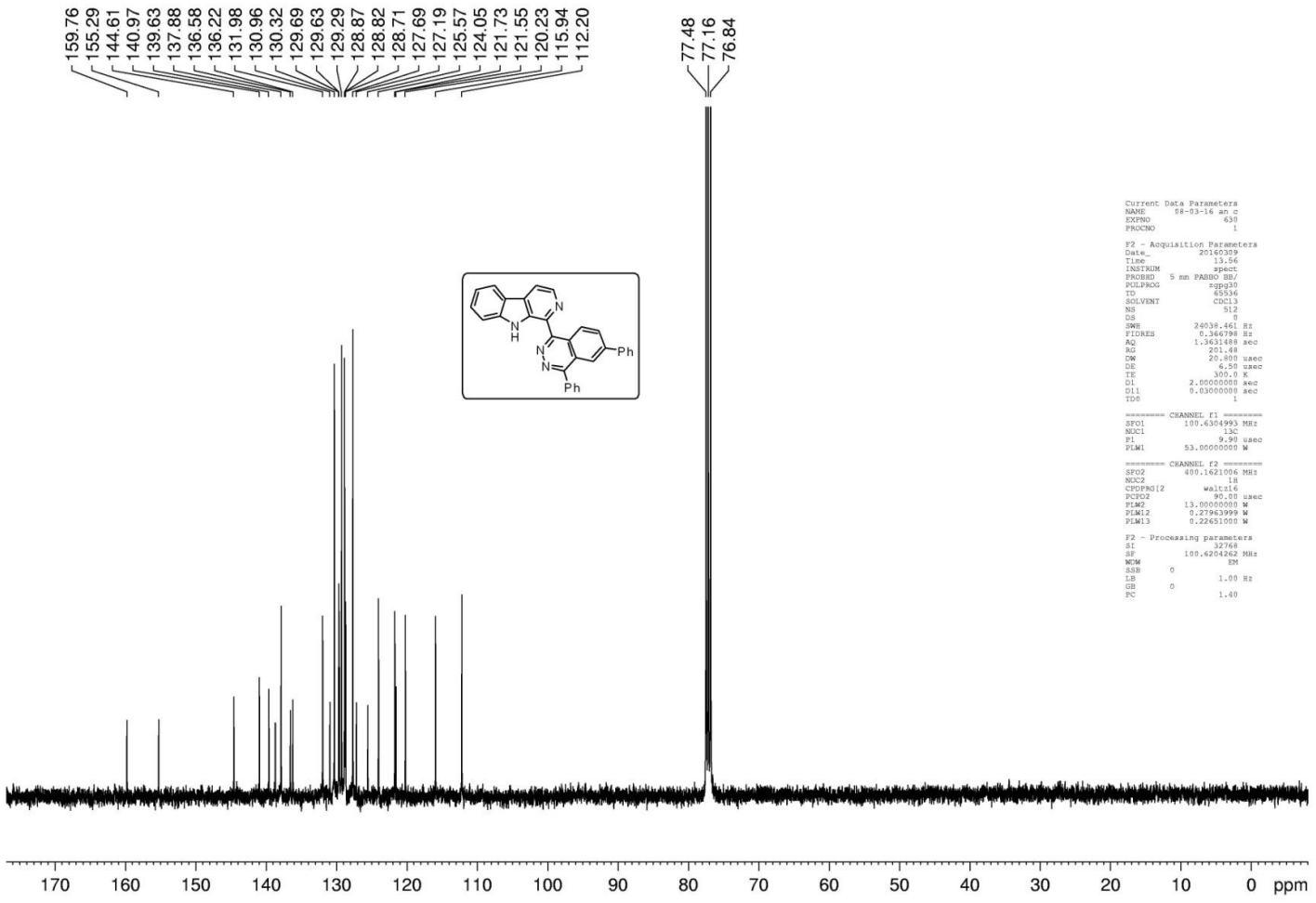



**Figure.** S-56**:** $^{13}$C-NMR spectrum of 1-(4,6-Diphenylphthalazin-1-yl)-9*H*-pyrido[3,4-*b*]indole **(5da)**.

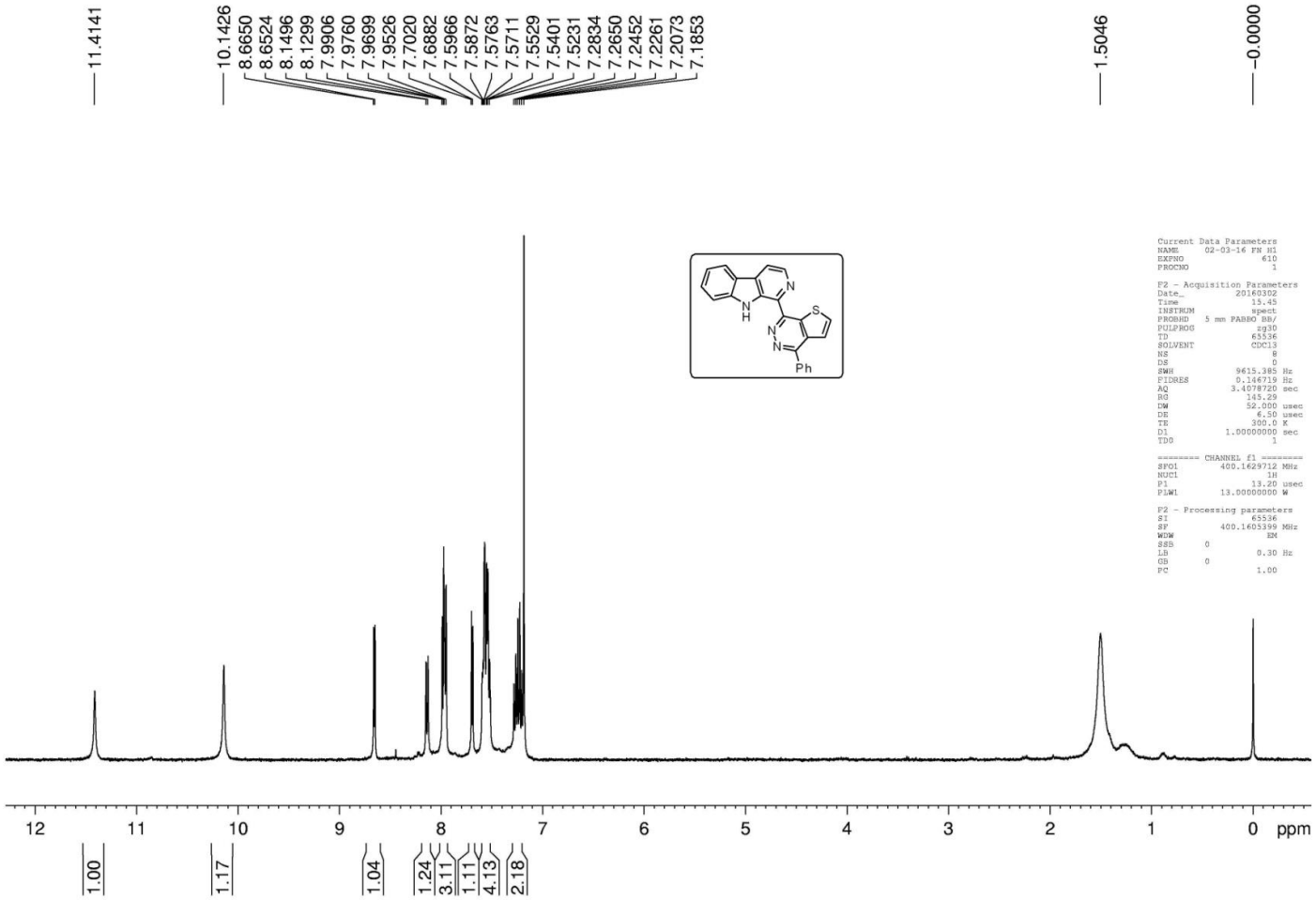



**Figure.** S-57**:** $^{1}$H-NMR spectrum of 4-Phenyl-7-(9*H*-pyrido[3,4-*b*]indol-1-yl)thieno[2,3-*d*]pyridazine **(5ka)**.

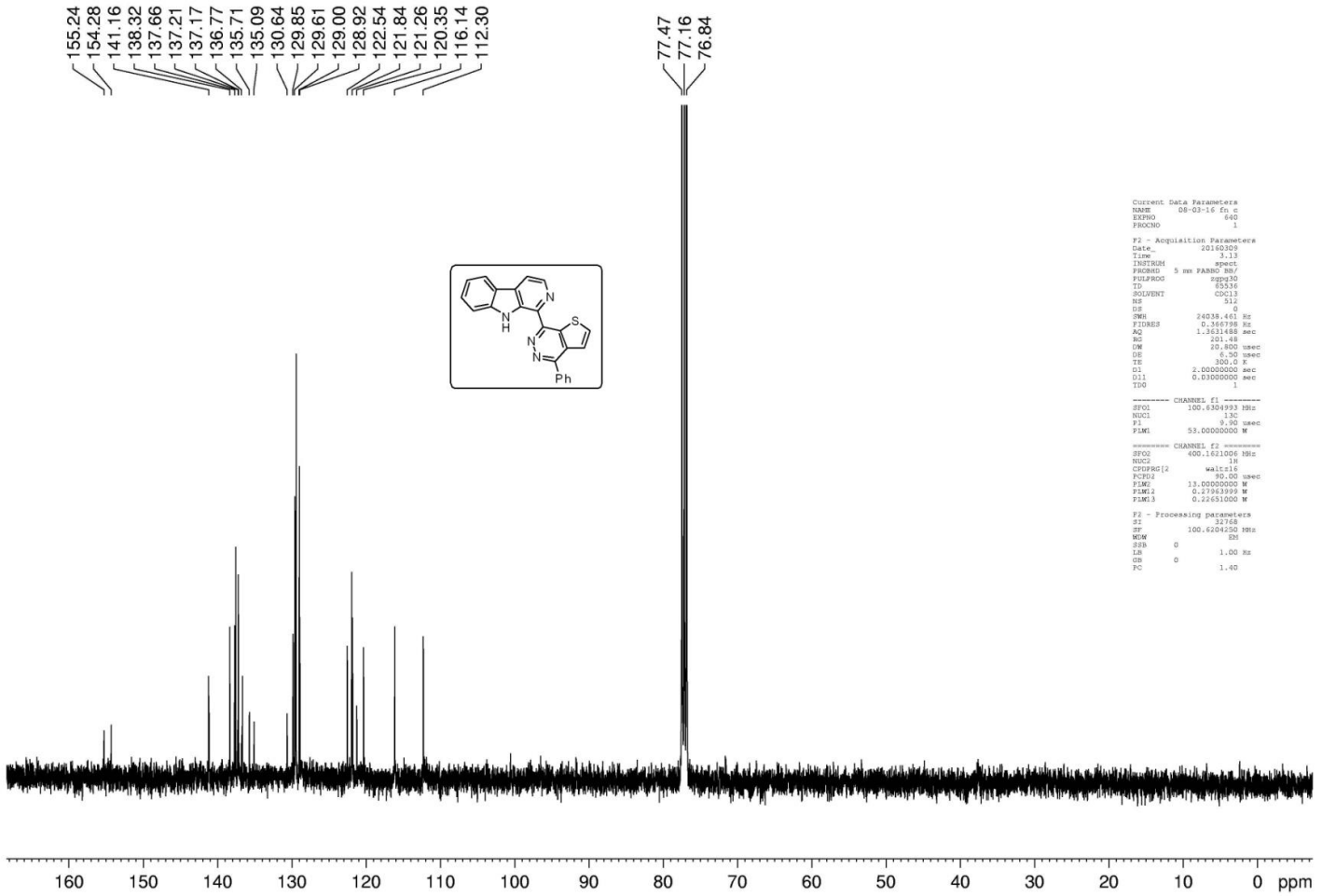



**Figure.** S-58**:** $^{13}$C-NMR spectrum of 4-Phenyl-7-(9*H*-pyrido[3,4-*b*]indol-1-yl)thieno[2,3-*d*]pyridazine **(5ka)**.

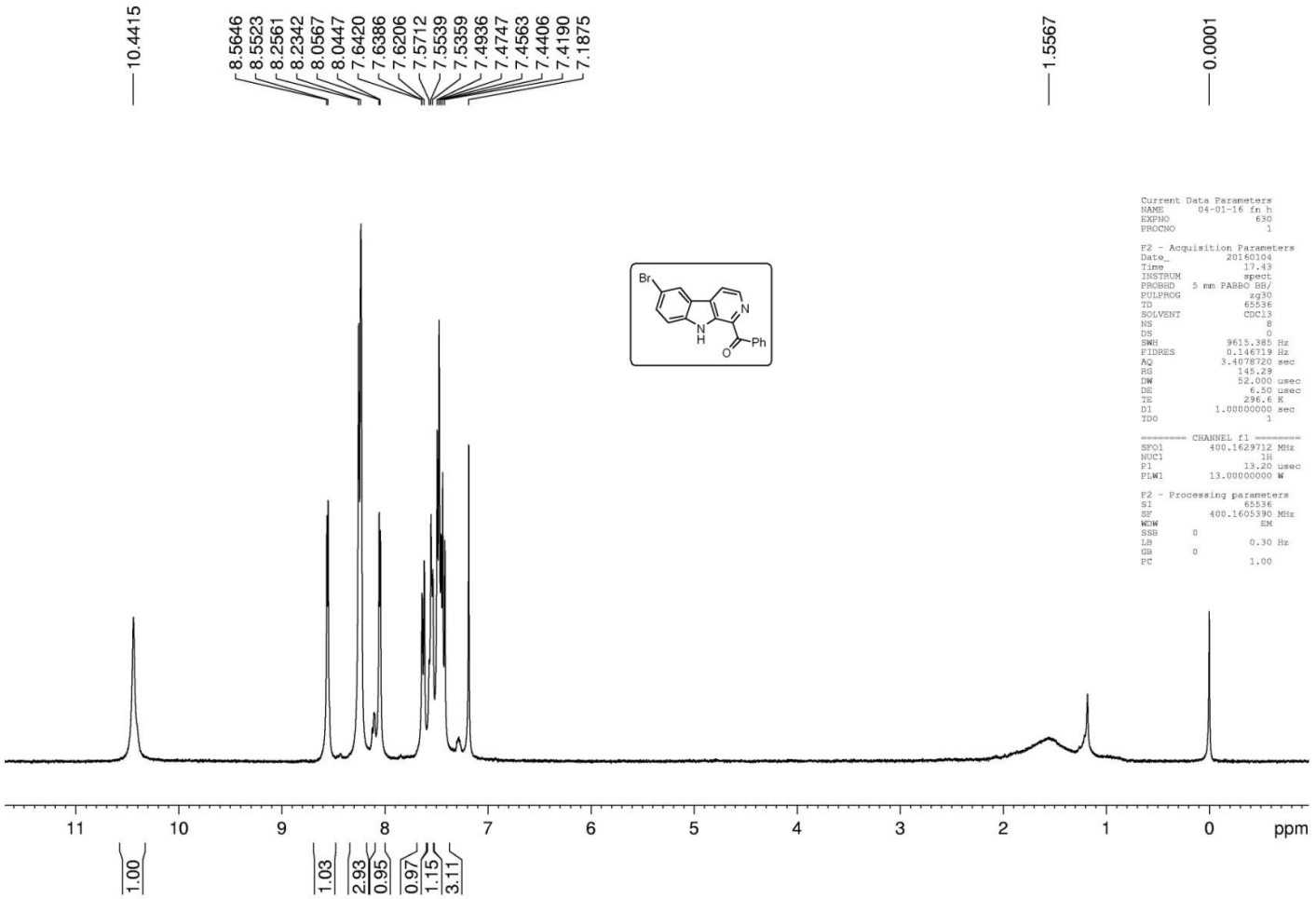



**Figure.** S-59**:** $^{1}$H-NMR spectrum of (6-Bromo-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone **(1m)**.

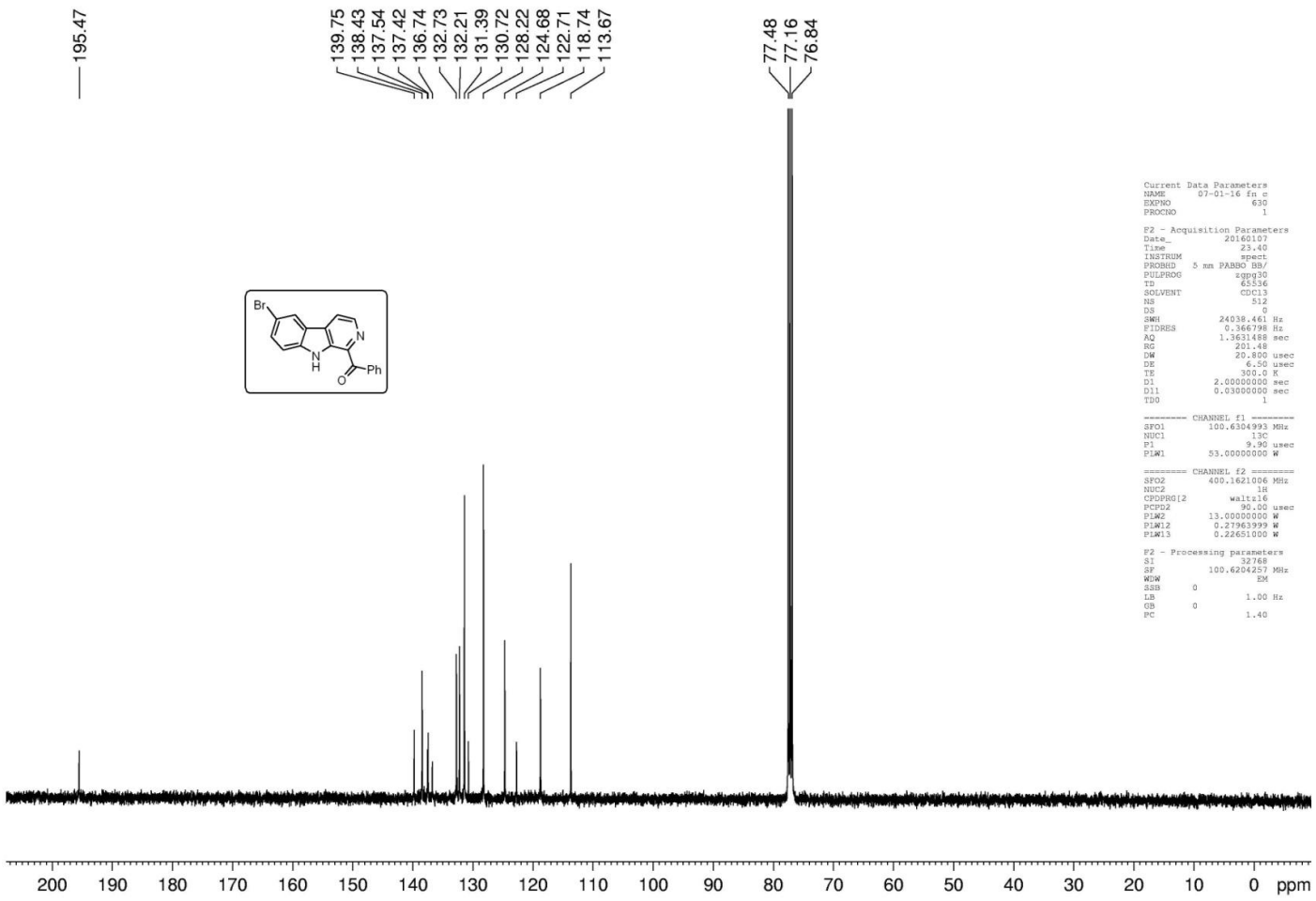
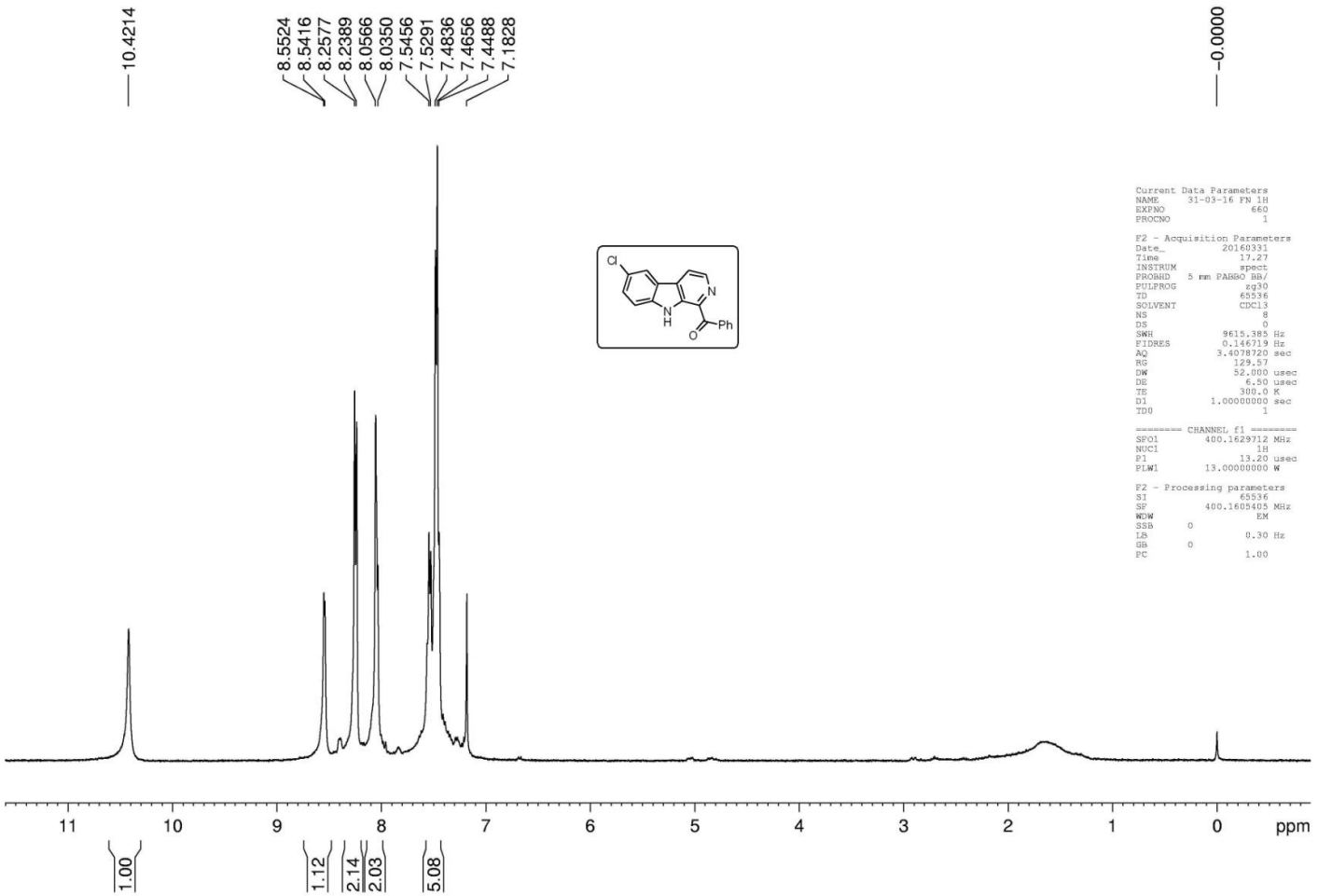



**Figure.** S-60**:** $^{13}$C-NMR spectrum of (6-Bromo-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone **(1m)**.

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PROCNO 1

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FIDRES 0.146719 Hz
AQ 3.4078720 sec
RG 129.57
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DE 6.50 usec
TE 300.0 K
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TD0 1

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NUC1 1H
P1 13.20 usec
PLW1 13.00000000 W

F2 - Processing parameters
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WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

**Figure.** S-61**:** $^{1}$H-NMR spectrum of (6-Chloro-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone **(1n)**.

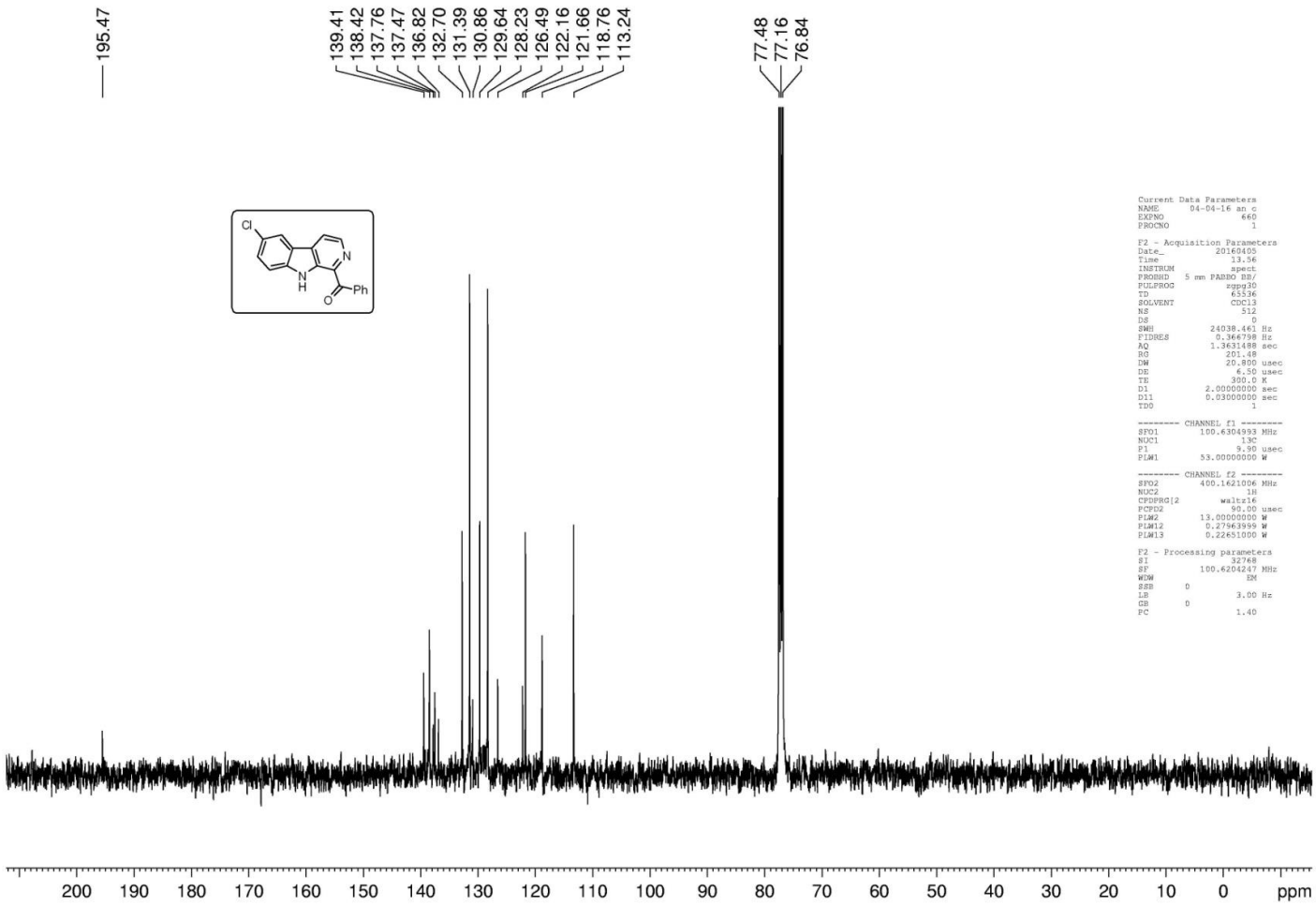


**Figure.** S-62**:** $^{13}$C-NMR spectrum of (6-Chloro-9*H*-pyrido[3,4-*b*]indol-1-yl)(phenyl)methanone **(1n)**.

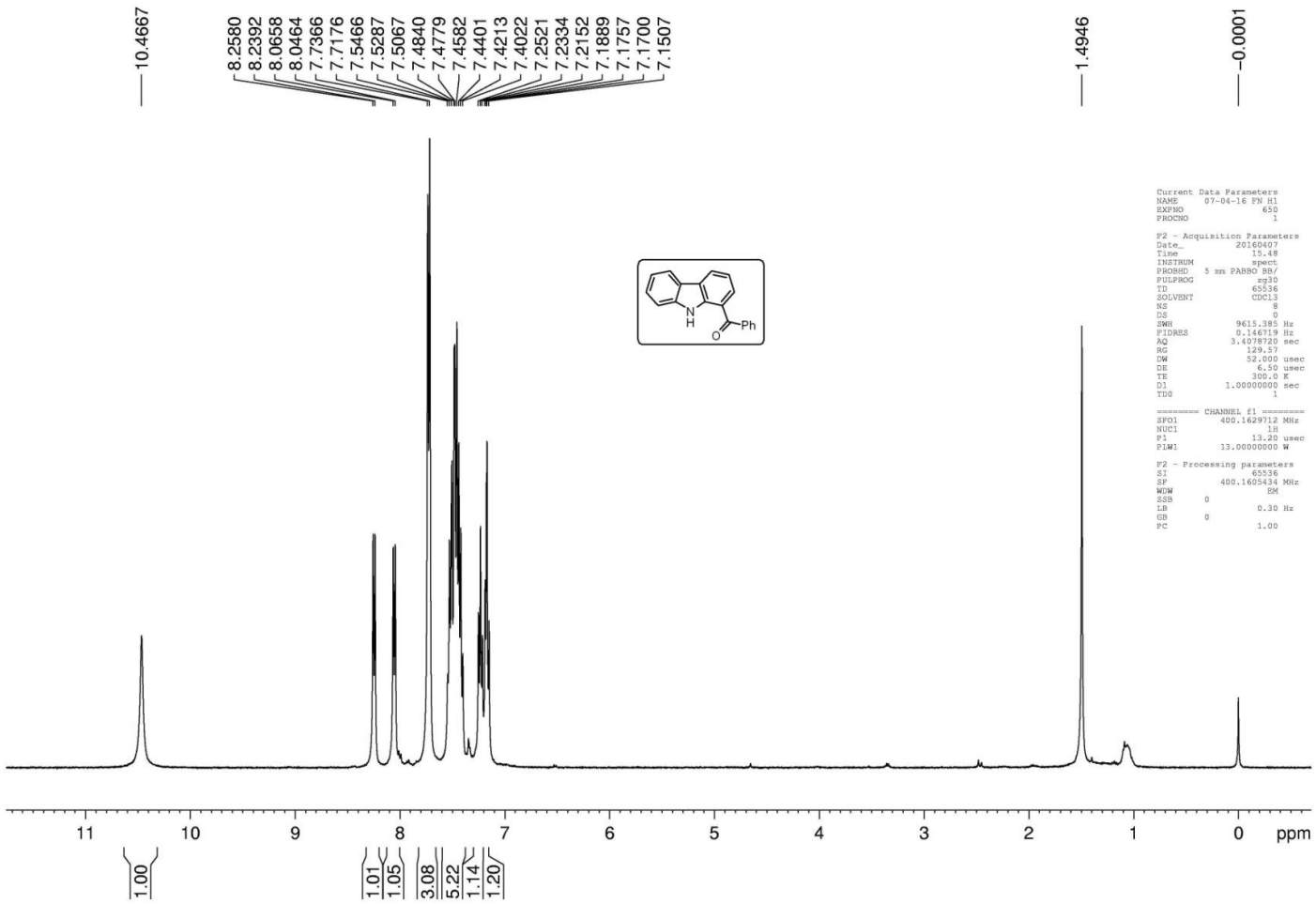


**Figure.** S-63**:** $^{1}$H-NMR spectrum of (9*H*-carbazol-1-yl)(phenyl)methanone **(4).**

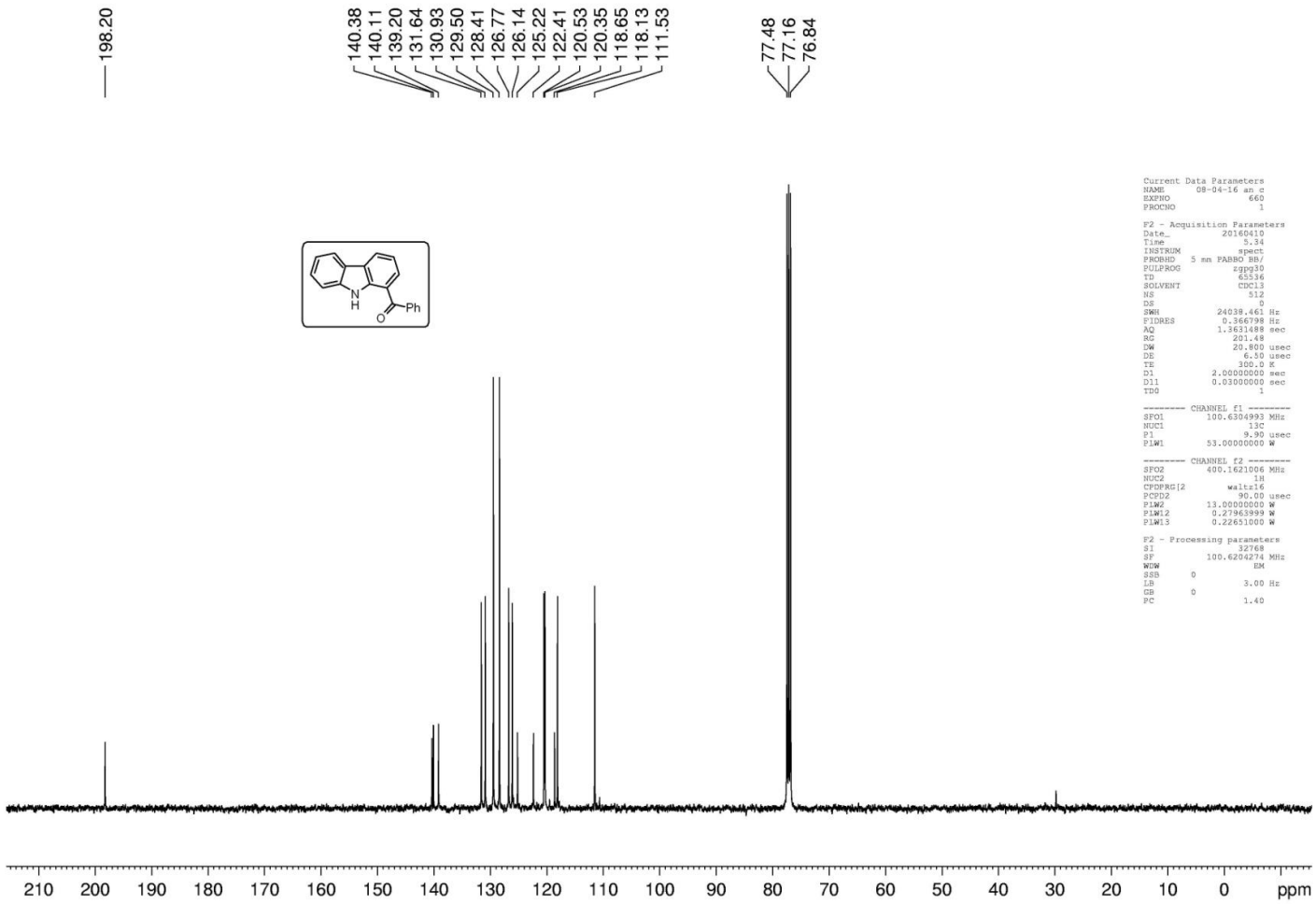


**Figure.** S-64**:** $^{13}$C-NMR spectrum of (9*H*-carbazol-1-yl)(phenyl)methanone **(4).**