Electronic Supplementary Material (ESI) for Chemical Communications

Palladium-catalyzed *ortho*-acylation of 2-aryl pyridine derivatives using benzylamines as new acyl sources

Qian Zhang, Fan Yang*, Yangjie Wu*

The College of Chemistry and Molecular Engineering, Henan Key Laboratory of Chemical Biology and Organic Chemistry, Key Laboratory of Applied Chemistry of Henan Universities, Zhengzhou University, Zhengzhou 450052, People's Republic of China

Tel/Fax: (+86)-371-6797-9408. E-mail: yangf@zzu.edu.cn; wyj@zzu.edu.cn

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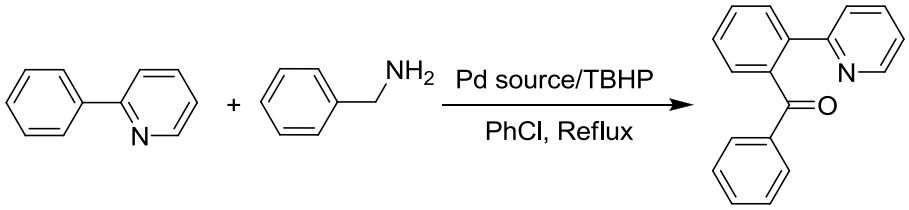
Optimization process data in detail

Table 1. Optimization of the Reaction Conditions[a]



1a **2a** **3a**

Entry	Palladium source	**1a**:**2a**	T (^{o}C)	t (h)	Additive (mol%)	Oxidant (equiv)	Solvent	Yield (%)[b]
1	$PdCl_2$(5)	1:2	reflux	8	-	O_2	chlorobenzene	<5
2	$PdCl_2$(5)	1:2	reflux	8	-	H_2O_2 (3.5)	chlorobenzene	<5
3	$PdCl_2$(5)	1:2	reflux	8	-	DDQ (3.5)	chlorobenzene	<5
4	$PdCl_2$(5)	1:2	reflux	8	-	Ag_2O (3.5)	chlorobenzene	<5
5	$PdCl_2$(5)	1:2	reflux	8	-	$Cu(OAc)_2$ (3.5)	chlorobenzene	<5
6	$PdCl_2$(5)	1:2	reflux	8	-	TBHP (3.5)	chlorobenzene	47
7	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	xylene	21
8	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	N,N-dimethyl aniline	<5
9	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	DMSO	<5
10	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	DMF	<5
11	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	DME	<5
12	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	NMP	17
13	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	nitrobenzene	<5
14	$PdCl_2$(5)	1:2	140	8	-	TBHP (3.5)	--	40
15	$PdCl_2$(5)	1:2	reflux	8	-	TBHP (3.5)	bromobenzene	37
16	$PdCl_2$(5)	1:2	reflux	8	-	TBHP (3.5)	1,4-dioxane	<5
17	$PdCl_2$(5)	1:2	reflux	8	TsOH (1equiv)	TBHP (3.5)	toluene	7
18	$PdCl_2$(5)	1:2	reflux	8	HOAc (1 equiv)	TBHP (3.5)	toluene	<5
19	$PdCl_2$(5)	1:2	reflux	8	-	TBHP (3.5)	toluene	16
20	$PdCl_2$(5)	1:2	reflux	8	PPh_3 (10)	TBHP (3.5)	chlorobenzene	40
21	$PdCl_2$(5)	1:2	reflux	8	Dppf (5)	TBHP (3.5)	chlorobenzene	35
22	$PdCl_2$(5)	1:2	reflux	8	1,10-Phenanthroline monohydrate (5)	TBHP (3.5)	chlorobenzene	21
23	$PdCl_2$(5)	1:2	reflux	8	DMEDA (5)	TBHP (3.5)	chlorobenzene	20
24	$PdCl_2$(5)	1:2	reflux	8	AgOAc (10)	TBHP (3.5)	chlorobenzene	20

25	$PdCl_2$(5)	1:2	reflux	8	CuBr (10)	TBHP (3.5)	chlorobenzene	15
26	$PdCl_2$(5)	1:2	reflux	8	$FeCl_3$ (10)	TBHP (3.5)	chlorobenzene	16
27	$PdCl_2$(5)	1:2	reflux	8	$AlCl_3$ (10)	TBHP (3.5)	chlorobenzene	<5
28	$PdCl_2$(5)	1:2	reflux	8	HOAc (10)	TBHP (3.5)	chlorobenzene	<5
29	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (3.5)	chlorobenzene	50
30	$PdCl_2$(10)	1:2	reflux	4	-	TBHP (3.5)	chlorobenzene	38
31	$PdCl_2$(10)	1:2	reflux	6	-	TBHP (3.5)	chlorobenzene	47
32	$PdCl_2$(10)	1:2	reflux	10	-	TBHP (3.5)	chlorobenzene	52
33	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (1)	chlorobenzene	<5
34	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (2.5)	chlorobenzene	24
35	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (3.5)	chlorobenzene	56
36	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (5)	chlorobenzene	58
37	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (7)	chlorobenzene	31
38	$PdCl_2$(10)	1:1.1	reflux	8	-	TBHP (3.5)	chlorobenzene	46
39	$PdCl_2$(10)	1:1.2	reflux	8	-	TBHP (3.5)	chlorobenzene	56 (46)
40	$PdCl_2$(10)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	69 (57)
41	$PdCl_2$(10)	1:1.6	reflux	8	-	TBHP (3.5)	chlorobenzene	54
42	$PdCl_2$(10)	1:2	reflux	8	-	TBHP (3.5)	chlorobenzene	50
43	$PdCl_2$(10)	1:3	reflux	8	-	TBHP (3.5)	chlorobenzene	37
44[c]	$PdCl_2$(10)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	76
45[d]	**$PdCl_2$(10)**	**1:1.4**	**reflux**	**8**	**-**	**TBHP (3.5)**	**chlorobenzene**	**81 (68)**
46[e]	$PdCl_2$(10)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	35
47[d]	$Pd(OAc)_2$ (10)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	47
48[d]	$Pd_2(dba)_3$ (5)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	55
49[d]	$Pd(PPh_3)_2Cl_2$ (10)	1:1.4	reflux	8	-	TBHP (3.5)	chlorobenzene	40

[a] Reaction conditions: **1a** (0.2 mmol), benzylamine, palladium catalyst, TBHP in 2 mL solvent at refluxing temperature for 8 h. [b] GC yield. [c] 1 mL solvent. [d] Under nitrogen atmosphere and 1 mL solvent. [e] At 110 ^{o}C, under nitrogen atmosphere and 1 mL solvent.

Experimental Section

General details

^{1}H NMR, ^{13}C NMR spectra were recorded on a Bruker DPX-400 spectrometer with $CDCl_3$ as the solvent and TMS as an internal standard. Melting points were measured by using a WC-1 microscopic apparatus. GC analysis was performed on Agilent 4890D gas chromatograph. Mass spectra were measured on an LC-MSD-Trap-XCT instrument. High resolution mass spectra were

measured on a UHPLC Q-TOF HR-MS. The single crystal X-ray diffraction study was measured on a Xcalibur, Eos, Gemini diffractometer. Dichloromethane, ethyl acetate and hexane were used for column chromatography without further purification, and other solvents were purified according to the standard methods. The chemicals were obtained from commercial sources and used as-received unless otherwise noted.

General procedure for the palladium-catalyzed acylation of 2-arylpyridines

To a solution of 2-arylpyridines (0.2 mmol) in chlorobenzene (1 mL), arylmethyl amines (0.28 mmol), $PdCl_2$ (10 mol%) and TBHP (0.7 mmol) were added. The resulting mixture was heated at refluxing temperature for 8 h. After the reaction was complete, the mixture was added into H_2O (25 mL) and extracted with ethyl acetate (10 mL) for three times. The combined organic layer was dried over anhydrous Na_2SO_4 and filtered. After removal of the solvent *in vacuo*, the residue was purified by column chromatography (ethyl acetate/hexane) to afford the pure product.

2-[(2-benzoyl)phenyl]pyridine (**3a**)[1]

Light yellow solid, mp 101–103 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 7.01 (t, J = 5.8 Hz, 1H), 7.28–7.30 (m, 2H), 7.36–7.42 (m, 1H), 7.49–7.63 (m, 5H), 7.71 (d, J = 7.52 Hz, 2H), 7.79 (d, J = 7.64 Hz, 1H), 8.37 (d, J = 4.08 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.9, 122.7, 128.0, 128.5, 128.8, 129.1, 129.5, 130.2, 132.3, 136.3, 137.9, 139.5, 139.7, 149.0, 156.8, 198.2; HRMS-ESI (m/z): calcd for $C_{18}H_{14}NO$ ($M+H^+$): 260.1070, found 260.1076.

2-{[2-benzoyl-4-(*tert*-butyl)]phenyl}pyridine (**3b**)

Light yellow solid, mp 74–76 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 1.37 (s, 9H), 6.96 (t, J = 5.86 Hz, 1H), 7.22–7.27 (m, 2H), 7.36 (t, J = 7.2 Hz, 1H), 7.46 (d, J = 7.76 Hz, 1H), 7.49–7.56 (m, 2H), 7.62 (d, J = 8.16 Hz, 1H), 7.67–7.72 (m, 3H), 8.33 (d, J = 4.16 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 31.2, 34.9, 121.7, 122.5, 126.1, 127.3, 128.0, 128.4, 129.5, 132.2, 136.2, 136.8, 138.0, 139.1, 149.0, 151.9, 156.7, 198.7; HRMS-ESI (m/z): calcd for $C_{22}H_{22}NO$ ($M+H^+$): 316.1696, found 316.1700.

2-{[2-benzoyl-4-(*tert*-butyl)]phenyl}-3-methylpyridine (**3c**)

Light yellow solid, mp 73–75 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 1.37 (s, 9H), 2.23 (s, 3H), 6.94 (dd, J = 7.50 Hz, 4.80 Hz, 1H), 7.24-7.30 (m, 2H), 7.32-7.42 (m, 3H), 7.59-7.67 (m, 4H), 8.24 (d, J = 4.28 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 31.3, 34.8, 44.0, 122.0, 126.6, 127.5, 127.8, 128.5, 129.6, 129.7, 131.5, 132.3, 137.7, 137.9, 138.8, 146.4, 150.8, 157.7, 198.2; HRMS-ESI (m/z): calcd for $C_{23}H_{24}NO$ ($M+H^+$): 330.1852, found 330.1857.

2-[(2-benzoyl-4-methyl)phenyl]pyridine (**3d**)[1]

Light yellow solid, mp 131–133 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 2.45 (s, 3H), 6.97 (dd, J = 6.64 Hz, 5.04 Hz, 1H), 7.22-7.28 (m, 2H), 7.34-7.42 (m, 3H), 7.46 (d, J = 7.84 Hz, 1H), 7.50-7.56 (m, 1H), 7.65-7.70 (m, 3H), 8.33 (d, J = 4.28 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.2, 121.7, 122.4, 128.0, 128.6, 129.4, 129.6, 130.9, 132.2, 136.2, 136.8, 138.0, 138.7, 139.4, 149.0, 156.7, 198.5; HRMS-ESI (m/z): calcd for $C_{19}H_{16}NO$ ($M+H^+$): 274.1226, found 274.1231.

2-[(2-benzoyl-5-methyl)phenyl]-4-methylpyridine (**3e**)

Light yellow solid, mp 134–136 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 2.24 (s, 3H), 2.49 (s, 3H),

6.80 (d, J = 4.96 Hz, 1H), 7.21-7.27 (m, 3H), 7.29-7.36 (m, 2H), 7.46 (d, J = 7.72 Hz, 1H), 7.56 (s, 1H), 7.63-7.67 (m, 2H), 8.22 (d, J = 5.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.0, 21.5, 122.9, 124.1, 128.0, 129.0, 129.4, 129.5, 129.6, 132.2, 136.6, 138.2, 140.1, 140.6, 147.2, 148.9, 156.9, 198.4; HRMS-ESI (m/z): calcd for $C_{20}H_{18}NO$ ($M+H^+$): 288.1383, found 288.1389.

2-[(2-benzoyl-5-methyl)phenyl]-5-methylpyridine (**3f**)
White solid, mp 150–152 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.20 (s, 3H), 2.48 (s, 3H), 7.23-7.34 (m, 5H), 7.35-7.44 (m, 2H), 7.56 (s, 1H), 7.68 (d, J = 7.68 Hz, 2H), 8.21 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.1, 21.5, 122.4, 128.0, 128.8, 129.2, 129.5, 129.6, 131.4, 132.2, 136.5, 136.7, 138.1, 139.9, 140.5, 149.5, 154.3, 198.4; HRMS-ESI (m/z): calcd for $C_{20}H_{18}NO$ ($M+H^+$): 288.1383, found 288.1387.

2-[(2-benzoyl-5-methyl)phenyl]-3-methylpyridine (**3g**)
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.18 (s, 3H), 2.46 (s, 3H), 6.98 (t, J = 6.0 Hz, 1H), 7.27- 7.31 (m, 4H), 7.34-7.41 (m, 2H), 7.52 (d, J = 7.56 Hz, 1H), 7.65 (d, J = 7.44 Hz, 2H), 8.29 (d, J = 3.76 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 21.5, 122.1, 127.9, 128.3, 129.8, 130.0, 130.7, 131.5, 132.3, 136.0, 137.6, 137.9, 141.0, 141.2, 146.4, 158.1, 197.5; HRMS-ESI (m/z): calcd for $C_{20}H_{18}NO$ ($M+H^+$): 288.1383, found 288.1390.

2-[(2-benzoyl-4-methoxy)phenyl]pyridine (**3h**)[1]
Light yellow solid, mp 113–115 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.87 (s, 3H), 6.94 (t, J = 6.0 Hz, 1H), 7.05 (d, J = 1.84 Hz, 1H), 7.09-7.14 (m, 1H), 7.22-7.28 (m, 2H), 7.34-7.39 (m, 1H), 7.42-7.54 (m, 2H), 7.67-7.74 (m, 3H), 8.29 (d, J = 4.24 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6, 114.0, 116.1, 121.4, 122.0, 128.0, 129.4, 129.9, 132.0, 132.3, 136.2, 137.8, 140.8, 148.8, 156.3, 159.9, 197.9; HRMS-ESI (m/z): calcd for $C_{19}H_{16}NO_2$ ($M+H^+$): 290.1176, found 290.1180.

2-[(2-benzoyl-6-methoxy)phenyl]pyridine (**3i**)
Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.85 (s, 3H), 6.94-6.99 (m, 1H), 7.11-7.16 (m, 2H), 7.22-7.28 (m, 2H), 7.35-7.40 (m, 1H), 7.46 (t, J = 7.96 Hz, 1H), 7.50-7.58 (m, 2H), 7.64-7.68 (m, 2H), 8.34 (d, J = 4.72 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.0, 113.0, 121.2, 121.7, 126.0, 127.9, 128.7, 129.4, 129.6, 132.3, 135.4, 137.8, 141.9, 148.7, 154.3, 156.7, 197.2; HRMS-ESI (m/z): calcd for $C_{19}H_{16}NO_2$ ($M+H^+$): 290.1176, found 290.1181.

2-[(2-benzoyl-5-methoxy)phenyl]pyridine (**3j**)
Light yellow solid, mp 101–104 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.92 (s, 3H), 6.98-7.05 (m, 2H), 7.21-7.26 (m, 3H), 7.32-7.41 (m, 2H), 7.49-7.57 (m, 2H), 7.65 (d, J = 7.52 Hz, 2H), 8.40 (d, J = 4.16 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6, 113.8, 114.6, 122.0, 123.3, 128.0, 130.0, 131.5, 131.8, 132.1, 136.2, 138.3, 142.3, 149.1, 157.1, 161.2, 197.5; HRMS-ESI (m/z): calcd for $C_{19}H_{16}NO_2$ ($M+H^+$): 290.1176, found 290.1180.

2-[(2-benzoyl-5-methoxy)phenyl]-3-methylpyridine (**3k**)
Light yellow solid, mp 89–91 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.18 (s, 3H), 3.89 (s, 3H), 6.97-7.03 (m, 3H), 7.29 (t, J = 7.14 Hz, 2H), 7.36-7.43 (m, 2H), 7.59-7.67 (m, 3H), 8.32 (d, J = 4.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.4, 55.6, 113.0, 115.5, 127.9, 129.3, 129.8, 131.1,

131.4, 132.1, 132.4, 137.6, 138.2, 143.3, 146.4, 158.0, 161.5, 196.8; HRMS-ESI (m/z): calcd for $C_{20}H_{18}NO$ ($M+H^+$): 304.1332, found 304.1338.

2-(2-benzoylphenyl)-3-methylpyridine (**3l**)
Yellow solid, mp 93–96 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.21 (s, 3H), 6.97 (dd, J = 7.04 Hz, 5.0 Hz, 1H), 7.25-7.31 (m, 2H), 7.35-7.41 (m, 2H), 7.45-7.51 (m, 2H), 7.56-7.63 (m, 2H), 7.66 (d, J = 7.52 Hz, 2H), 8.26 (d, J = 3.96 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 122.2, 127.7, 127.9, 129.5, 129.7, 129.9, 130.4, 131.5, 132.5, 137.7, 137.8, 139.1, 140.7, 146.4, 157.7, 197.7; HRMS-ESI (m/z): calcd for $C_{19}H_{16}NO$ ($M+H^+$): 274.1226, found 274.1230.

2-[(2-benzoyl-4-bromo)phenyl]pyridine (**3m**)[1]
Yellow solid, mp 106–108 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (dd, J = 6.72 Hz, 5.16Hz, 1H), 7.28 (t, J = 7.36 Hz, 2H), 7.40 (t, J = 7.36Hz, 1H), 7.48 (d, J = 7.88Hz, 1H), 7.57 (td, J = 7.74 Hz, 1.6Hz, 1H), 7.63-7.75 (m, 5H), 8.33 (d, J = 4.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.3, 122.4, 122.9, 128.2, 129.4, 130.2, 131.8, 132.7, 133.1, 136.5, 137.3, 138.4, 141.2, 149.1, 155.6, 196.5; HRMS-ESI (m/z): calcd for $C_{18}H_{13}BrNO$ ($M+H^+$): 338.0181, found 338.0180.

2-[(2-benzoyl-4-bromo)phenyl]-3-methylpyridine (**3n**)
Light yellow solid, mp 57–59 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.21 (s, 3H), 6.97 (s, 1H), 7.26-7.37 (m, 5H), 7.63 (d, J = 6.72 Hz, 2H), 7.69-7.75 (m, 2H), 8.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 122.5, 127.0, 128.1, 129.6, 131.5, 131.6, 132.2, 132.8, 133.2, 137.1, 138.0, 139.4, 141.1, 146.5, 156.4, 195.9; HRMS-ESI (m/z): calcd for $C_{19}H_{15}BrNO$ ($M+H^+$): 352.0337, found 352.0335.

2-[(2-benzoyl-5-ethoxycarbonyl)phenyl]pyridine (**3o**)
White solid, mp 111–113 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.44 (t, J = 7.12 Hz, 3H), 4.45 (dd, J = 14.24Hz, 7.12 Hz, 2H), 7.05 (dd, J = 8.78 Hz, 4.40 Hz, 1H), 7.28 (t, J = 6.96 Hz, 2H), 7.41 (t, J = 7.36 Hz, 1H), 7.57-7.70 (m, 5H), 8.19 (dd, J = 7.90 Hz, 1.16 Hz, 1H), 8.35 (d, J = 4.72 Hz, 1H), 8.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.4, 61.5, 122.4, 122.5, 128.2, 129.1, 129.3, 129.5, 129.7, 132.0, 132.6, 136.6, 137.4, 139.6, 143.5, 149.9, 155.7, 165.8, 197.4; HRMS-ESI (m/z): calcd for $C_{21}H_{18}NO_3$ ($M+H^+$): 332.1281, found 332.1286.

2-[(2-benzoyl-5-ethoxycarbonyl)phenyl]-5-methylpyridine (**3p**)
Light yellow solid, mp 95–97 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.44 (t, J = 7.1 Hz, 3H), 2.21 (s, 3H), 4.45 (dd, J = 14.18 Hz, 7.04Hz, 2H), 7.29 (t, J = 8.20 Hz, 2H), 7.39-7.45 (m, 2H), 7.54 (t, J = 8.24 Hz, 2H), 7.69 (d, J = 7.56 Hz, 2H), 8.14-8.18 (m, 2H), 8.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.4, 18.1, 61.4, 121.8, 128.2, 128.9, 129.2, 129.3, 129.5, 131.9, 132.0, 132.6, 137.1, 137.5, 139.6, 143.4, 149.4, 152.8, 165.9, 197.5; HRMS-ESI (m/z): calcd for $C_{22}H_{20}NO_3$ ($M+H^+$): 346.1438, found 346.1442.

2-[(2-benzoyl-4-fluoro)phenyl]pyridine (**3q**)
Light yellow solid, mp 150–152 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.02 (dd, J = 7.02 Hz, 1H), 7.22-7.33 (m, 4H), 7.37-7.49 (m, 2H), 7.55-7.69 (m, 3H), 7.77 (dd, J = 8.52 Hz, 1H), 8,35 (d, J = 4.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 116.2 (d, J = 22.9 Hz), 117.1 (d, J = 21.4 Hz),

122.0, 122.4, 128.2, 129.4, 130.7 (d, J = 8.0 Hz), 132.7, 135.7 (d, J = 2.8 Hz), 136.5, 137.3, 141.5 (d, J = 6.1 Hz), 149.0, 155.7, 162.6 (d, J = 249.3 Hz), 196.6; HRMS-ESI (m/z): calcd for $C_{18}H_{13}FNO$ ($M+H^+$): 278.0981, found 278.0981.

2-[2-(3-benzoyl)thienyl]pyridine (**3r**)
Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.07 (t, J = 5.86 Hz, 1H), 7.23 (d, J = 5.0 Hz, 1H), 7.32-7.38 (m, 3H), 7.42-7.49 (m, 3H), 7.82 (d, J = 7.52 Hz, 2H), 8.47 (d, J = 3.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.4, 122.5, 126.6, 128.4, 129.9, 130.0 , 133.1, 136.3, 137.5, 137.8, 145.8, 149.4, 151.3, 193.8; HRMS-ESI (m/z): calcd for $C_{16}H_{12}NOS$ ($M+H^+$): 266.0634, found 266.0639.

2-[2-(3-benzoyl)thienyl]-5-methylpyridine (**3s**)
Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.24 (s, 3H), 7.21 (d, J = 5.16 Hz, 1H), 7.27 (s,2H), 7.32-7.41 (m, 3H), 7.48 (t, J = 7.36 Hz, 1H), 7.82 (d, J = 7.44 Hz, 2H), 8.31 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 18.2, 122.1, 126.1, 128.4, 129.9, 130.0, 132.2, 133.1, 136.8, 137.3, 137.6, 146.1, 148.6, 149.8, 193.8; HRMS-ESI (m/z): calcd for $C_{17}H_{14}NOS$ ($M+H^+$): 280.0791, found 280.0795.

10-benzoylbenzo[h]quinoline (**3t**)[1]
Yellow solid, mp 145–147 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27-7.37 (m, 3H), 7.38-7.46 (m, 1H), 7.64-7.67 (m, 1H), 7.73-7.83 (m, 4H), 7.91 (d, J = 8.8 Hz, 1H), 8.04-8.12 (m, 2H), 8.52 (dd, J = 4.36 Hz, 1.56 Hz, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.7, 126.2, 126.4, 126.6, 127.0, 127.8, 127.9, 128.1, 128.5, 128.7, 129.0, 131.8, 133.8, 135.3, 138.9, 139.3, 144.6, 147.1; HRMS-ESI (m/z): calcd for $C_{20}H_{14}NO$ ($M+H^+$): 284.1070, found 284.1074.

2-[2-(3,4-dimethoxybenzoyl)phenyl]-3-methylpyridine (**3u**)
Light yellow solid, mp 124–126 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.14 (s, 3H), 3.78 (s, 3H), 3.81 (s, 3H), 6.67 (d, J = 8.36 Hz, 1H), 6.94 (dd, J = 6.94Hz, 4.80 Hz, 1H), 7.19-7.23(m, 1H), 7.25-7.27 (m, 1H), 7.32-7.43 (m, 3H), 7.48-7.52 (m, 2H), 8.21 (d, J = 4.12 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.6, 55.9, 56.0, 109.5, 111.3, 122.2, 125.7, 127.5, 129.3, 129.9, 130.1, 130.5, 131.7, 137.7, 139.2, 140.5, 146.4, 148.6, 152.9, 157.9, 196.2; HRMS-ESI (m/z): calcd for $C_{21}H_{20}NO_3$ ($M+H^+$): 334.1438, found 334.1442.

3-methyl-2-[2-(4-methylbenzoyl)phenyl]pyridine (**3v**)
Light yellow solid, mp 82–84 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.21 (s, 3H), 2.34 (s, 3H), 7.0 (dd, J = 7.68 Hz, 4.80 Hz, 1H), 7.11 (d, J = 8.08 Hz, 2H), 7.26 (s, 1H), 7.39 (d, J = 7.72 Hz, 1H), 7.44-7.51 (m, 2H), 7.55-7.61 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.6, 21.7, 122.2, 127.6, 128.7, 129.5, 130.0, 130.1, 130.3, 131.6, 135.1, 137.8, 139.3, 140.7, 143.4, 146.5, 157.9, 197.3; HRMS-ESI (m/z): calcd for $C_{20}H_{18}NO$ ($M+H^+$): 288.1383, found 288.1388.

2-[2-(3,4-dicholobenzoyl)phenyl]-3-methylpyridine (**3w**)
Light yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.26 (s, 3H), 7.0 (dd, J = 7.20 Hz, 4.84 Hz, 1H), 7.35 (d, J = 8.24 Hz, 1H), 7.42 (d, J = 7.36 Hz, 1H), 7.46-7.55 (m, 3H), 7.59-7.64 (m, 2H), 7.68 (s, 1H), 8.25 (d, J = 3.72 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 122.4, 128.0, 128.6,

129.5, 130.0, 130.1, 130.8, 131.3, 131.6, 132.4, 136.8, 137.4, 138.1, 138.3, 140.6, 146.5, 157.0, 195.4; HRMS-ESI (m/z): calcd for $C_{19}H_{14}Cl_2NO$ ($M+H^+$): 342.0452, found 342.0450.

2-[2-(4-bromobenzoyl)phenyl]-3-methylpyridine (**3x**)

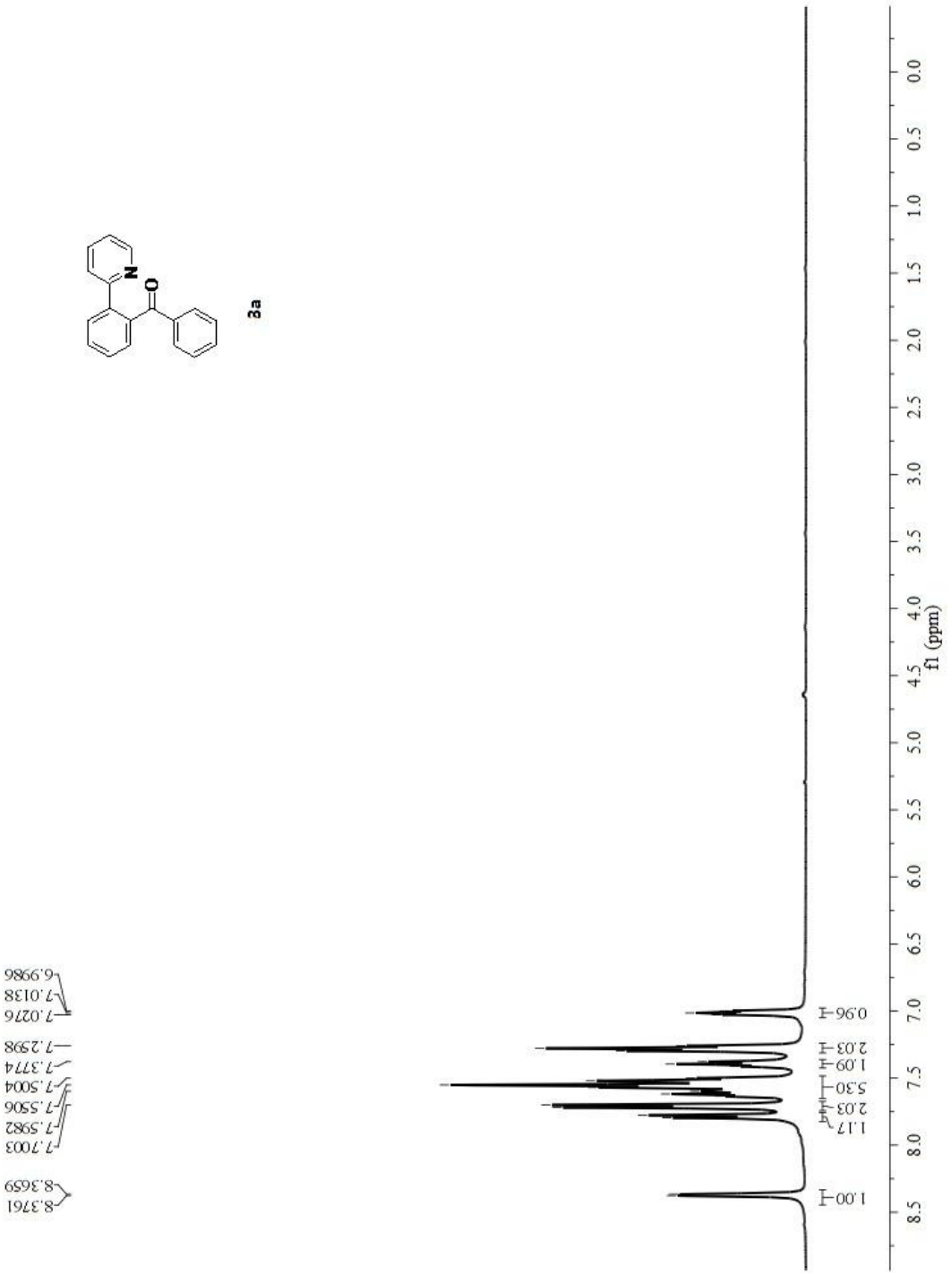
Light yellow solid, mp 118–120 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 2.13 (s, 3H), 6.91 (dd, J = 6.98 Hz, 4.96 Hz, 1H), 7.30-7.35 (m, 3H), 7.37-7.45 (m, 4H), 7.48-7.54 (m, 2H), 8.17 (d, J = 3.72 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 122.3, 127.6, 127.8, 129.3, 130.0, 130.6, 131.2, 131.3, 131.6, 136.5, 137.9, 138.7, 140.6, 146.5, 157.4, 196.7; HRMS-ESI (m/z): calcd for $C_{19}H_{15}BrNO$ ($M+H^+$): 352.0337, found 352.0333.

3-methyl-2-[2-(4-trifluoromethylbenzoyl)phenyl]pyridine (**3y**)

Light yellow solid, mp 65–67 ^oC; ^1H NMR (400 MHz, $CDCl_3$): δ 2.25 (s, 3H), 6.99 (t, J = 4.94 Hz, 1H), 7.38-7.41 (m, 1H), 7.40-7.47 (m, 4H), 7.53 (d, J = 6.40 Hz, 2H), 7.74 (d, J = 7.52 Hz, 2H), 8.24 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.5, 122.2, 122.4, 124.9 (q, J = 3.7 Hz), 127.9, 128.0, 128.0 (q, J = 200.0 Hz), 129.7, 130.0, 130.9, 133.5 (q, J = 32.5 Hz), 138.0, 138.5, 140.8, 140.8, 146.5, 157.2, 196.8; HRMS-ESI (m/z): calcd for $C_{20}H_{15}F_3NO$ ($M+H^+$): 342.1106, found 342.1104.

Refrences:

1. F. H. Xiao, Q. Shuai, F. Zhao, O. Baslè, G. J. Deng and C. J. Li, *Org. Lett.*, 2011, **13**, 1614.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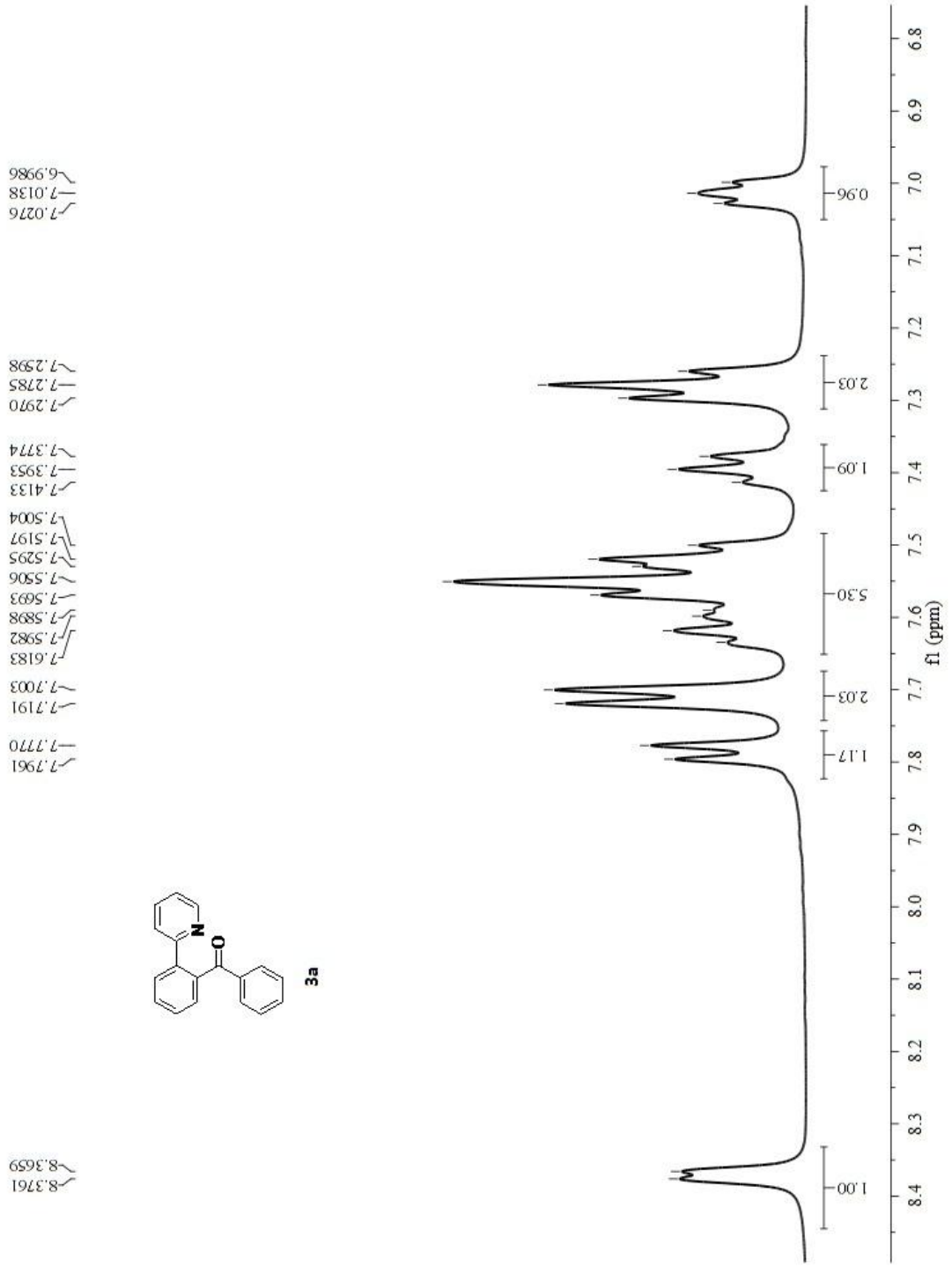
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2.03
1.17
5.30
2.03
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8.3
8.2
8.1
8.0
7.9
7.8
7.7
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7.3
7.2
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6.8
f1 (ppm)
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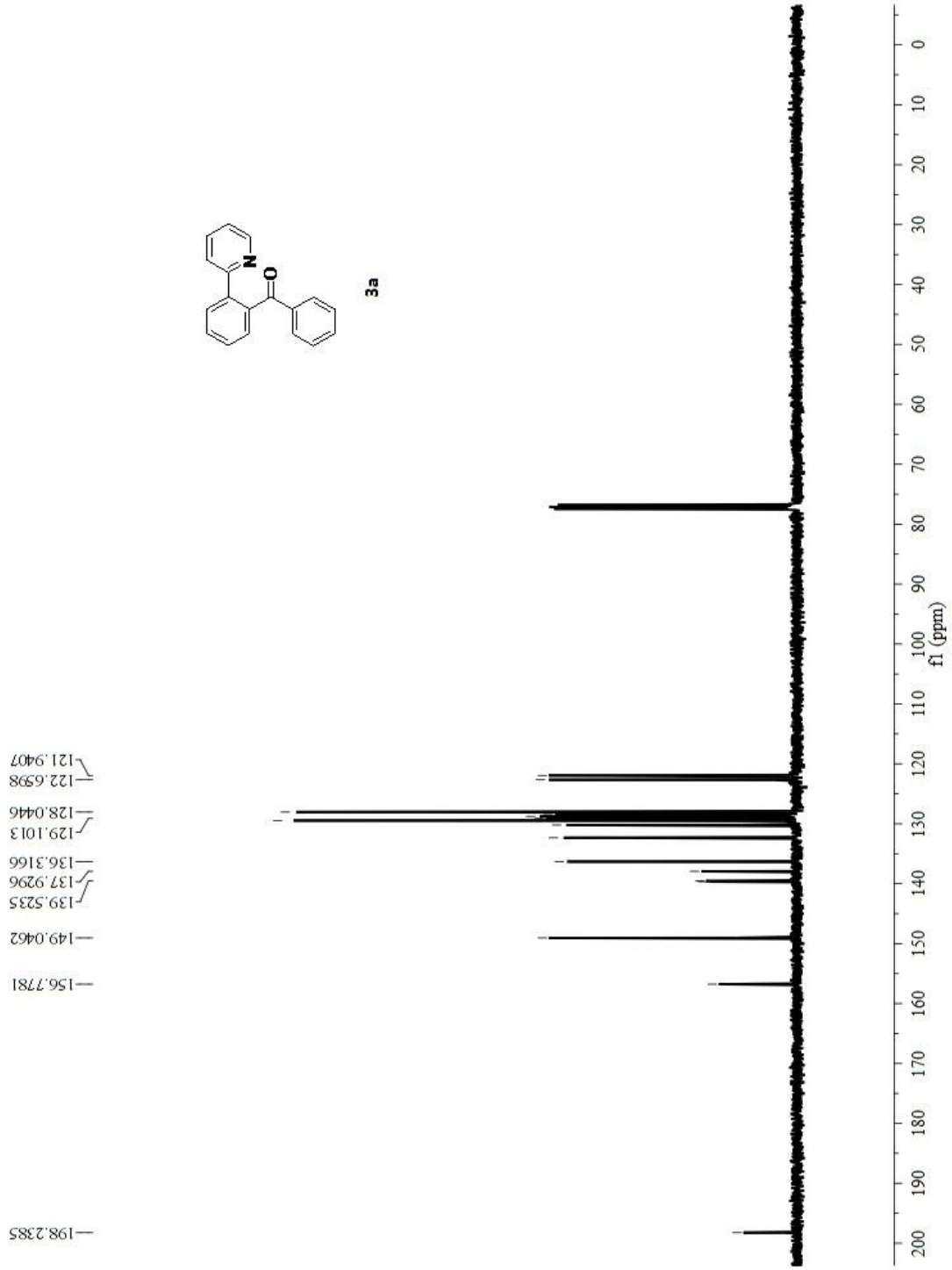
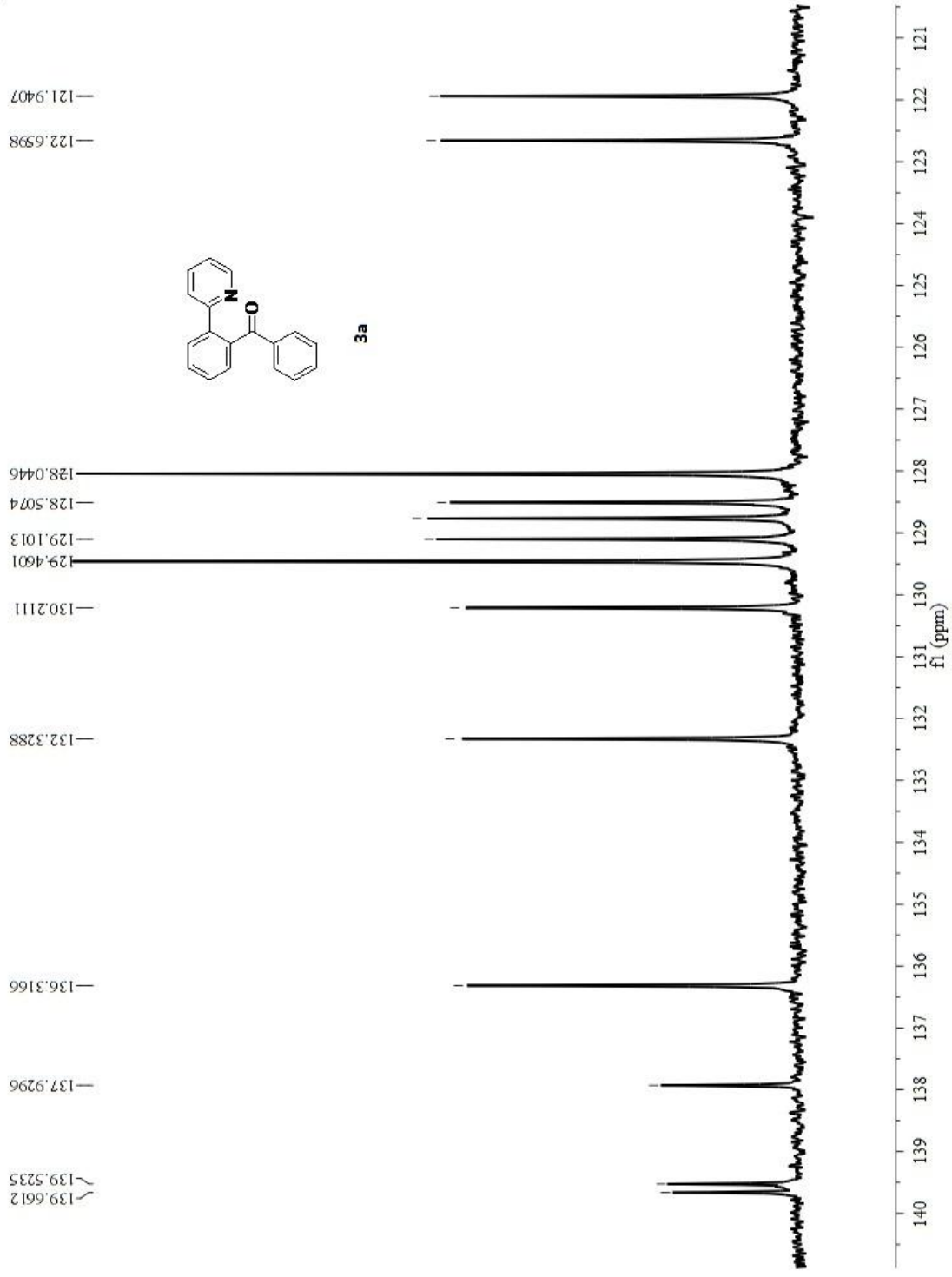
O
3a

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O
N
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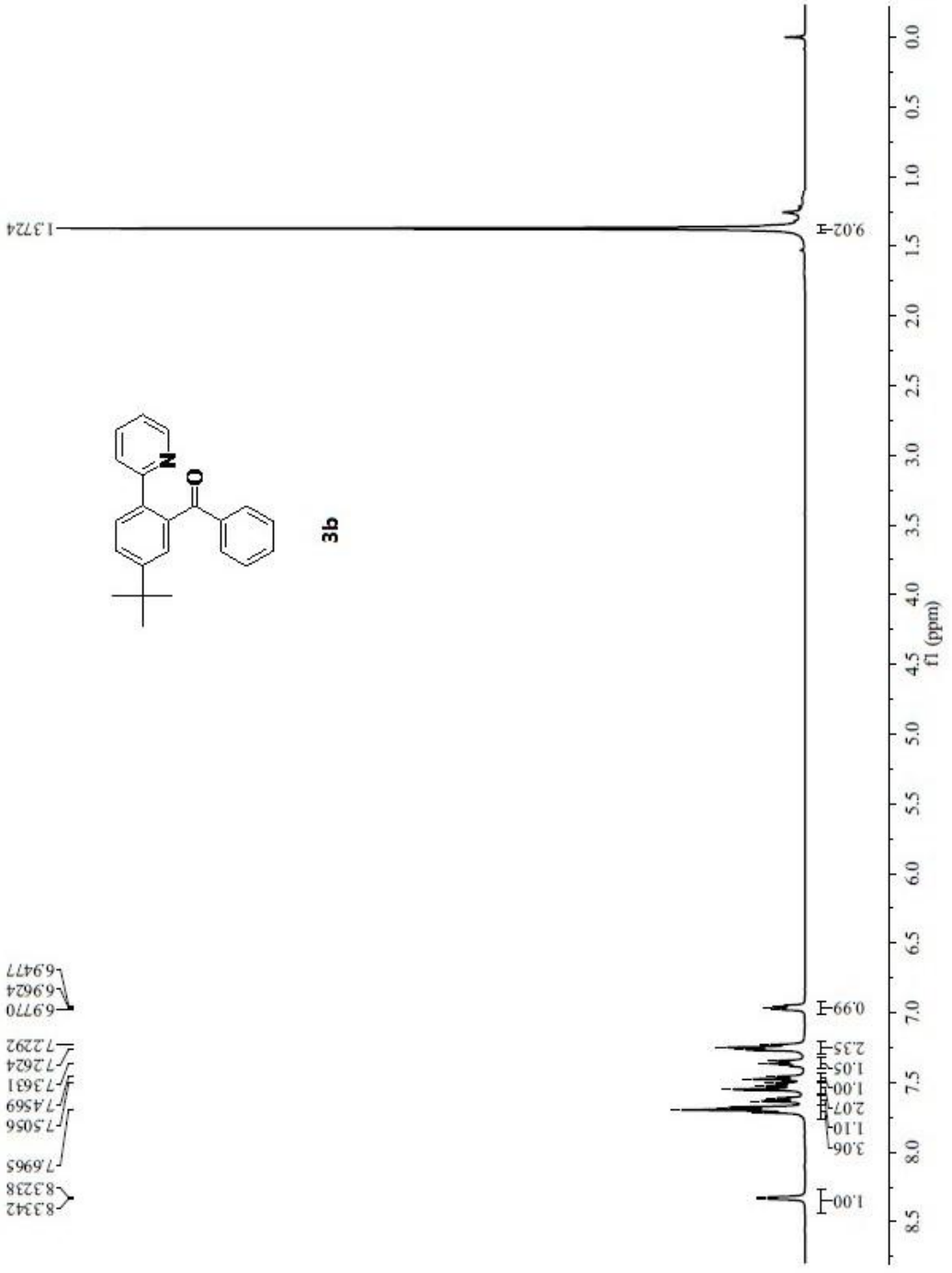
f1 (ppm)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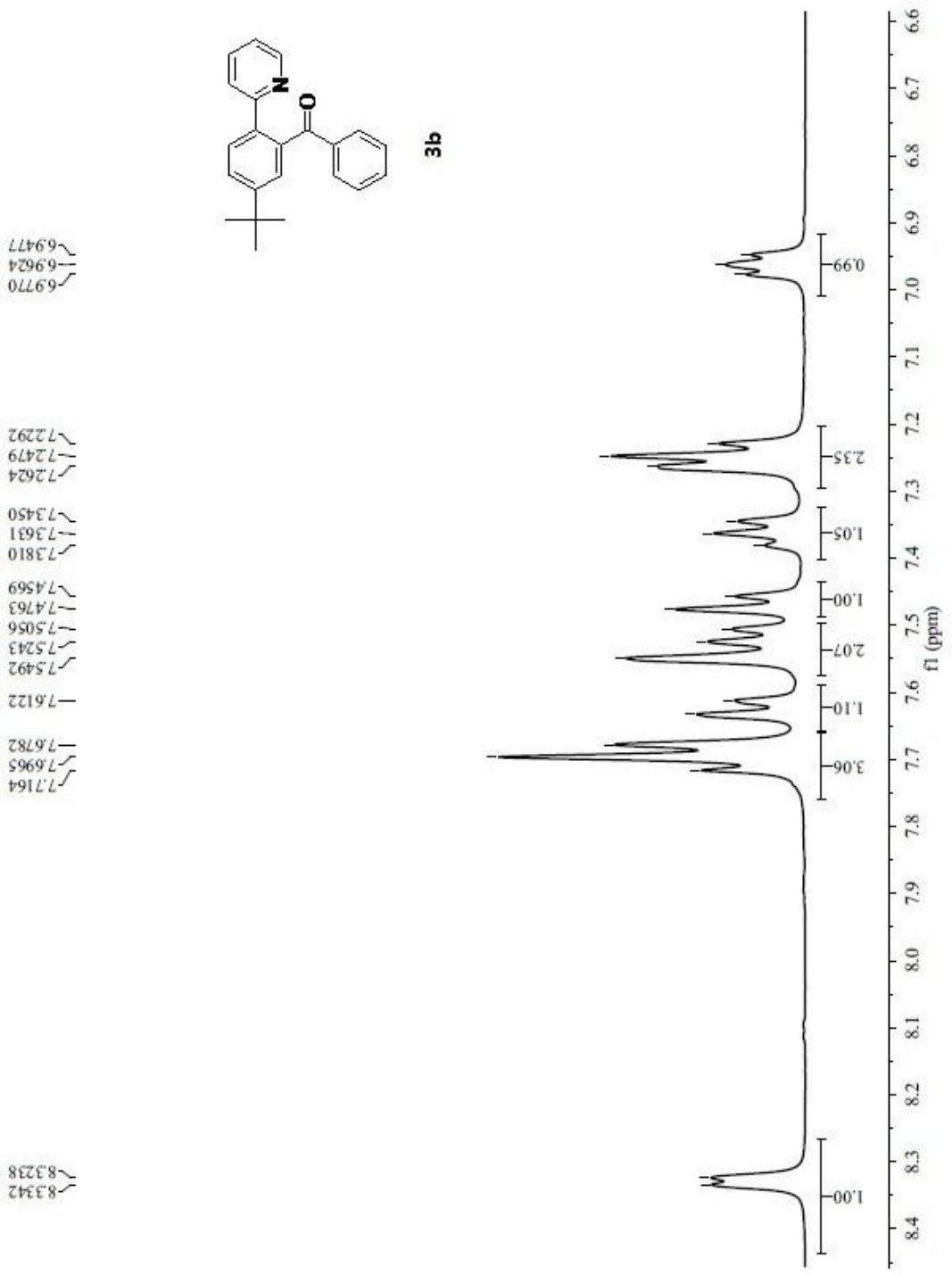
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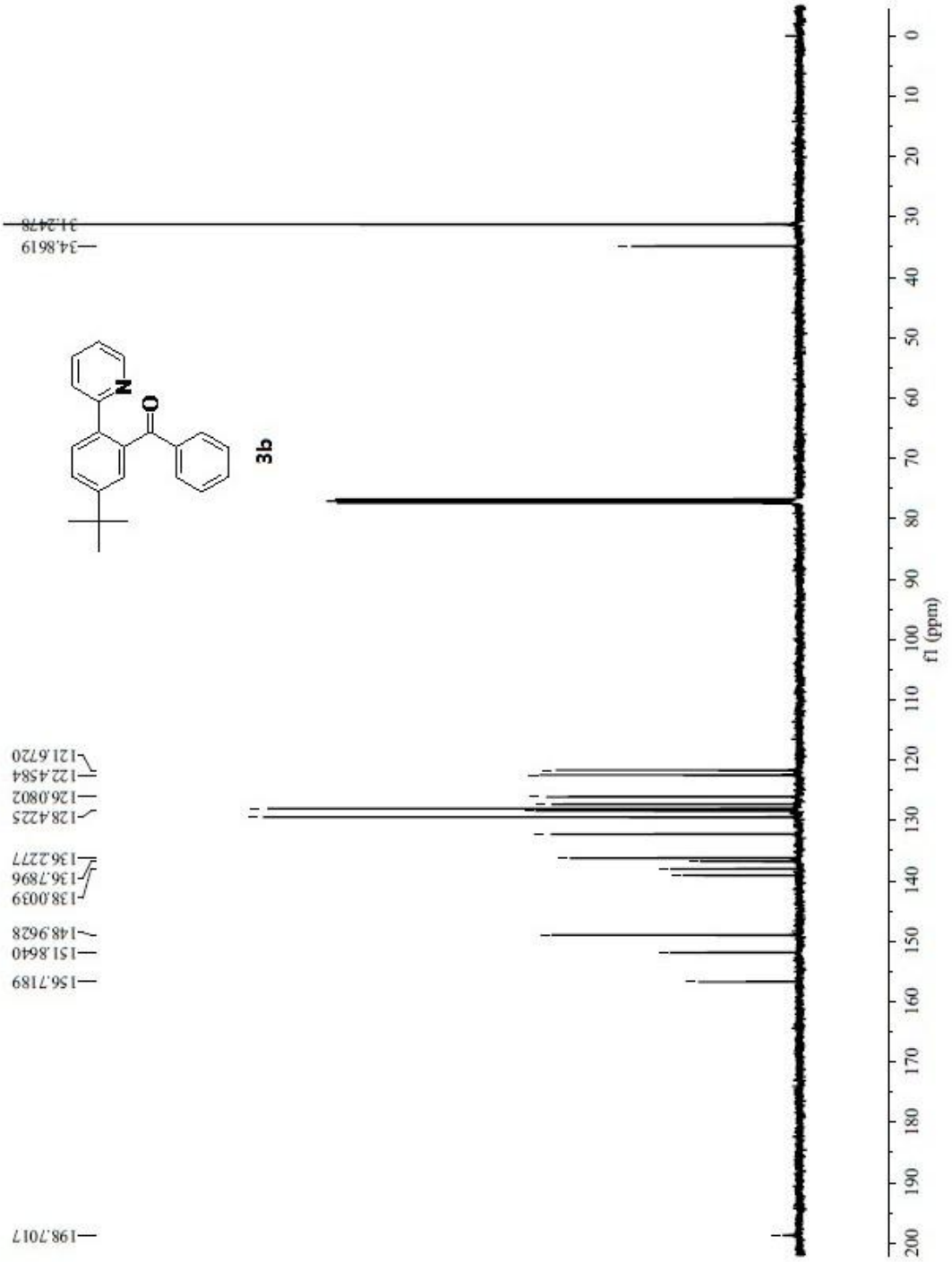

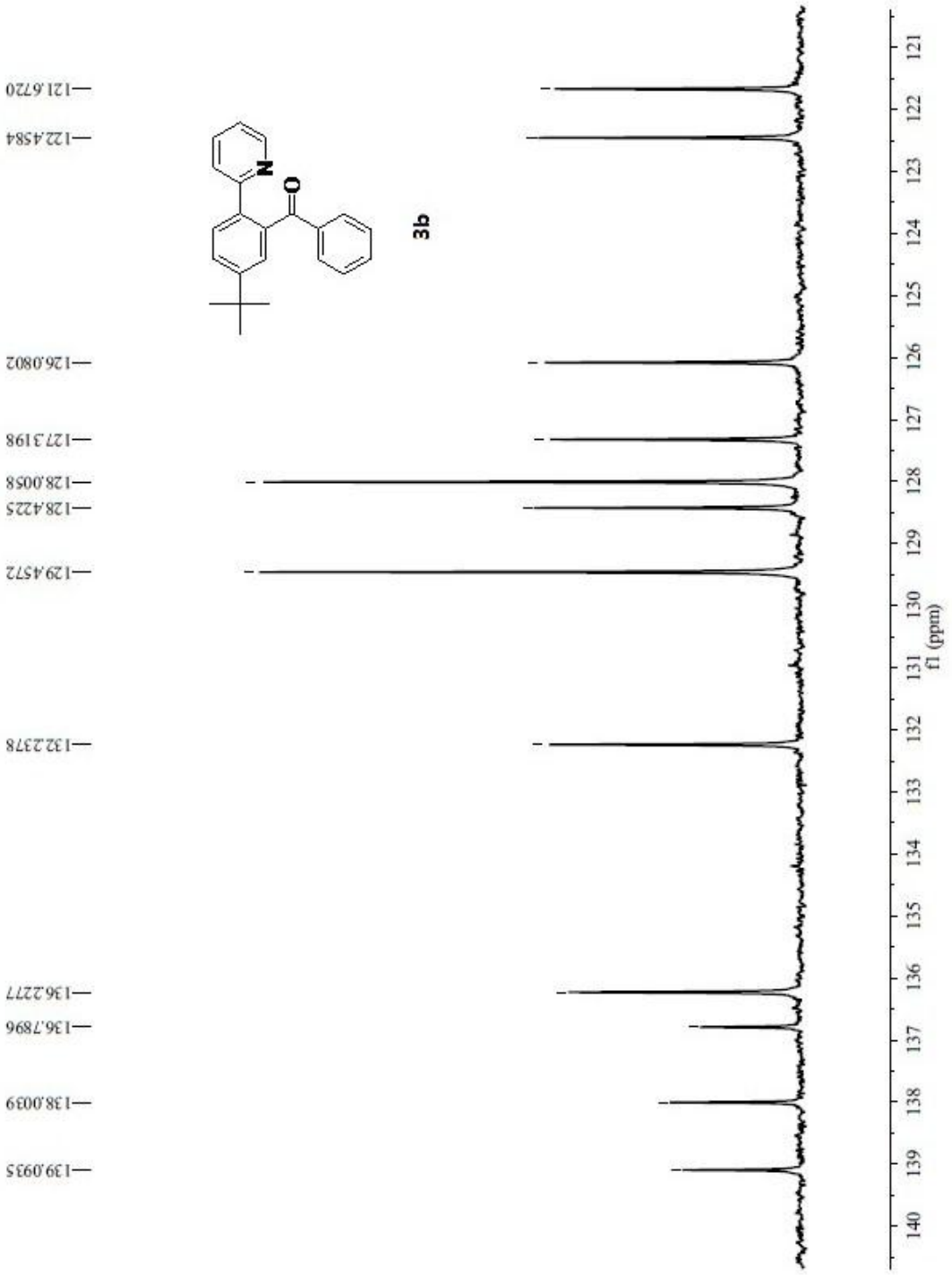
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O
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122
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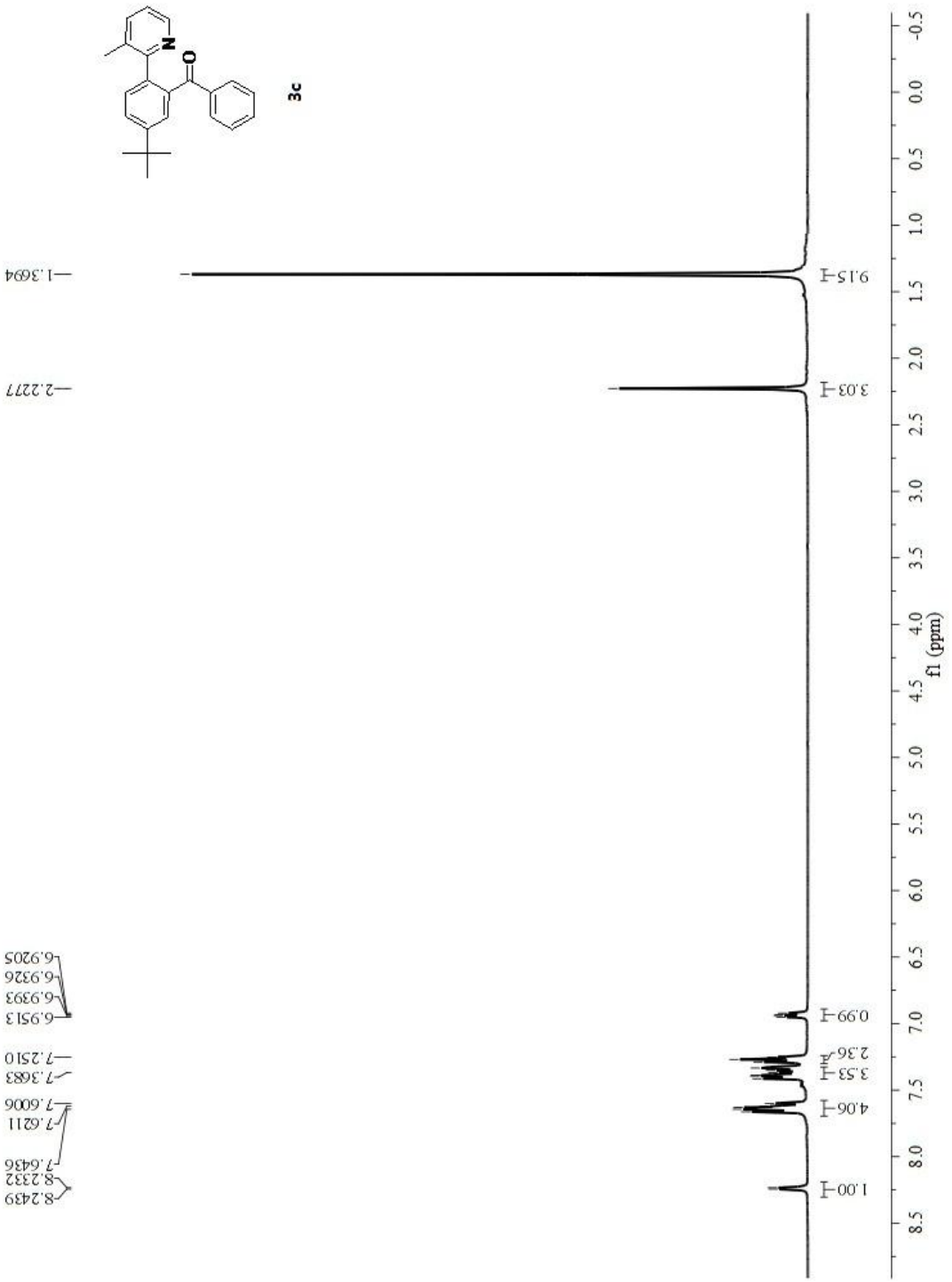
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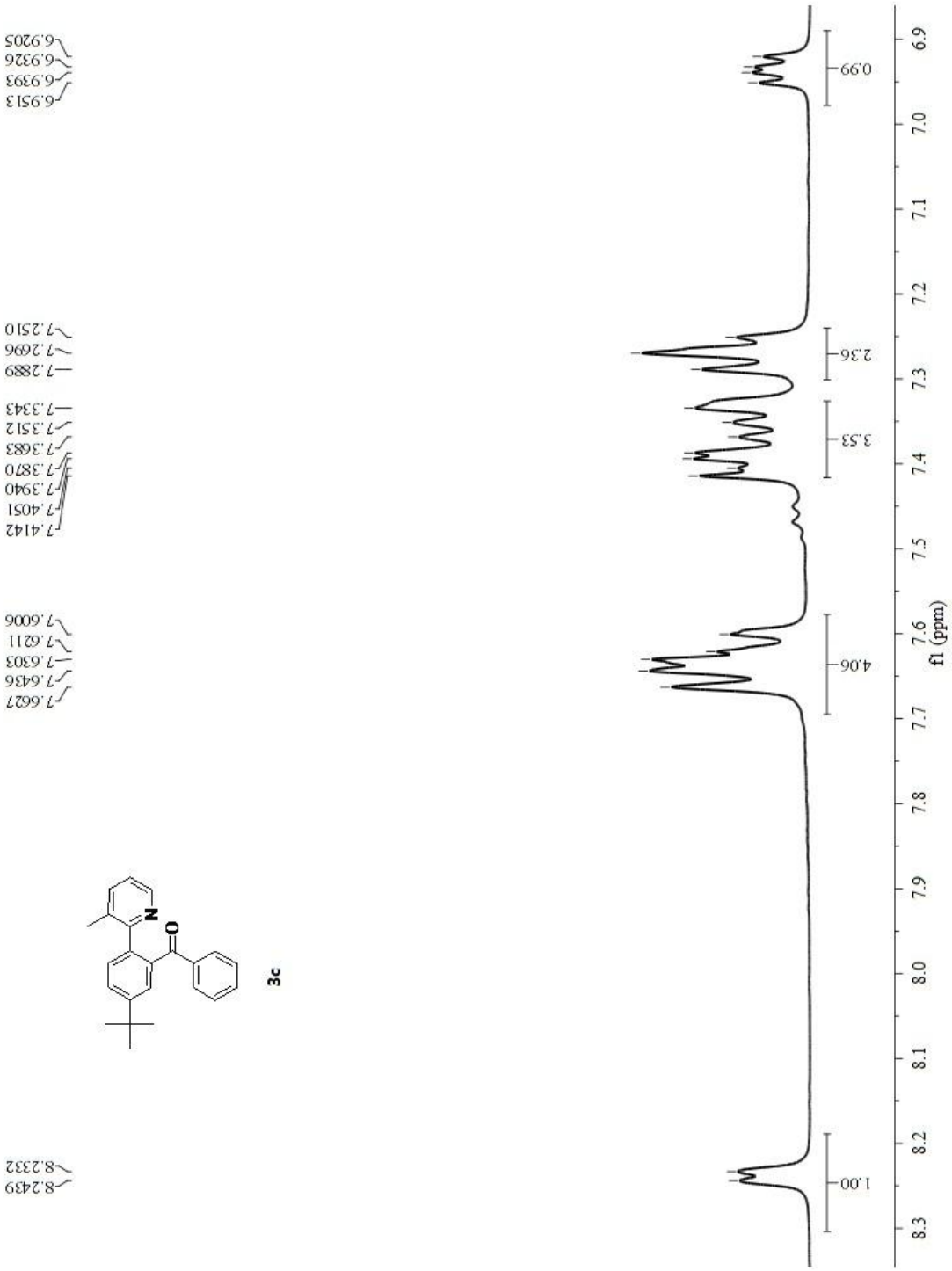
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6.9326
6.9205
3c
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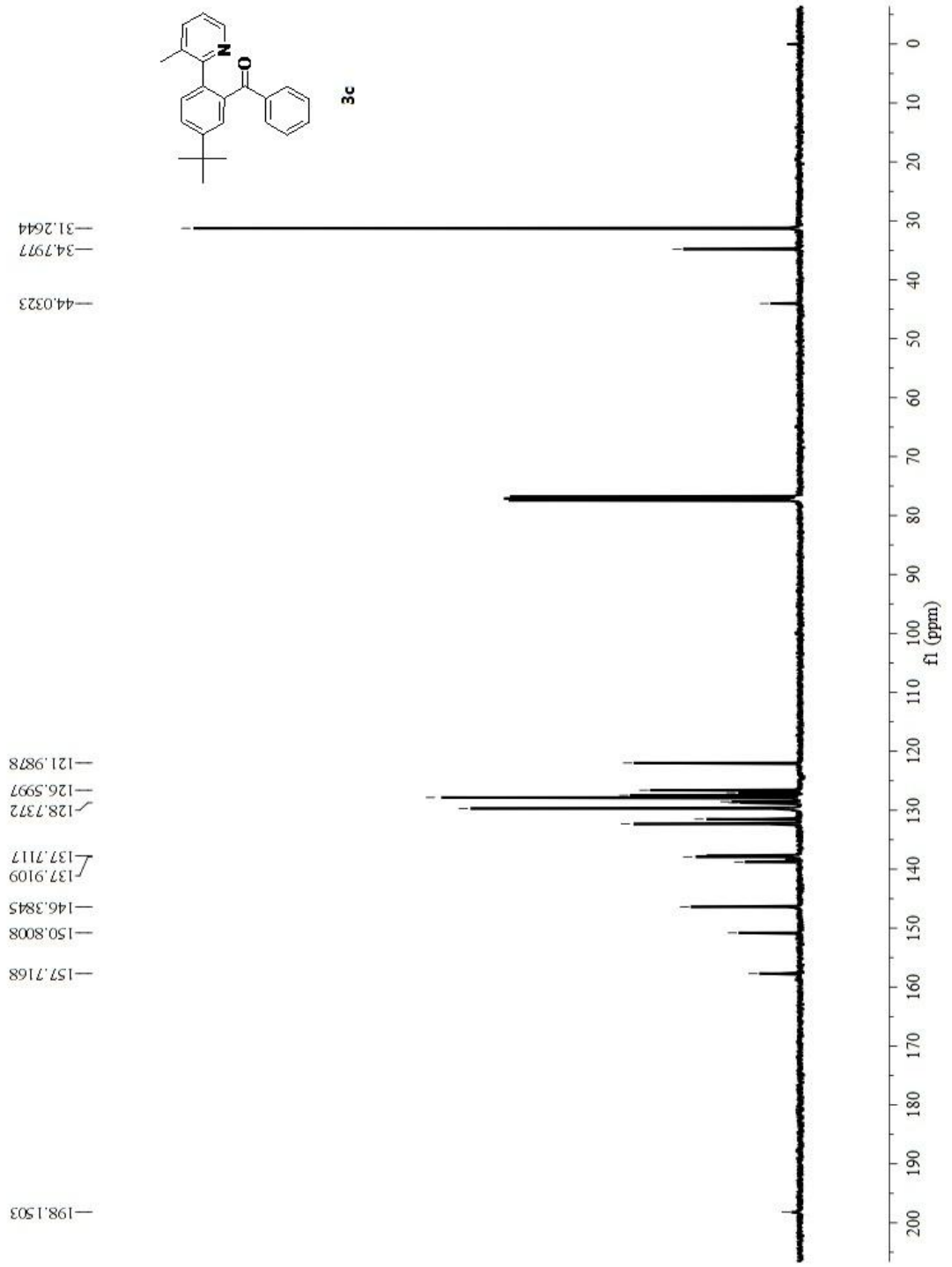

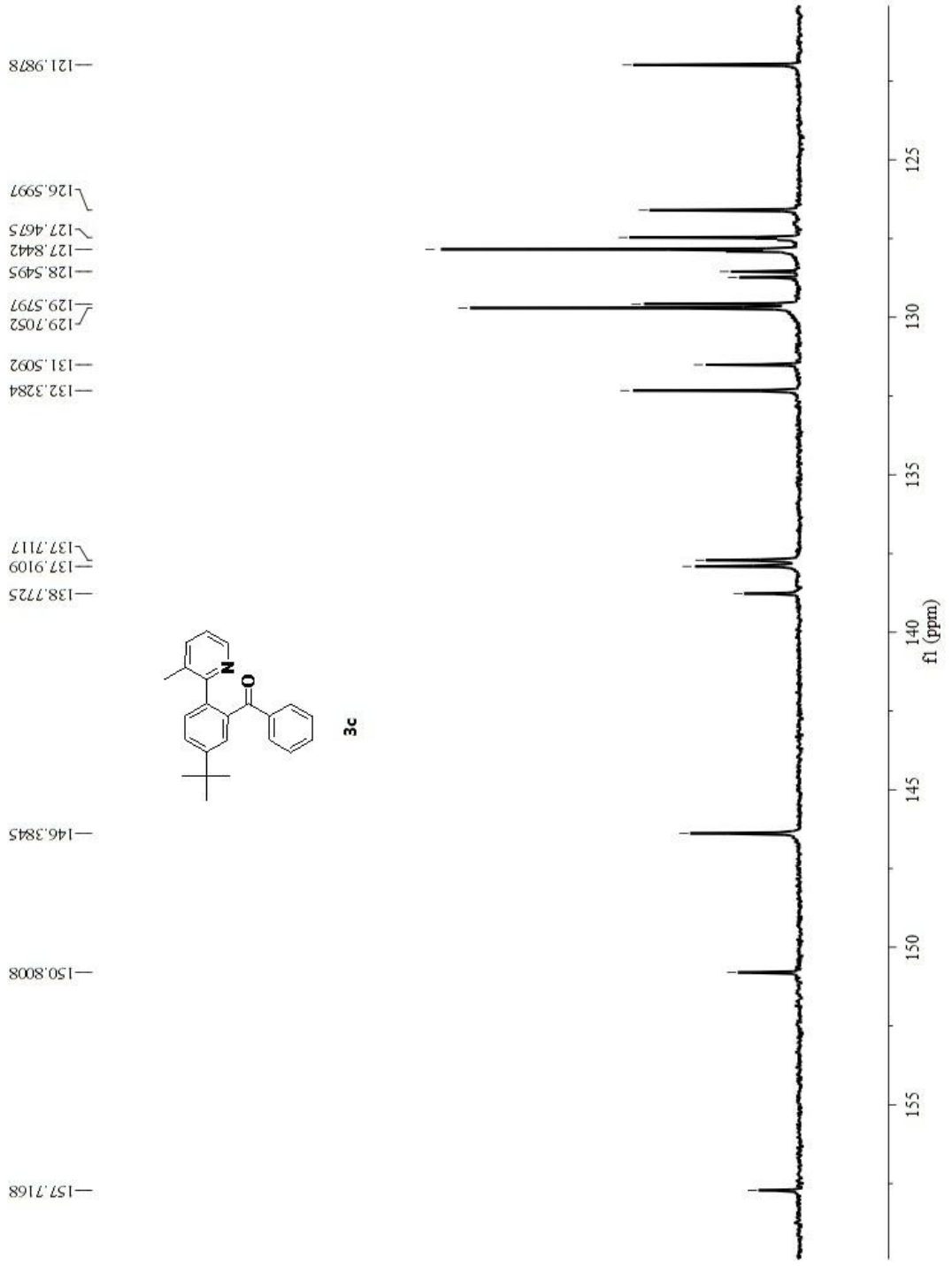
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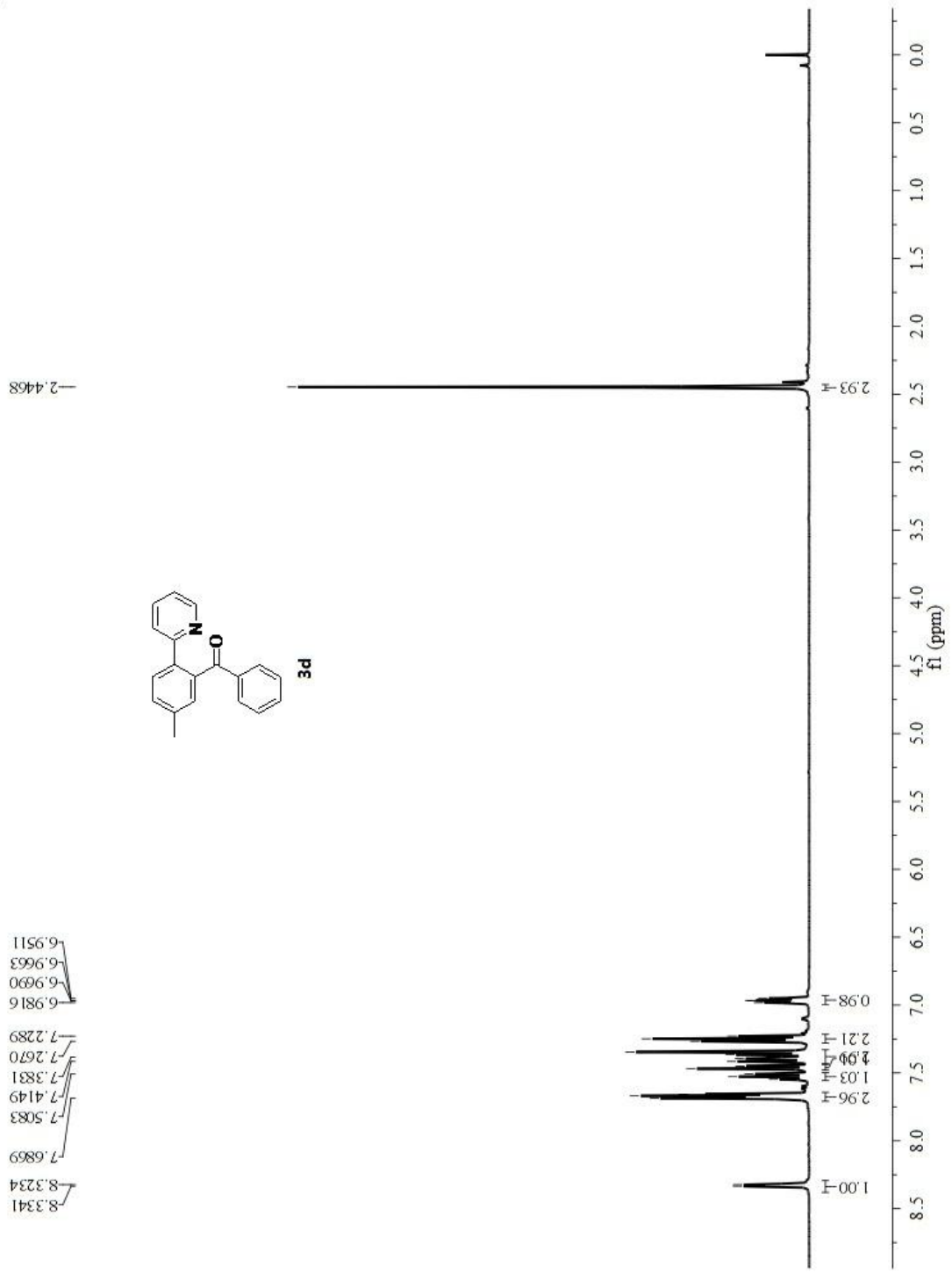
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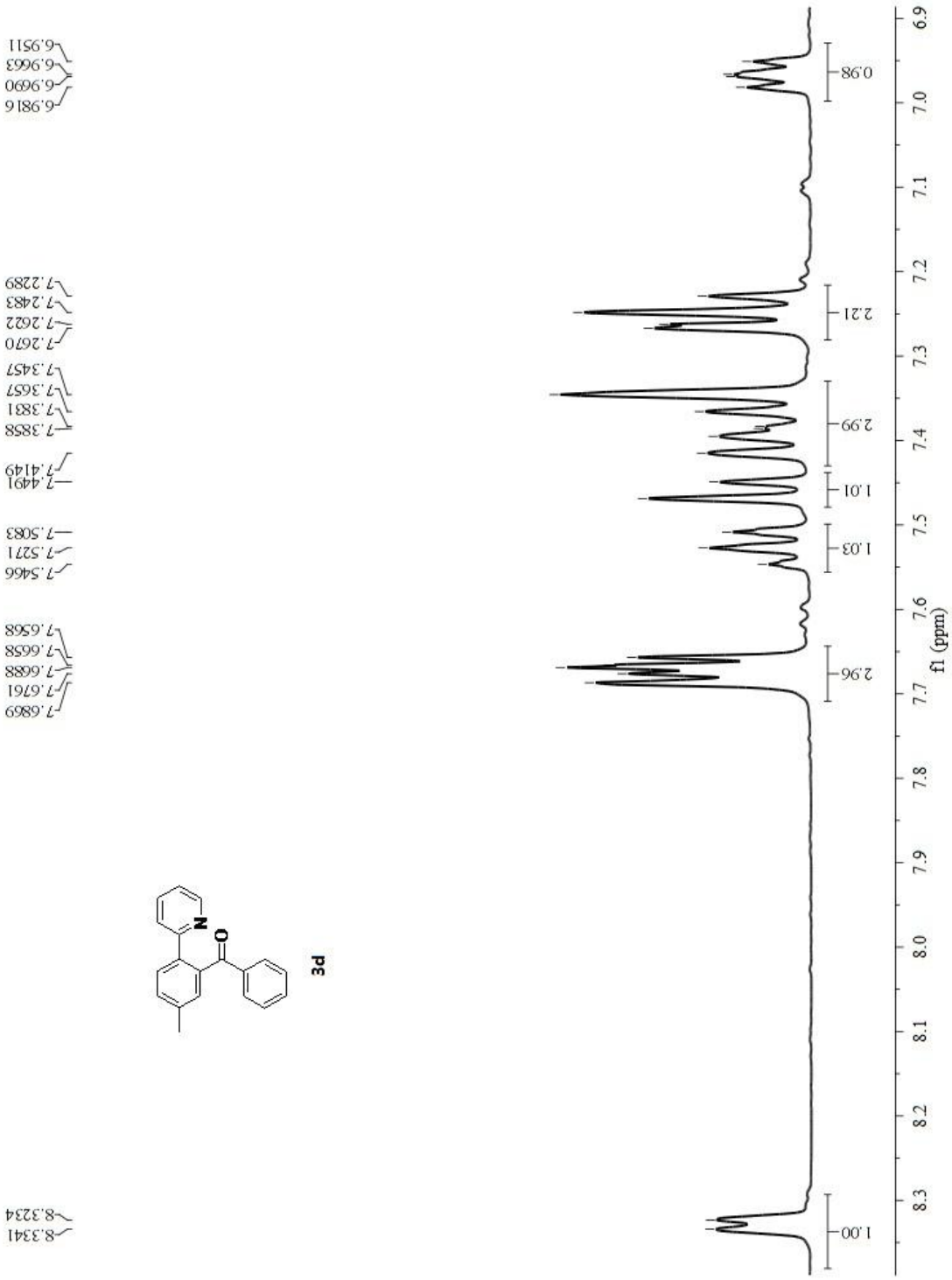
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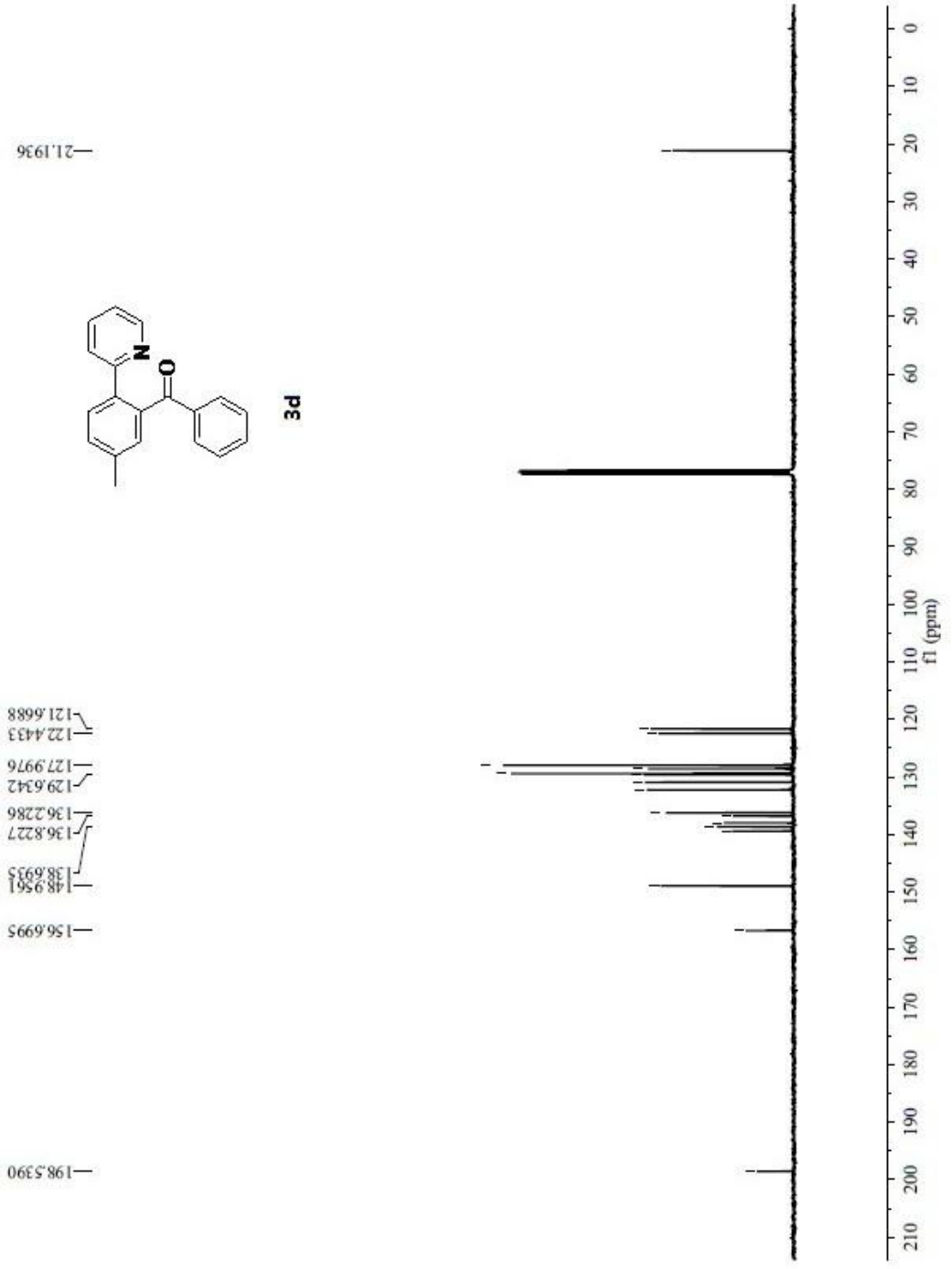
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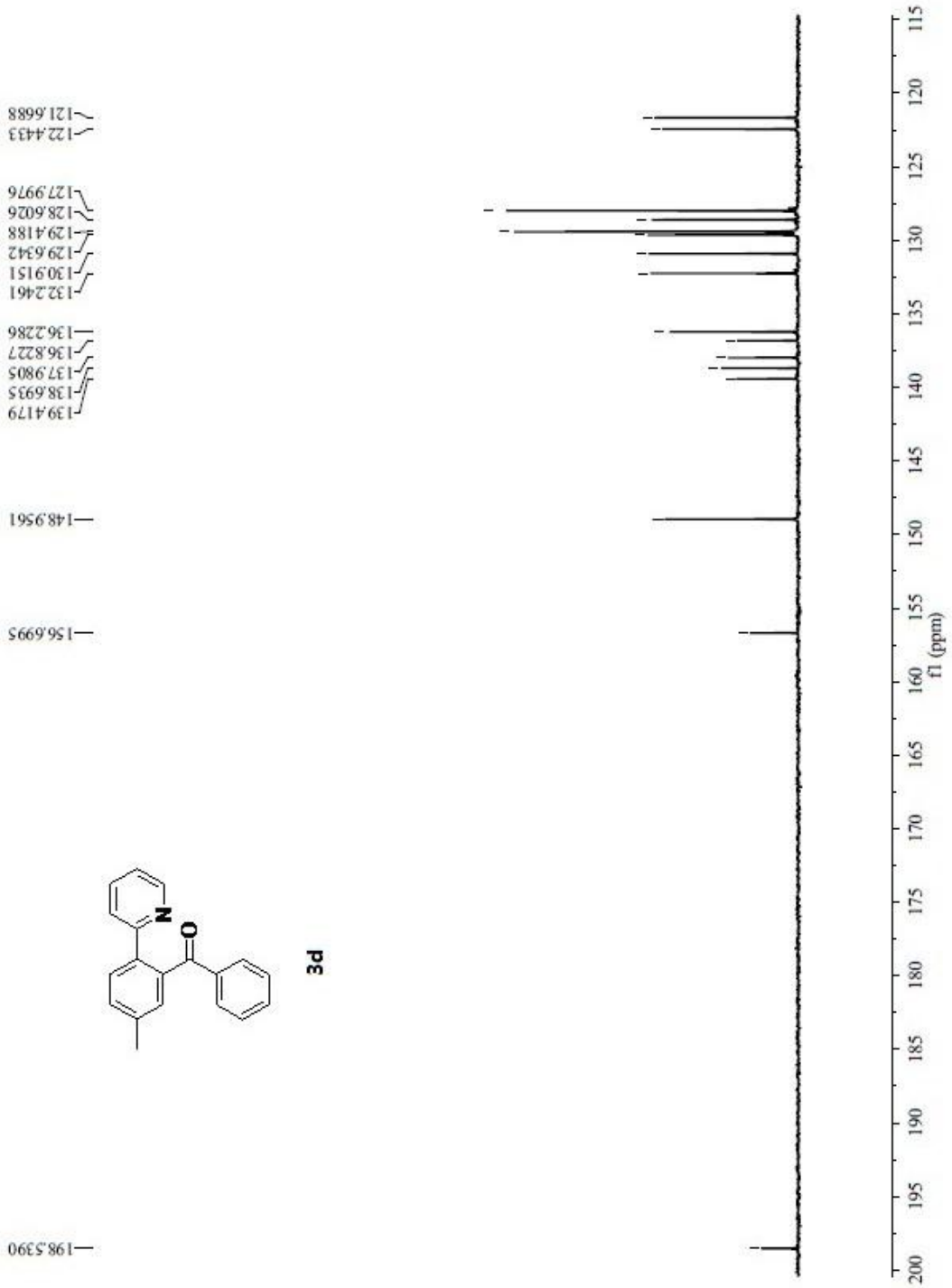
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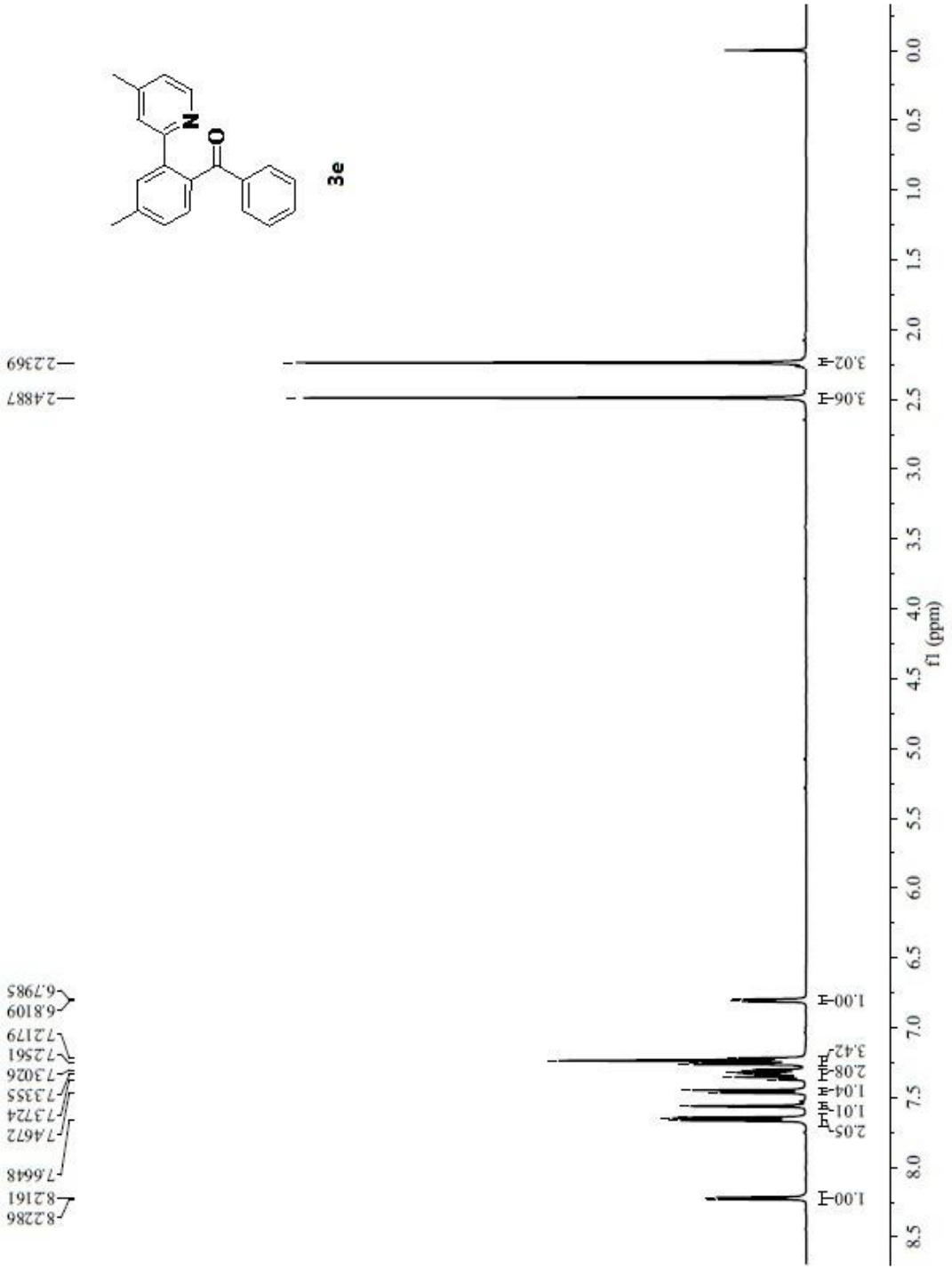
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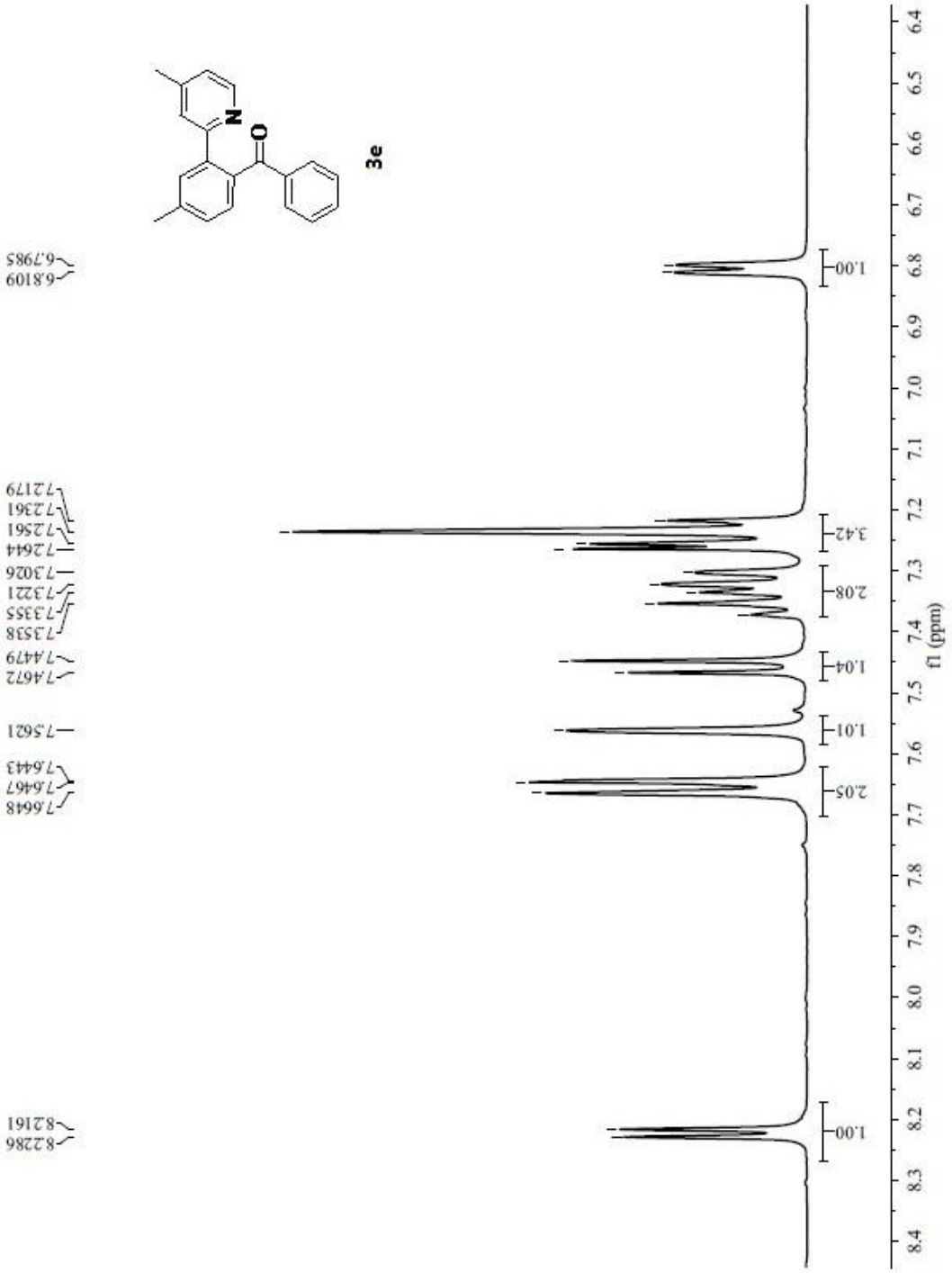

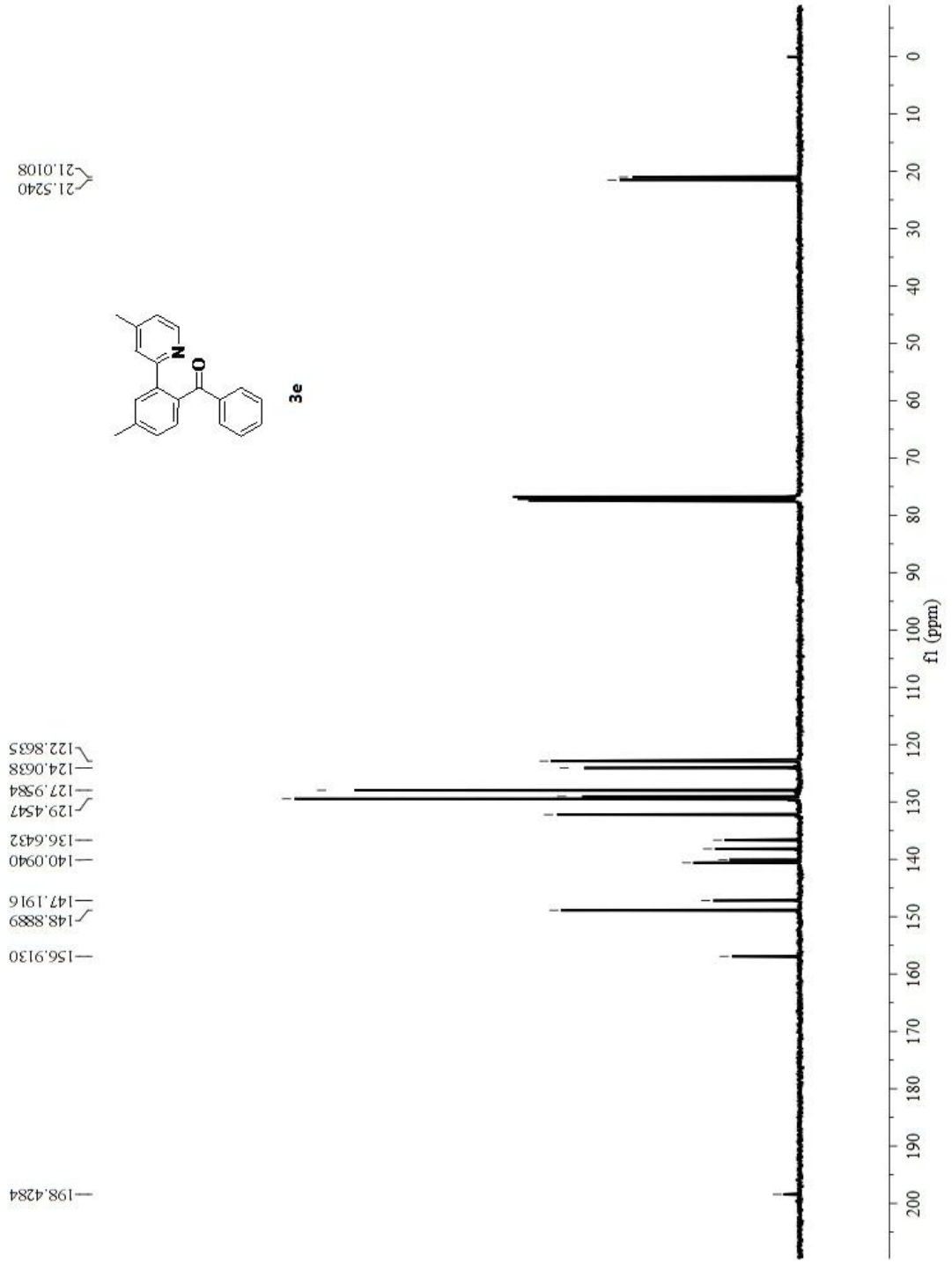
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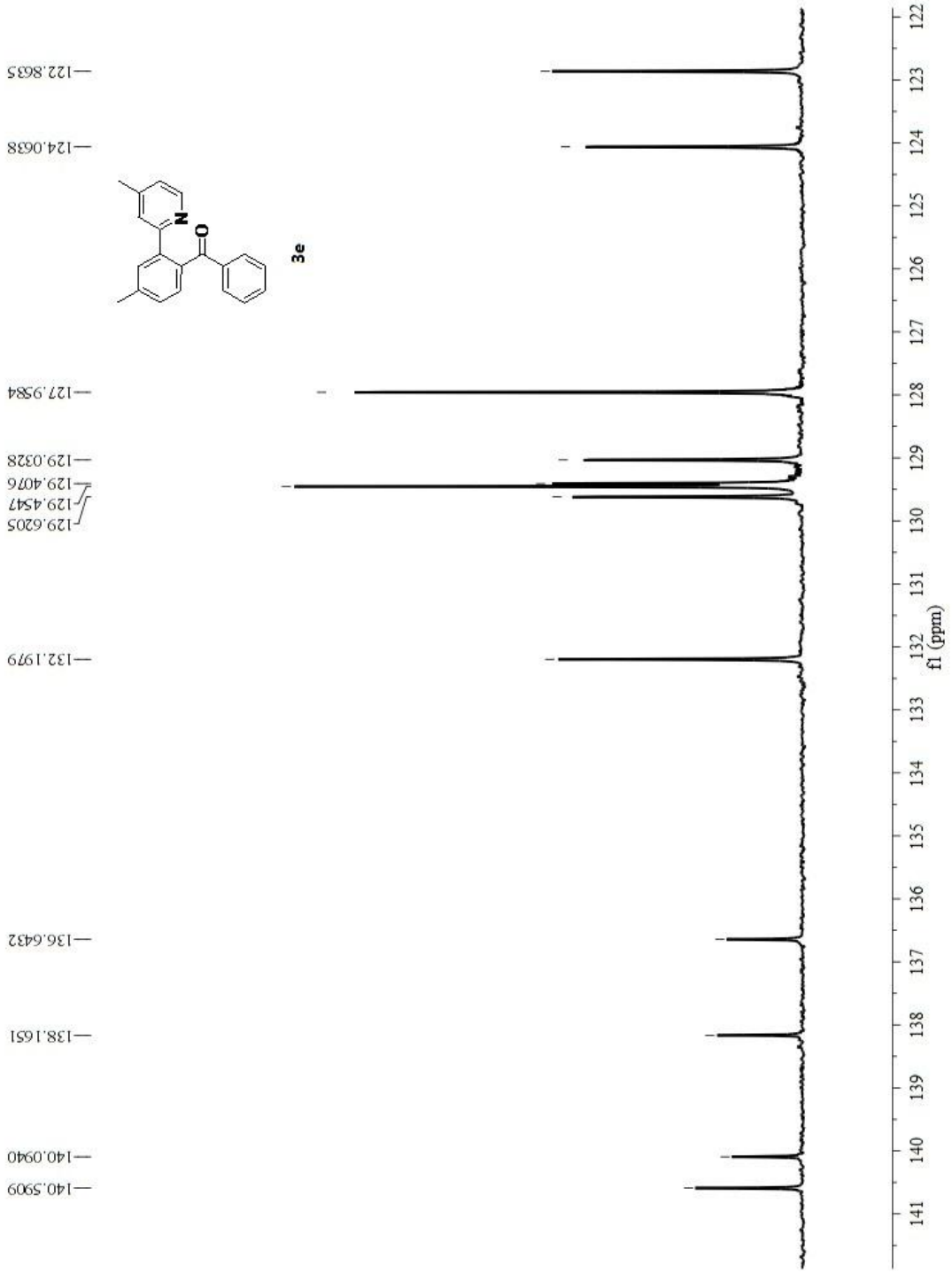
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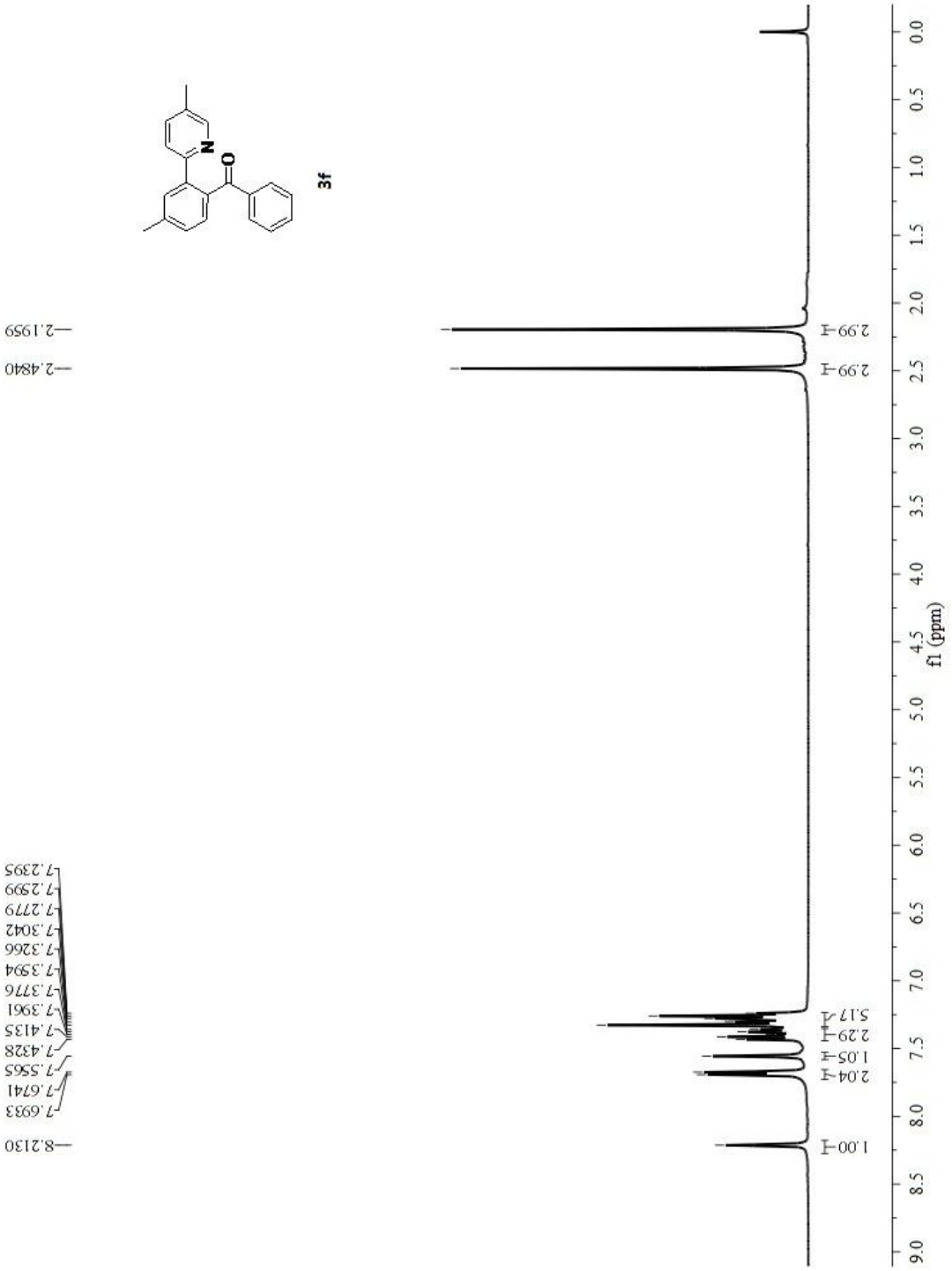
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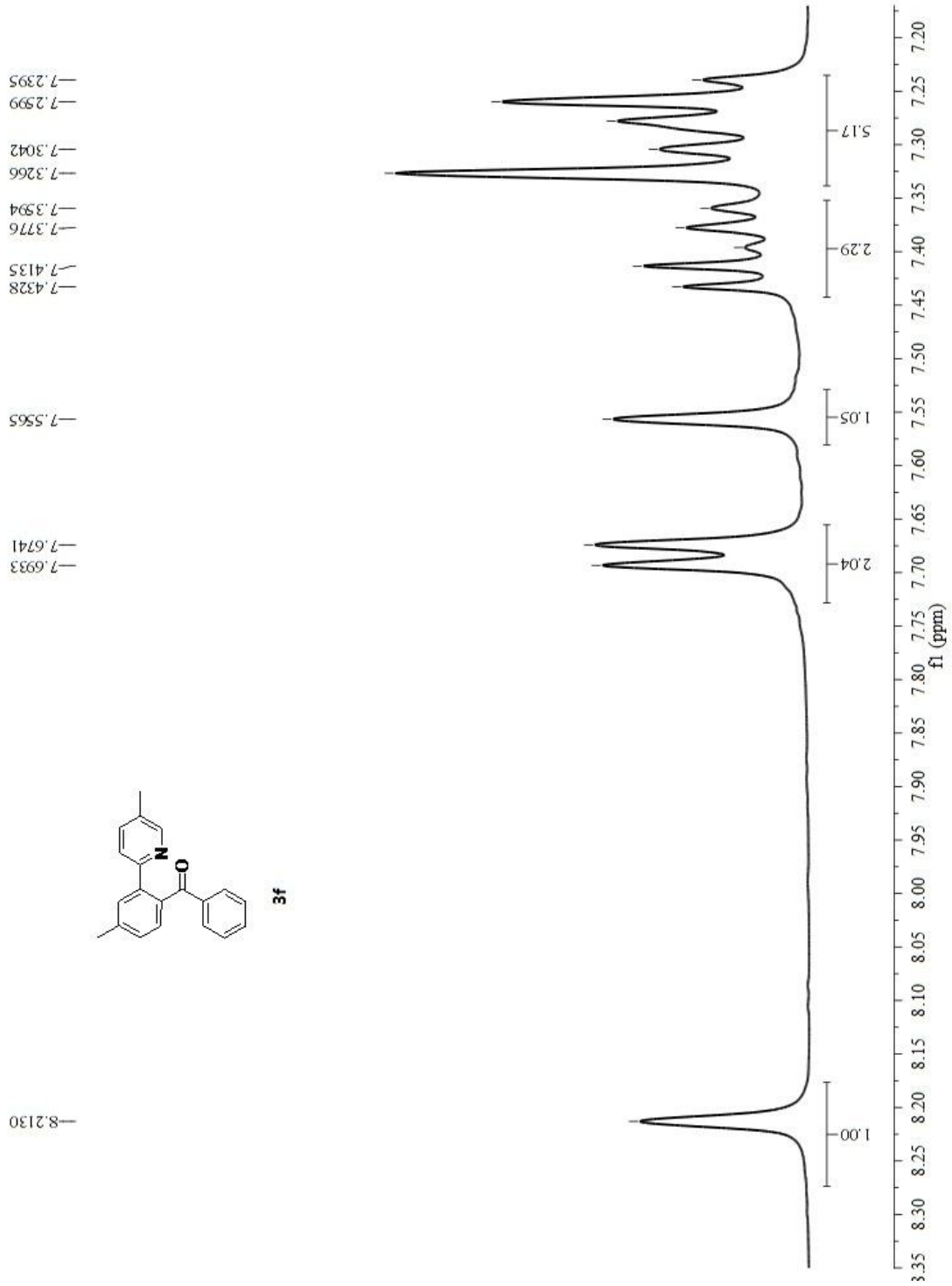
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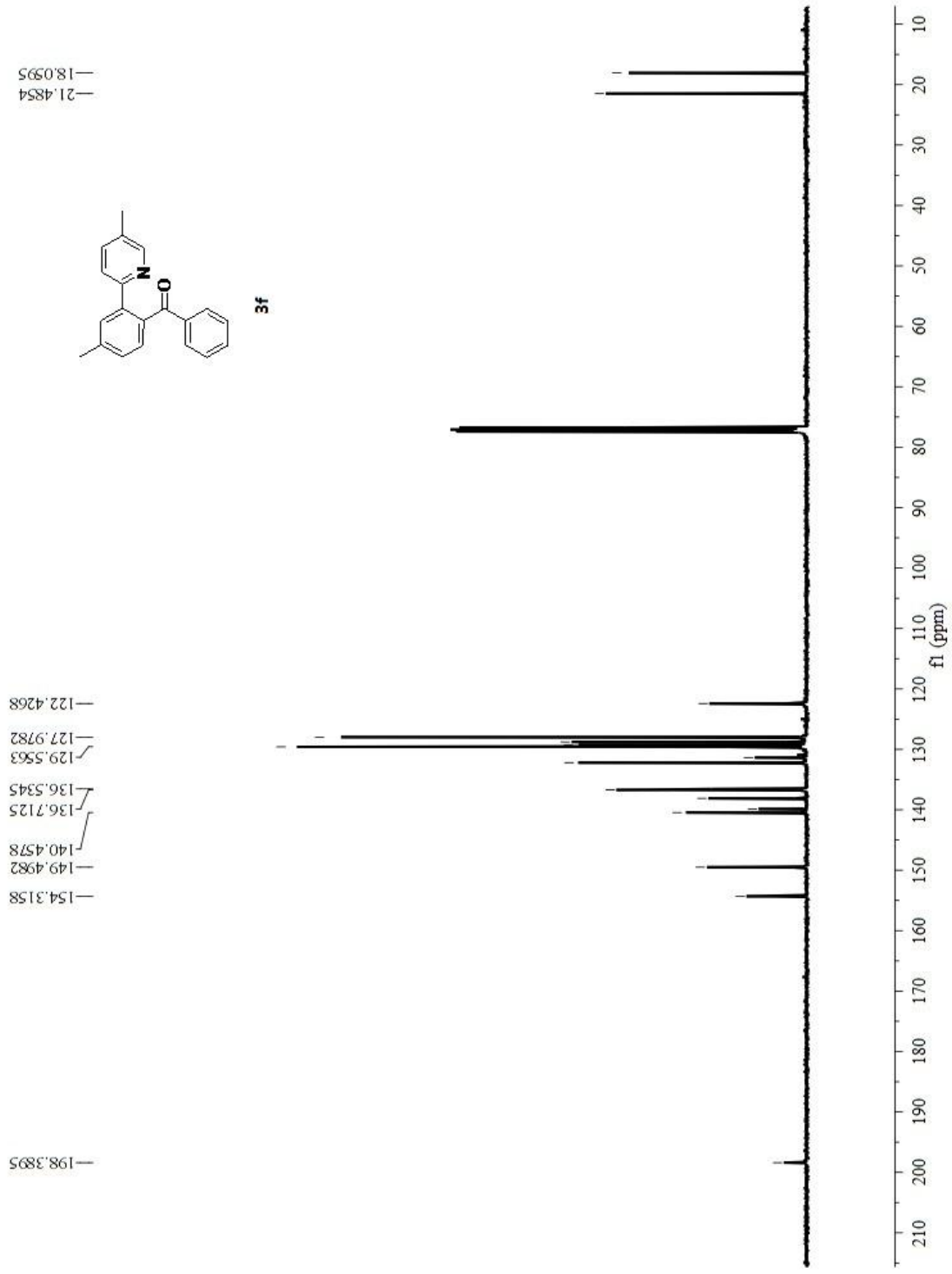
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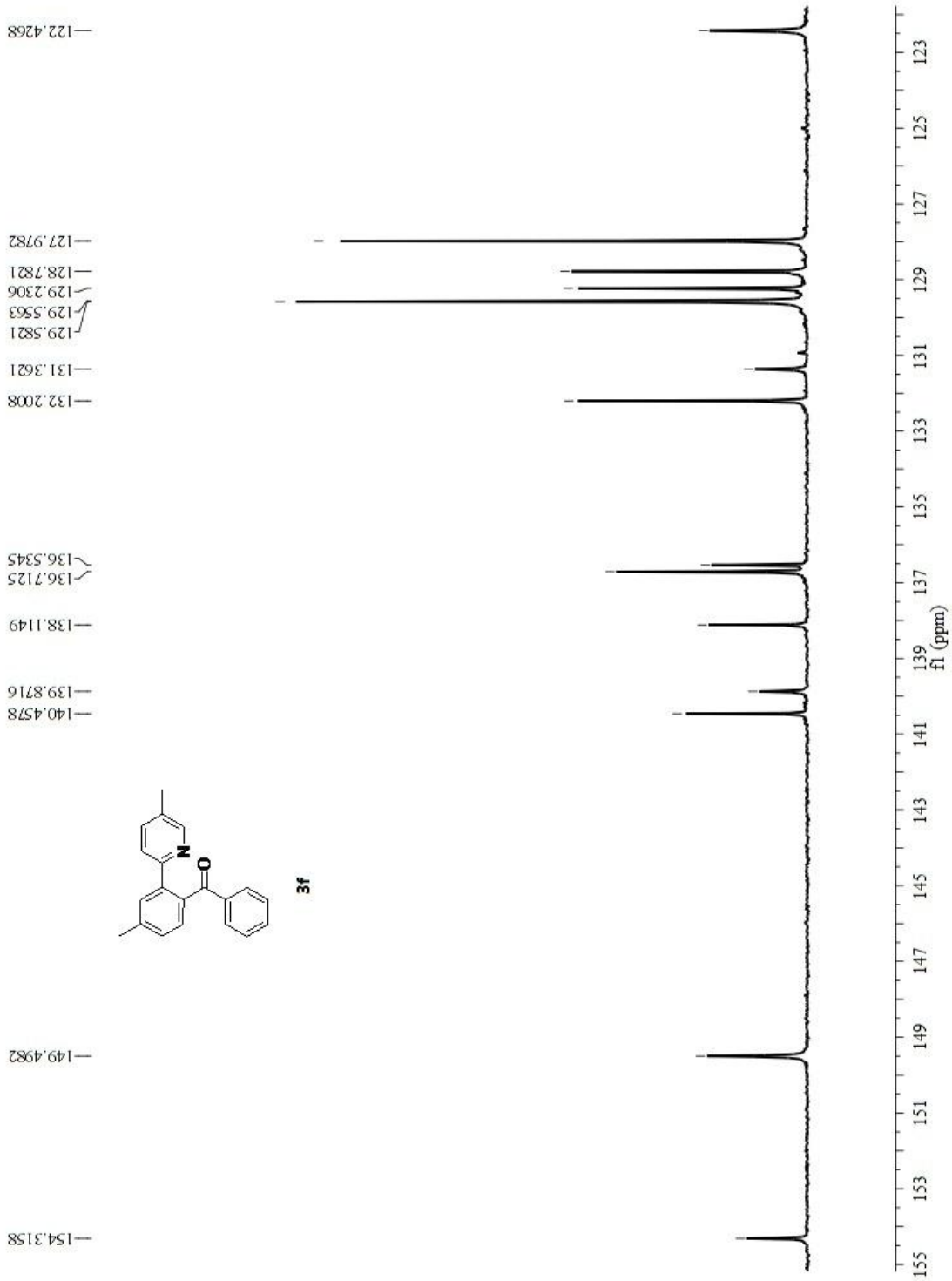
f1 (ppm)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129.5563
129.5821
131.3621
132.2008
136.5345
136.7125
138.1149
139.8716
140.4578
149.4982
154.3158
3f
O
N
123
125
127
129
131
133
135
137
139
141
143
145
147
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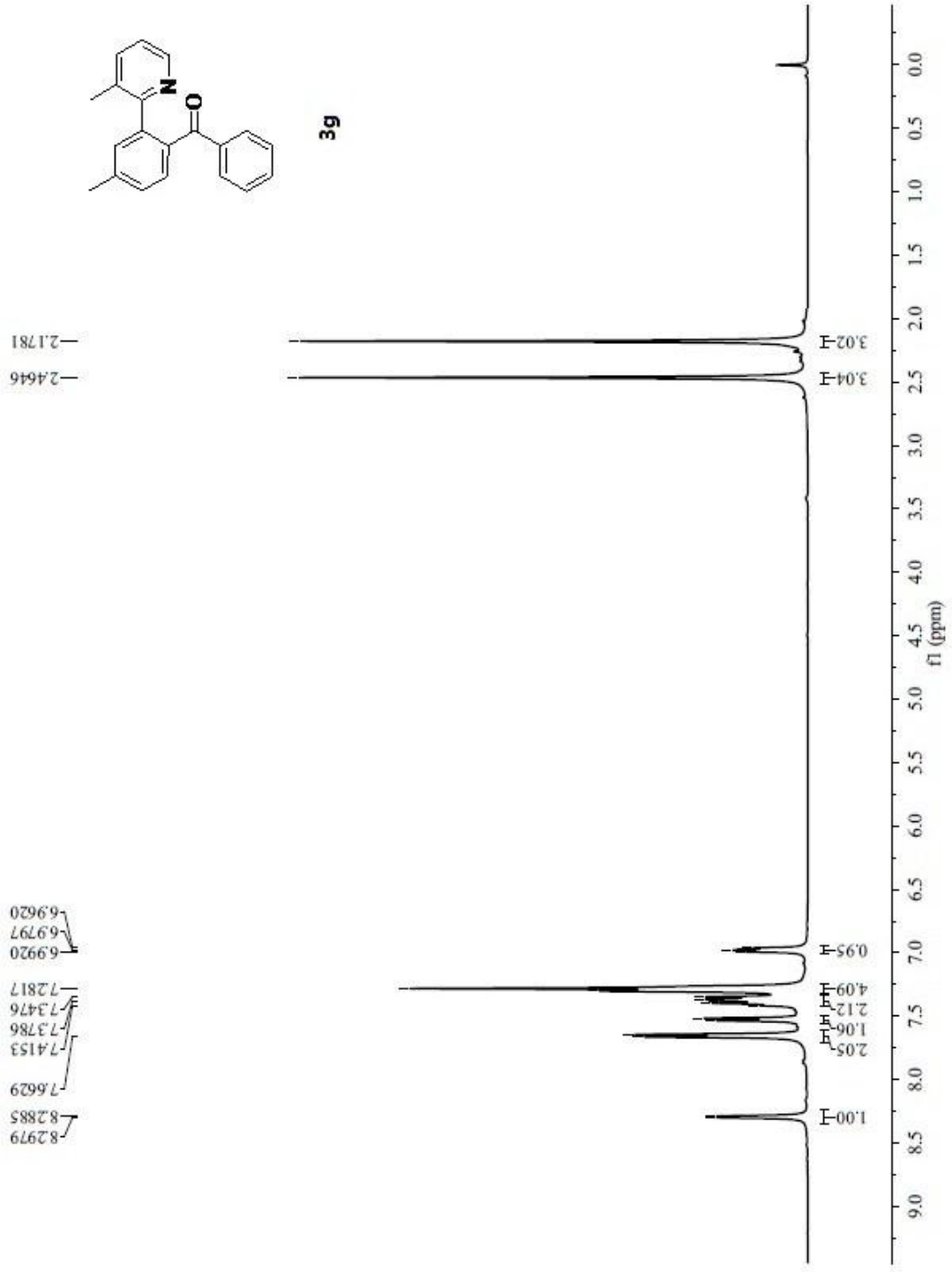
153
155
f1 (ppm)


3g
N
O
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2.4646
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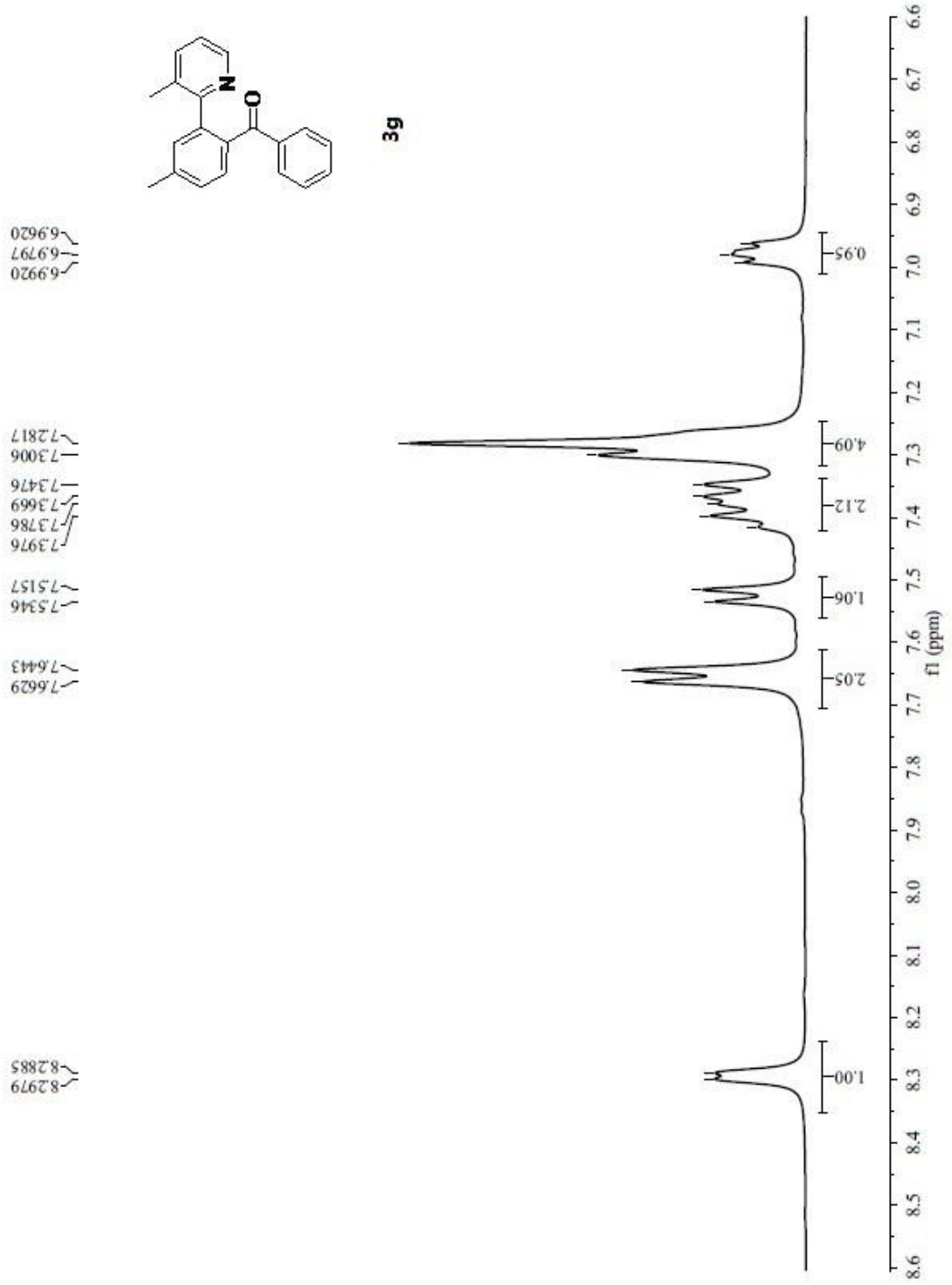
6.9797
6.9920
7.2817
7.3476
7.3786
7.4153
7.6629
8.2885
8.2979
3.02
3.04
0.95
4.09
2.12
1.06
2.05
1.00
f1 (ppm)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N
O
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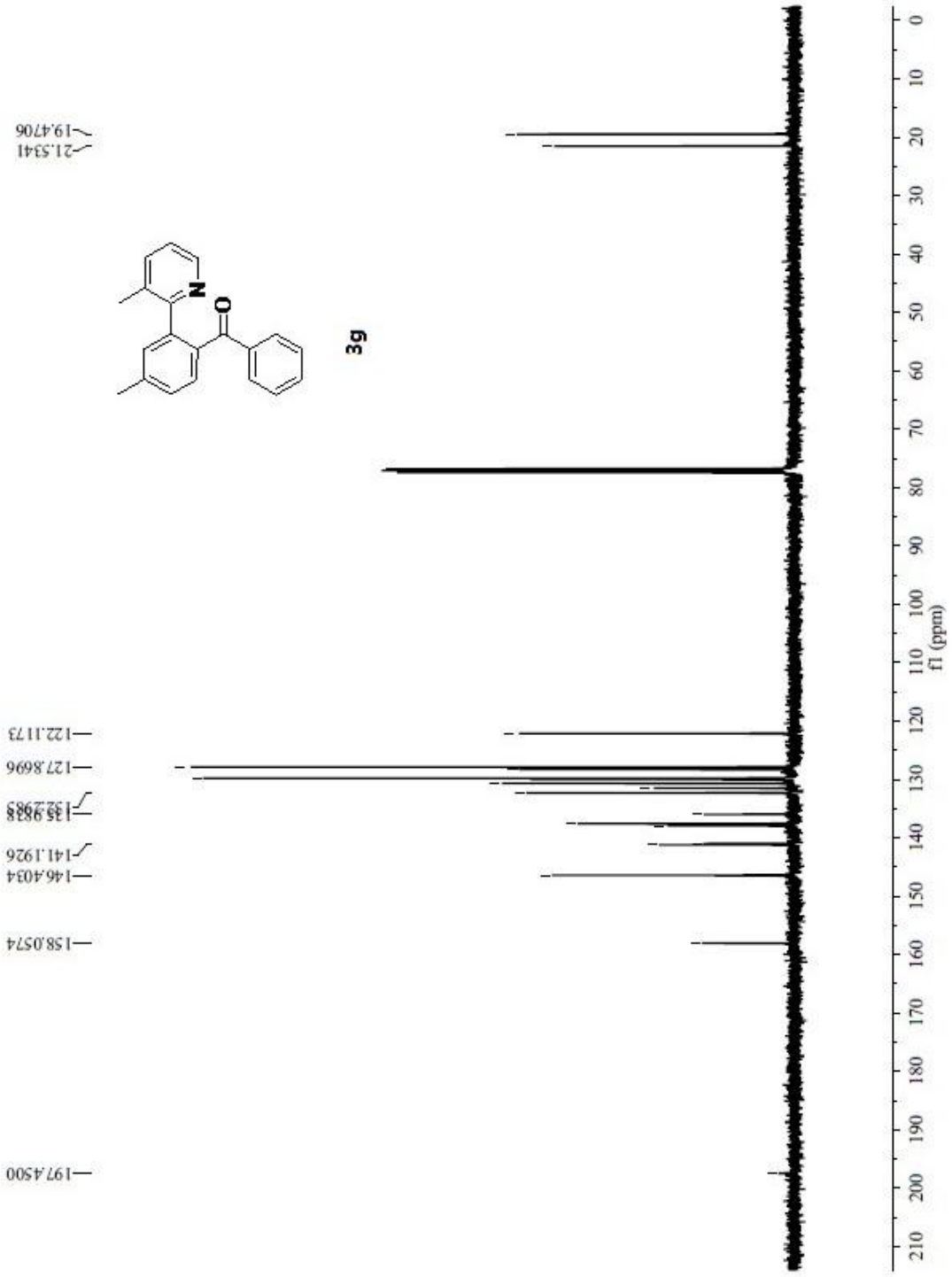
6.9797
6.9920
7.2817
7.3006
7.3476
7.3669
7.3786
7.3976
7.5157
7.5346
7.6443
7.6629
8.2885
8.2979
0.95
4.09
2.12
1.06
2.05
1.00
f1 (ppm)


19.4706
21.5341
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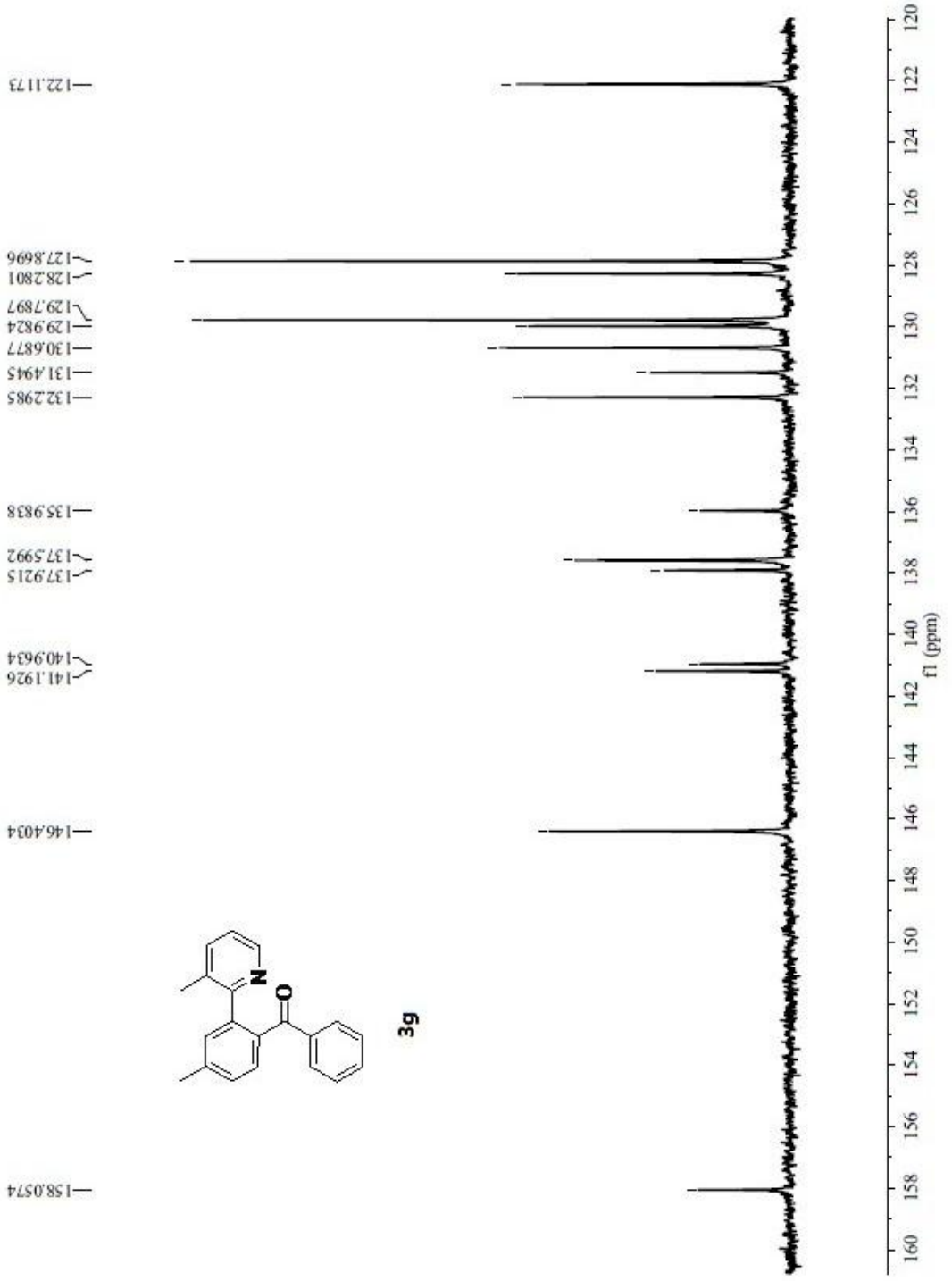
136.9838
139.2985
141.1926
146.4034
158.0574
197.4500
3g
f1 (ppm)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127.8696
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129.9824
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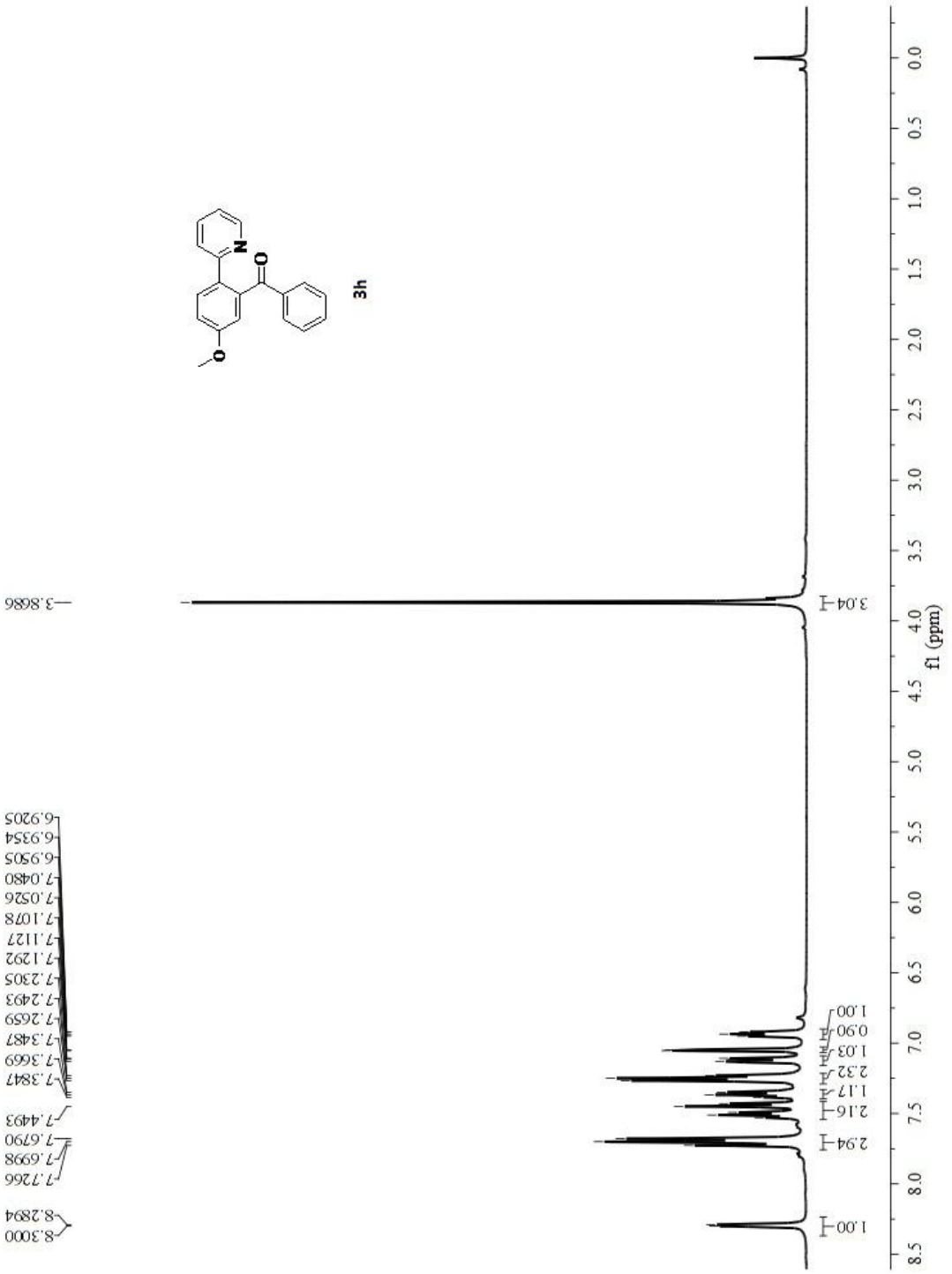
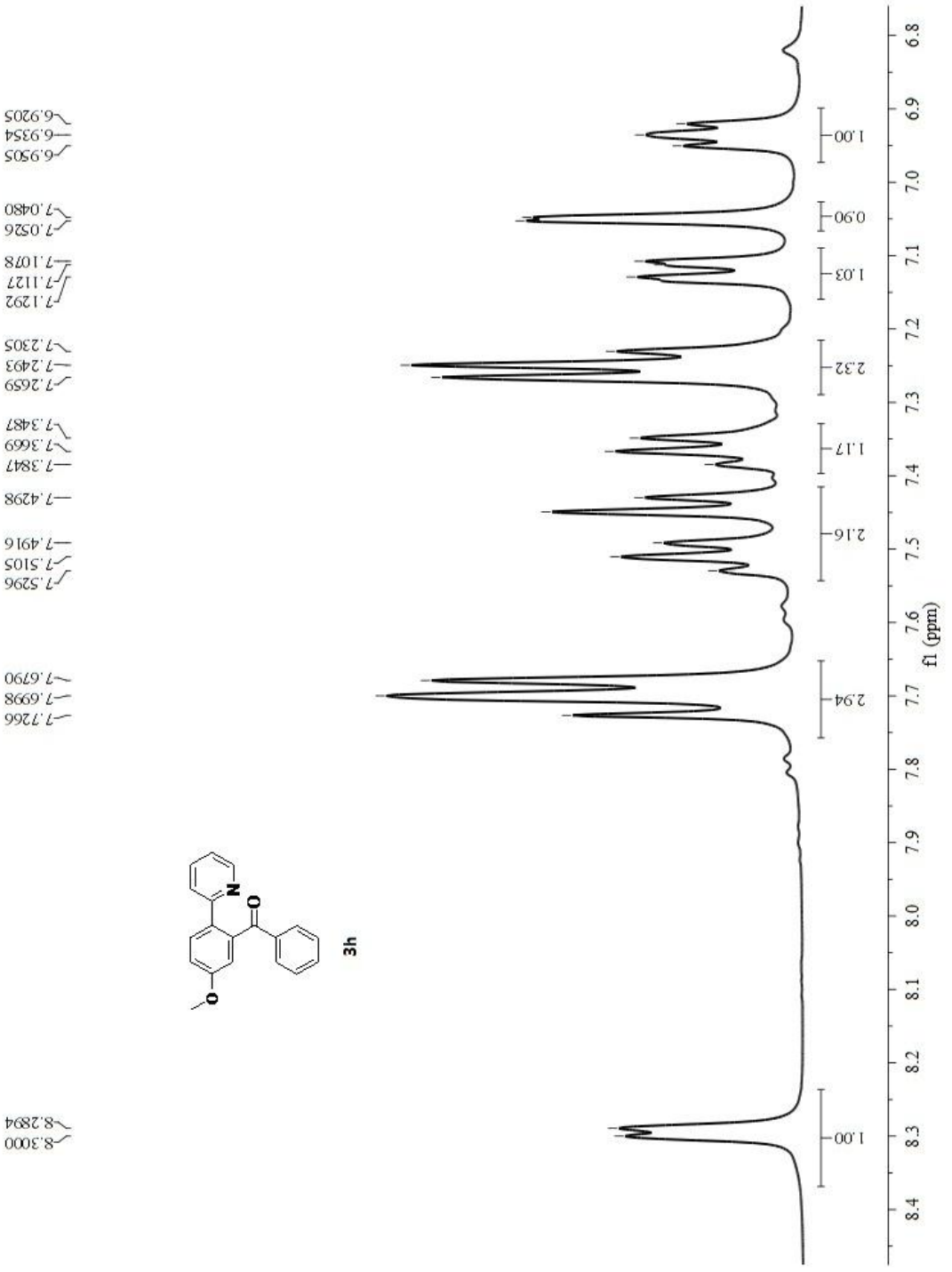
131.4945
132.2985
135.9838
137.5992
137.9215
140.9634
141.1926
146.4034
158.0574
3g
N
O
120
122
124
126
128
130
132
134
136
138
140
142
144
146
148
150
152
154
156
158
160
f1 (ppm)


3h
f1 (ppm)
3.8686
8.3000
8.2894
7.7266
7.6998
7.6790
7.4493
7.3847
7.3669
7.3487
7.2659
7.2493
7.2305
7.1292
7.1127
7.1078
7.0526
7.0480
6.9505
6.9354
6.9205
3.04
2.94
2.16
1.17
2.32
1.03
0.90
1.00
1.00


8.3000
8.2894
7.7266
7.6998
7.6790
7.4916
7.4298
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7.3669
7.3487
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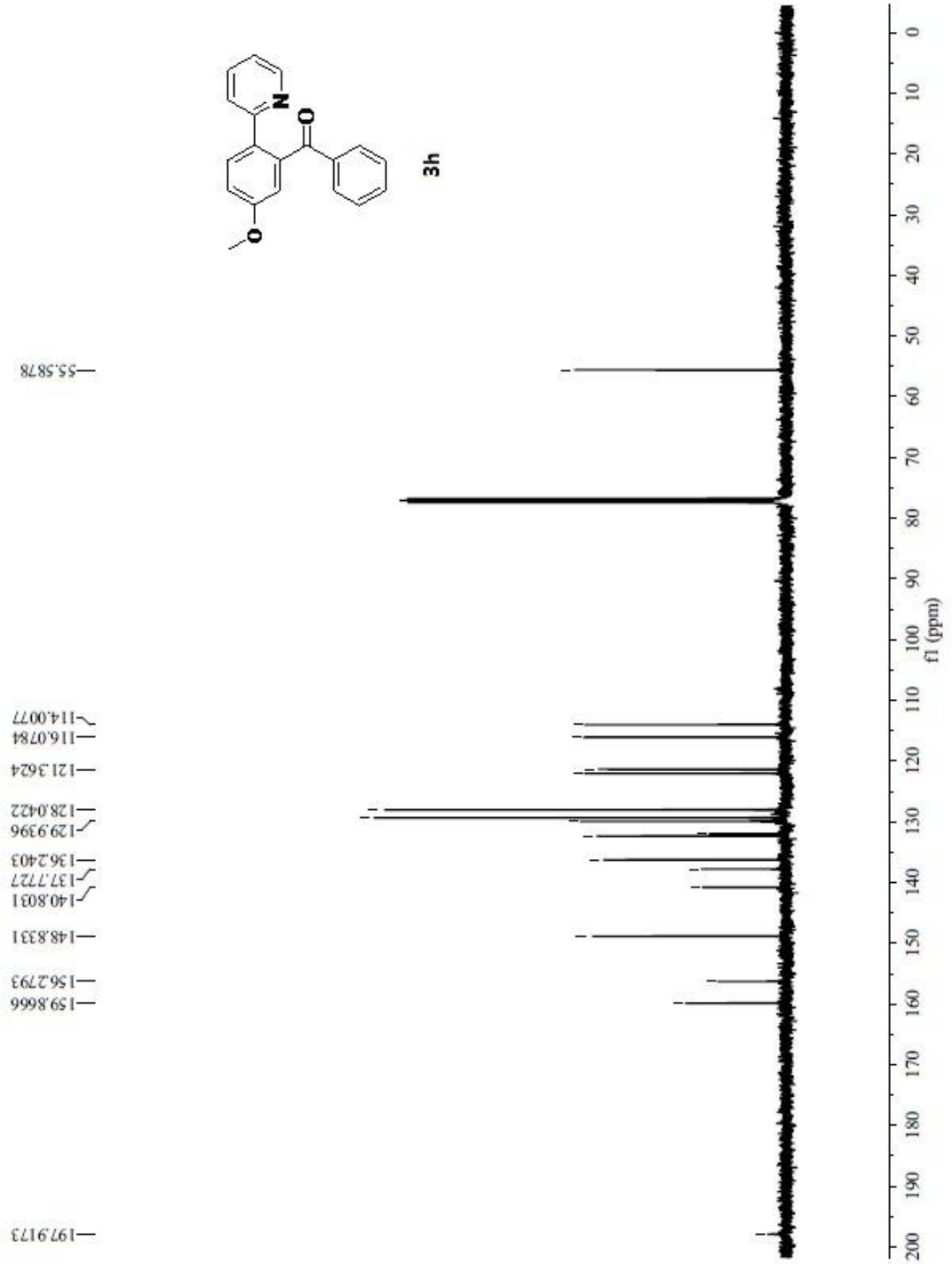
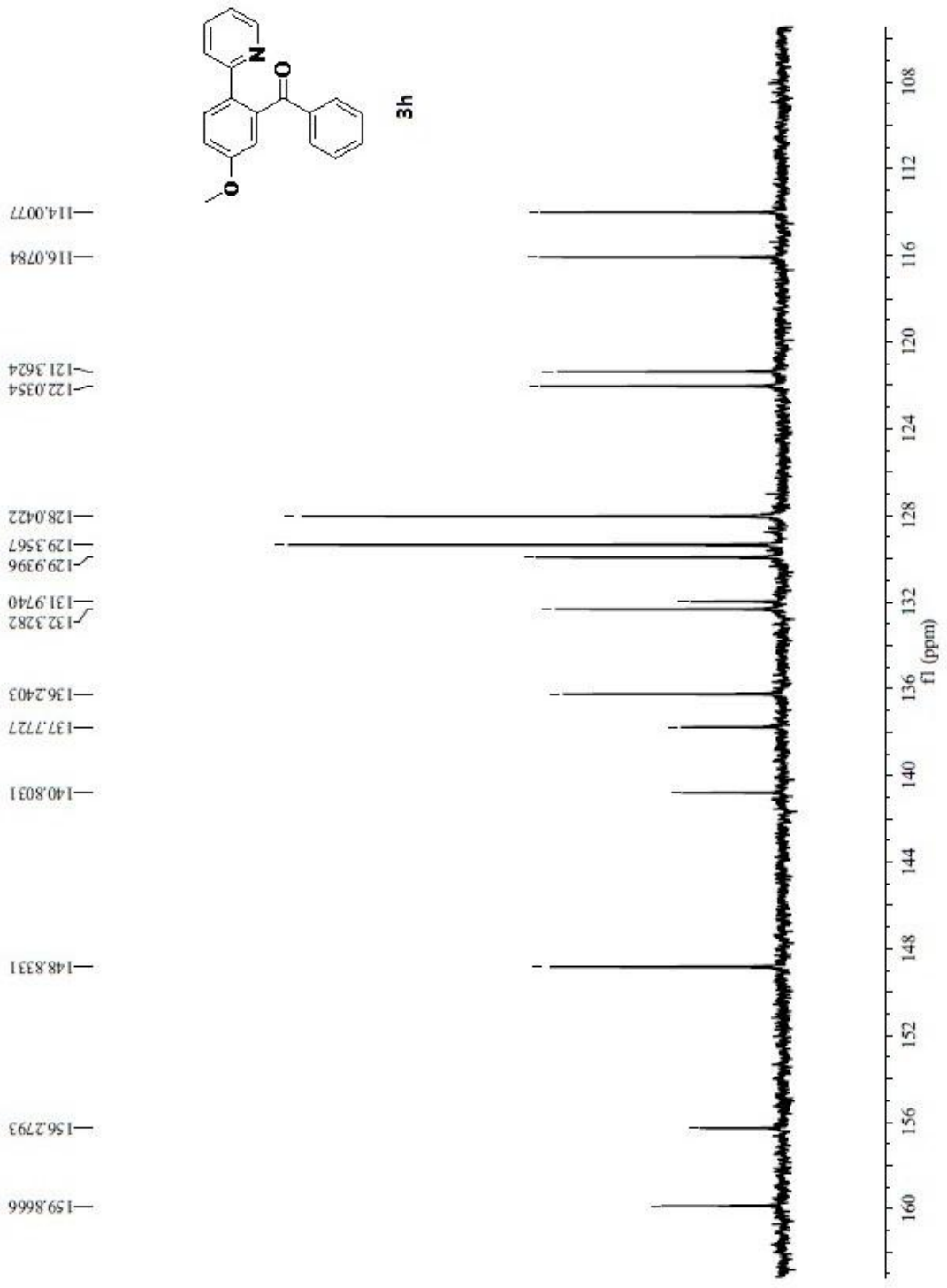
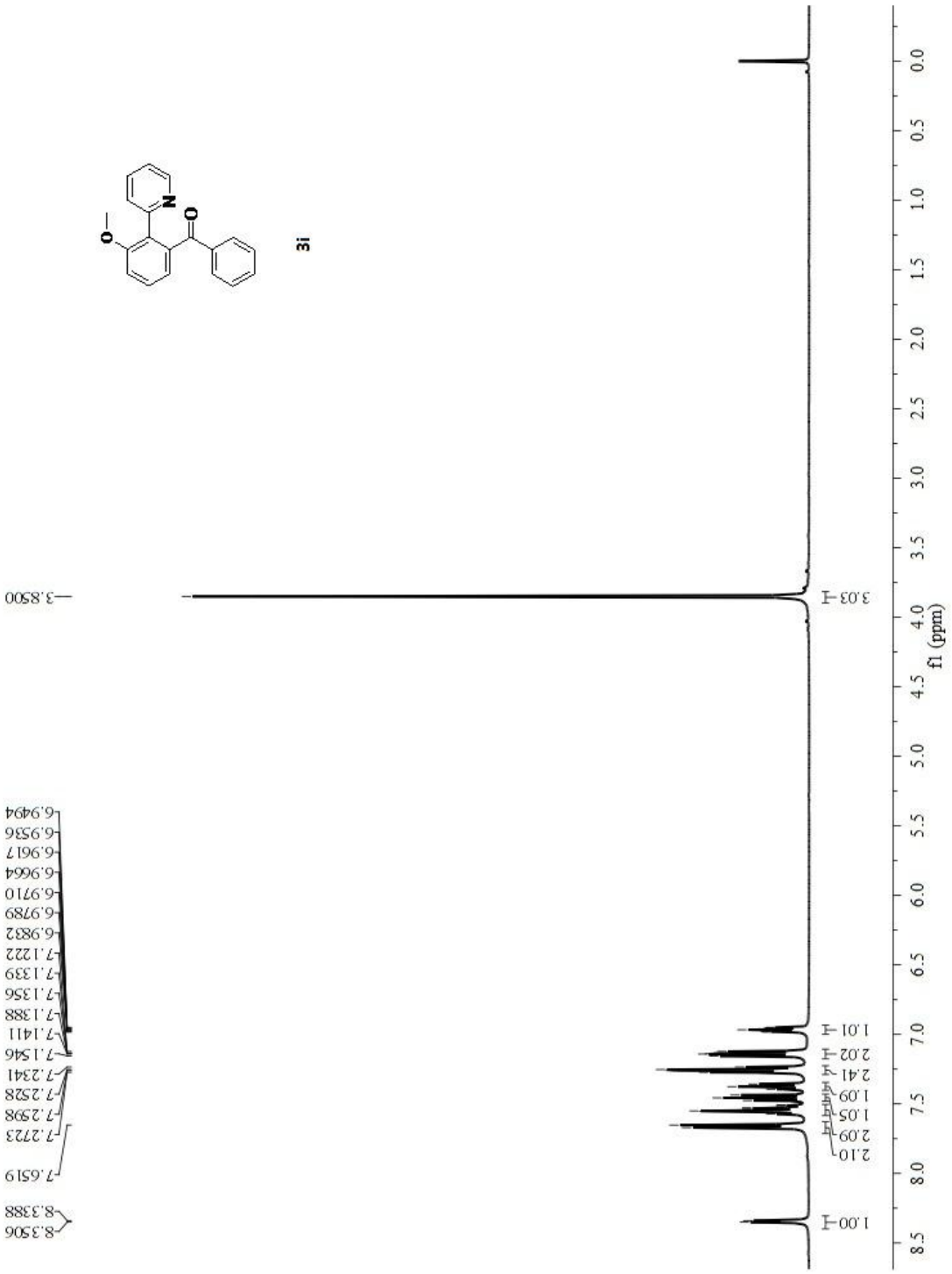
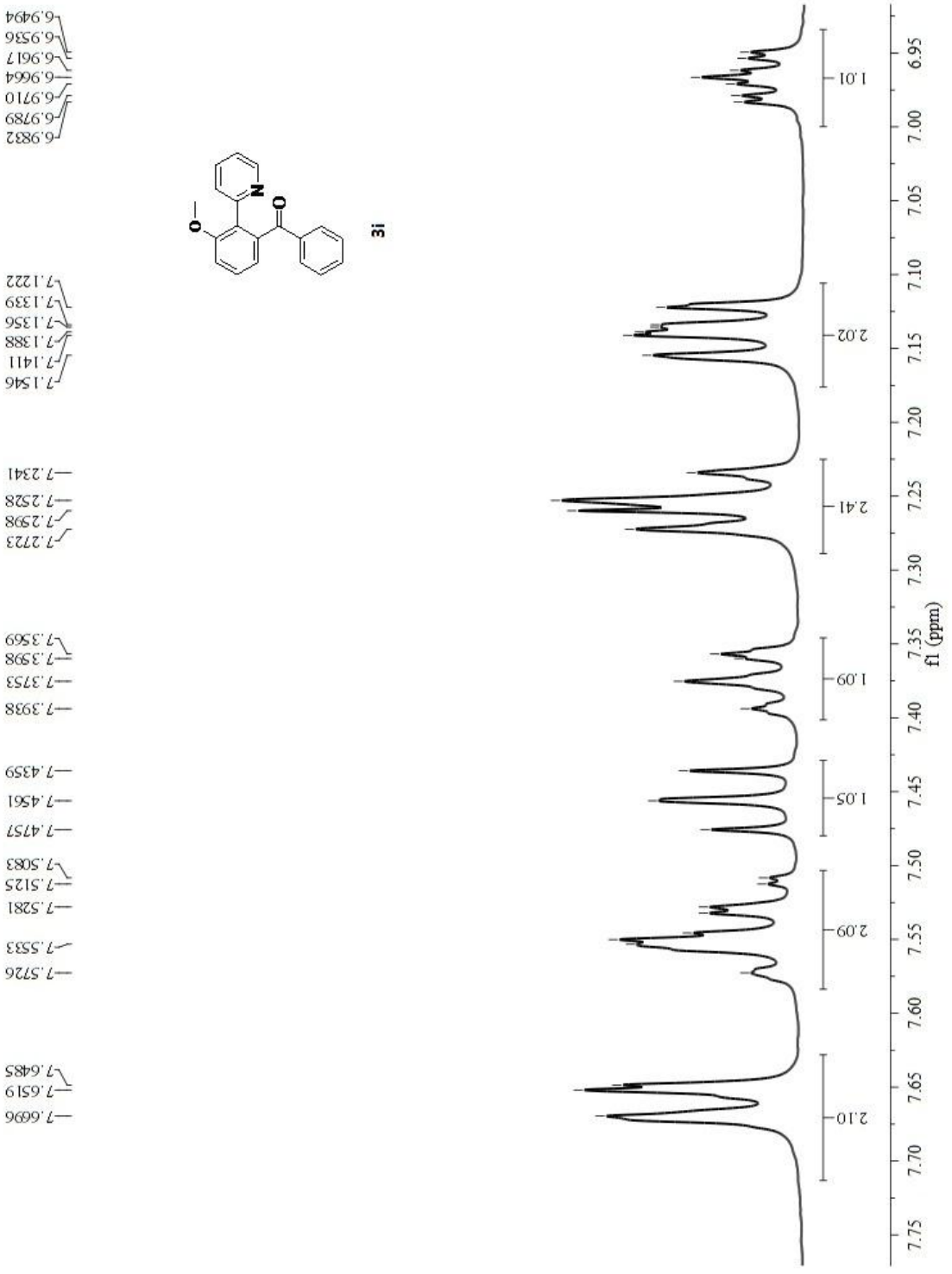
7.2493
7.2305
7.1292
7.1127
7.1078
7.0526
7.0480
6.9505
6.9354
6.9205
1.00
0.90
1.03
2.32
1.17
2.16
2.94
1.00
6.8
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
f1 (ppm)
N
O
O
3h


3h
55.5878
114.0077
116.0784
121.3624
128.0422
129.9396
136.2403
137.7727
140.8031
148.8331
156.2793
159.8666
197.9173
f1 (ppm)




3i
3.8500
8.3506
8.3388
7.6519
7.2723
7.2598
7.2528
7.2341
7.1546
7.1411
7.1388
7.1356
7.1339
7.1222
6.9832
6.9789
6.9710
6.9664
6.9617
6.9536
6.9494
3.03
1.01
2.02
2.41
1.09
1.05
2.09
2.10
1.00
f1 (ppm)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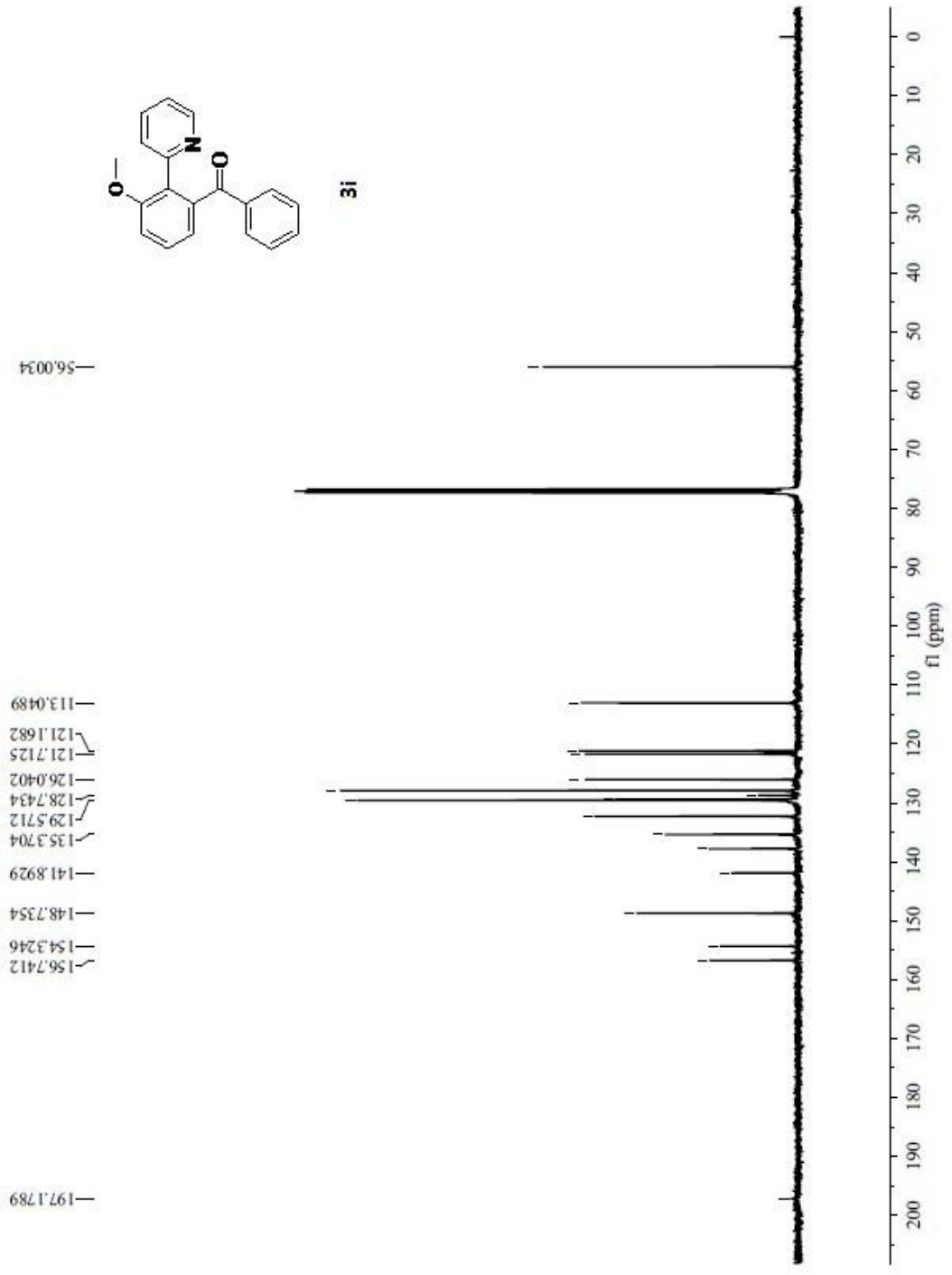
6.9536
6.9617
6.9664
6.9710
6.9789
6.9832
7.1222
7.1339
7.1356
7.1388
7.1411
7.1546
7.2341
7.2528
7.2598
7.2723
7.3569
7.3598
7.3753
7.3938
7.4359
7.4561
7.4757
7.5083
7.5125
7.5281
7.5533
7.5726
7.6485
7.6519
7.6696
O
N
O
3i
1.01
2.02
2.41
1.09
1.05
2.09
2.10
6.95
7.00
7.05
7.10
7.15
7.20
7.25
7.30
7.35
7.40
7.45
7.50
7.55
7.60
7.65
7.70
7.75
f1 (ppm)


3i
O
N
O
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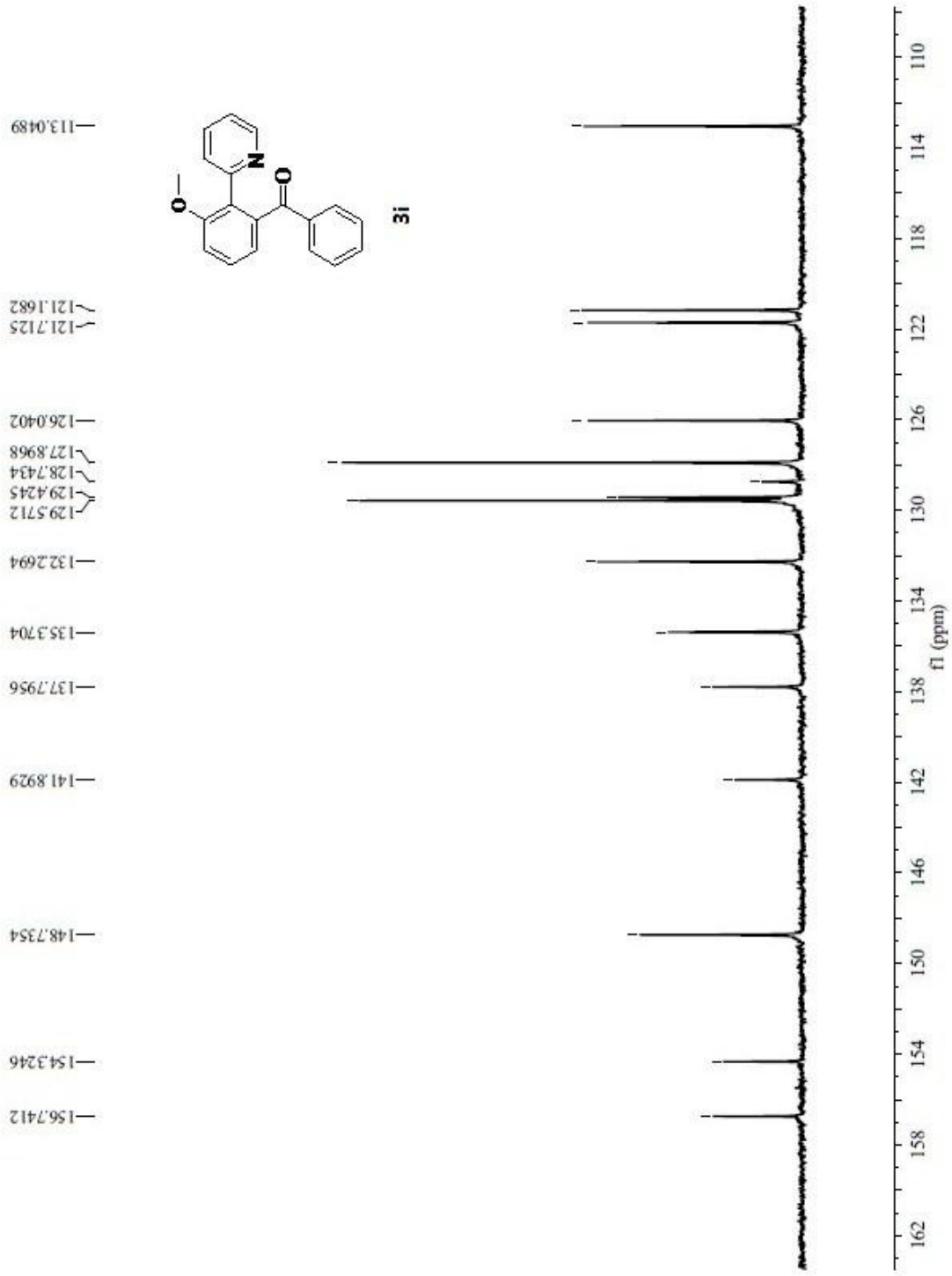
113.0489
121.1682
121.7125
126.0402
128.7434
129.5712
135.3704
141.8929
148.7354
154.3246
156.7412
197.1789
f1 (ppm)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121.7125
126.0402
127.8968
128.7434
129.4245
129.5712
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135.3704
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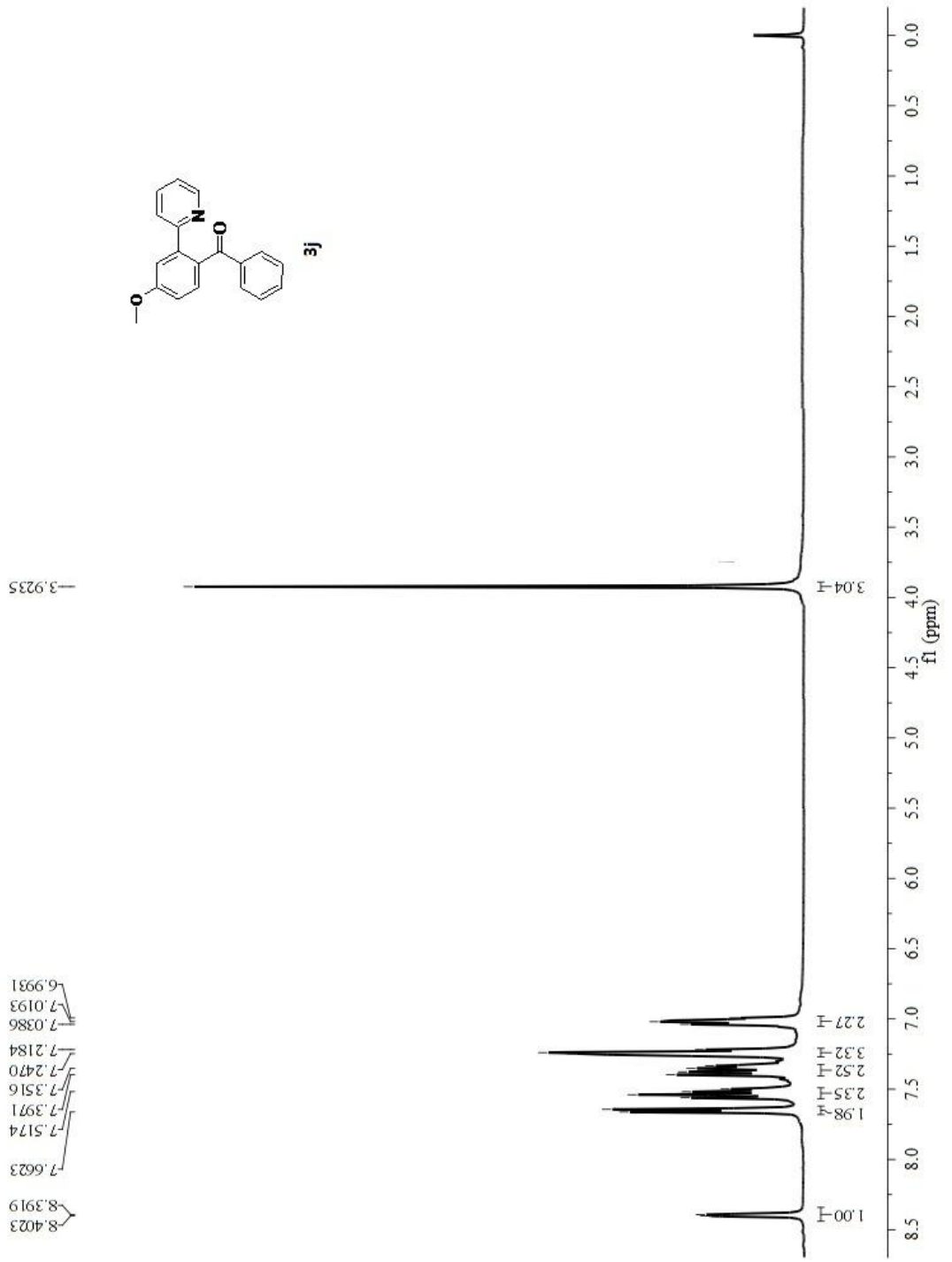
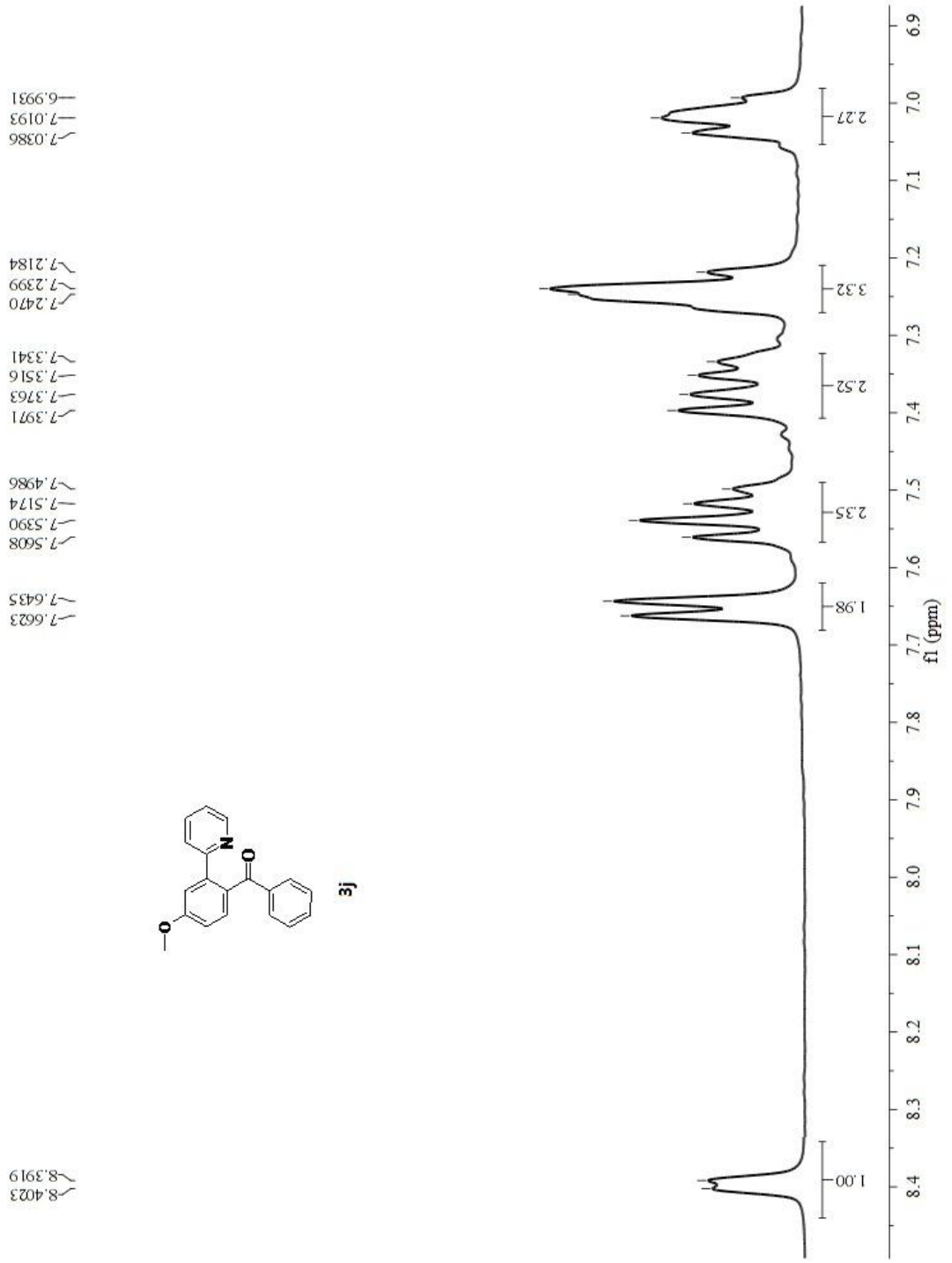
148.7354
154.3246
156.7412
3i
f1 (ppm)

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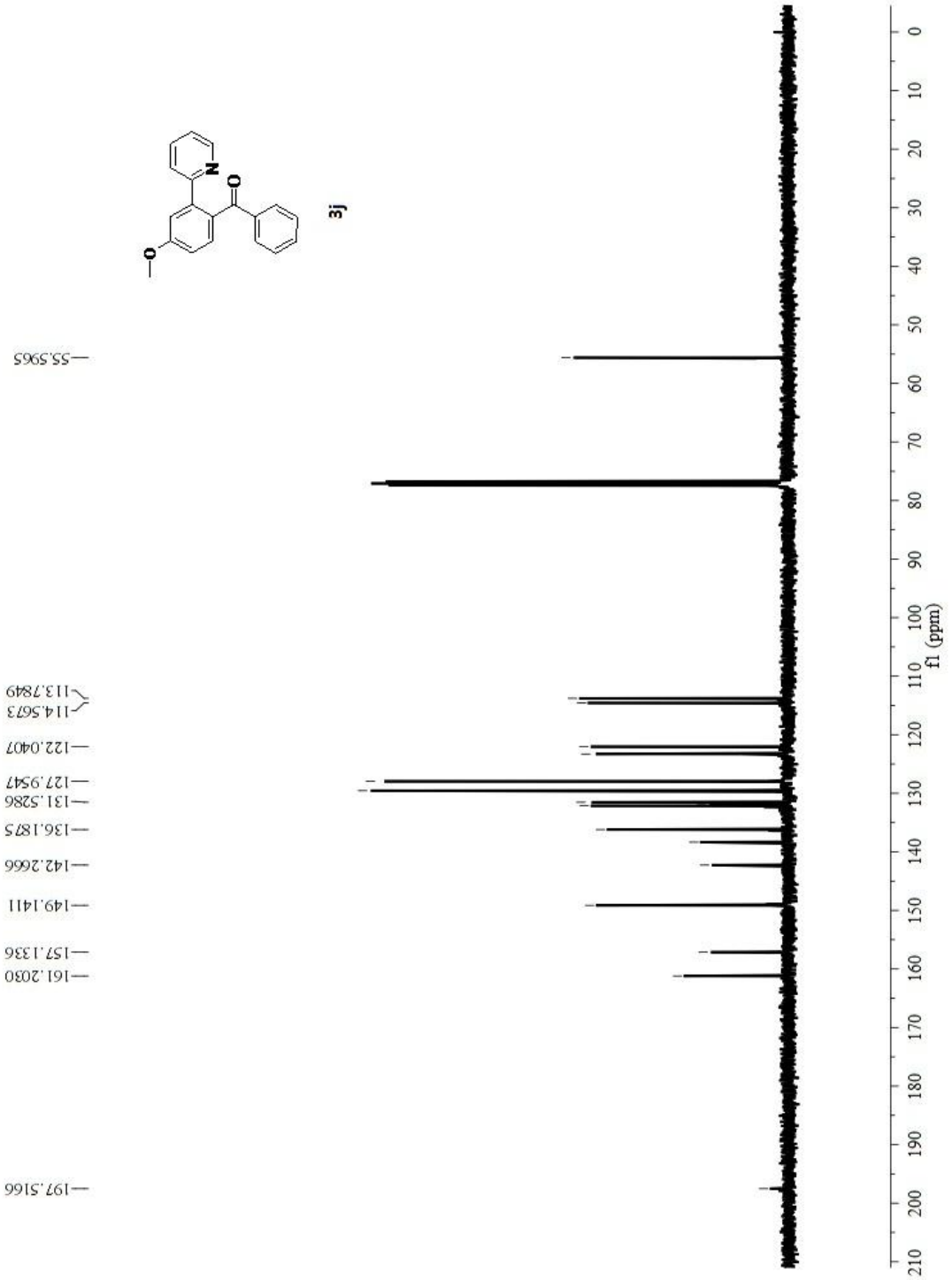
7.6623
7.6435
7.5608
7.5390
7.5174
7.4986
7.3971
7.3763
7.3516
7.3341
7.2470
7.2399
7.2184
7.0386
7.0193
6.9931
1.00
1.98
2.35
2.52
3.32
2.27
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
f1 (ppm)
N
O
O
3j


3j
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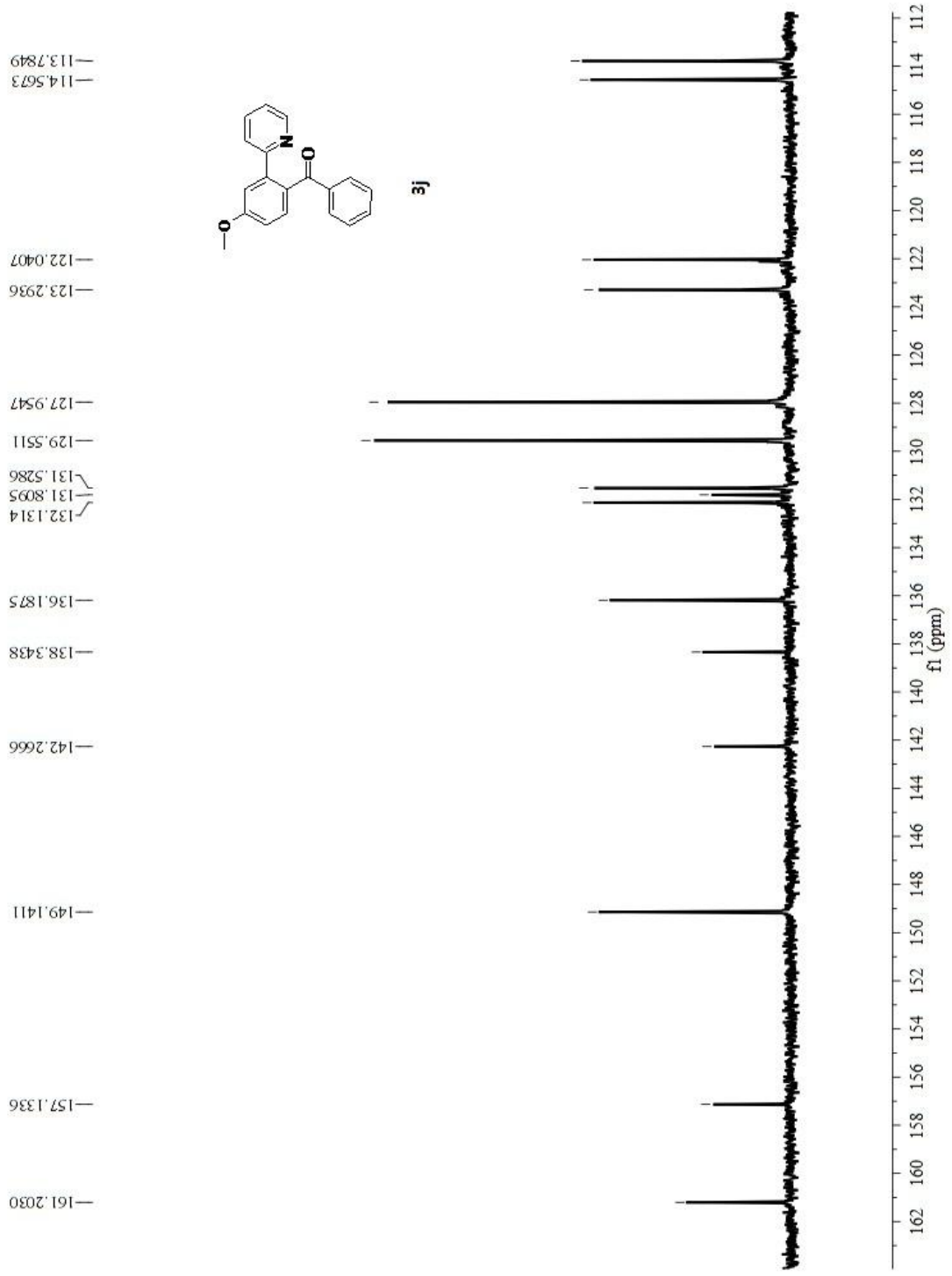
113.7849
114.5673
122.0407
127.9547
131.5286
136.1875
142.2666
149.1411
157.1336
161.2030
197.5166
f1 (ppm)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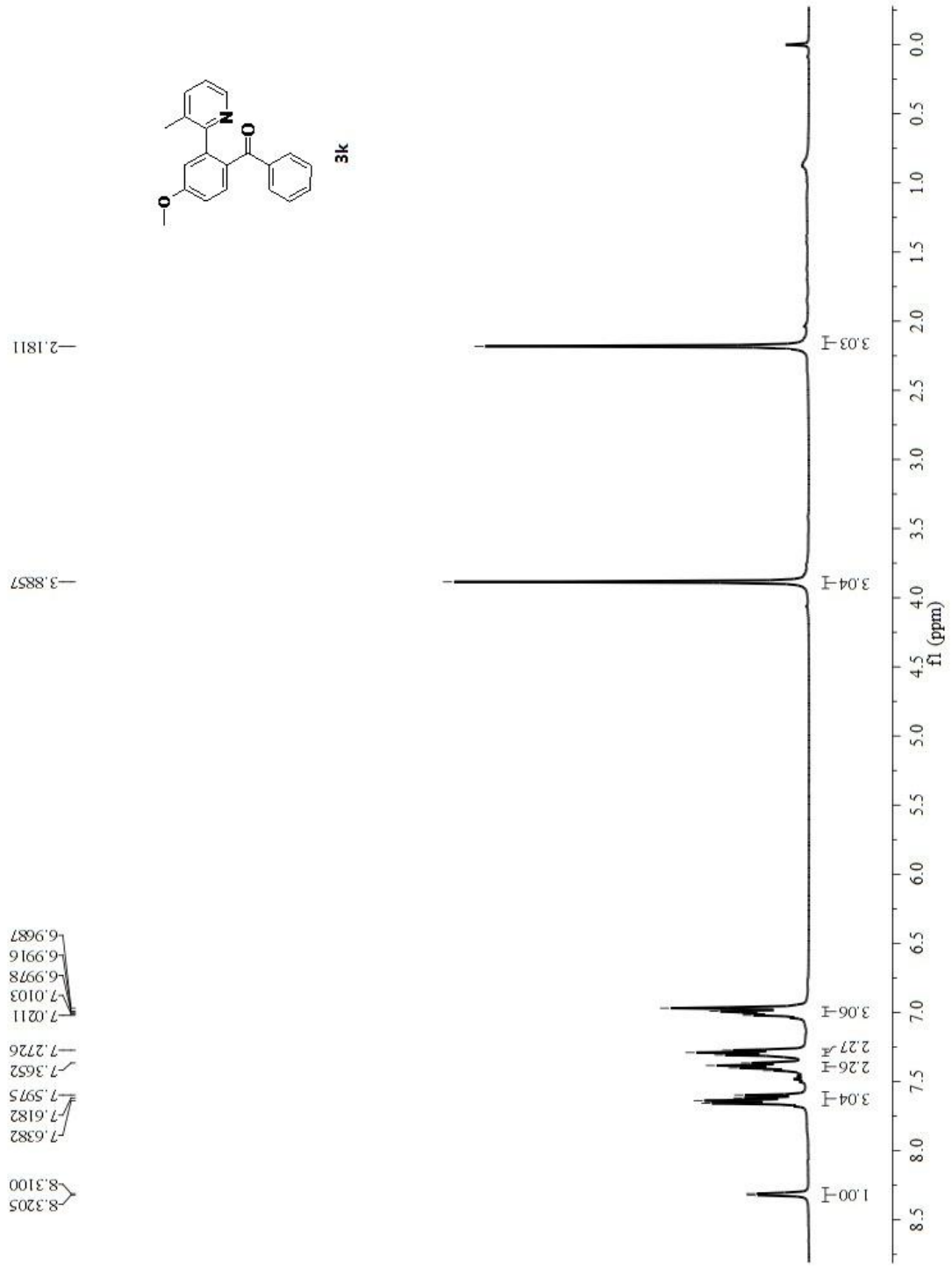
114.5673
122.0407
123.2936
127.9547
129.5511
131.5286
131.8095
132.1314
136.1875
138.3438
142.2666
149.1411
157.1336
161.2030
3j
O
N
O
O
112
114
116
118
120
122
124
126
128
130
132
134
136
138
140
142
144
146
148
150
152
154
156
158
160
162
f1 (ppm)


3k
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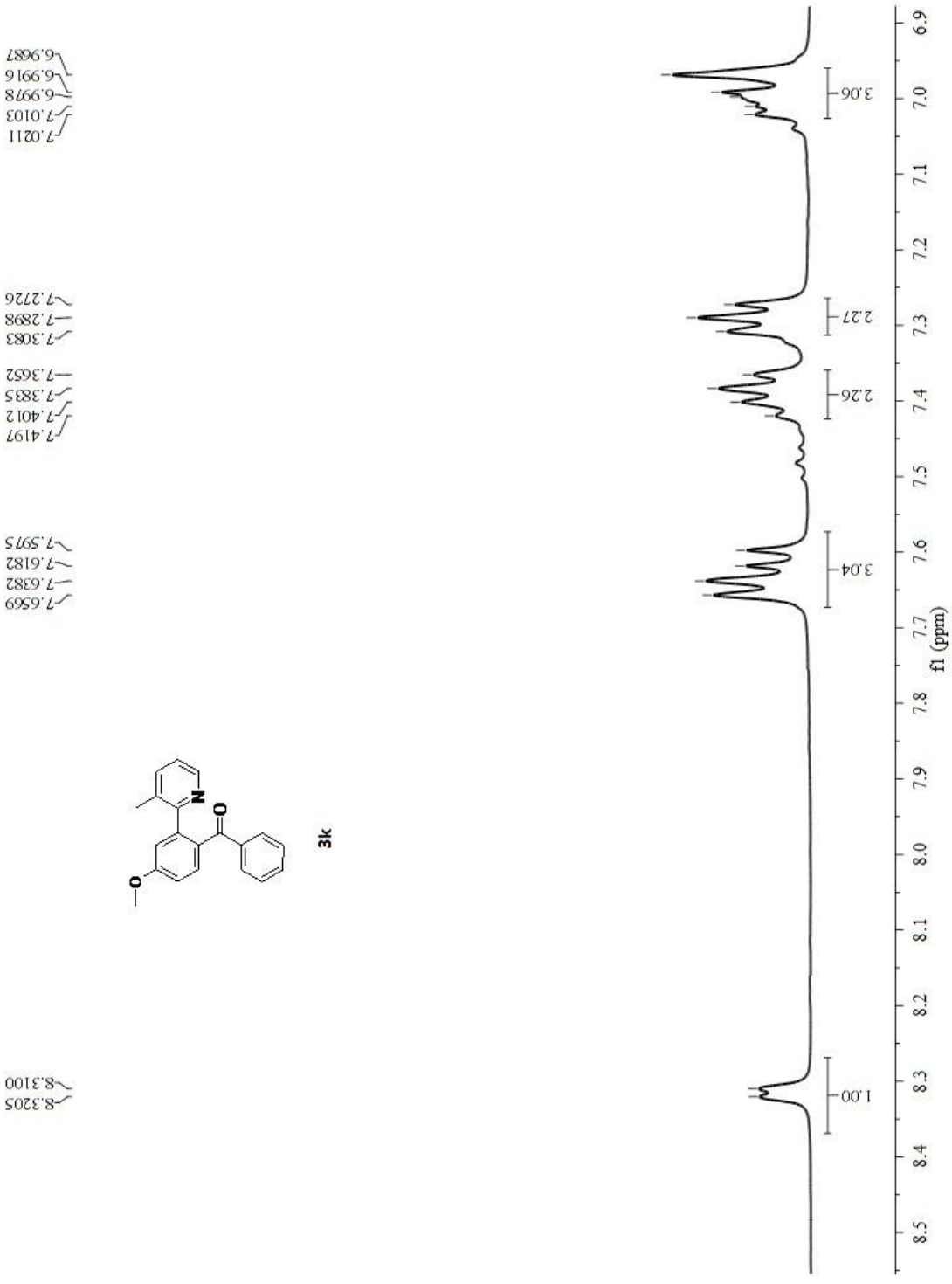
3.8857
8.3205
8.3100
7.6382
7.6182
7.5975
7.3652
7.2726
7.0211
7.0103
6.9978
6.9916
6.9687
3.03
3.04
3.06
2.27
2.26
3.04
1.00
f1 (ppm)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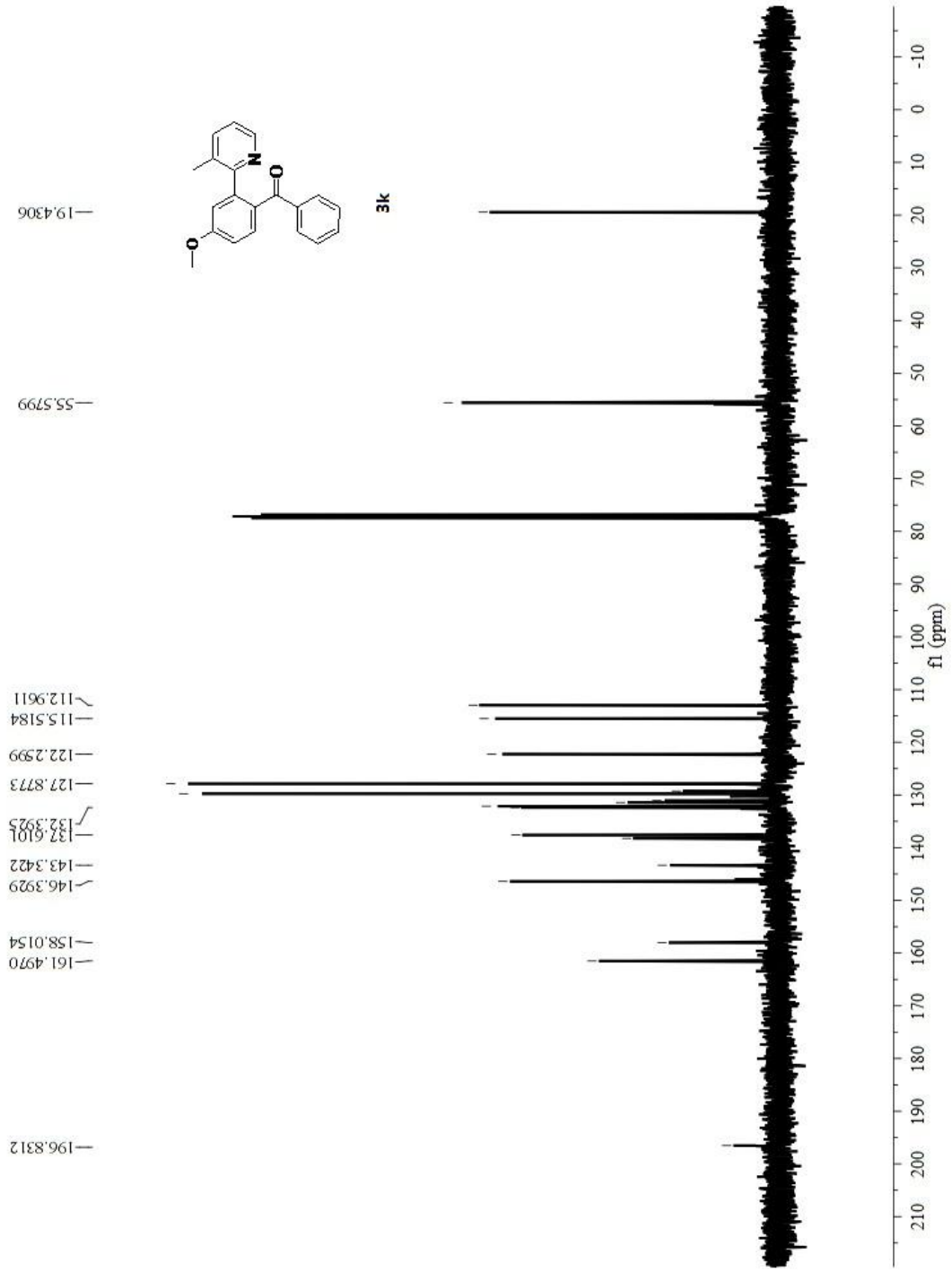
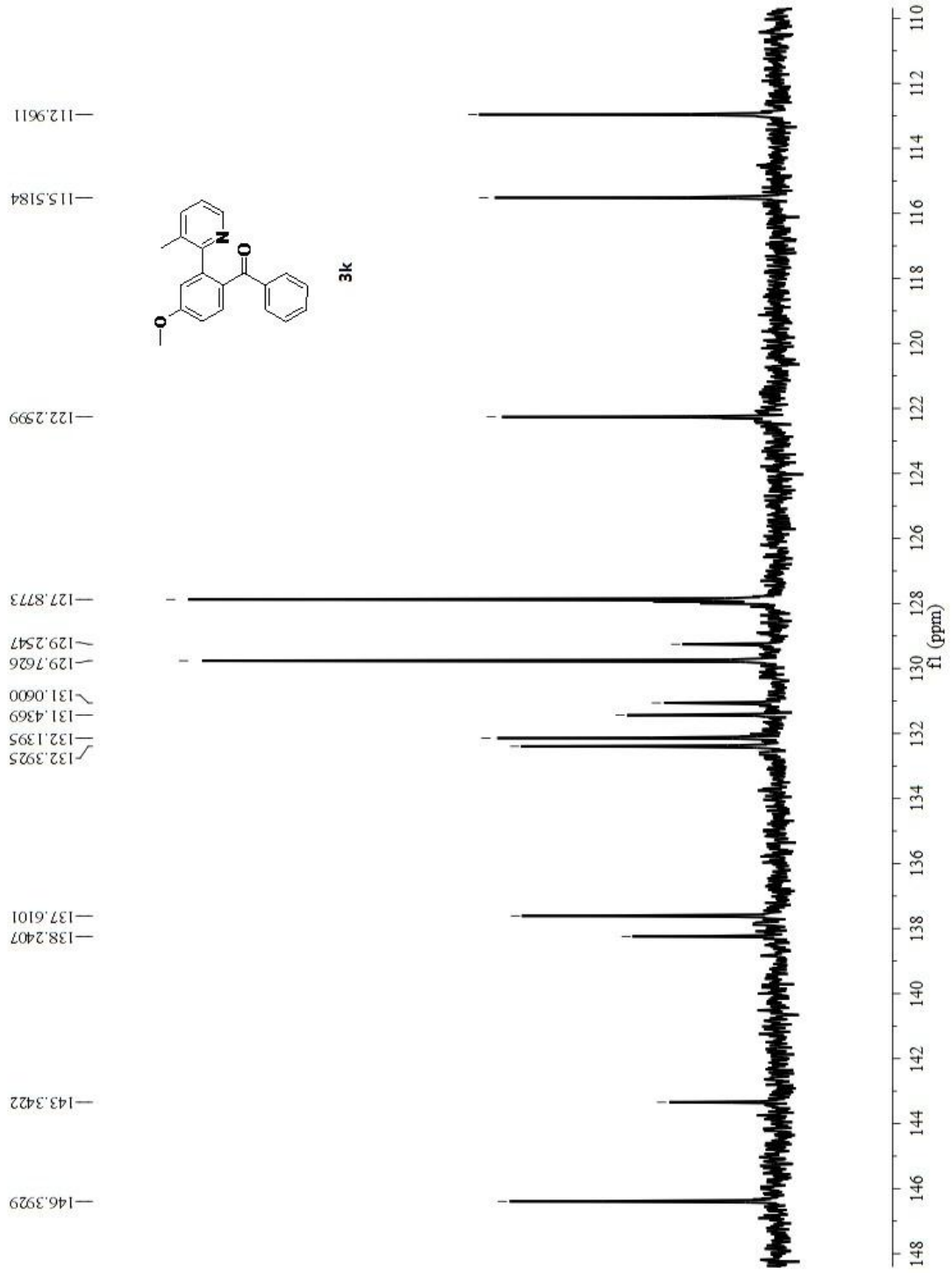
8.3100
7.6569
7.6382
7.6182
7.5975
7.4197
7.4012
7.3835
7.3652
7.3083
7.2898
7.2726
7.0211
7.0103
6.9978
6.9916
6.9687
3k
1.00
3.04
2.26
2.27
3.06
6.9
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
f1 (ppm)

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122.2599
127.8773
129.2547
129.7626
131.0600
131.4369
132.1395
132.3925
137.6101
138.2407
143.3422
146.3929
3k
O
N
O
110
112
114
116
118
120
122
124
126
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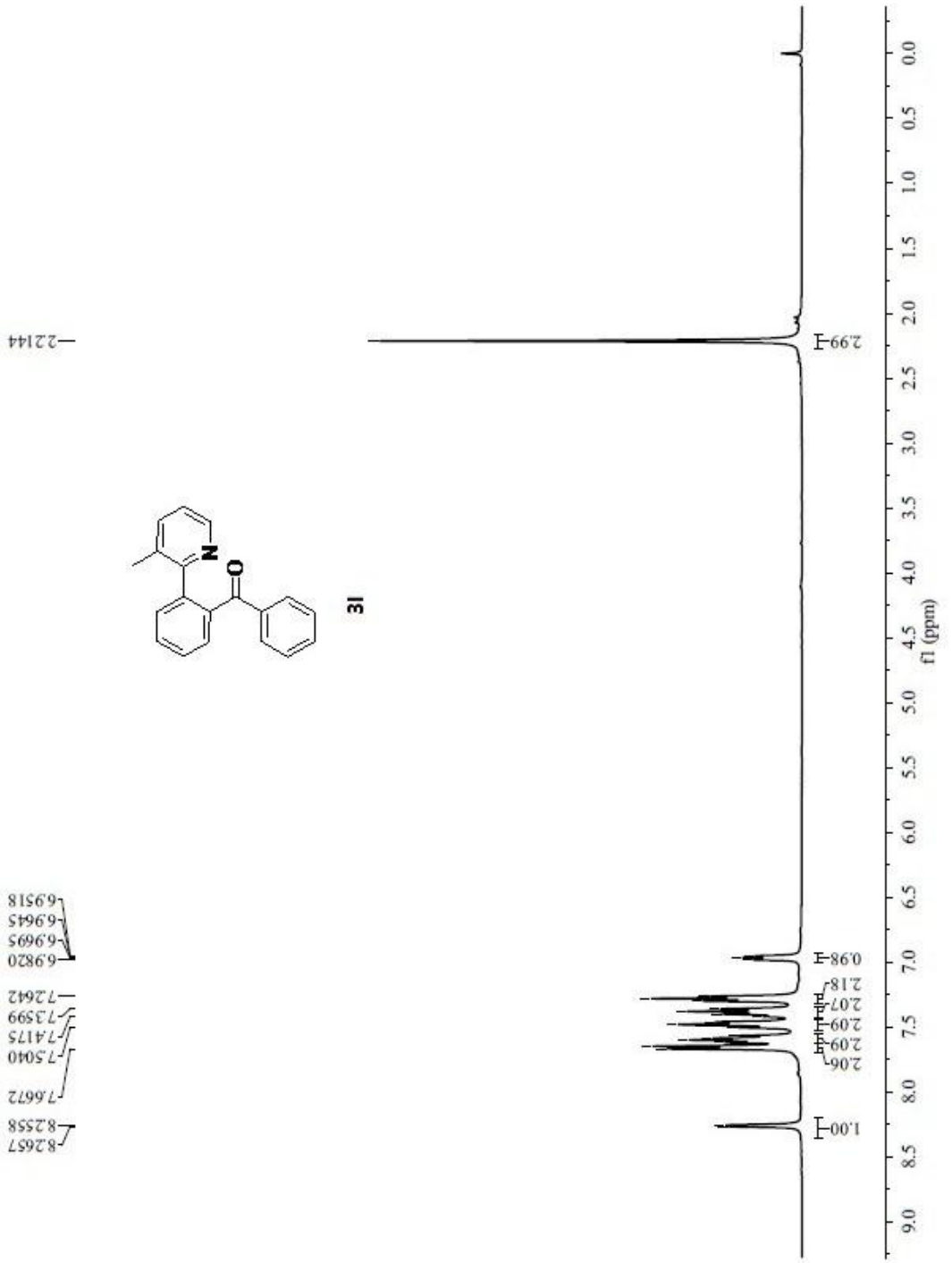
136
138
140
142
144
146
148
f1 (ppm)


3l
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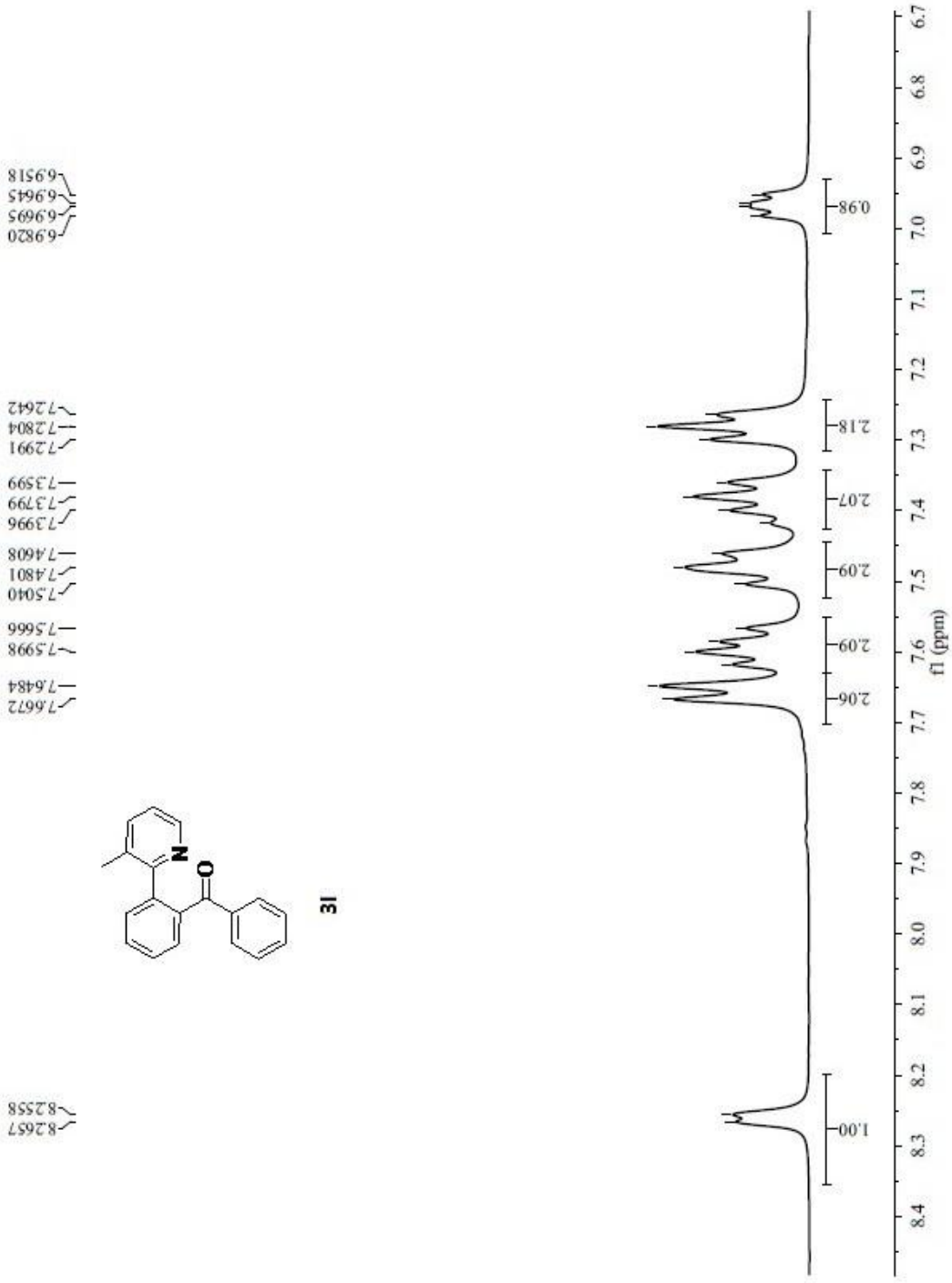
0.98
2.18
2.07
2.09
2.09
2.06
1.00
2.2144
8.2657
8.2558
7.6672
7.5040
7.4175
7.3599
7.2642
6.9820
6.9695
6.9645
6.9518
f1 (ppm)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8.2558
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7.6484
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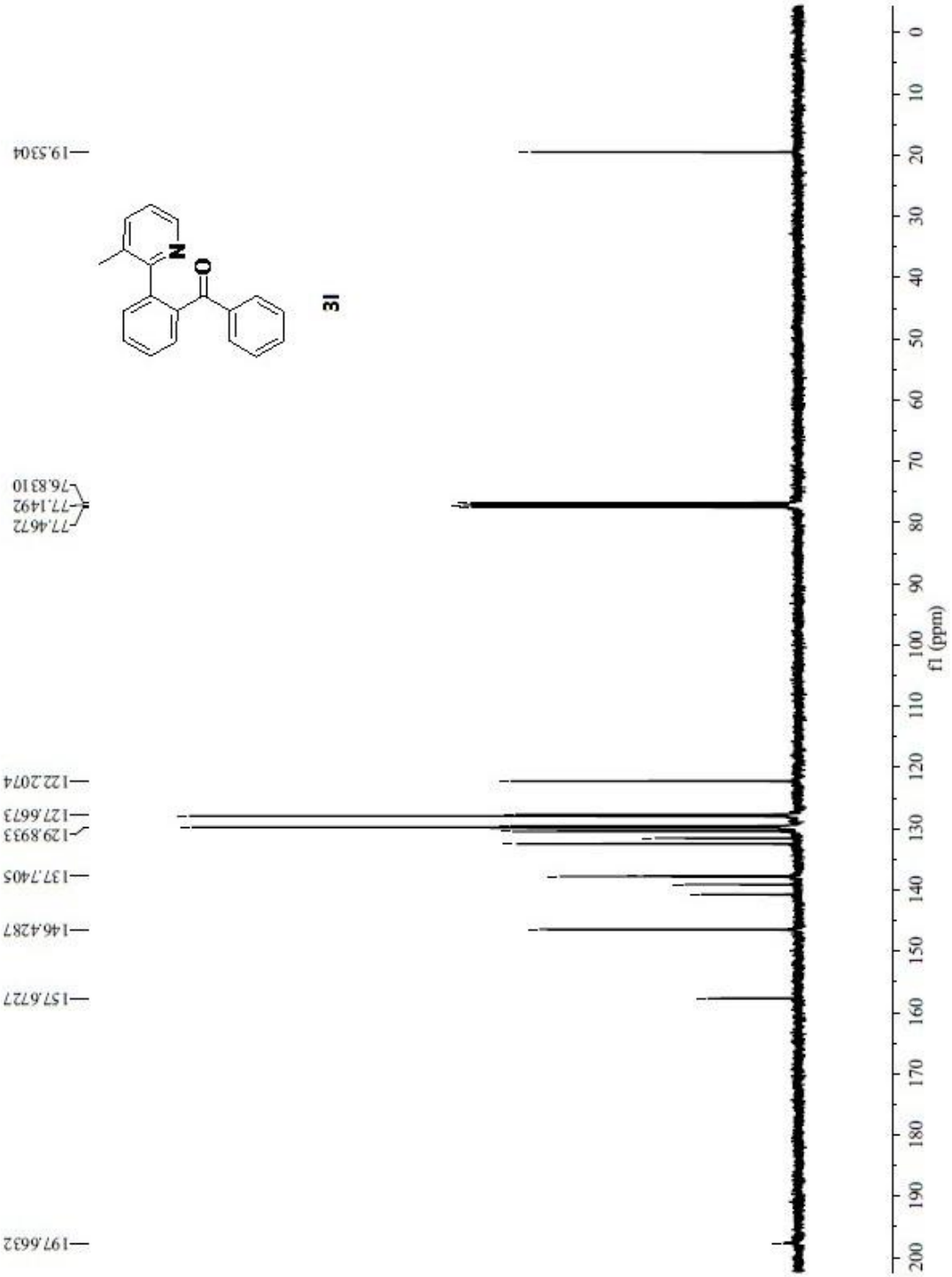
7.5666
7.5040
7.4801
7.4608
7.3996
7.3799
7.3599
7.2991
7.2804
7.2642
6.9820
6.9695
6.9645
6.9518
3l
1.00
2.06
2.09
2.09
2.07
2.18
0.98
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
f1 (ppm)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77.1492
77.4672
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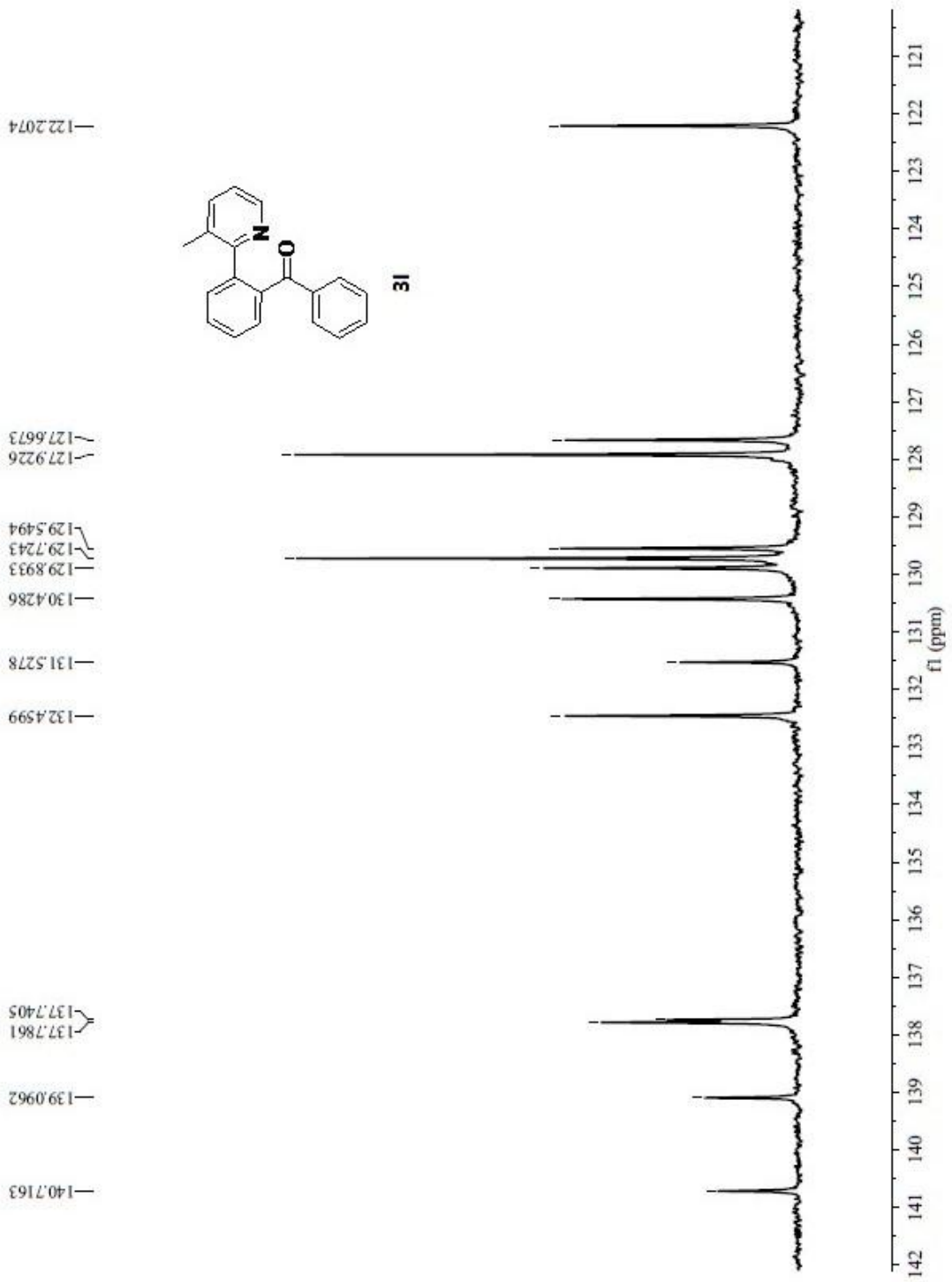
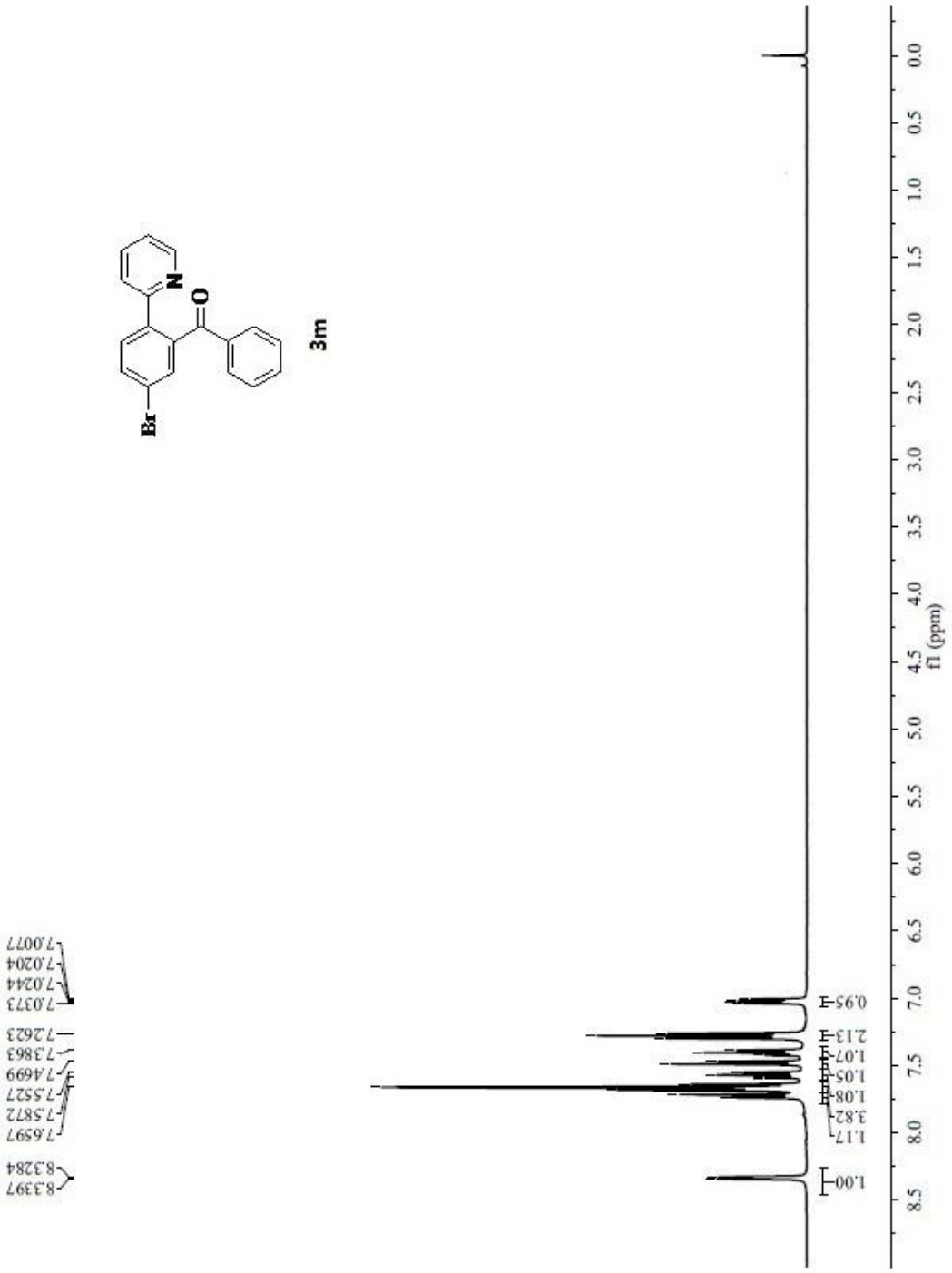
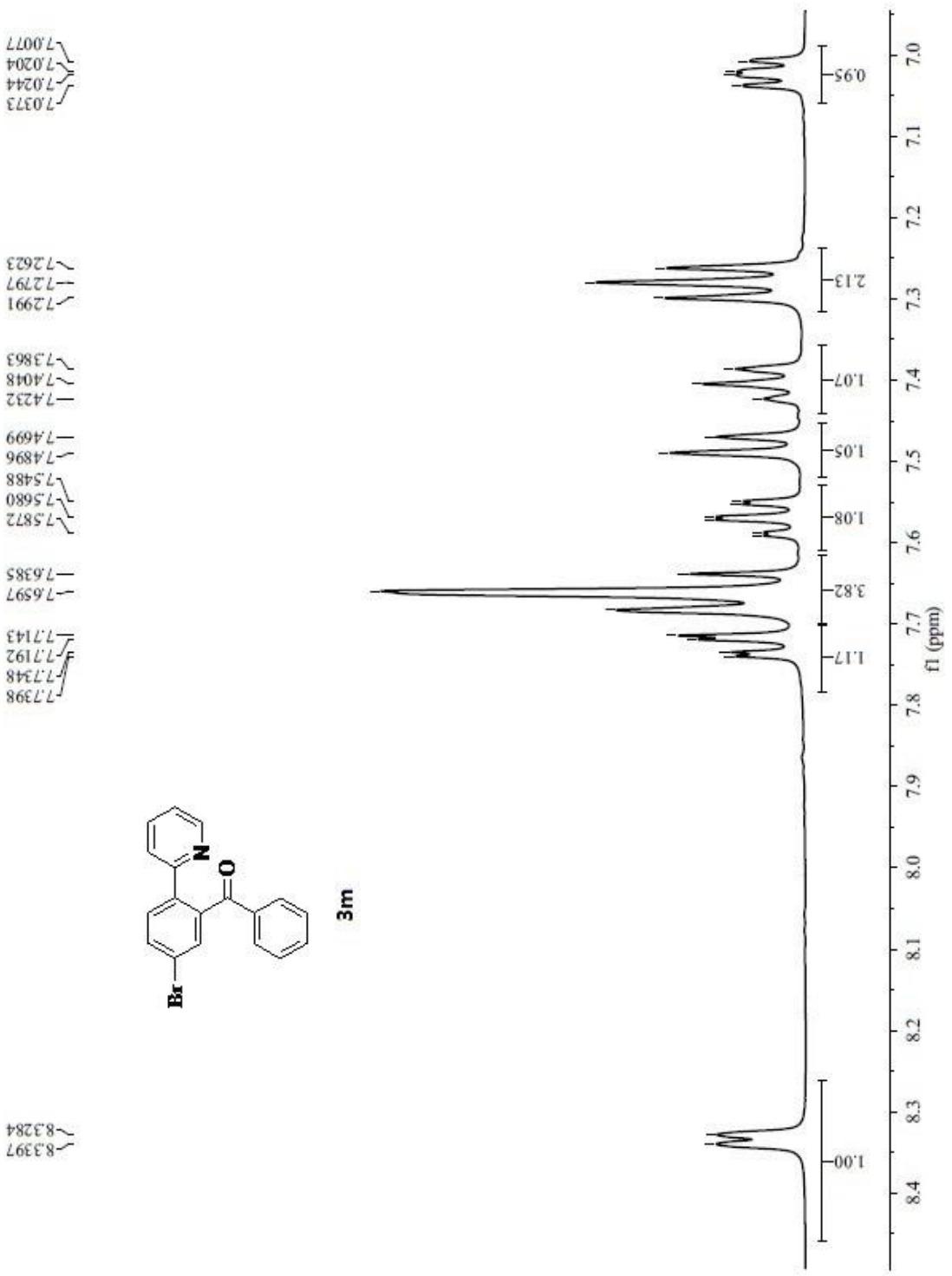
127.6673
129.8933
137.7405
146.4287
157.6727
197.6632
3l
f1 (ppm)




3m
Br
O
N
8.3397
8.3284
7.6597
7.5872
7.5527
7.4699
7.3863
7.2623
7.0373
7.0244
7.0204
7.0077
1.00
1.17
3.82
1.08
1.05
1.07
2.13
0.95
f1 (ppm)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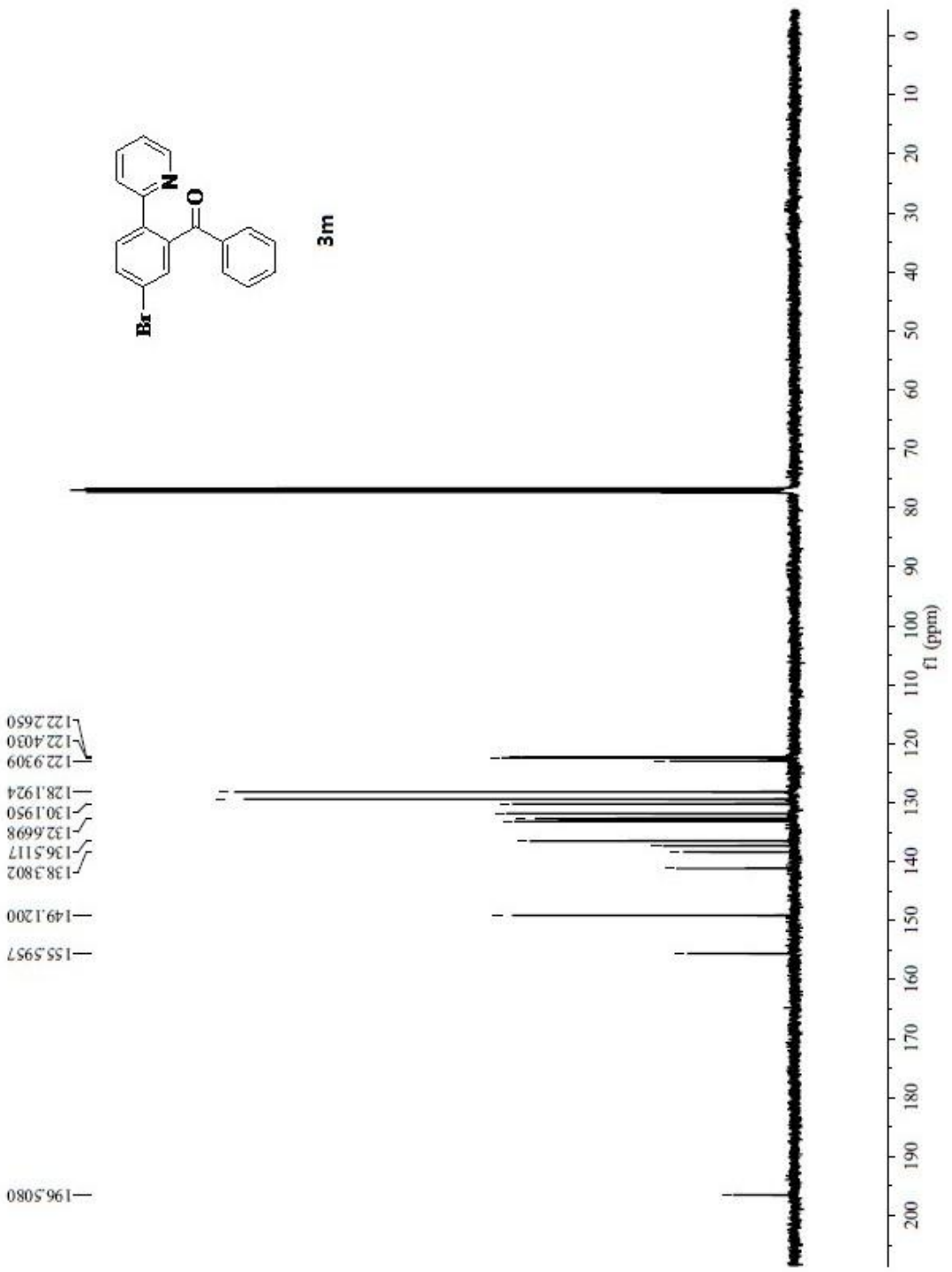
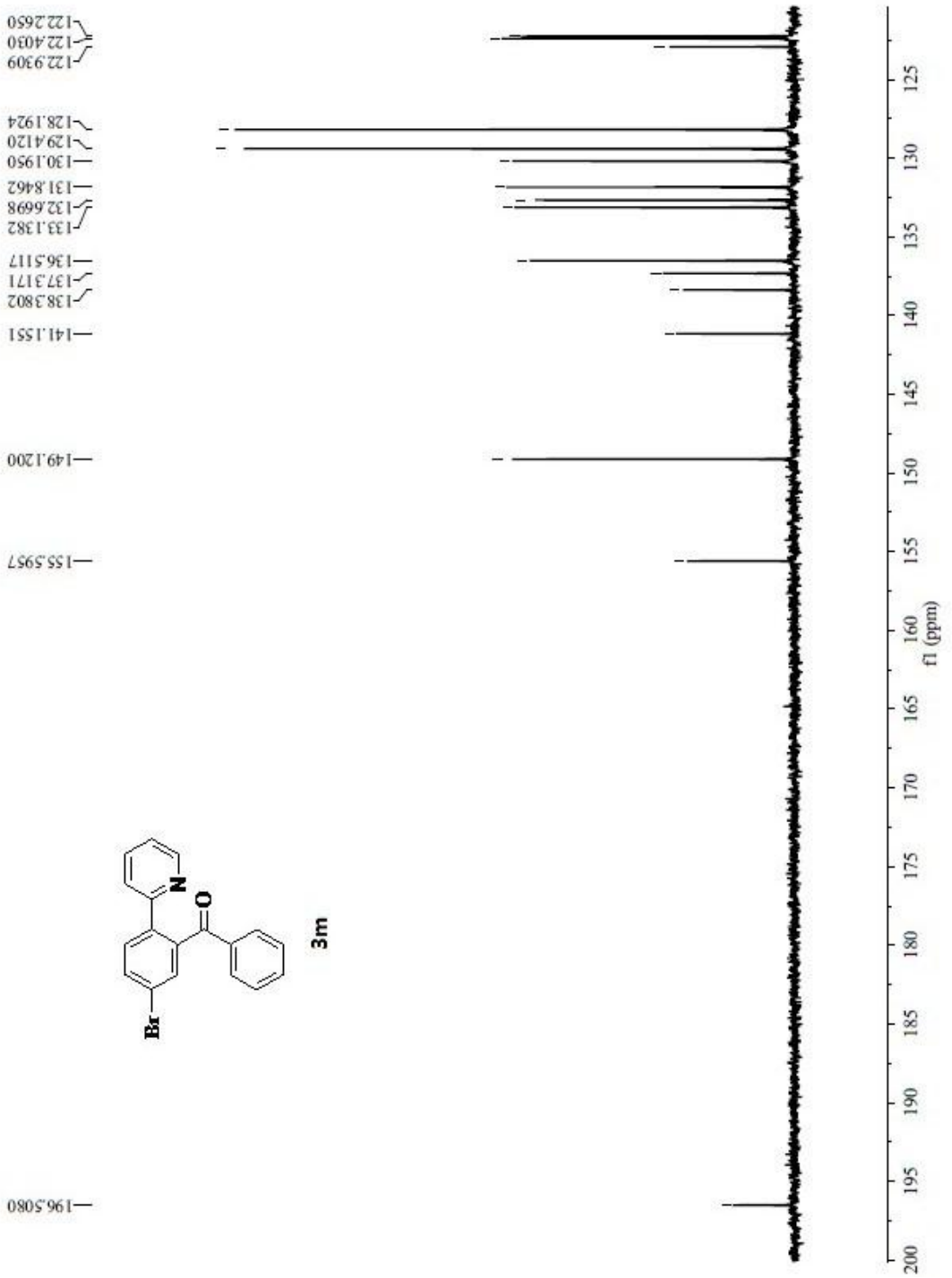
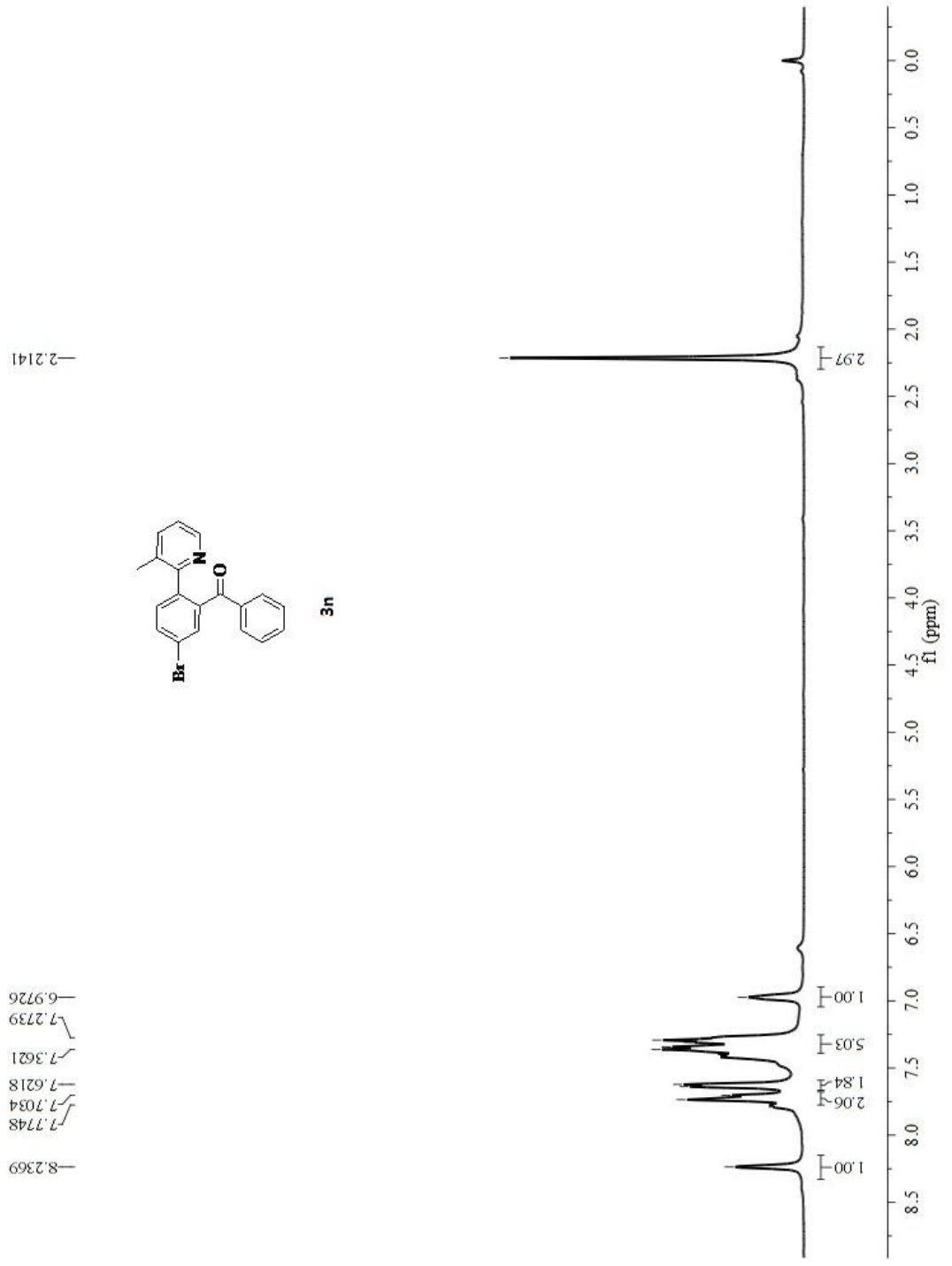
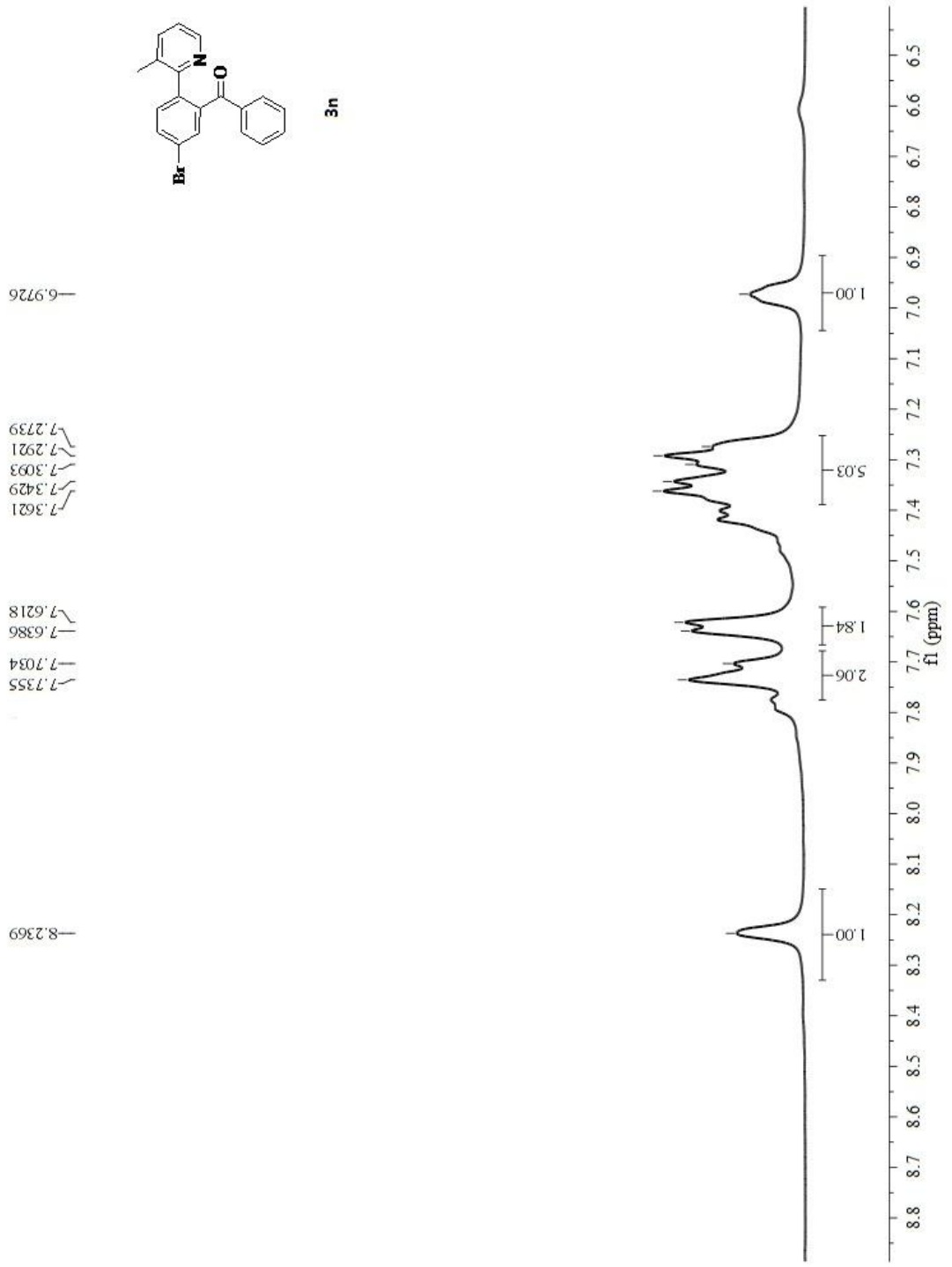
7.0204
7.0244
7.0373
7.2623
7.2797
7.2991
7.3863
7.4048
7.4232
7.4699
7.4896
7.5488
7.5680
7.5872
7.6385
7.6597
7.7143
7.7192
7.7348
7.7398
8.3284
8.3397
0.95
2.13
1.07
1.05
1.08
3.82
1.17
1.00
7.0
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
f1 (ppm)
N
O
Br
3m




122.2650
122.4030
122.9309
128.1924
129.4120
130.1950
131.8462
132.6698
133.1382
136.5117
137.3171
138.3802
141.1551
149.1200
155.5957
196.5080
3m
N
O
Br
125
130
135
140
145
150
155
160
165
170
175
180
185
190
195
200
f1 (ppm)


8.2369
7.7748
7.7034
7.6218
7.3621
7.2739
6.9726
2.2141
3n
Br
N
O
1.00
5.03
1.84
2.06
1.00
2.97
f1 (ppm)


3n
Br
N
O
8.2369
7.6973
7.6218
7.6386
7.7034
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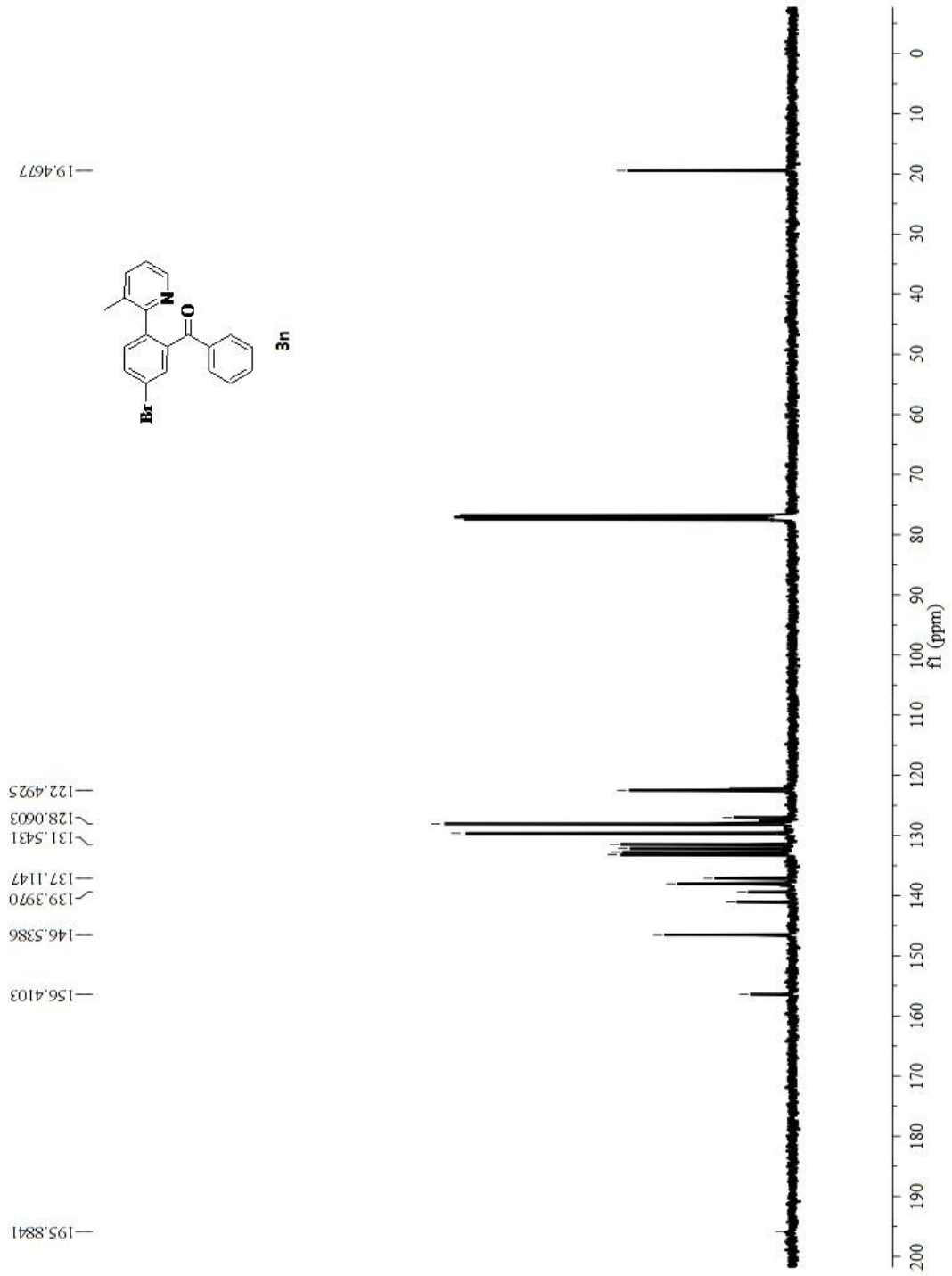
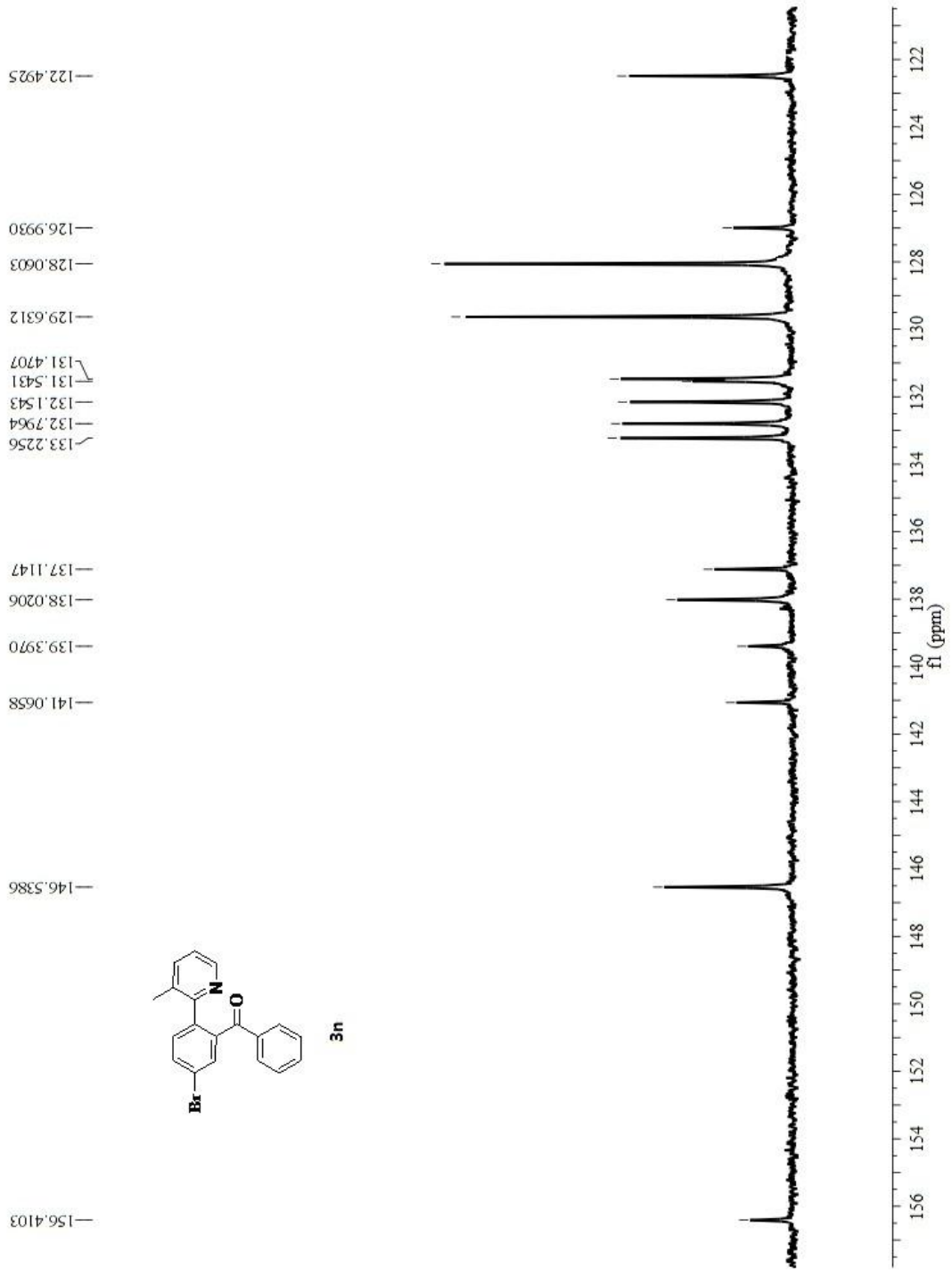
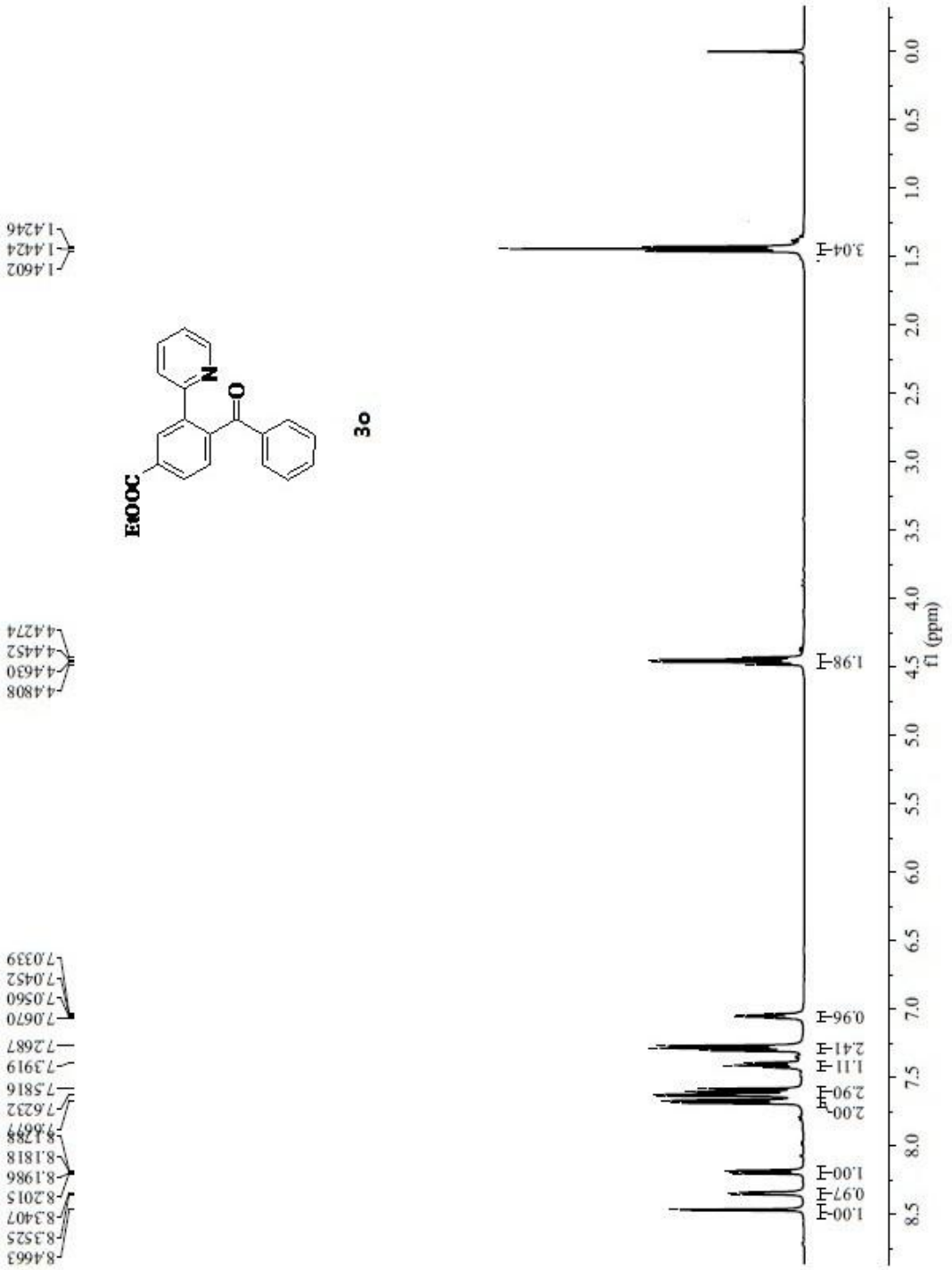
1.00
f1 (ppm)



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7.0670
7.2687
7.3919
7.5816
7.6232
7.8077
8.1288
8.1818
8.1986
8.2015
8.3407
8.3525
8.4663
EtOOC
N
O
3o
3.04
1.98
0.96
2.41
1.11
2.90
2.00
1.00
0.97
1.00
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
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6.0
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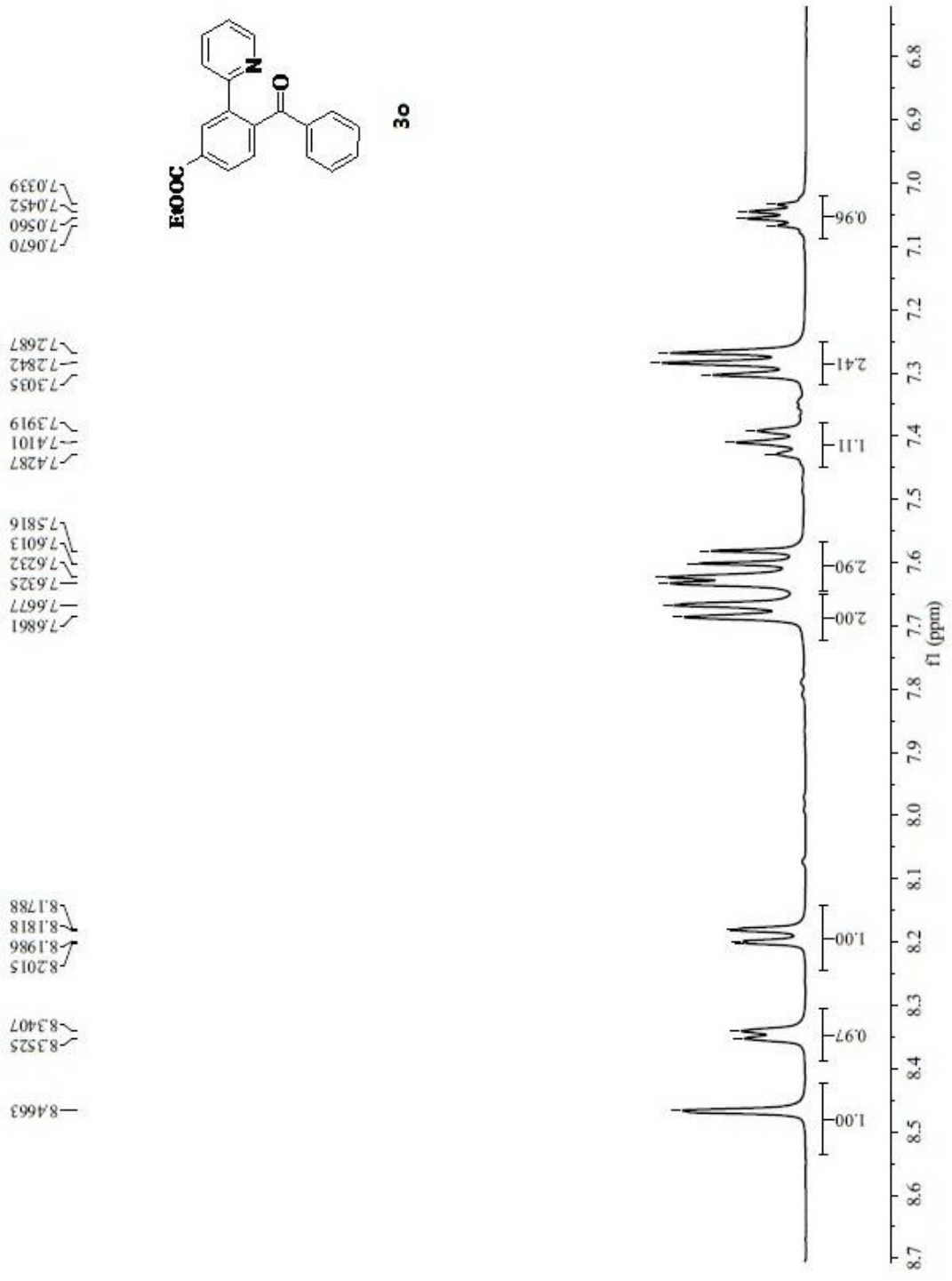
7.5
8.0
8.5
f1 (ppm)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O
3o
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7.6677
7.6325
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7.6013
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7.4287
7.4101
7.3919
7.3035
7.2842
7.2687
7.0670
7.0560
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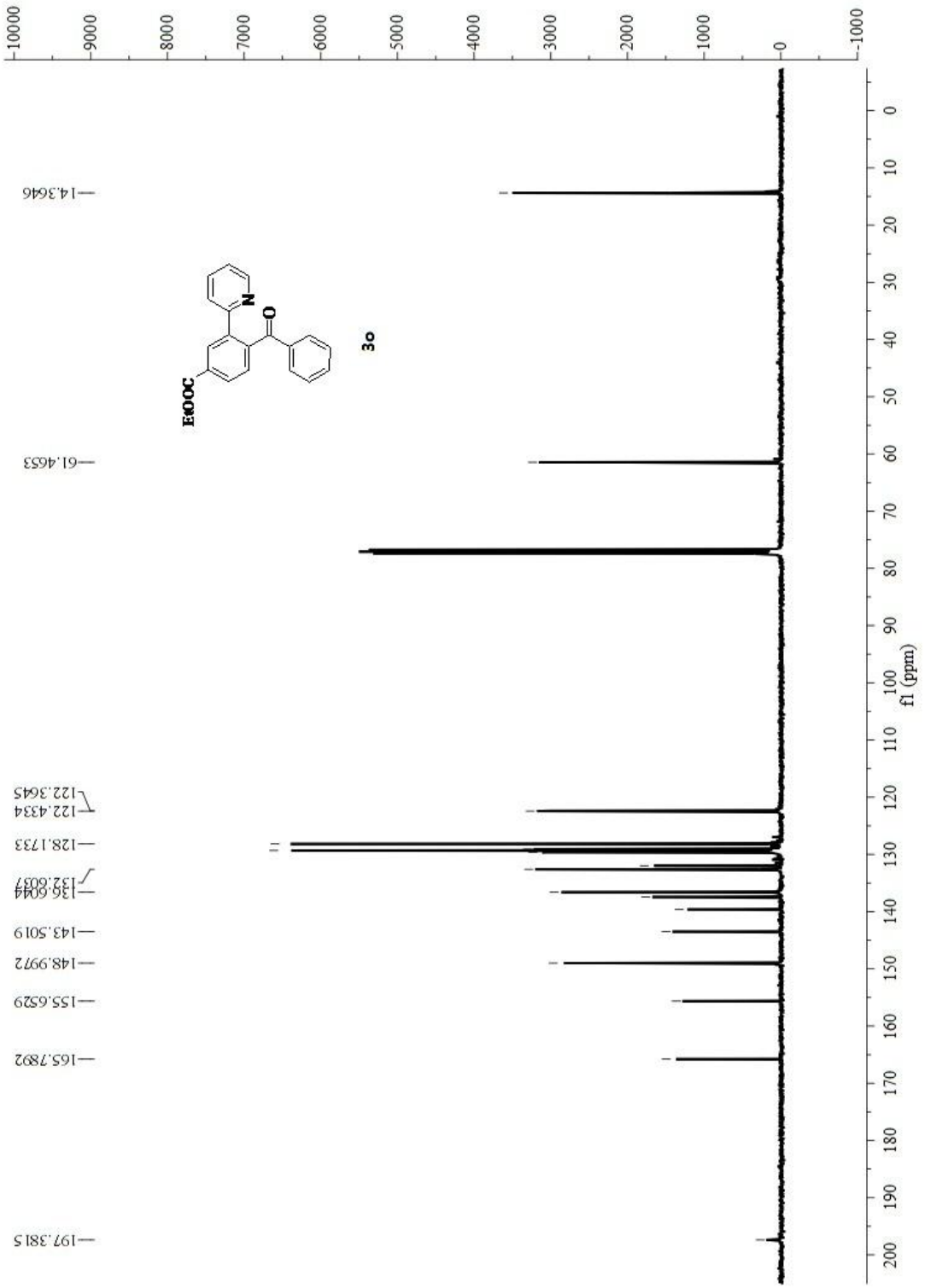
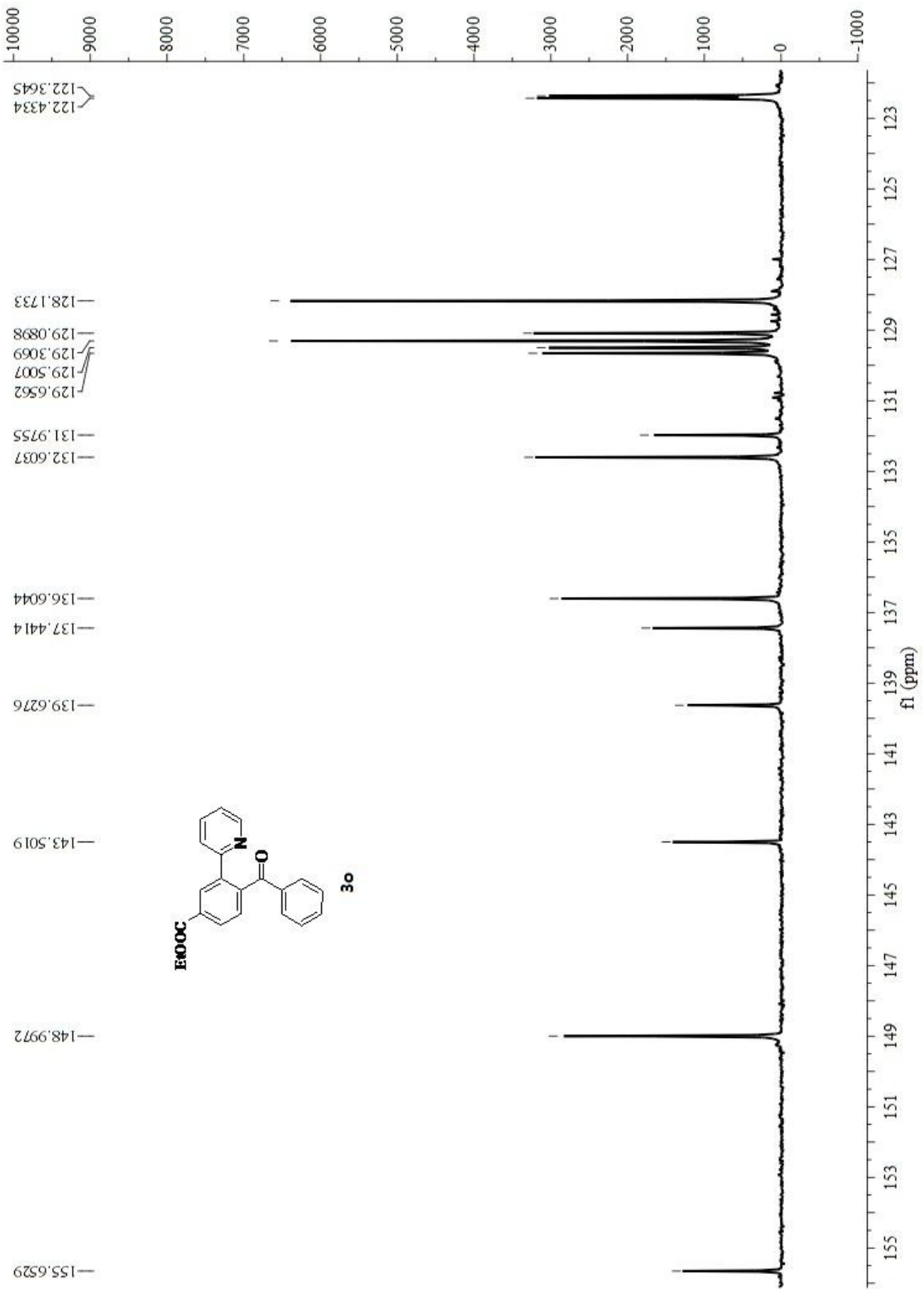
2.41
1.11
2.90
2.00
1.00
0.97
1.00
f1 (ppm)

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132.6037
136.6044
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139.6276
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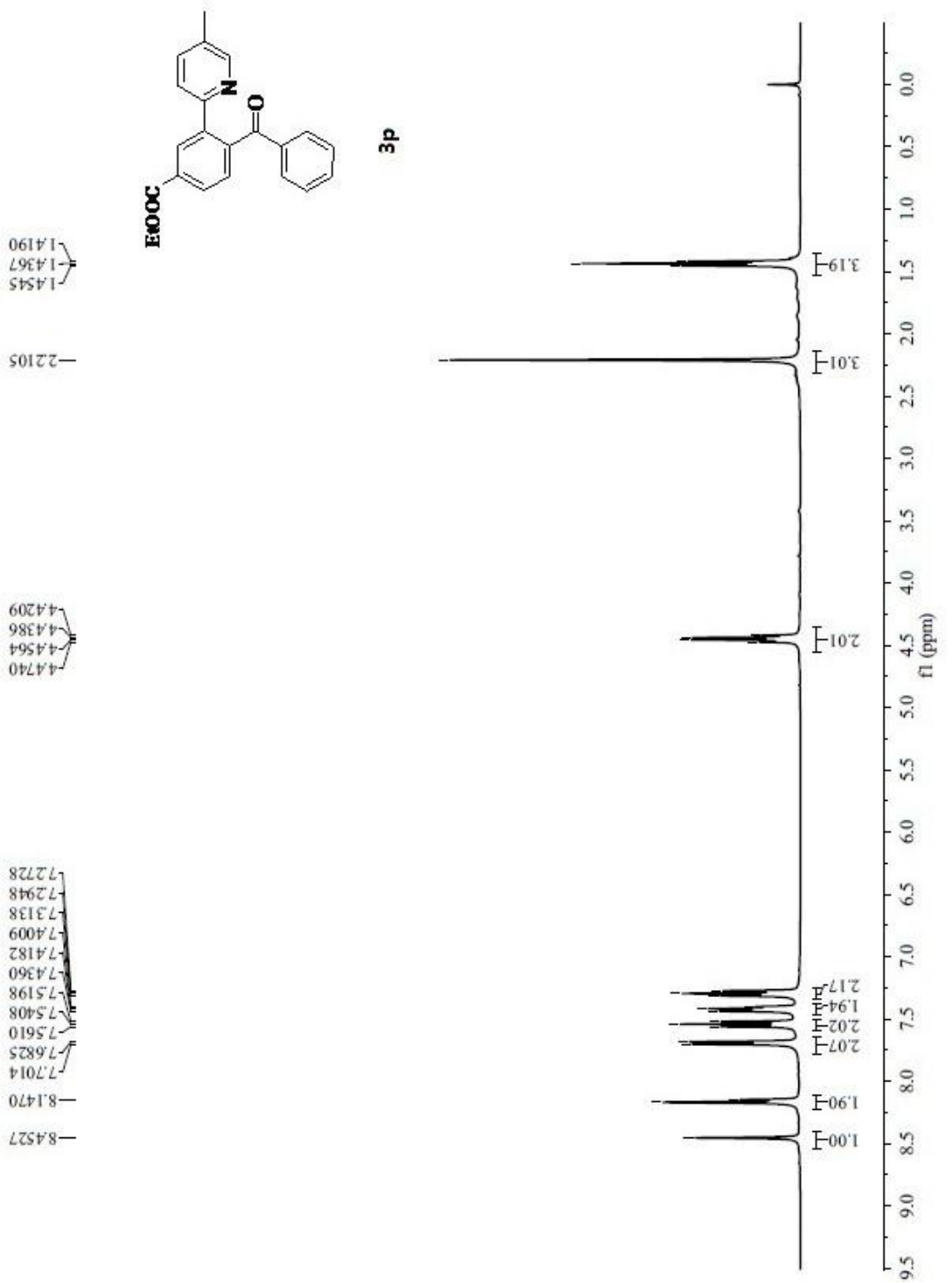
148.9972
155.6529
EtOOC
N
O
3o
f1 (ppm)


EtOOC
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O
3p
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1.4545
2.2105
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4.4386
4.4564
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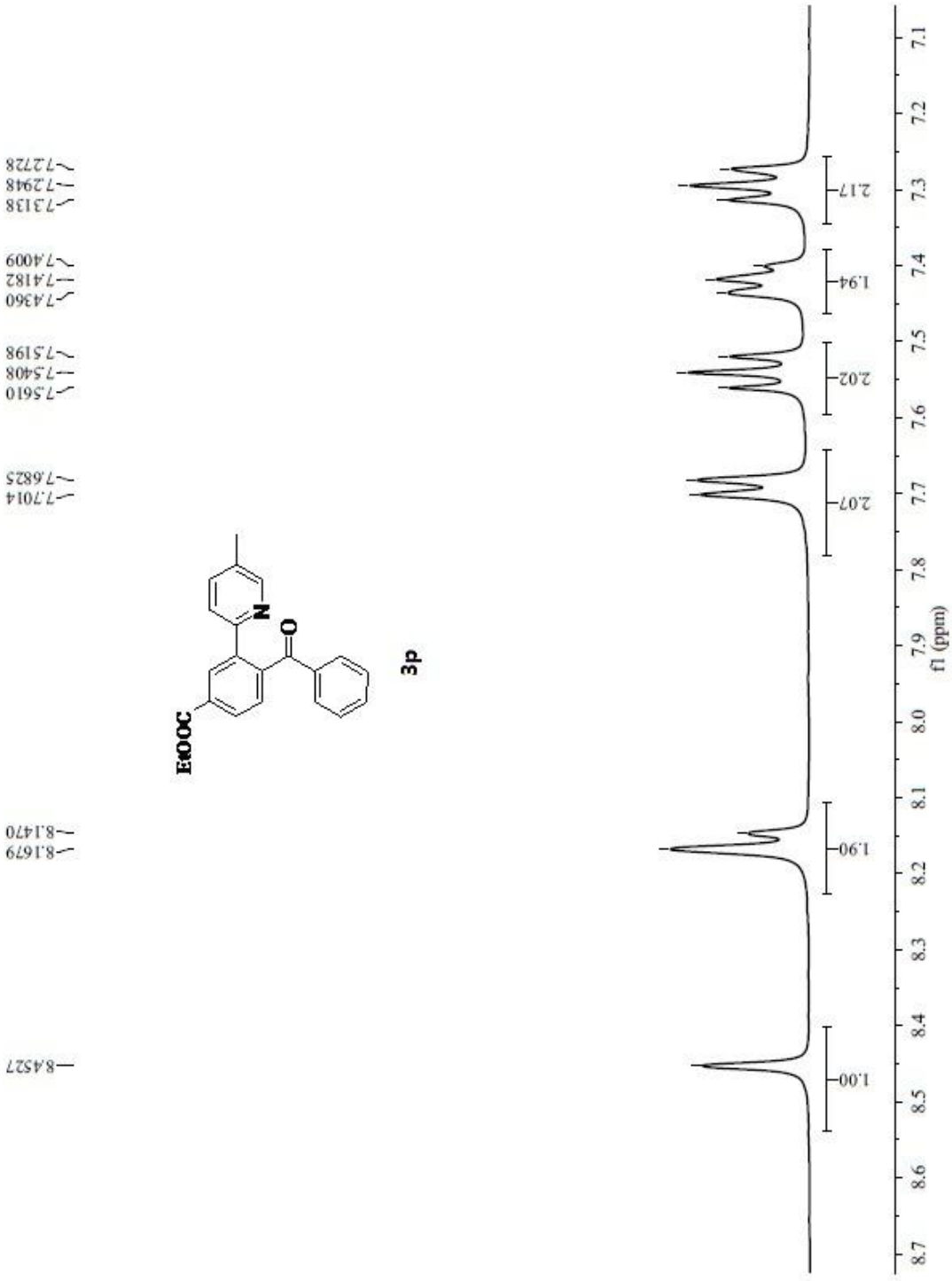
7.2728
7.2948
7.3138
7.4009
7.4182
7.4360
7.5198
7.5408
7.5610
7.6825
7.7014
8.1470
8.4527
3.19
3.01
2.01
2.17
1.94
2.02
2.07
1.90
1.00
f1 (ppm)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7.2948
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7.4182
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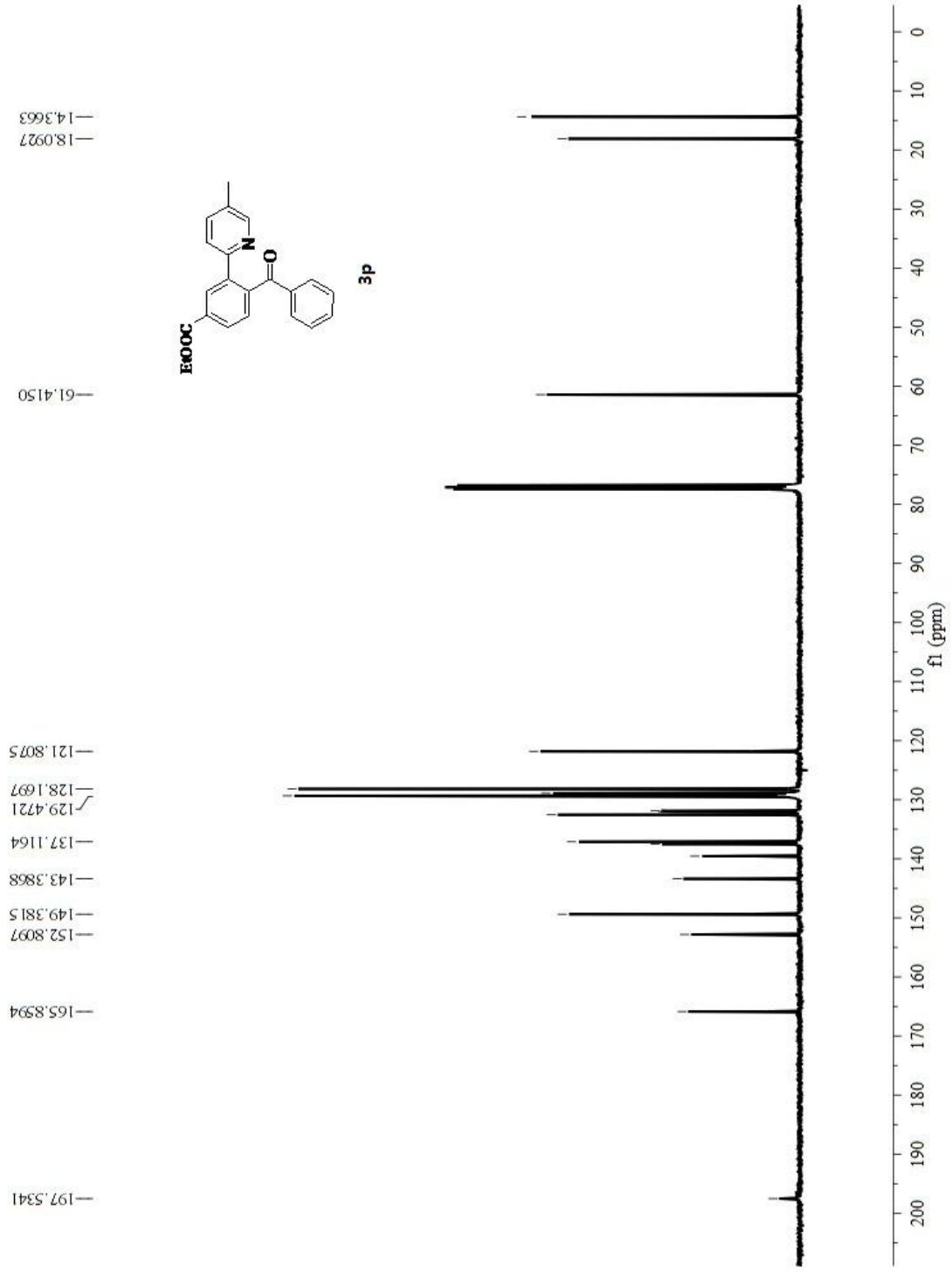
7.5198
7.5408
7.5610
7.6825
7.7014
8.1470
8.1679
8.4527
EtOOC
N
O
3p
2.17
1.94
2.02
2.07
1.90
1.00
7.1
7.2
7.3
7.4
7.5
7.6
7.7
7.8
7.9
8.0
8.1
8.2
8.3
8.4
8.5
8.6
8.7
f1 (ppm)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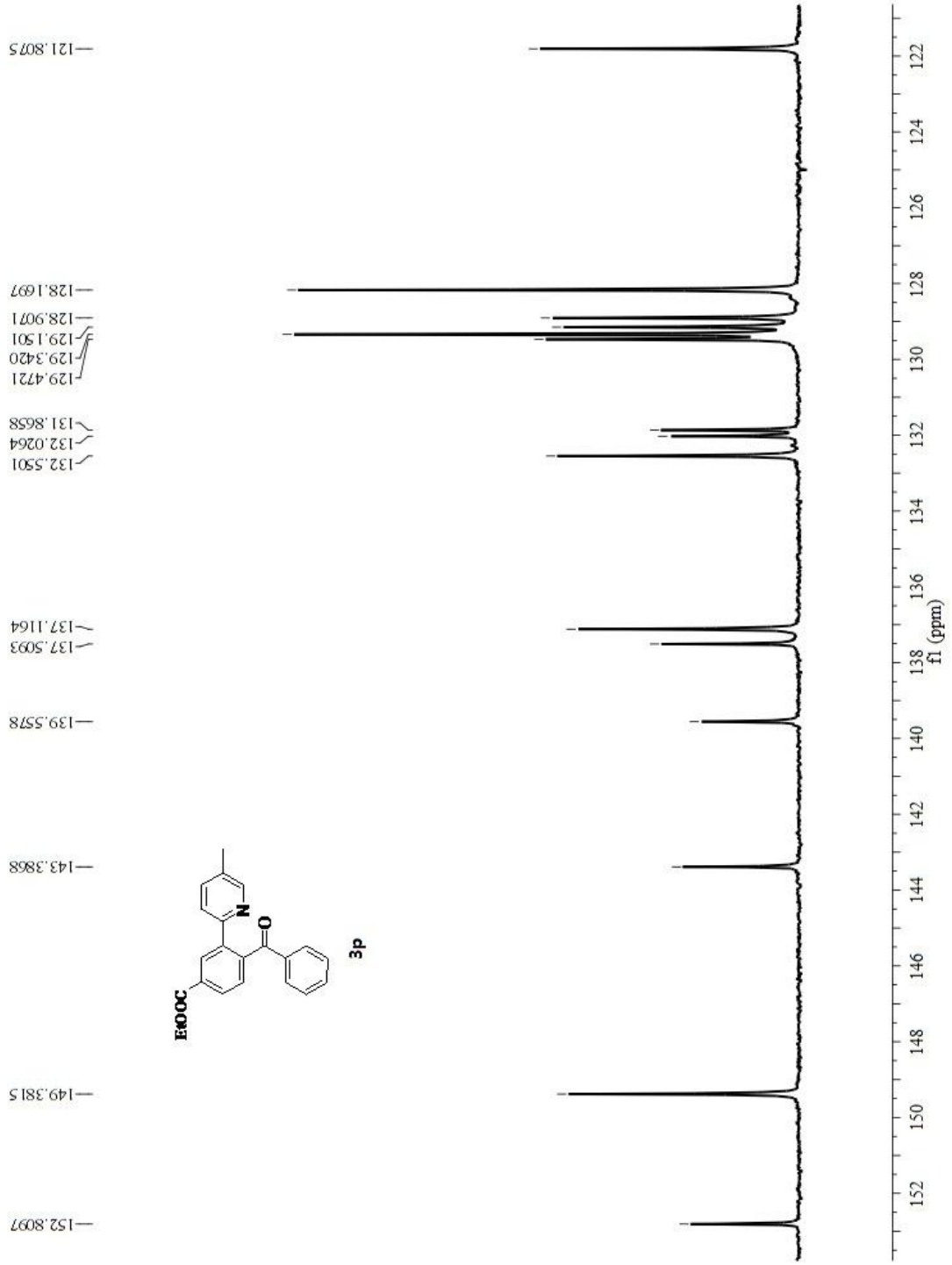
61.4150
121.8075
128.1697
129.4721
137.1164
143.3868
149.3815
152.8097
165.8594
197.5341
EtOOC
N
O
3p
f1 (ppm)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131.8658
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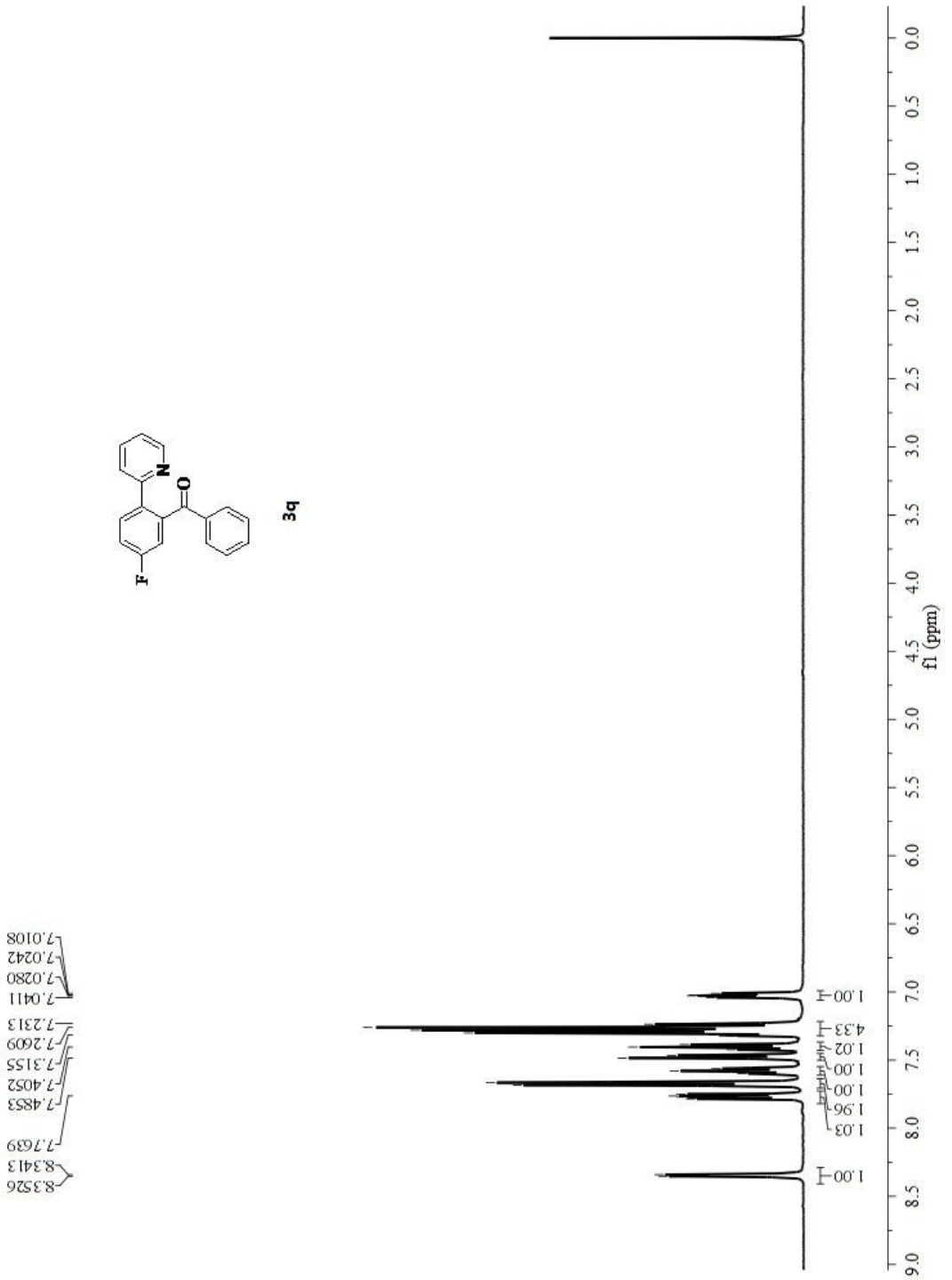
132.5501
137.1164
137.5093
139.5578
143.3868
149.3815
152.8097
f1 (ppm)
122
124
126
128
130
132
134
136
138
140
142
144
146
148
150
152
N
O
EtOOC
3p


3q
F
O
N
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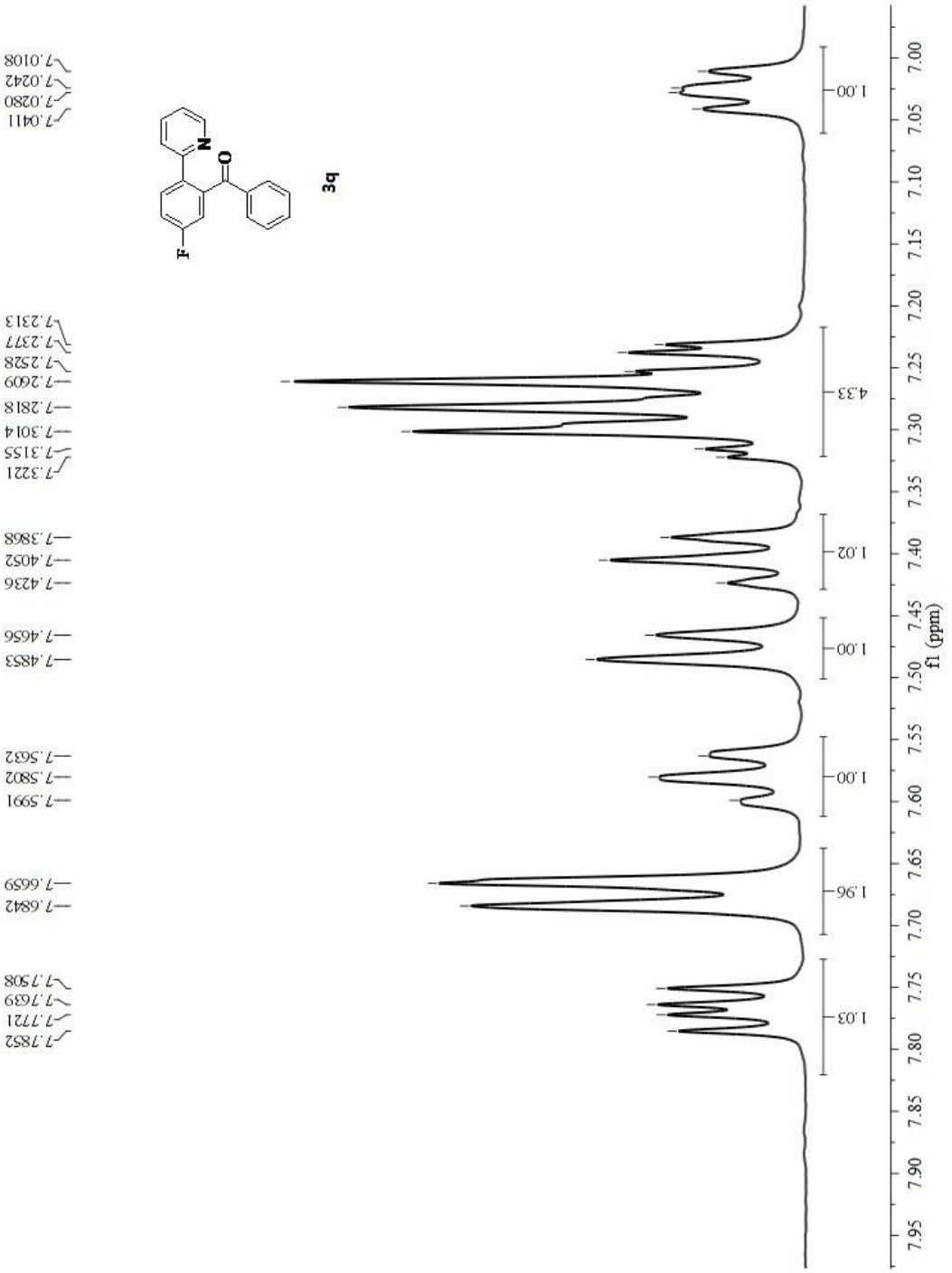
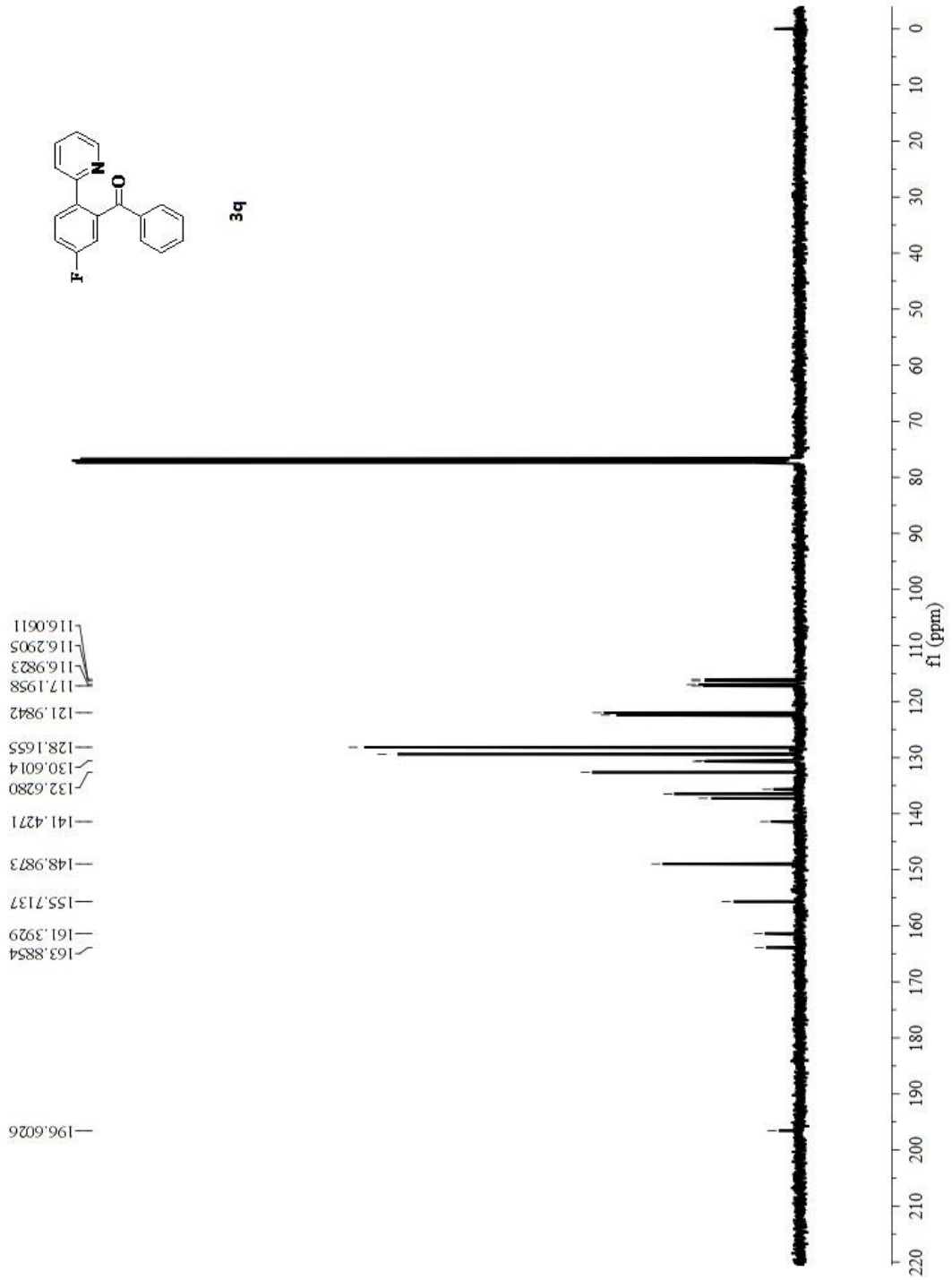
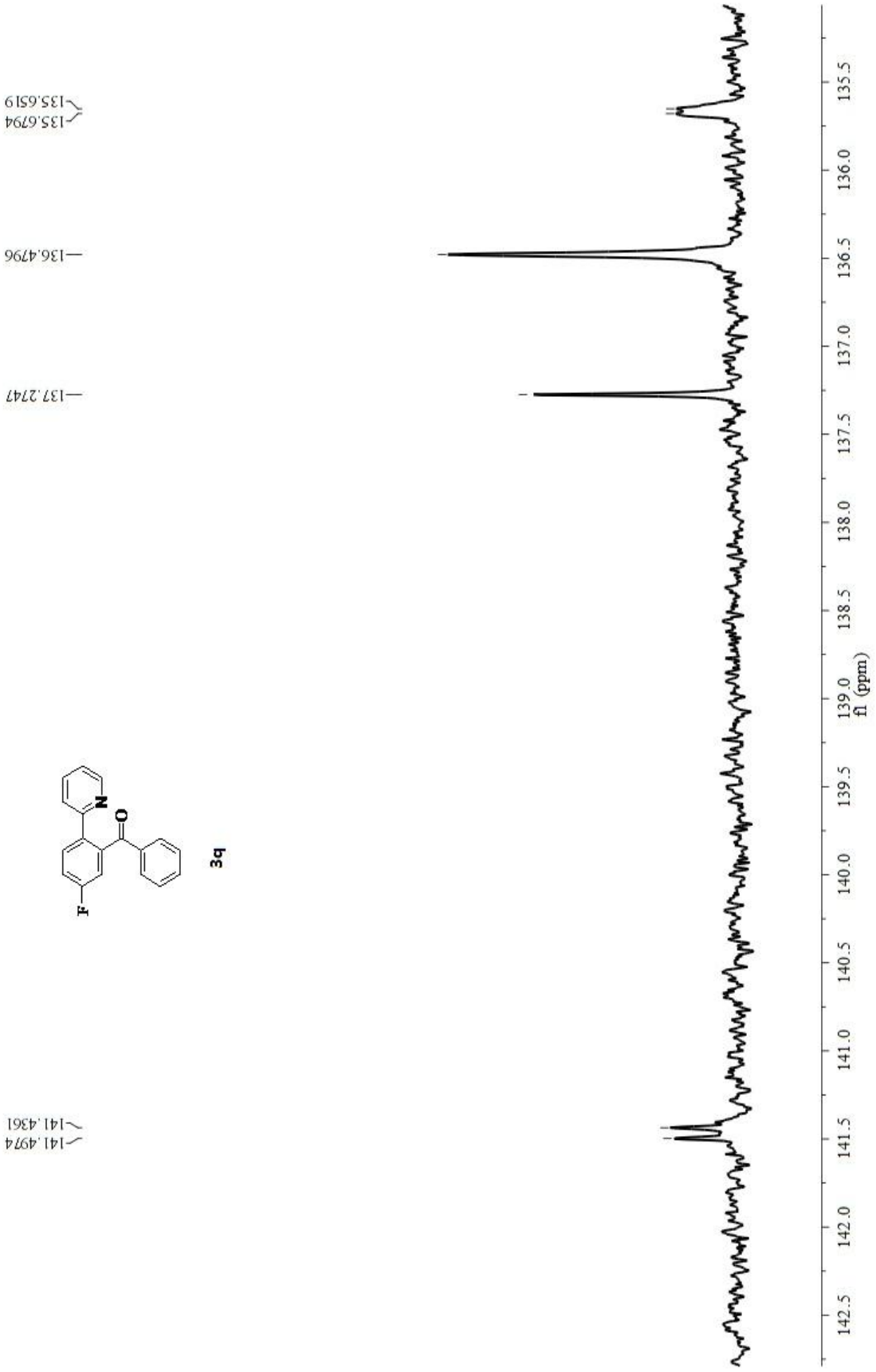
8.3413
7.7639
7.4853
7.4052
7.3155
7.2609
7.2313
7.0411
7.0280
7.0242
7.0108
1.00
1.03
1.96
1.00
1.00
1.02
4.33
1.00
f1 (ppm)



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141.4974
N
O
F
3q
135.5
136.0
136.5
137.0
137.5
138.0
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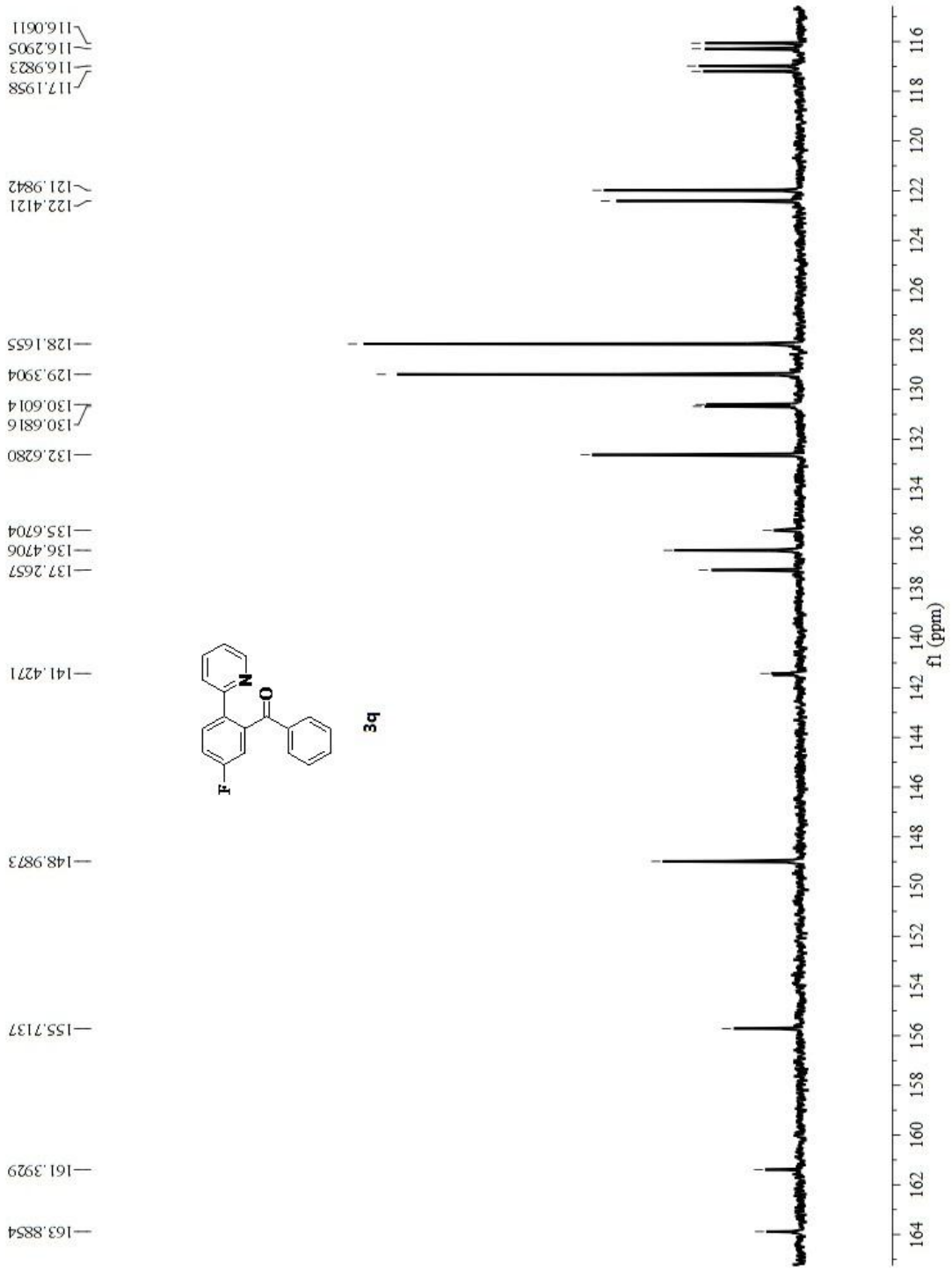
139.0
139.5
140.0
140.5
141.0
141.5
142.0
142.5
f1 (ppm)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116.9823
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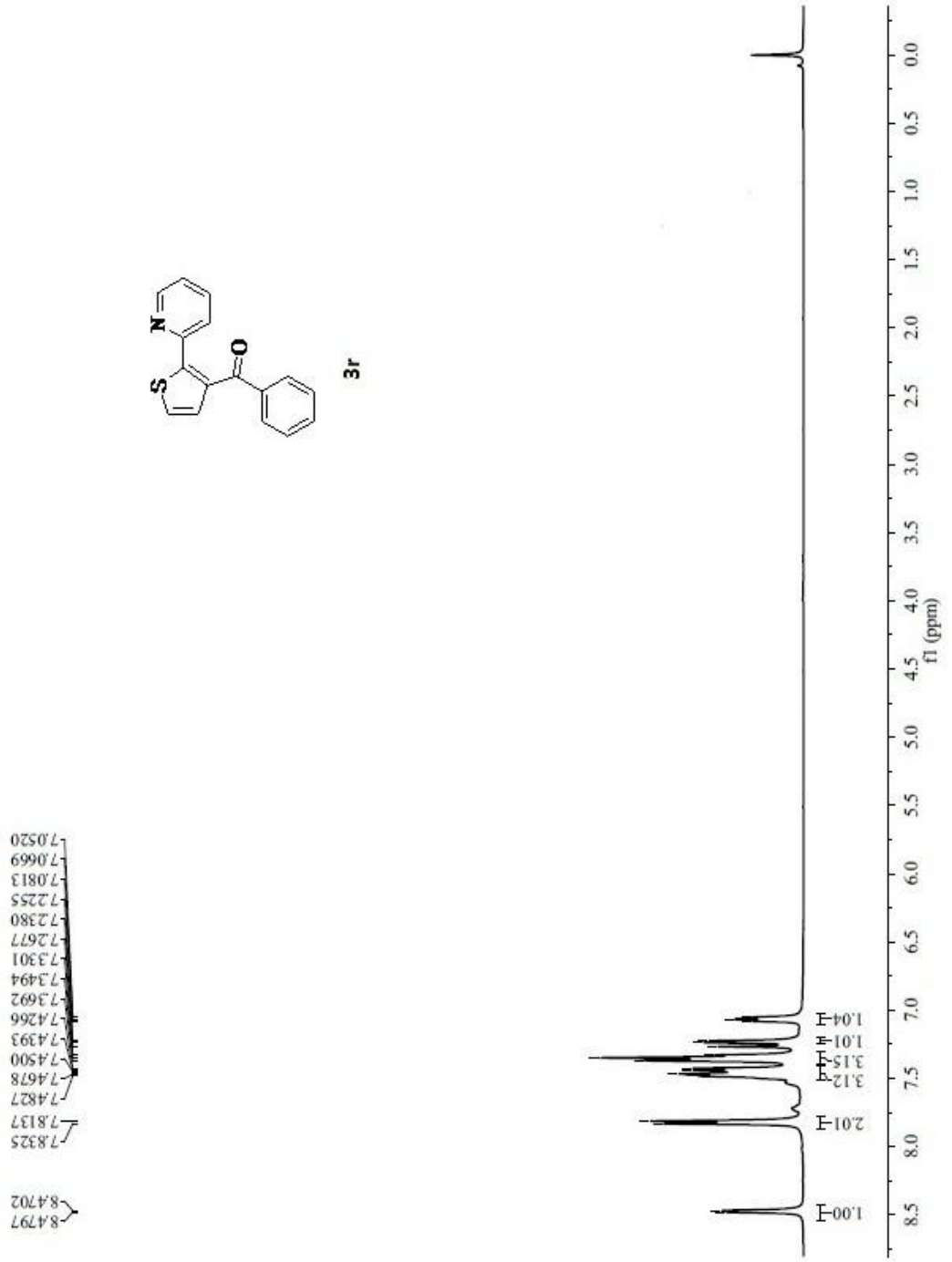
128.1655
129.3904
130.6014
130.6816
132.6280
135.6704
136.4706
137.2657
141.4271
148.9873
155.7137
161.3929
163.8854
3q
F
N
O
fl (ppm)


3r
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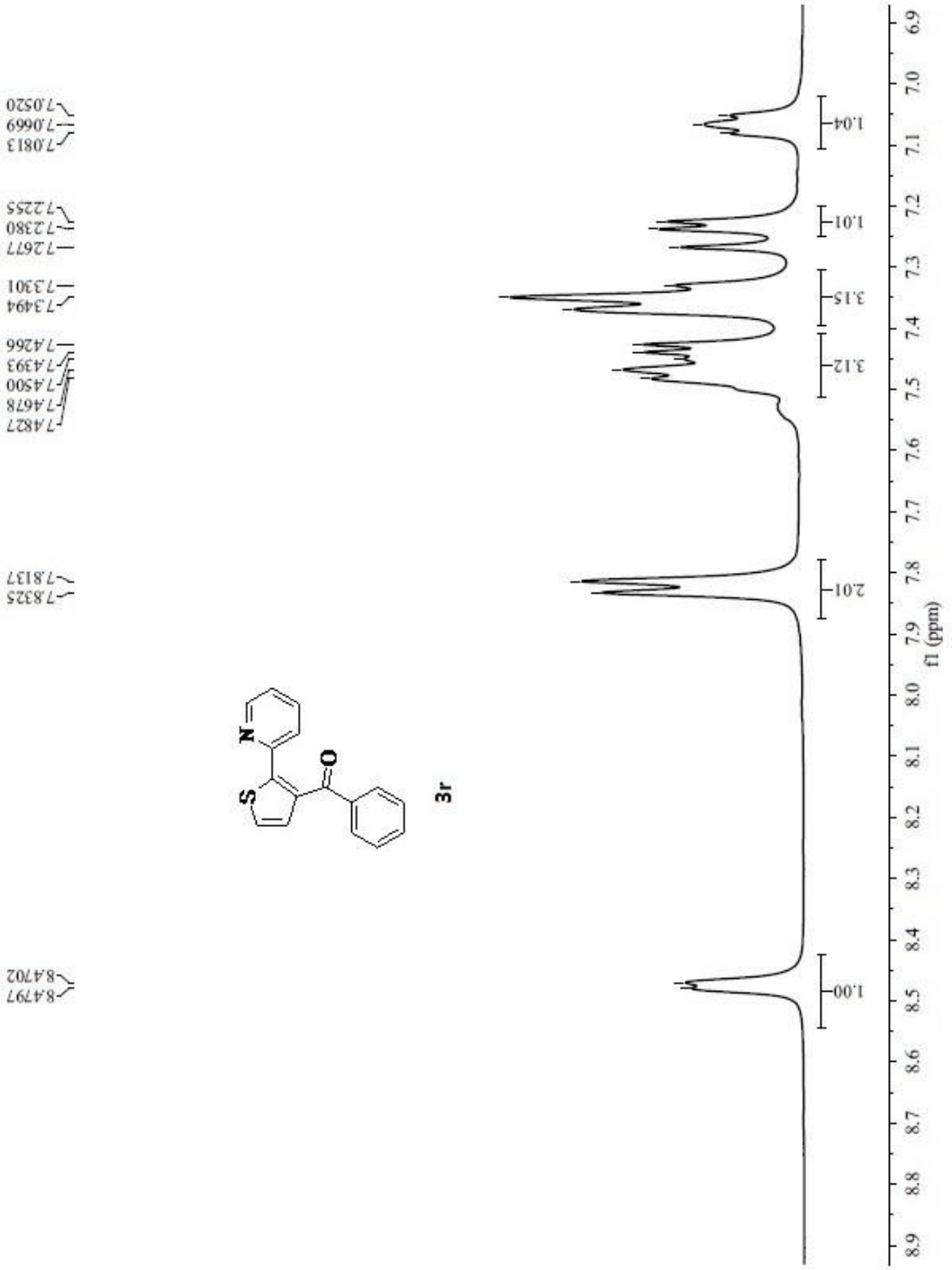
7.8325
7.8137
7.4827
7.4678
7.4500
7.4393
7.4266
7.3692
7.3494
7.3301
7.2677
7.2380
7.2255
7.0813
7.0669
7.0520
1.00
2.01
3.12
3.15
1.01
1.04
f1 (ppm)


8.4797
8.4702
7.8325
7.8137
7.4827
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7.4500
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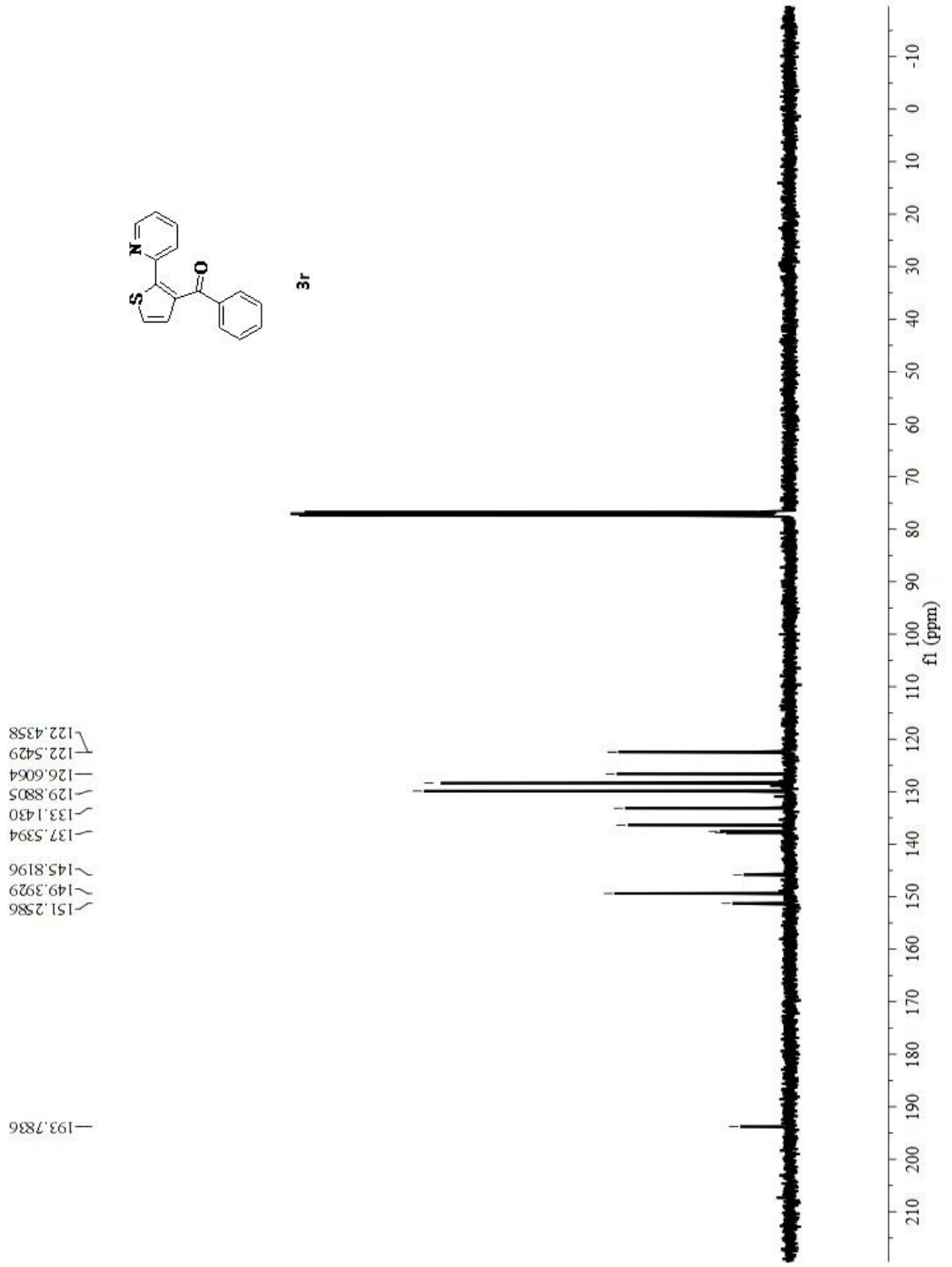
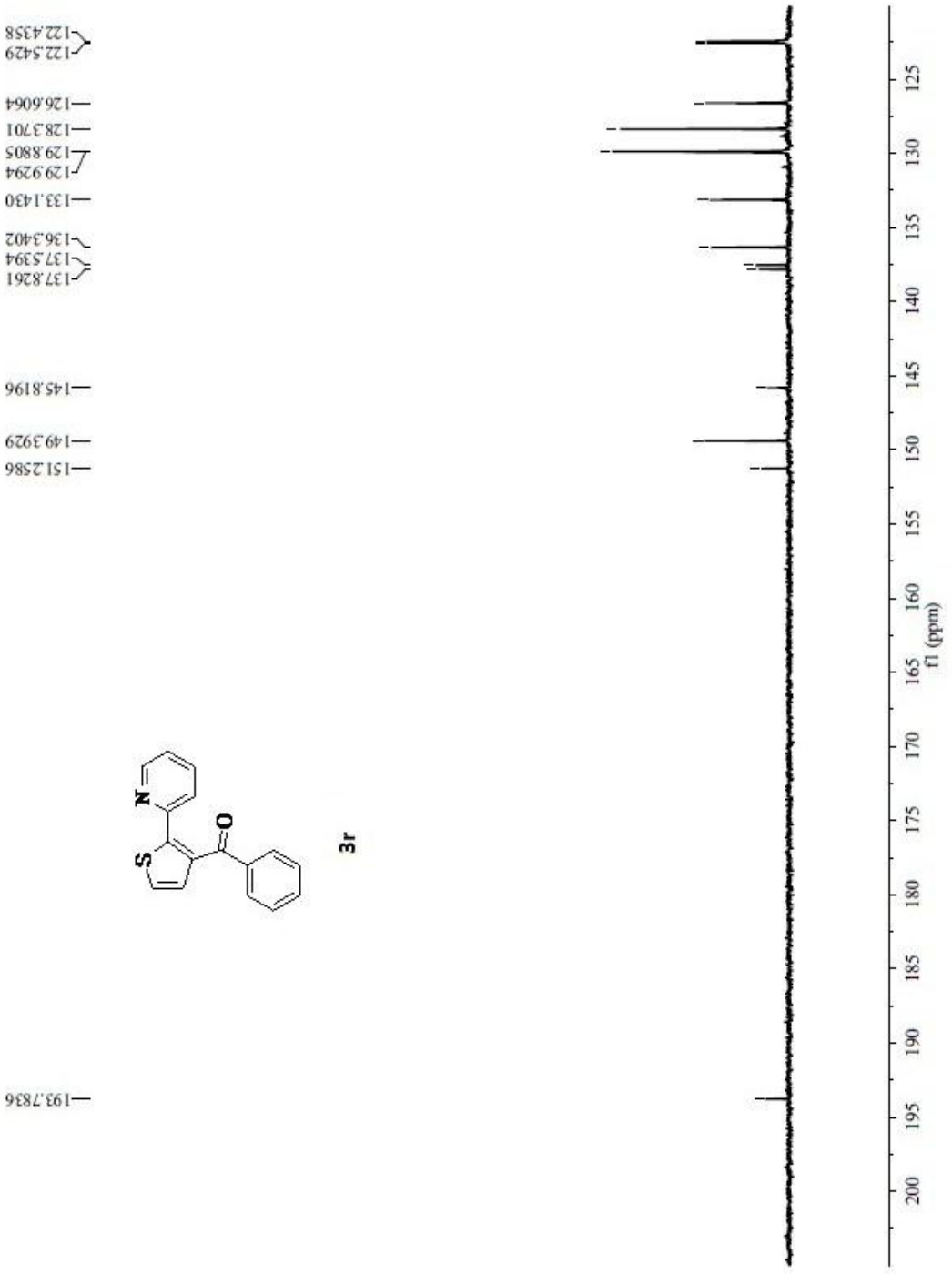
7.4266
7.3494
7.3301
7.2677
7.2380
7.2255
7.0813
7.0669
7.0520
1.00
2.01
3.12
3.15
1.01
1.04
f1 (ppm)
3r

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128.3701
129.8805
129.9294
133.1430
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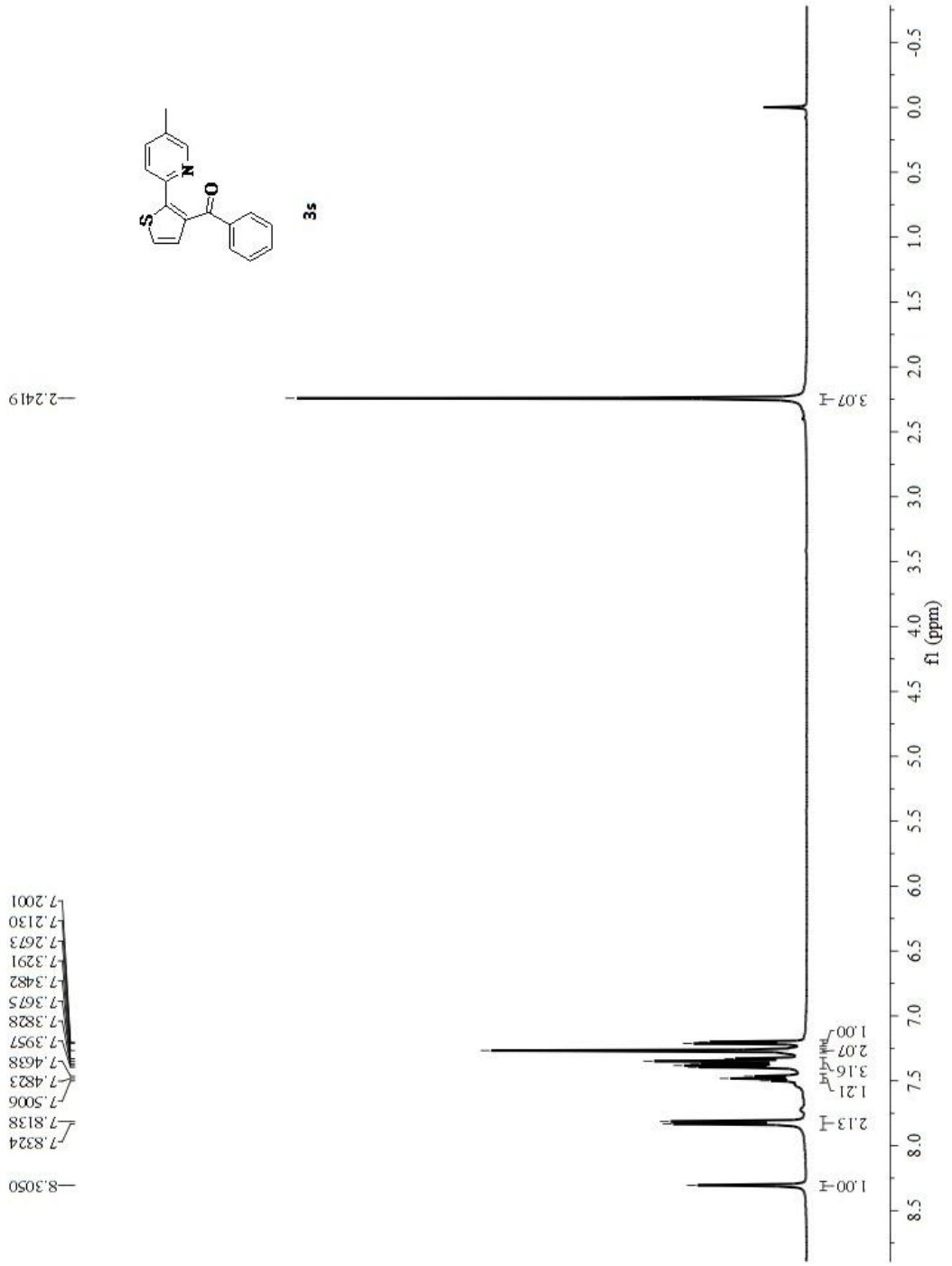
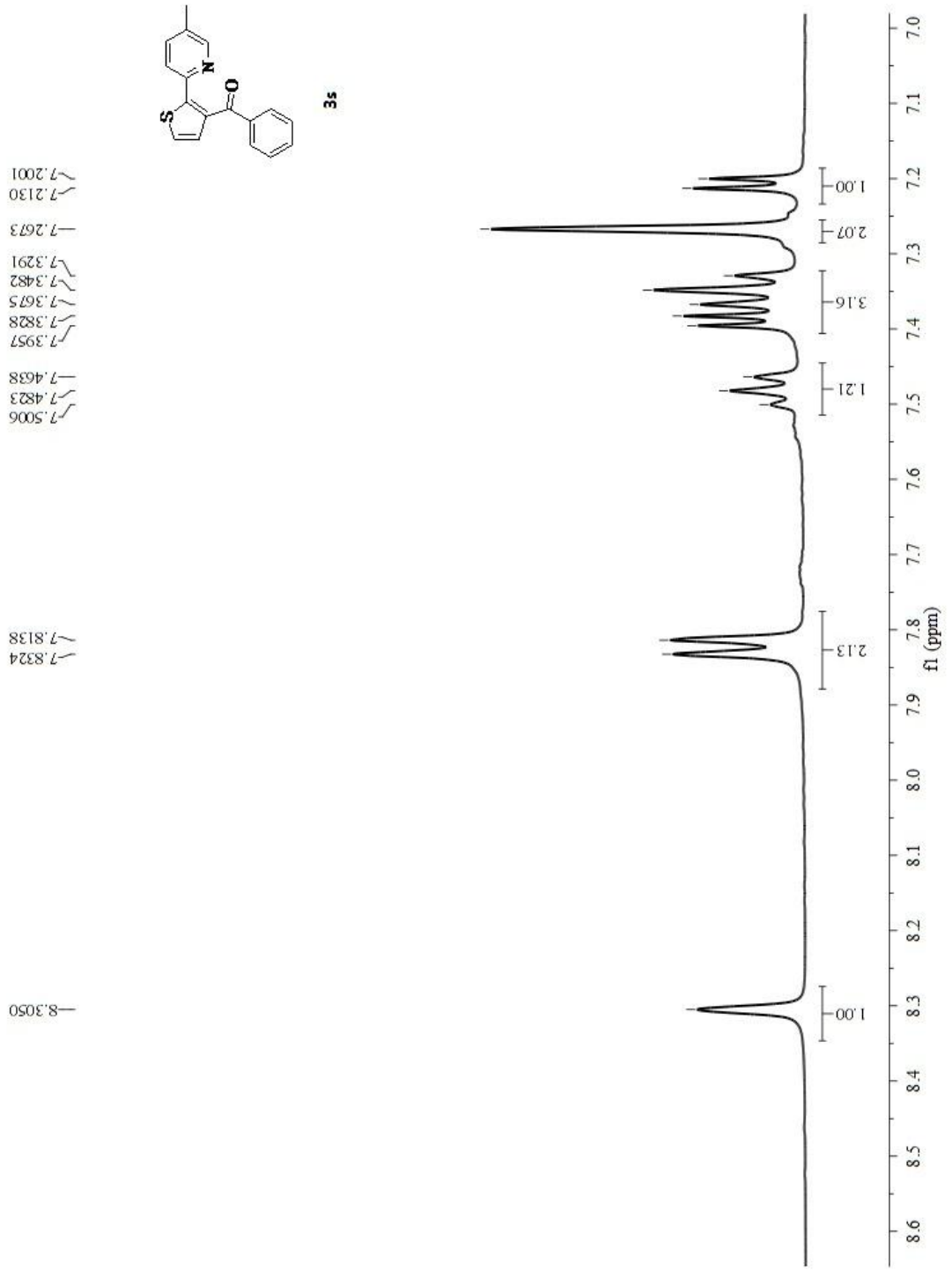
137.5394
137.8261
145.8196
149.3929
151.2586
193.7836
3r
f1 (ppm)


3s
f1 (ppm)


3s
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7.8138
7.4823
7.4638
7.3957
7.3828
7.3675
7.3482
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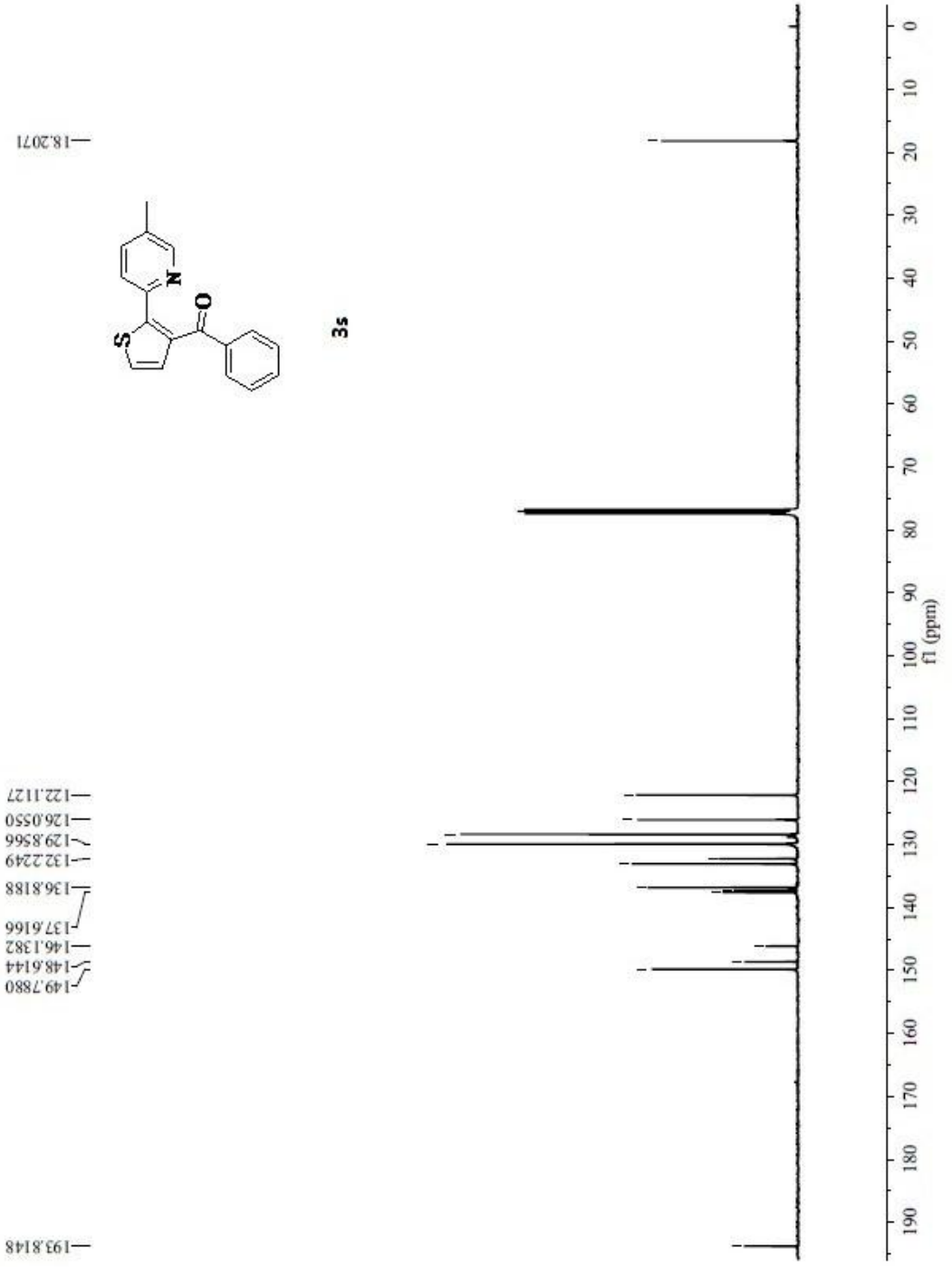
7.2130
7.2001
1.00
2.07
3.16
1.21
2.13
1.00
f1 (ppm)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126.0550
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149.7880
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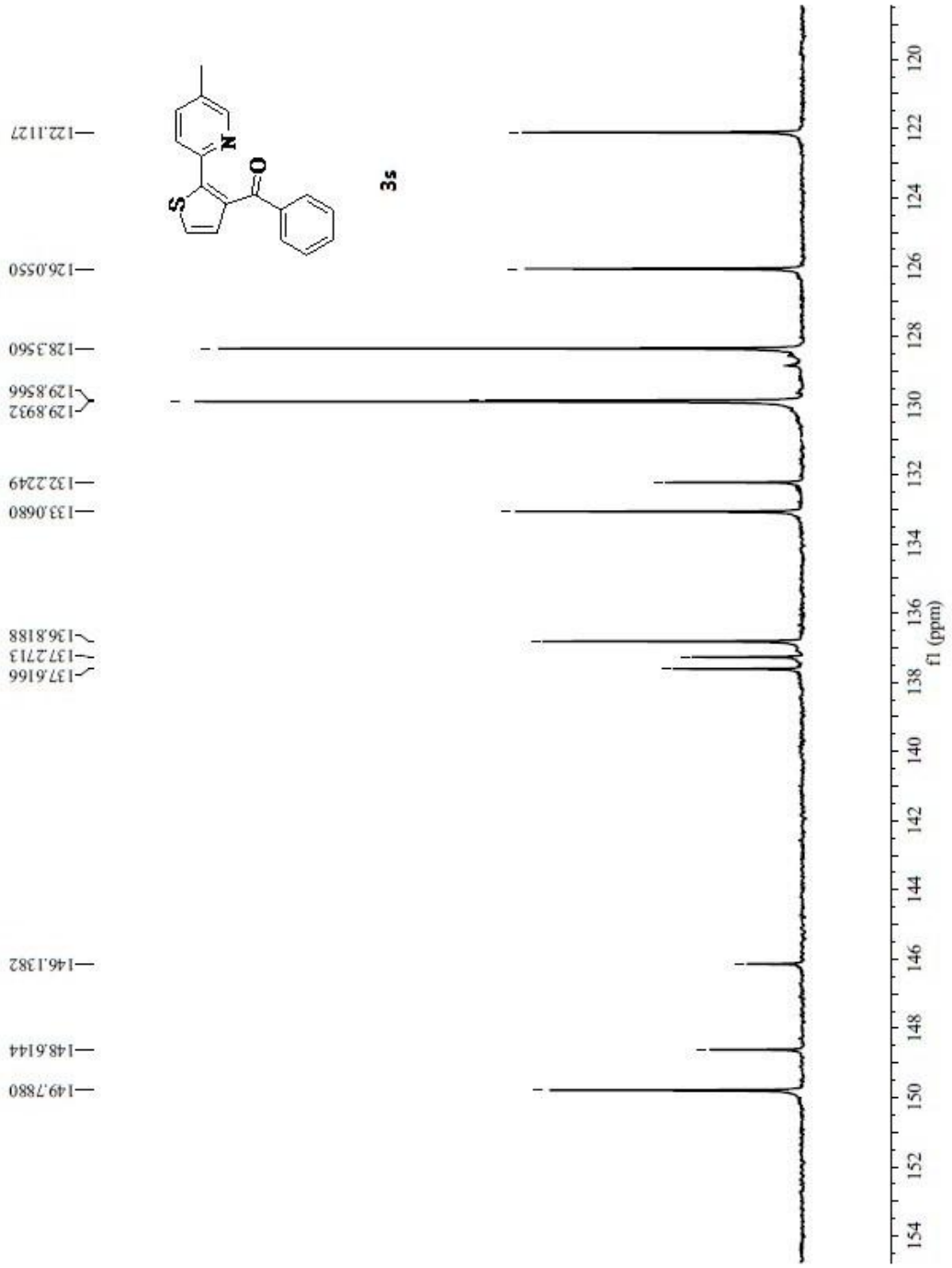
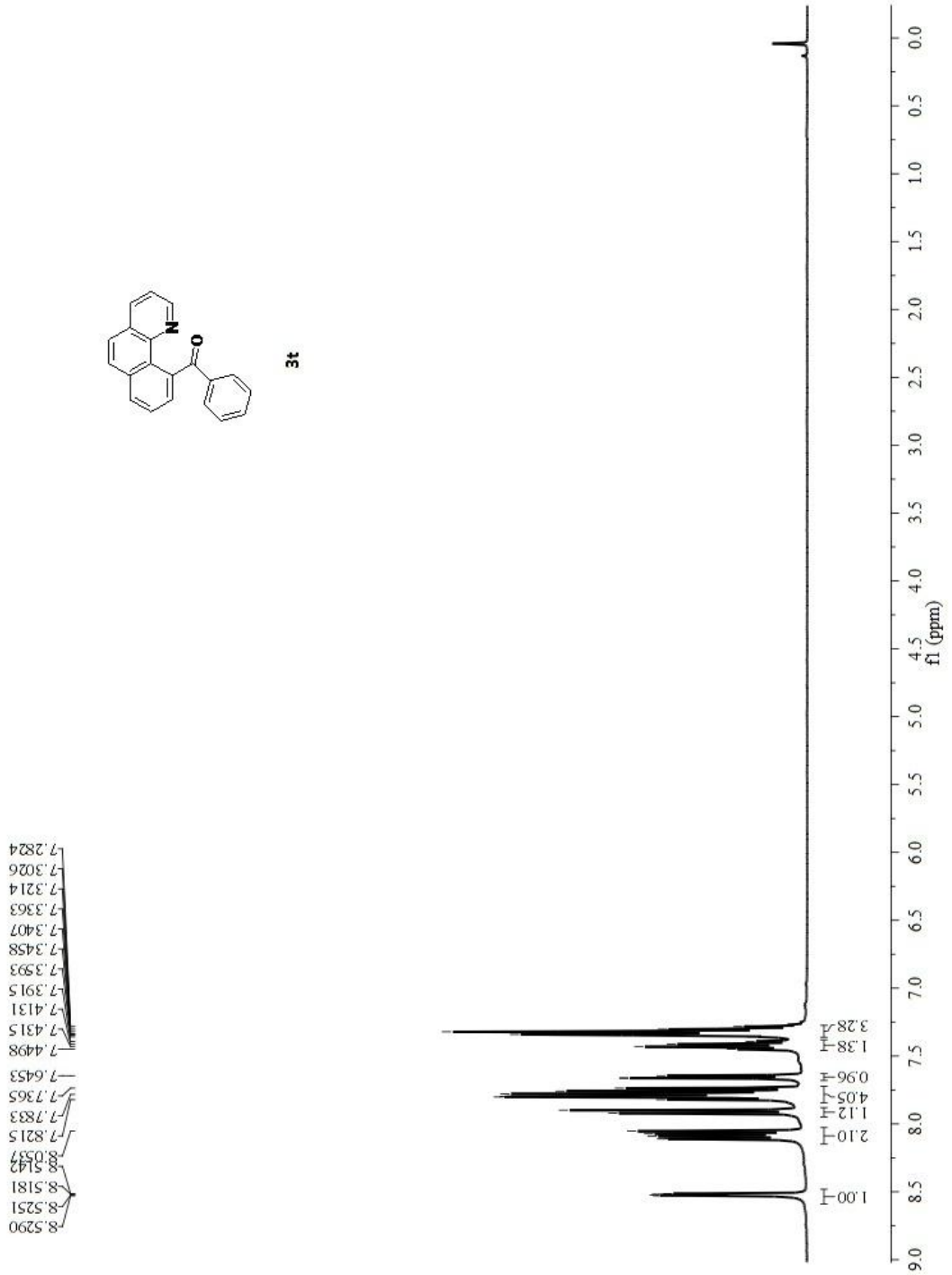
3s
f1 (ppm)




3t
f1 (ppm)
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8.0
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1.00
2.10
1.12
4.05
0.96
1.38
3.28
8.5290
8.5251
8.5181
8.5143
8.0537
7.8215
7.7833
7.7365
7.6453
7.4498
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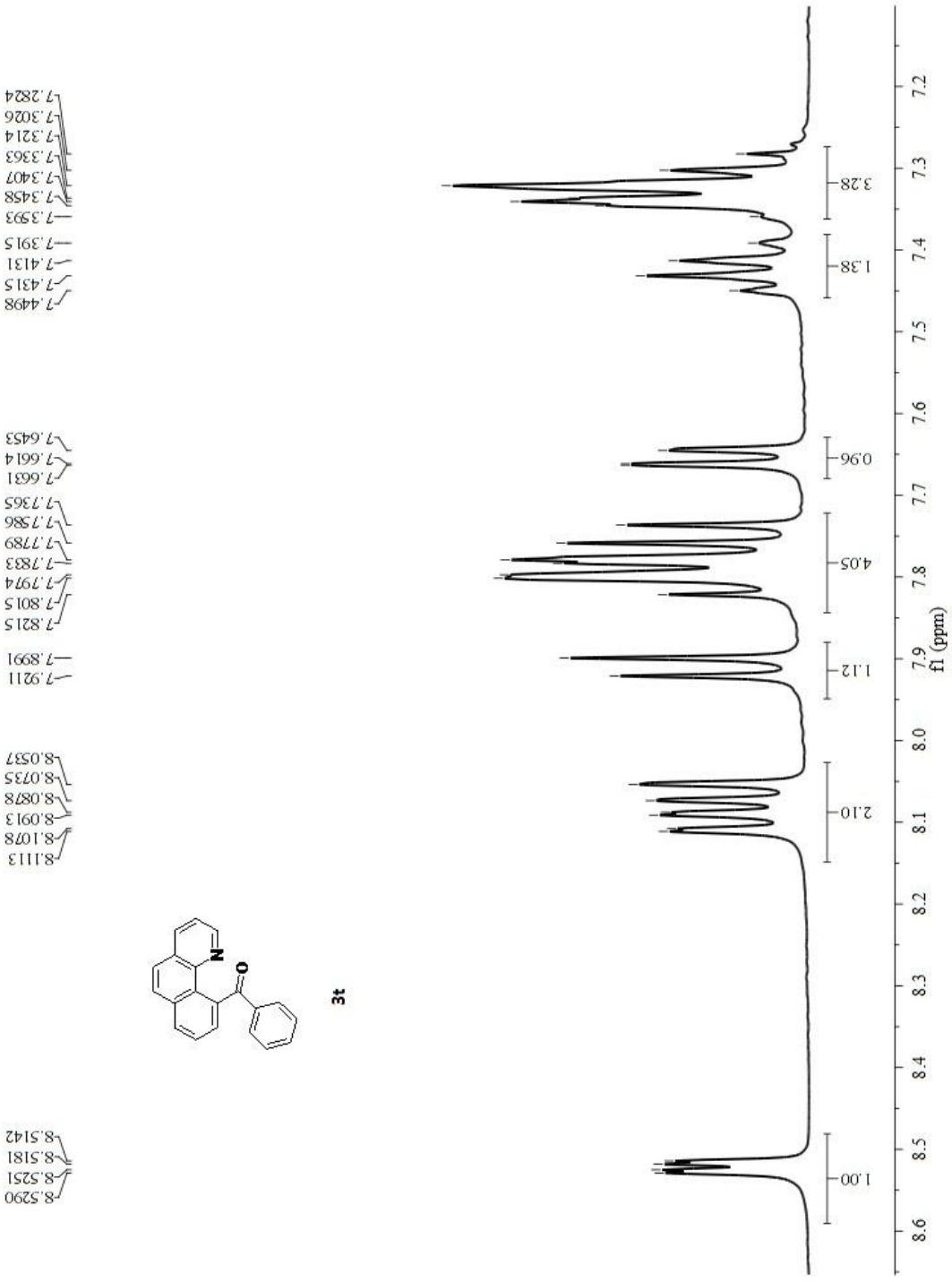
7.3915
7.3593
7.3458
7.3407
7.3363
7.3214
7.3026
7.2824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8.5251
8.5181
8.5142
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8.1078
8.0913
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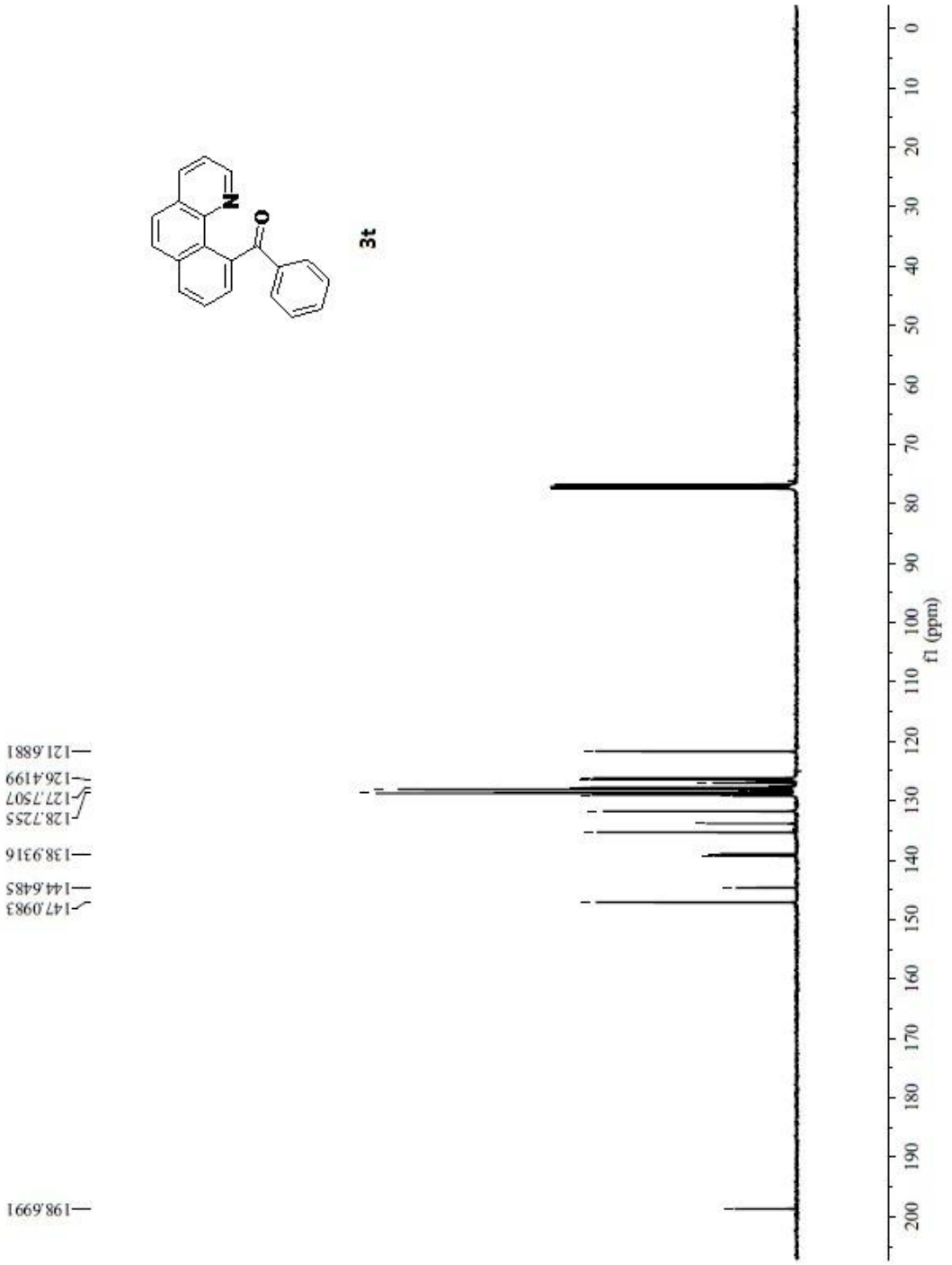
8.0735
8.0537
7.9211
7.8991
7.8215
7.8015
7.7974
7.7833
7.7789
7.7586
7.7365
7.6631
7.6614
7.6453
7.4498
7.4315
7.4131
7.3915
7.3593
7.3458
7.3407
7.3363
7.3214
7.3026
7.2824
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
f1 (ppm)
1.00
2.10
1.12
4.05
0.96
1.38
3.28
O
N
3t


3t
O
N
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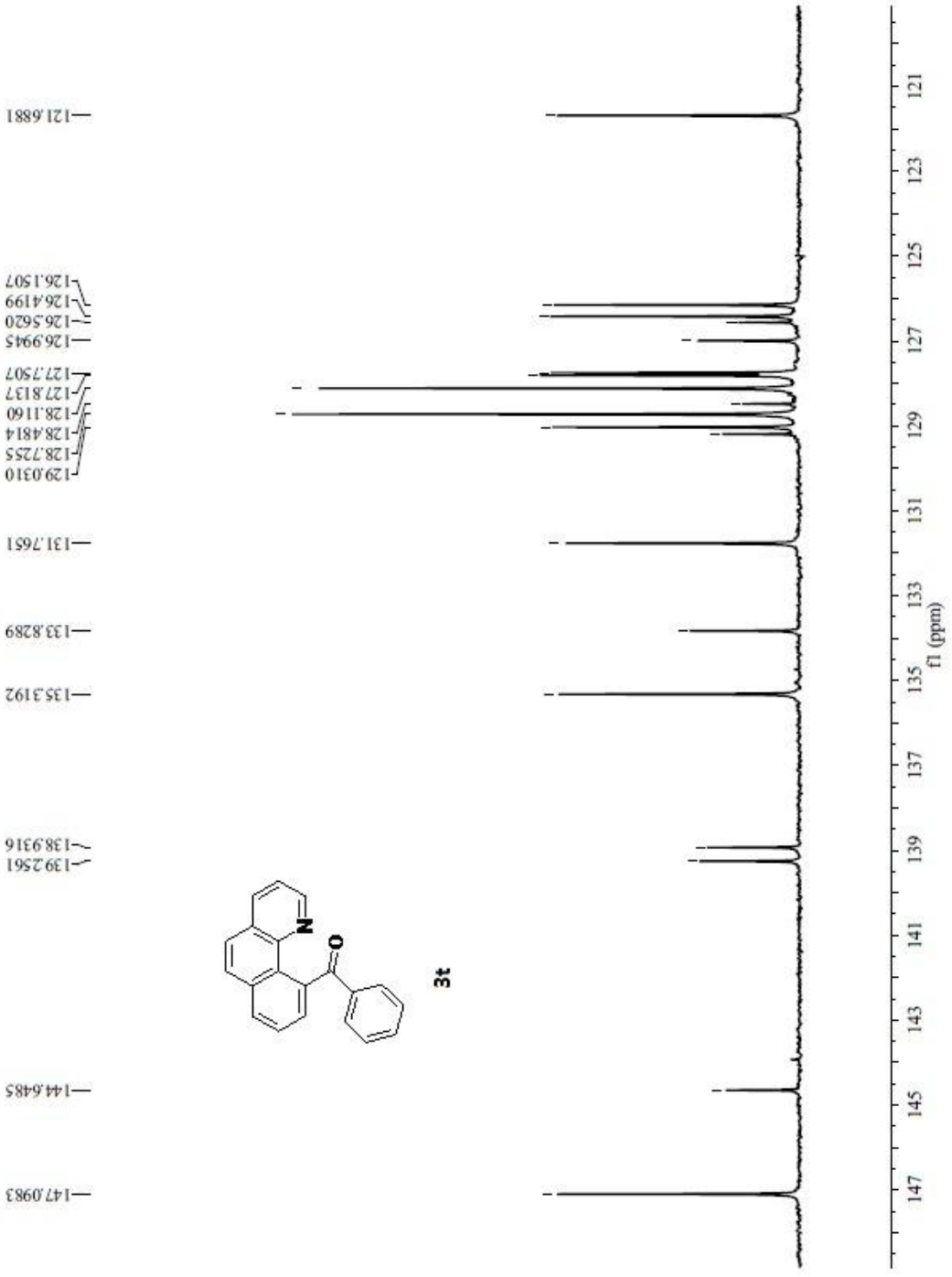
138.9316
128.7255
127.7507
126.4199
121.6881
f1 (ppm)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126.4199
126.5620
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127.7507
127.8137
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128.4814
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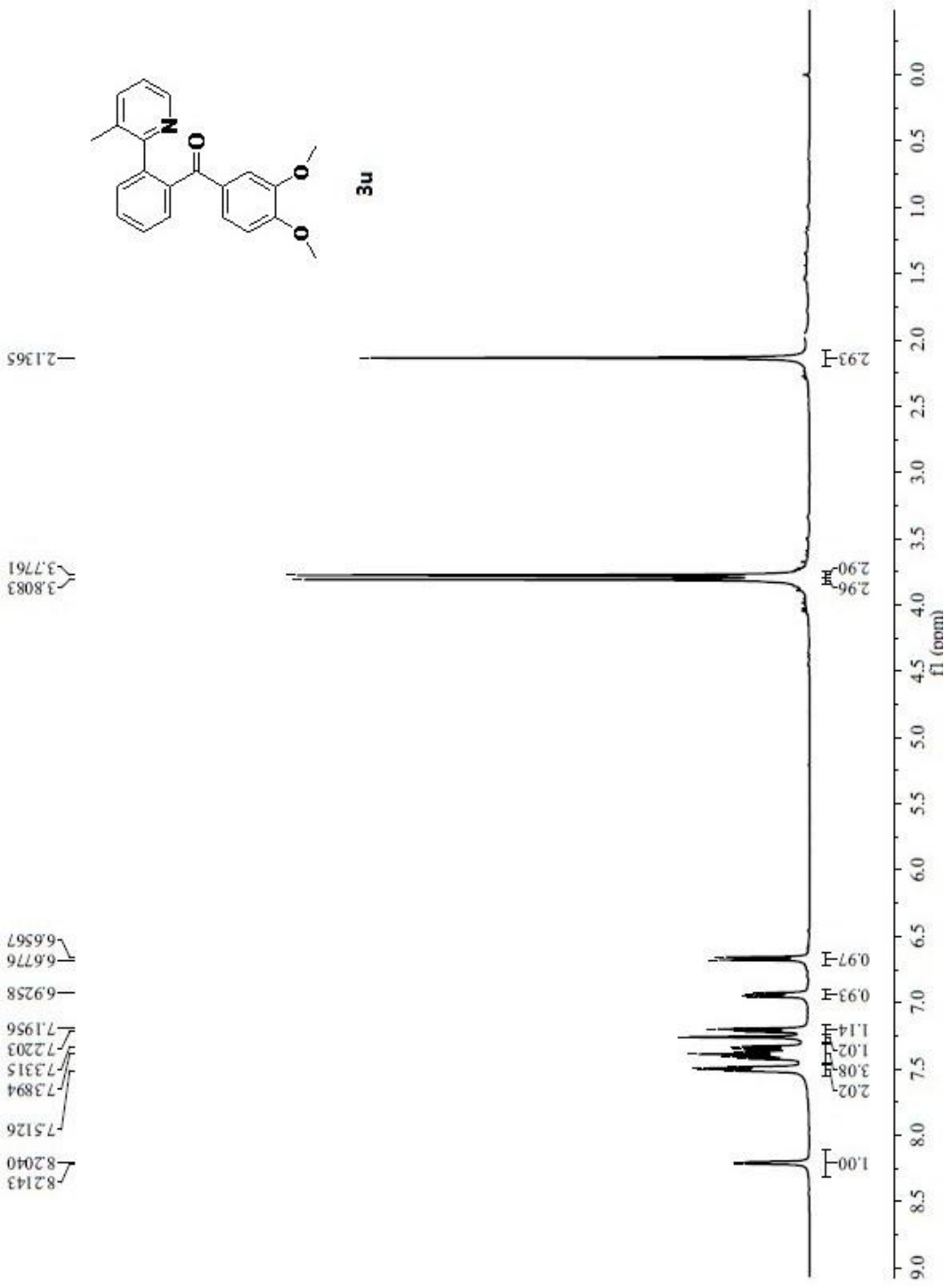
129.0310
131.7651
133.8289
135.3192
138.9316
139.2561
144.6485
147.0983
O
N
3t
121
123
125
127
129
131
133
135
137
139
141
143
145
147
f1 (ppm)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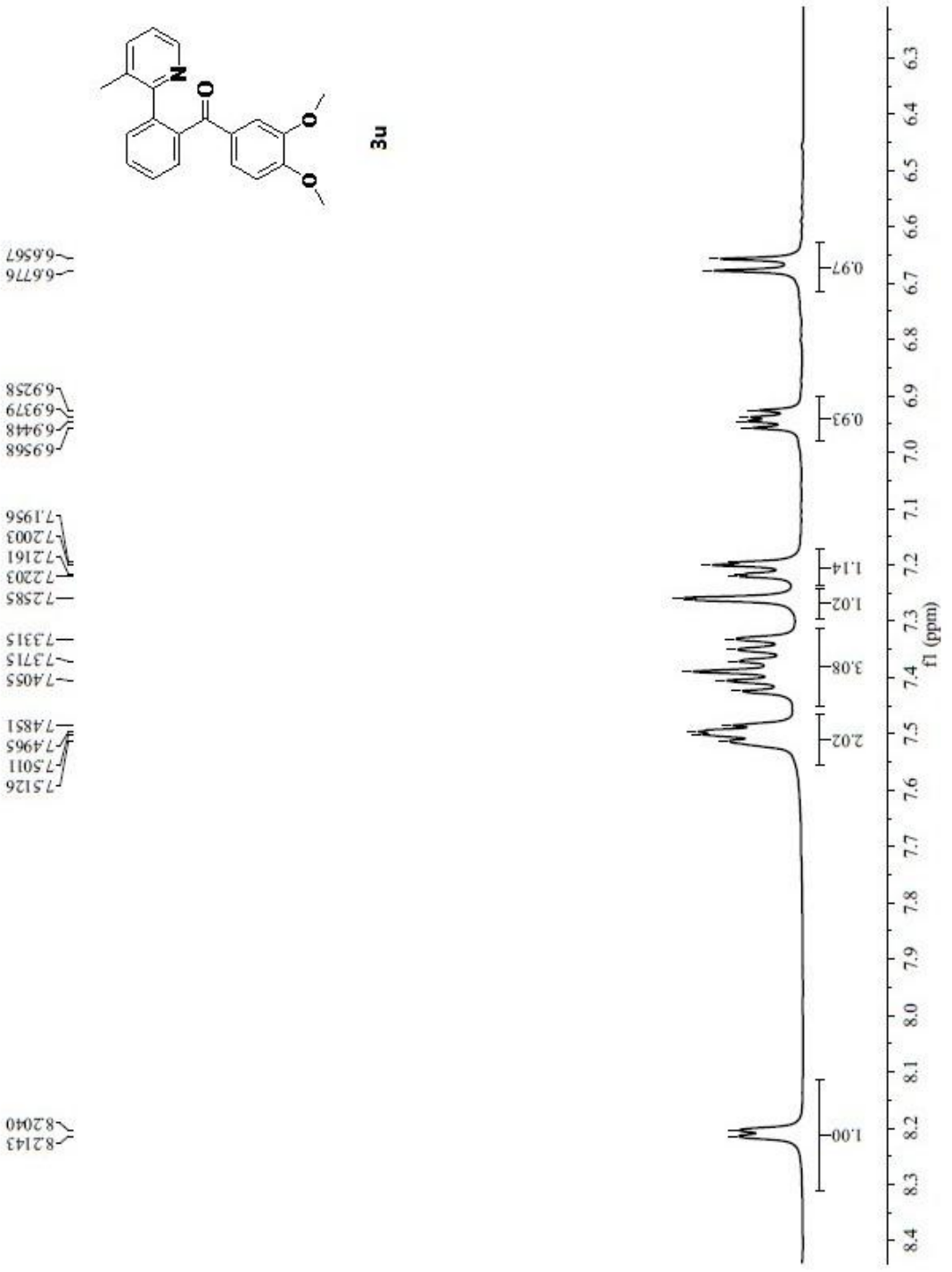
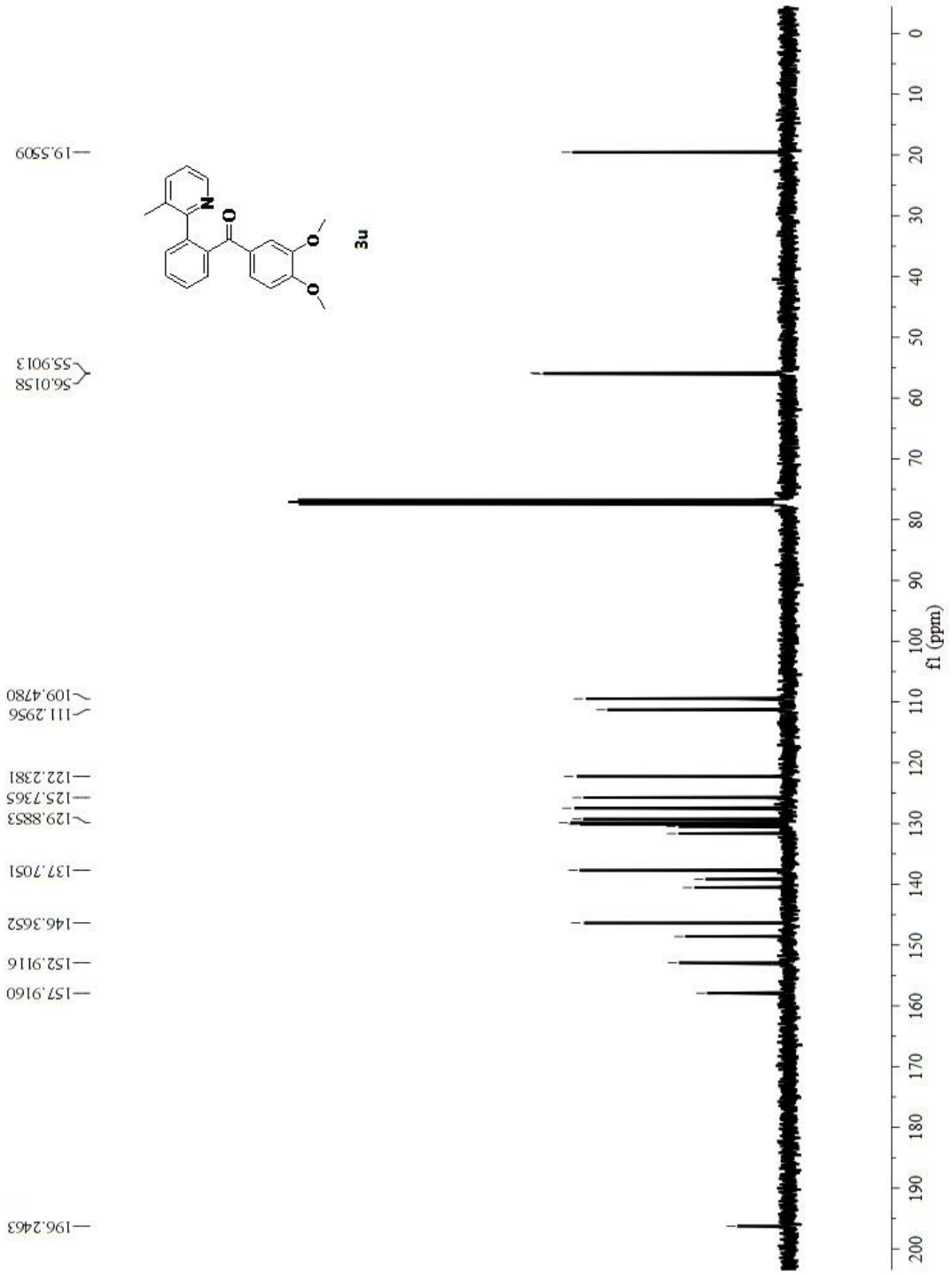
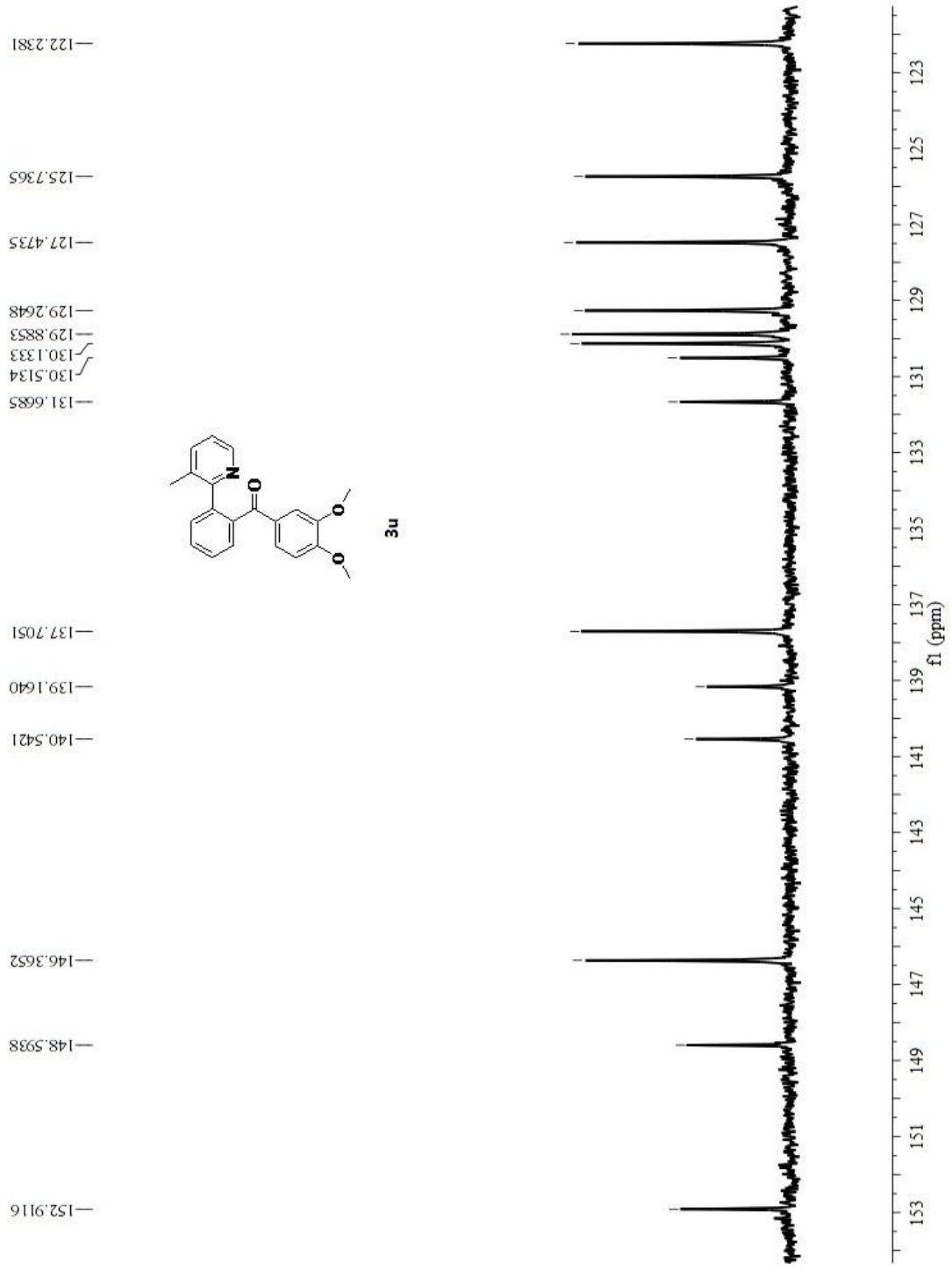
7.3894
7.3315
7.2203
7.1956
6.9258
6.6776
6.6567
3.8083
3.7761
2.1365
1.00
2.02
3.08
1.02
1.14
0.93
0.97
2.96
2.90
2.93
f1 (ppm)


3u
8.2040
8.2143
7.5126
7.5011
7.4965
7.4851
7.4055
7.3715
7.3315
7.2585
7.2203
7.2161
7.2003
7.1956
6.9568
6.9448
6.9379
6.9258
6.6776
6.6567
1.00
2.02
3.08
1.02
1.14
0.93
0.97
f1 (ppm)

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129.2648
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130.1333
130.5134
131.6685
137.7051
139.1640
140.5421
146.3652
148.5938
152.9116
3u
123
125
127
129
131
133
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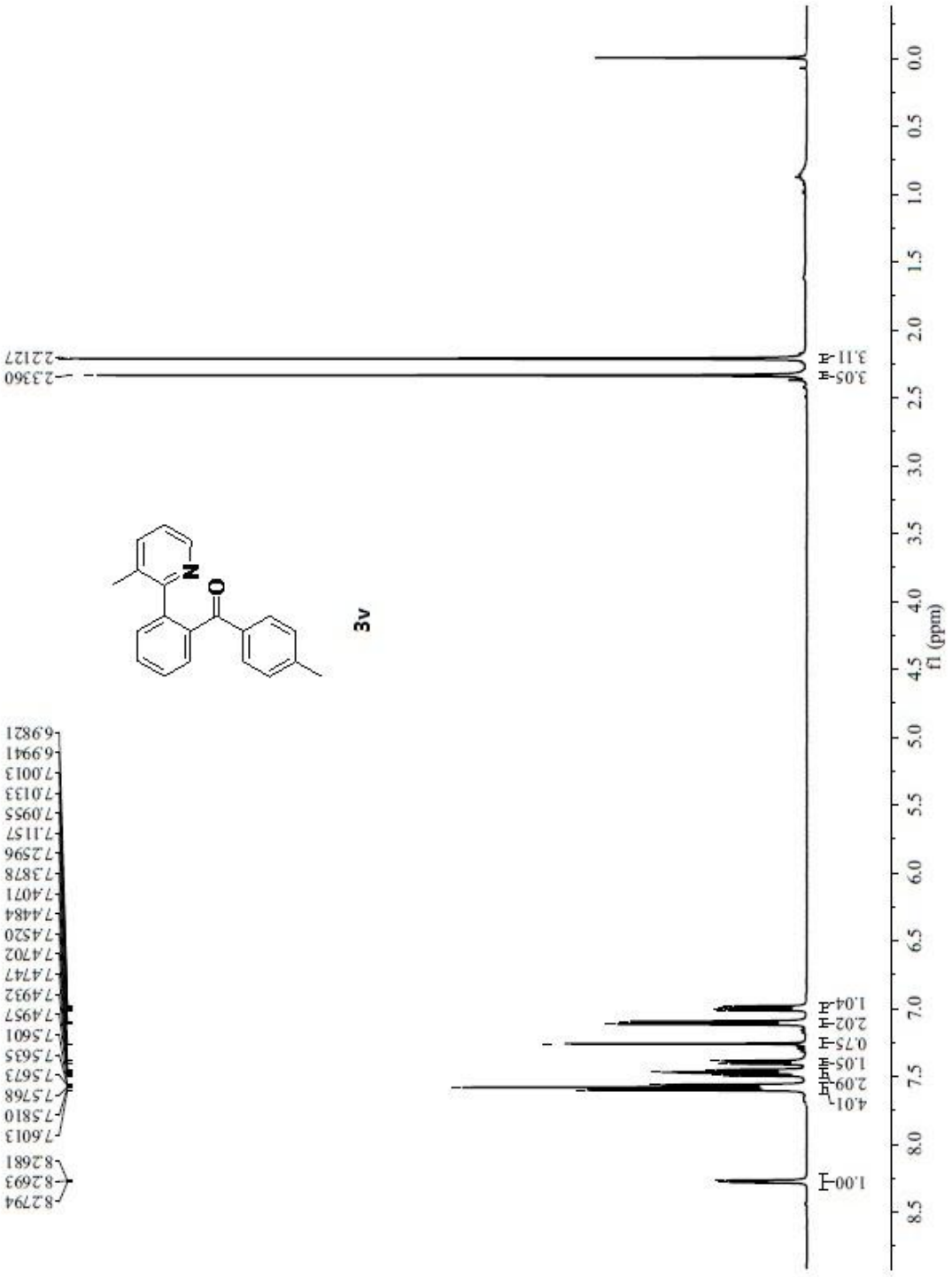
137
139
141
143
145
147
149
151
153
f1 (ppm)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3.11
3.05
1.04
2.02
0.75
1.05
2.09
4.01
1.00
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8.2693
8.2681
7.6013
7.5810
7.5768
7.5673
7.5635
7.5601
7.4957
7.4932
7.4747
7.4702
7.4520
7.4484
7.4071
7.3878
7.2596
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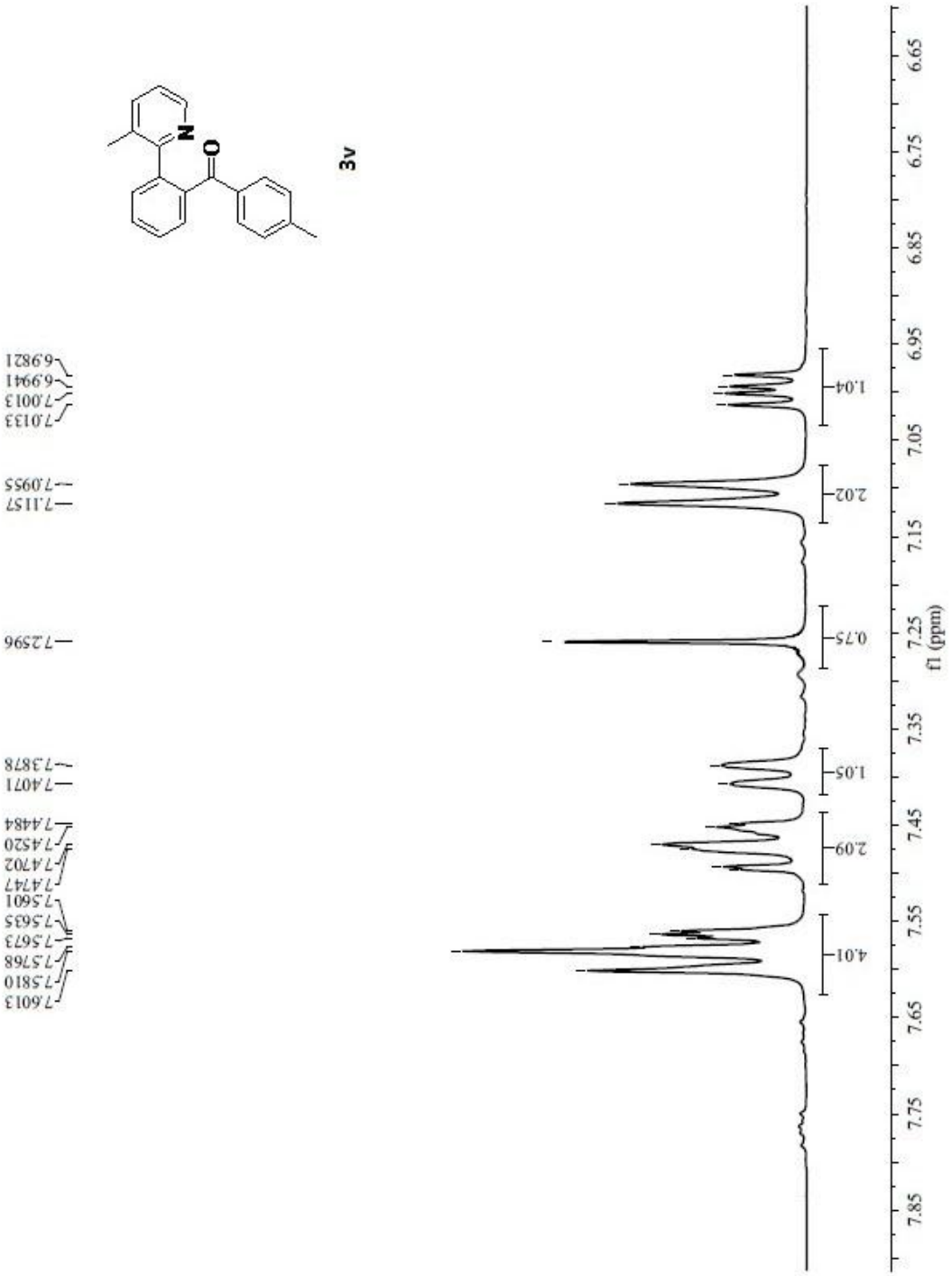
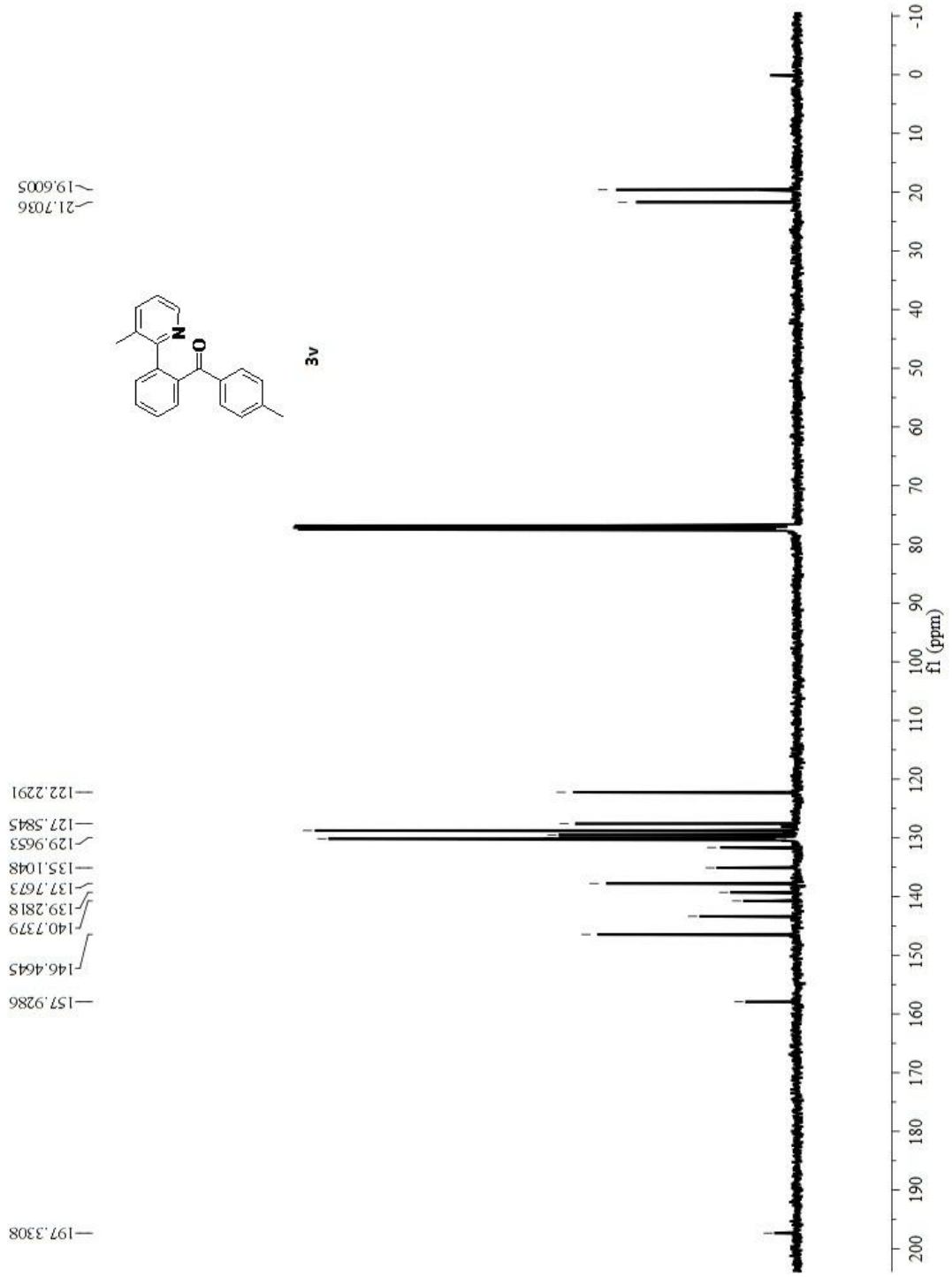
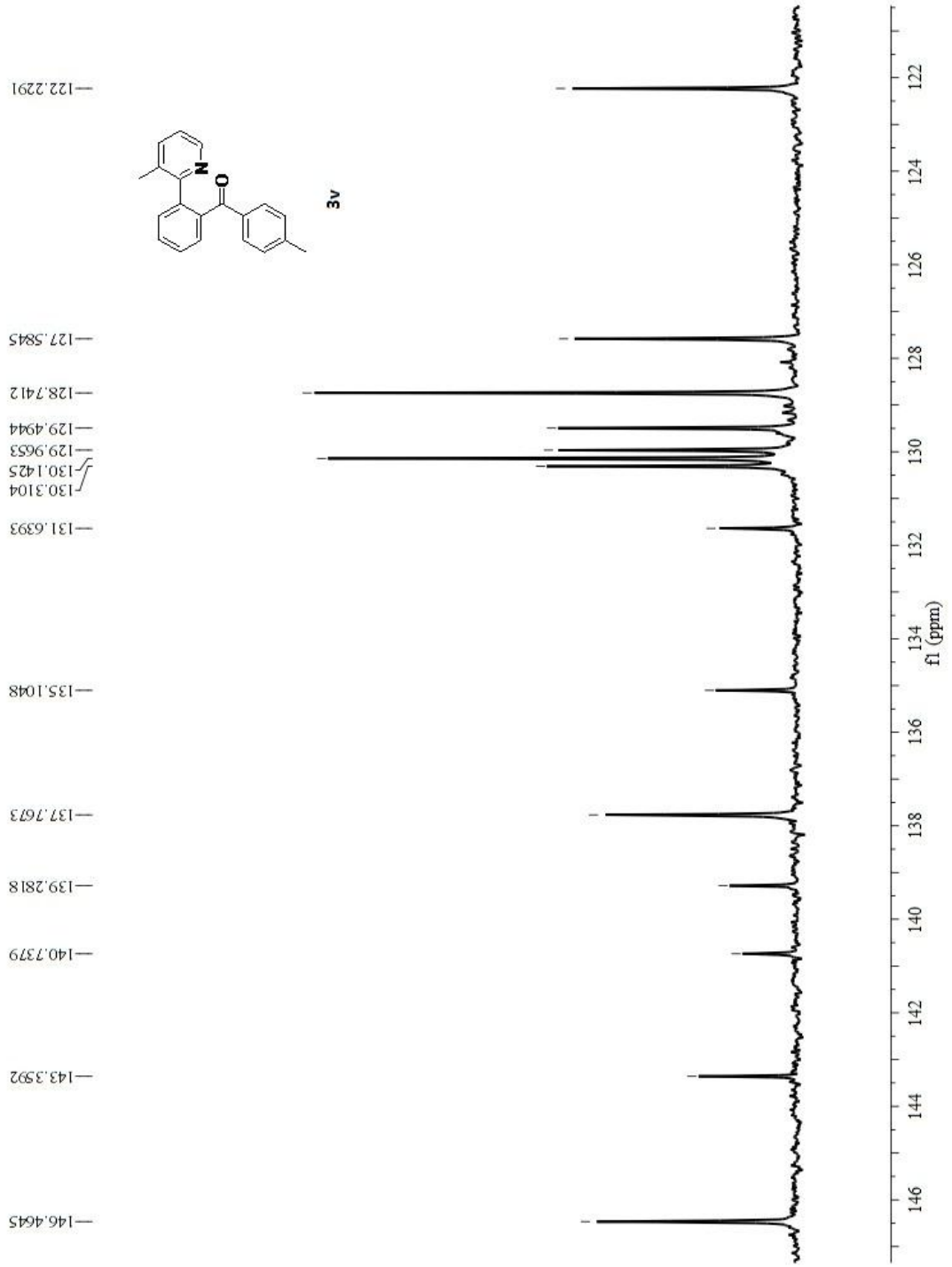
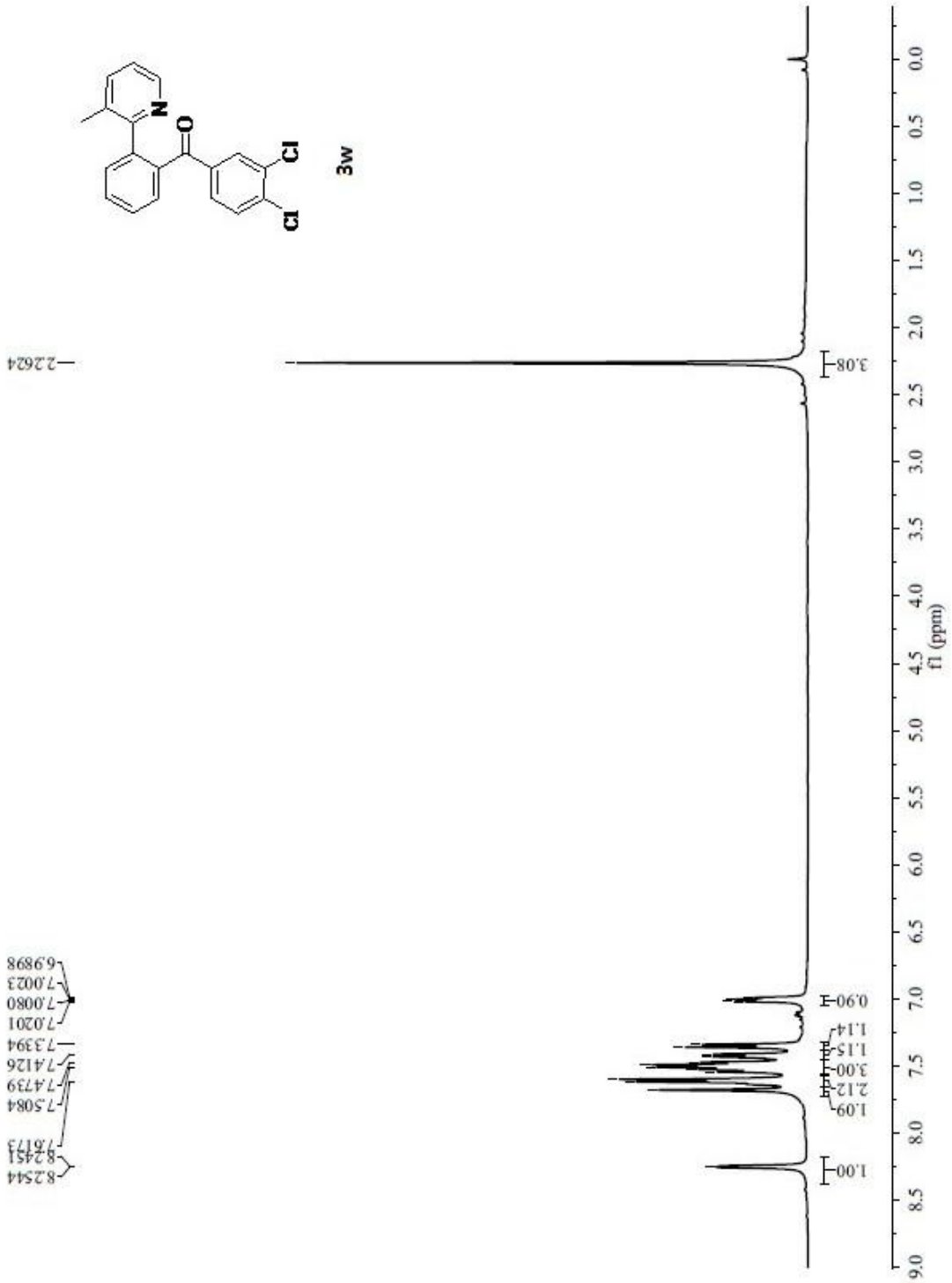
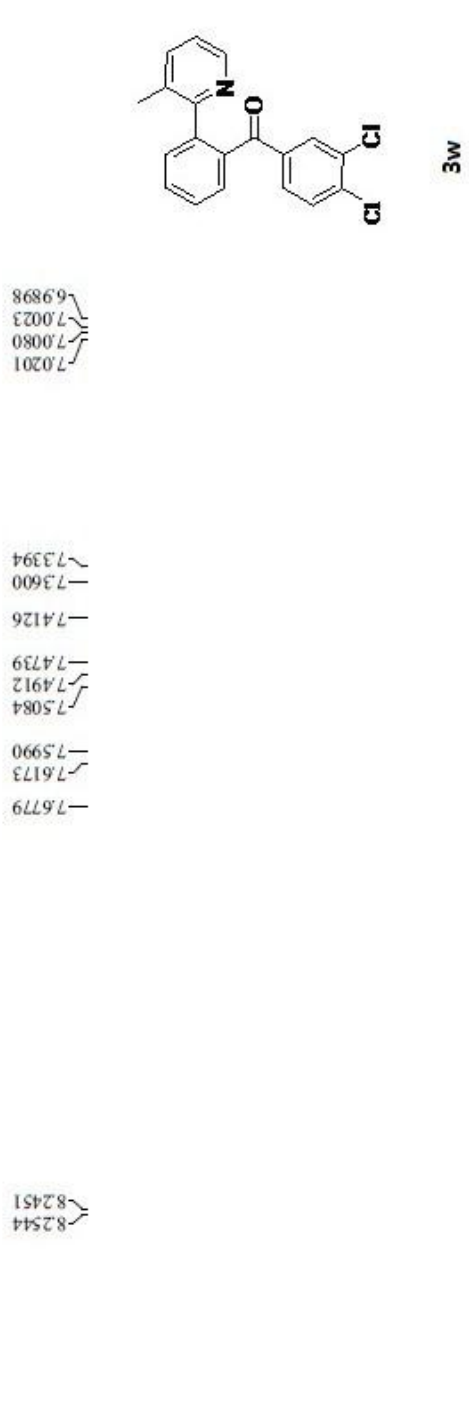
7.0955
7.0133
7.0013
6.9941
6.9821
N
O
3v
f1 (ppm)

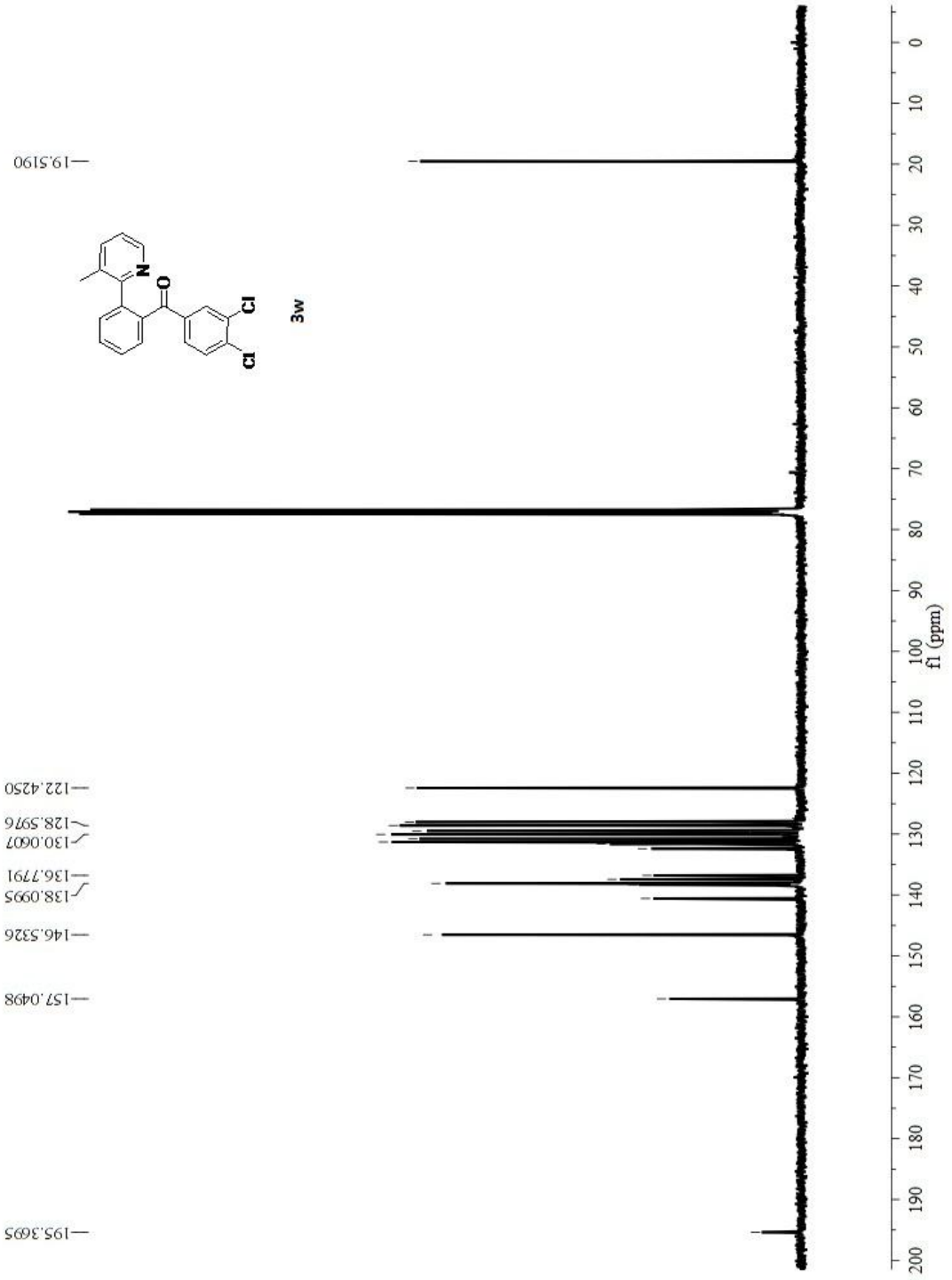

3v
N
O
7.6013
7.5810
7.5768
7.5673
7.5635
7.5601
7.4747
7.4702
7.4520
7.4484
7.4071
7.3878
7.2596
7.1157
7.0955
7.0133
7.0013
6.9941
6.9821
1.04
2.02
0.75
1.05
2.09
4.01
6.65
6.75
6.85
6.95
7.05
7.15
7.25
7.35
7.45
7.55
7.65
7.75
7.85
f1 (ppm)

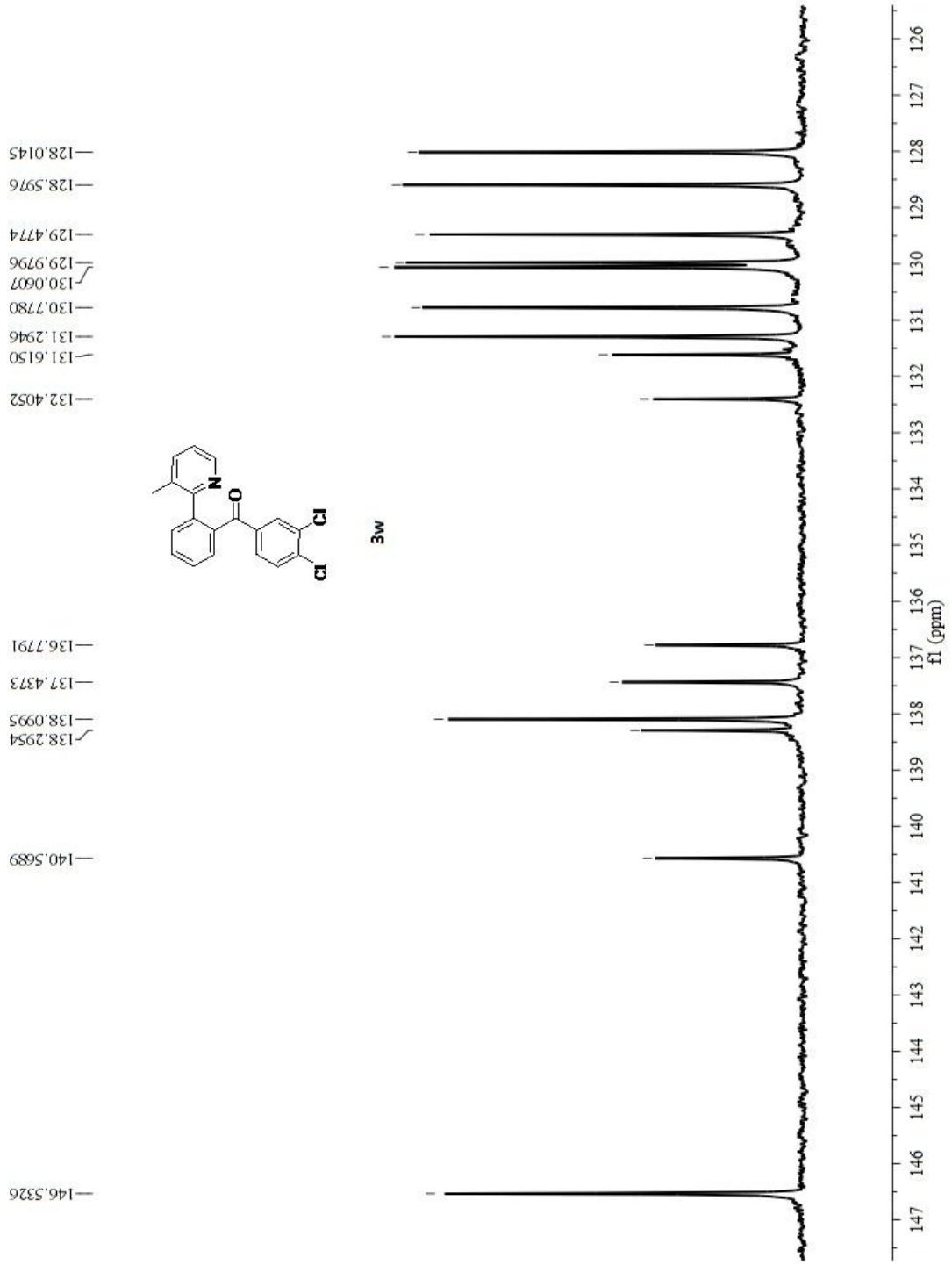

19.6005
21.7036
3v
122.2291
127.5845
129.9653
135.1048
137.7673
139.2818
140.7379
146.4645
157.9286
197.3308
f1 (ppm)

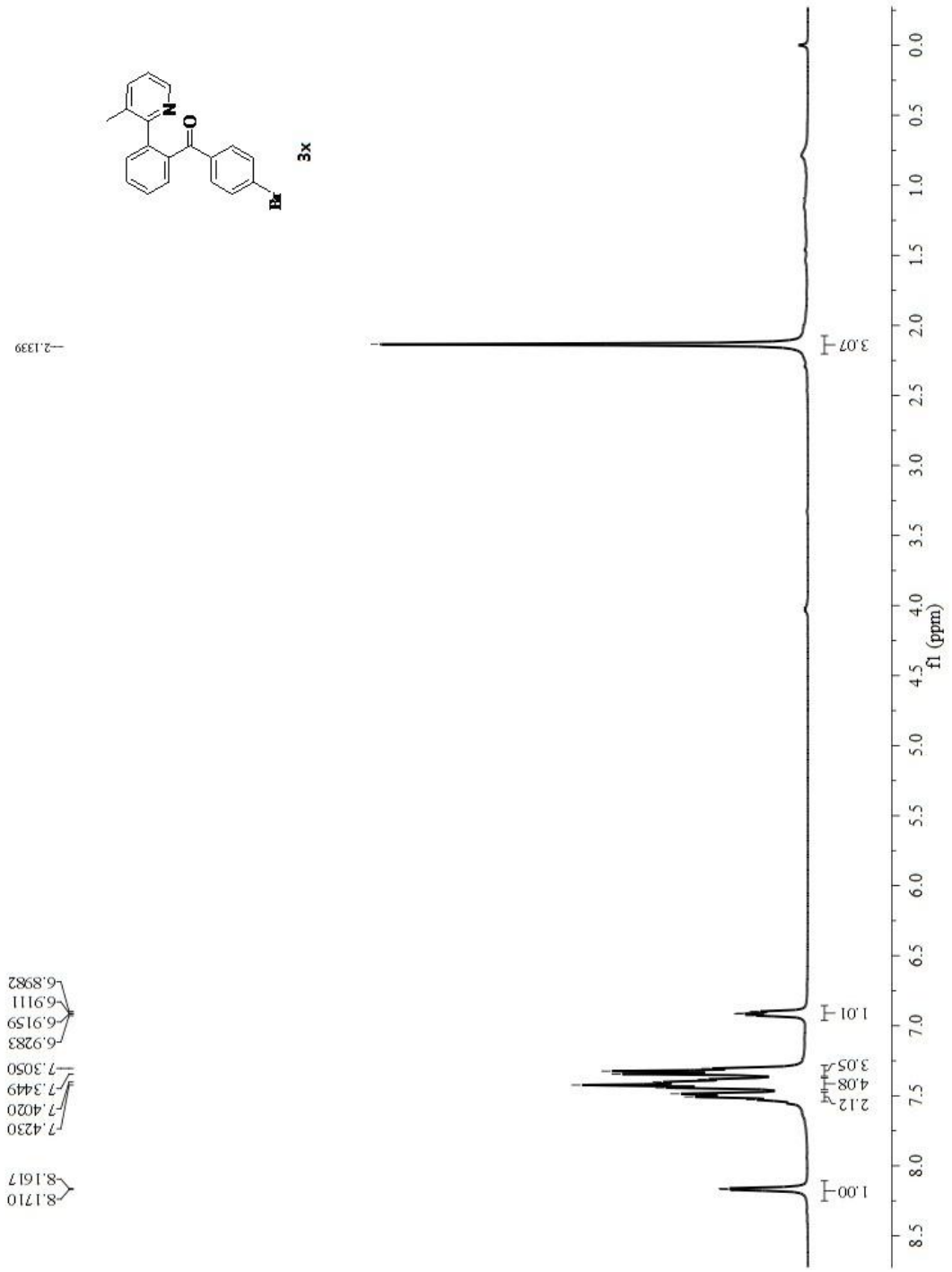


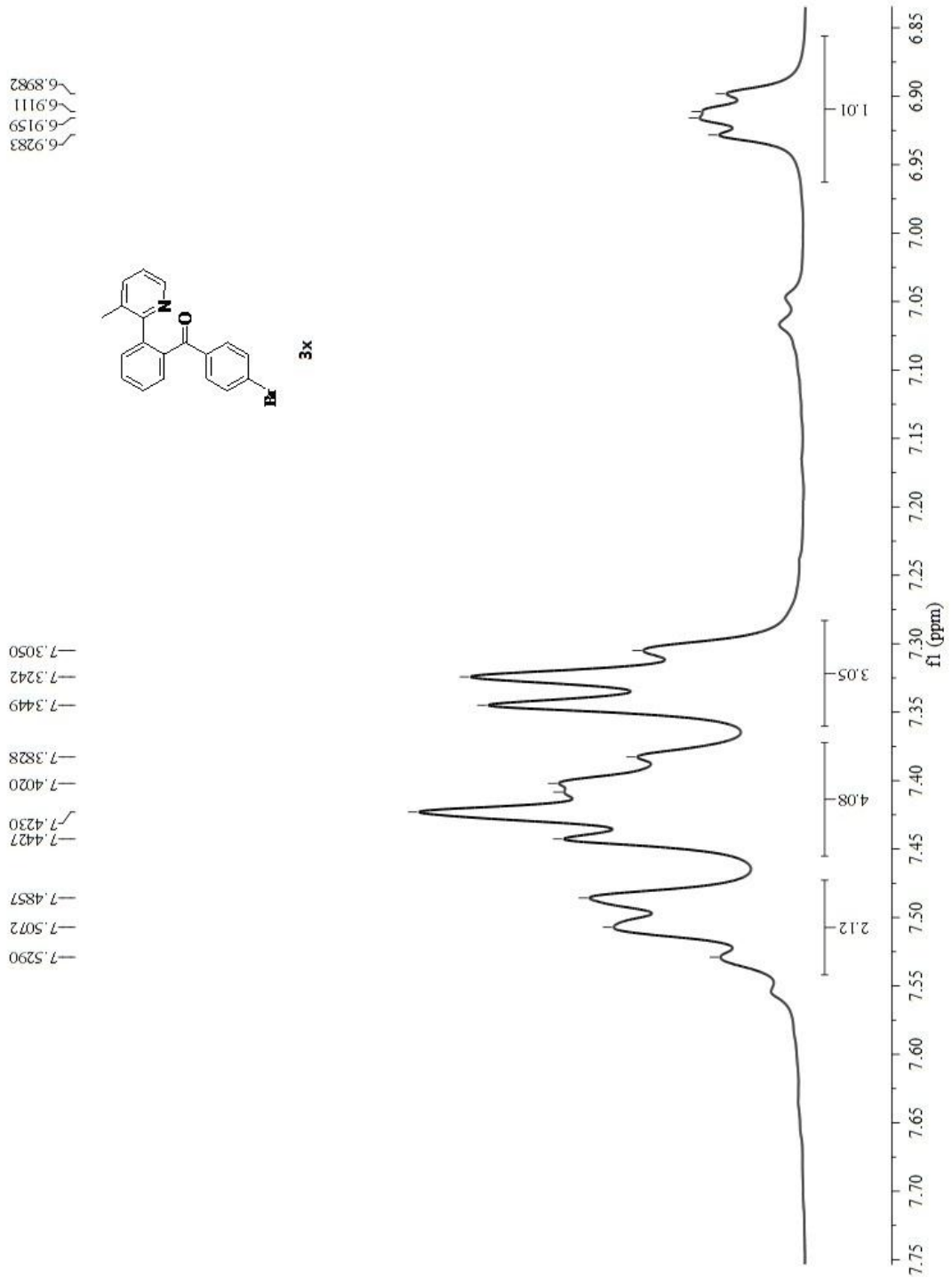

3w
Cl
Cl
O
N
2.2624
3.08
0.90
1.14
1.15
3.00
2.12
1.09
1.00
8.2544
8.2451
7.6173
7.5084
7.4739
7.4126
7.3394
7.0201
7.0080
7.0023
6.9898
f1 (ppm)

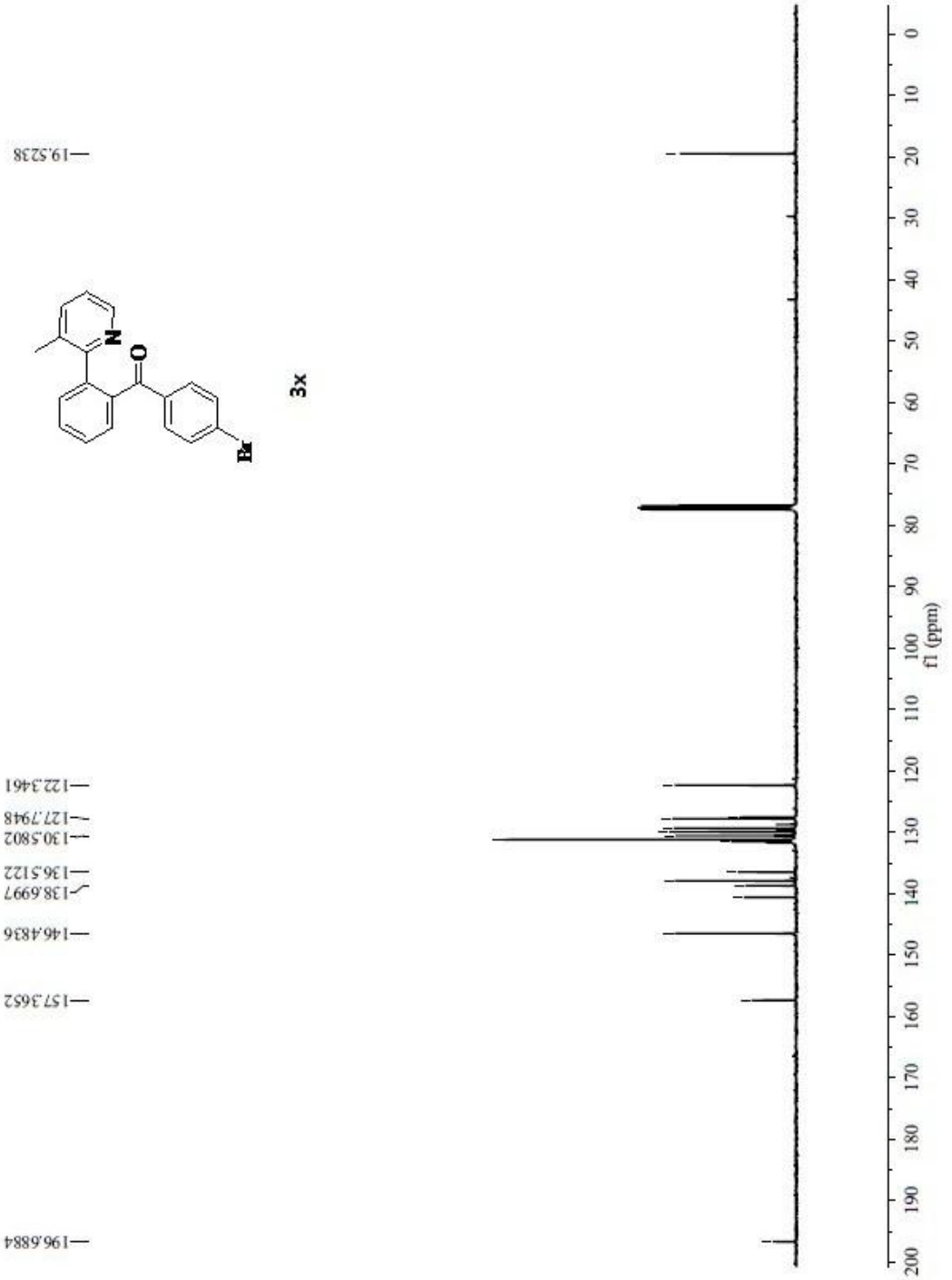


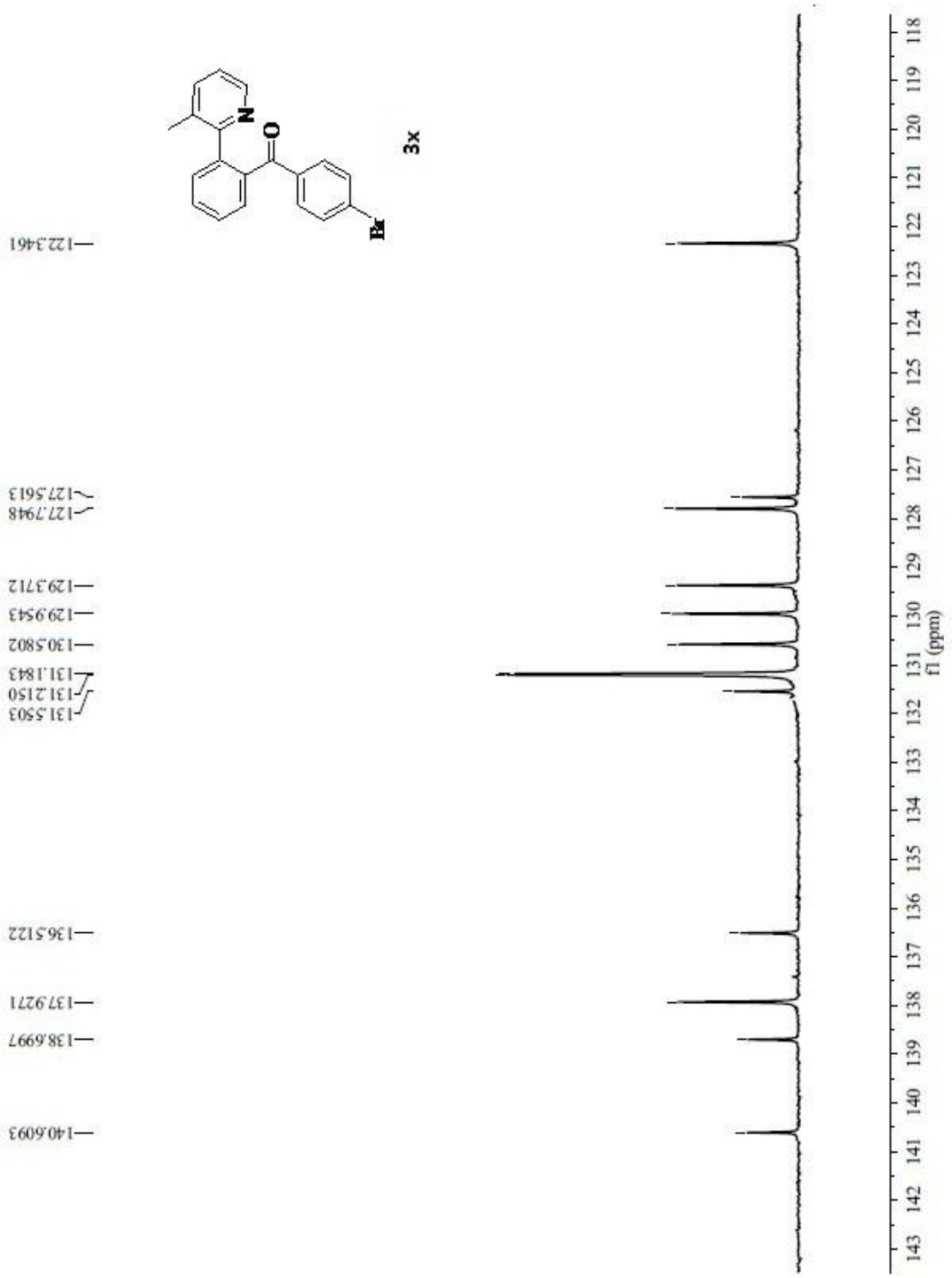


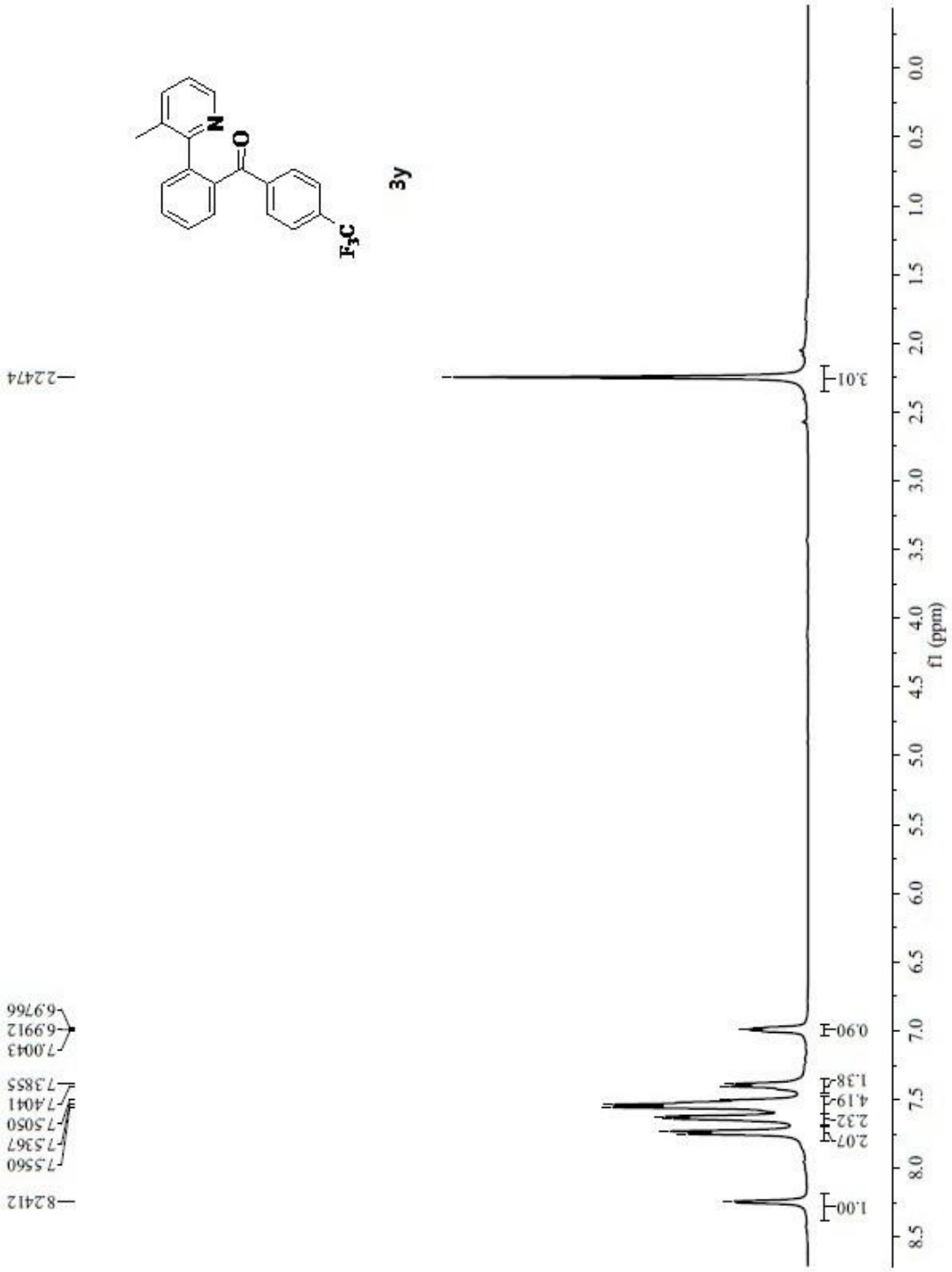

128.0145
128.5976
129.4774
129.9796
130.0607
130.7780
131.2946
131.6150
132.4052
136.7791
137.4373
138.0995
138.2954
140.5689
146.5326
3w
Cl
Cl
O
N
126
127
128
129
130
131
132
133
134
135
136
137
138
139
140
141
142
143
144
145
146
147
f1 (ppm)

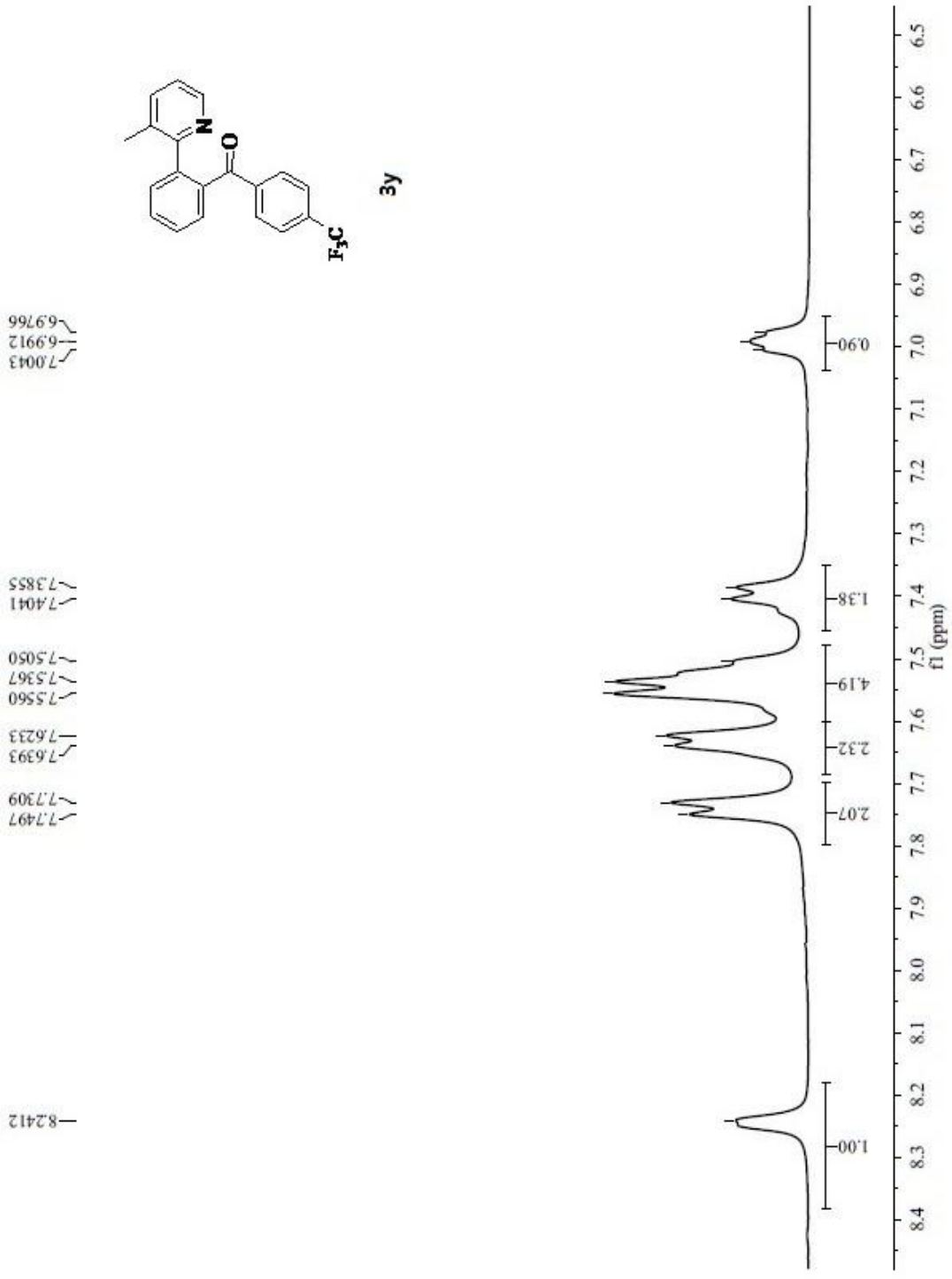


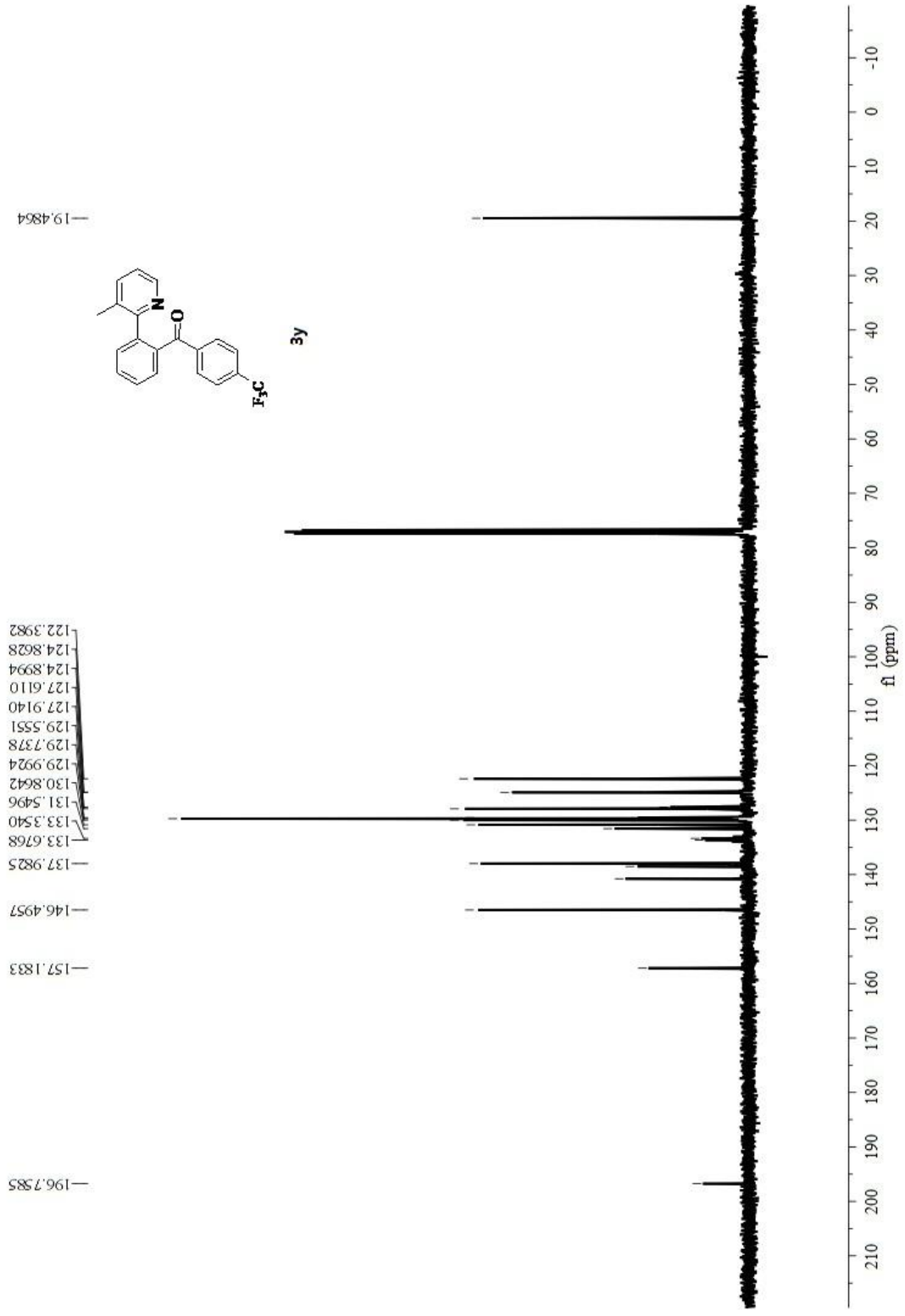

6.8982
6.9111
6.9159
6.9283
7.3050
7.3242
7.3449
7.3828
7.4020
7.4230
7.4427
7.4857
7.5072
7.5290
3x
Br
N
O
1.01
3.05
4.08
2.12
6.85
6.90
6.95
7.00
7.05
7.10
7.15
7.20
7.25
7.30
7.35
7.40
7.45
7.50
7.55
7.60
7.65
7.70
7.75
f1 (ppm)

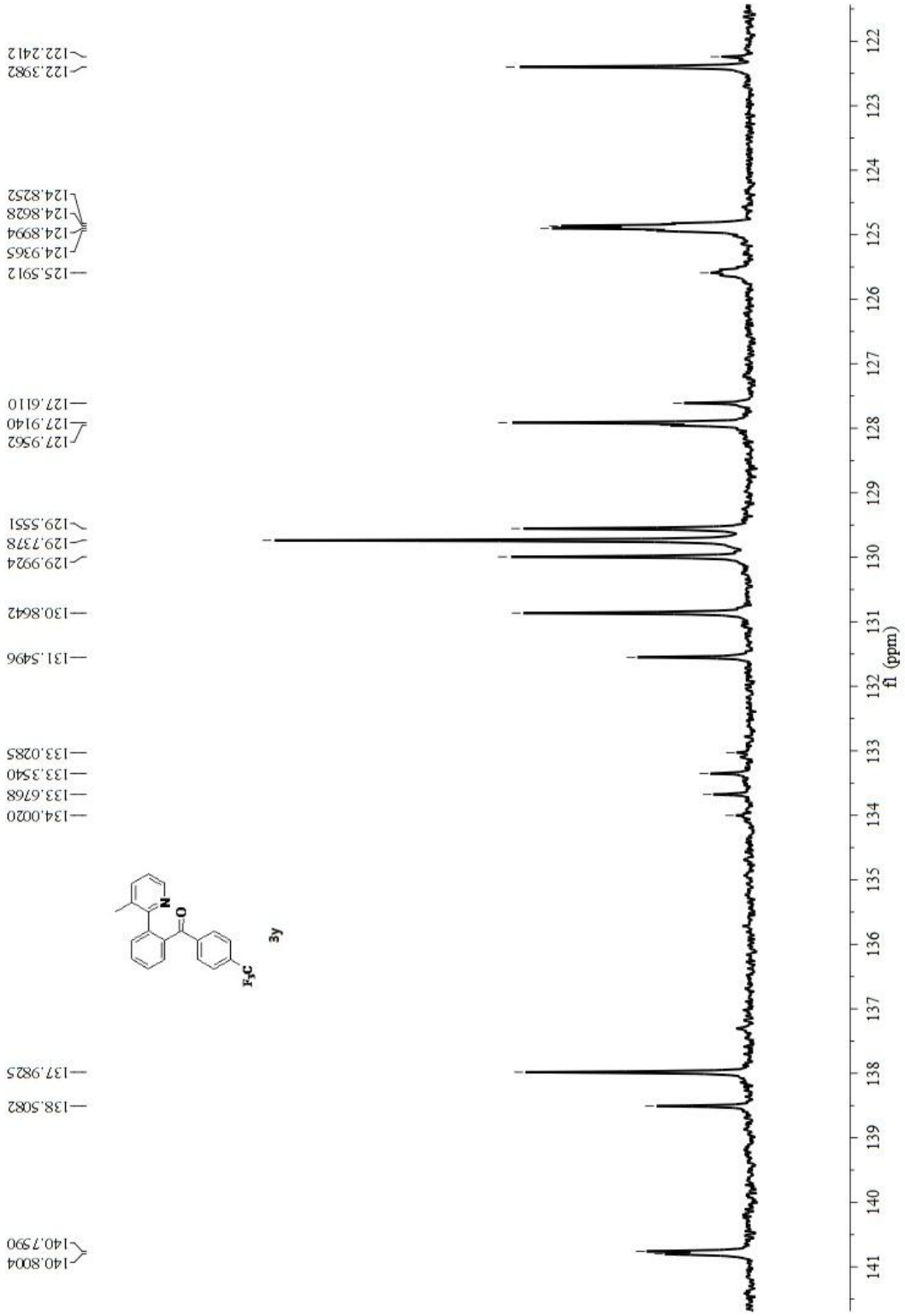

19.5238
122.3461
127.7948
130.5802
136.5122
138.6997
146.4836
157.3652
196.6884
N
O
Br
3x
f1 (ppm)

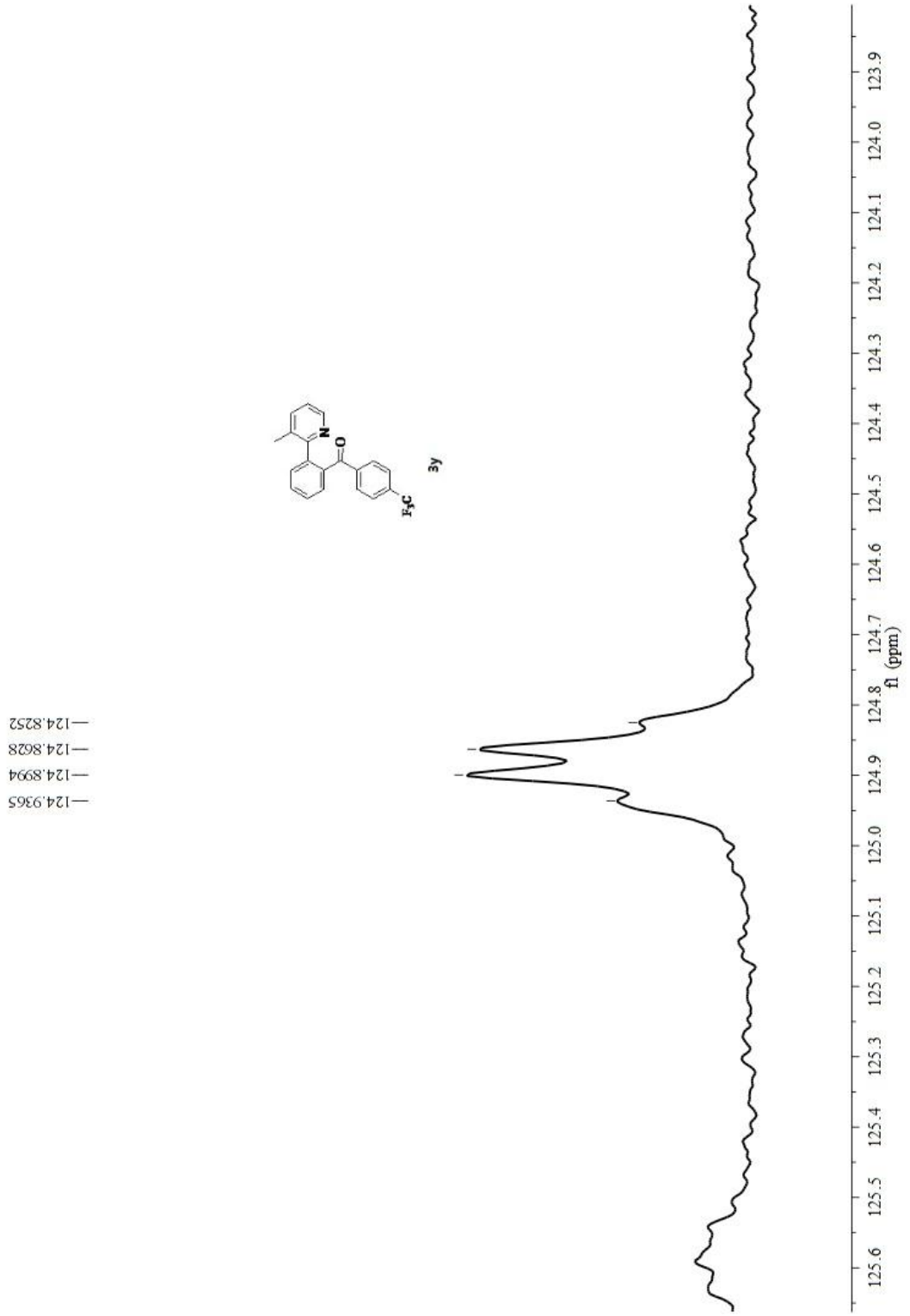



3y
F3C
O
N
8.2412
7.5560
7.5367
7.5050
7.4041
7.3855
7.0043
6.9912
6.9766
2.2474
3.01
0.90
1.38
4.19
2.32
2.07
1.00
f1 (ppm)




19.4864
122.3982
124.8628
124.8994
127.6110
127.9140
129.5551
129.7378
129.9924
130.8642
131.5496
133.3540
133.6768
137.9825
146.4957
157.1833
196.7585
N
O
F3C
3y
f1 (ppm)


140.8004
140.7590
138.5082
137.9825
134.0020
133.6768
133.3540
133.0285
131.5496
130.8642
129.9924
129.7378
129.5551
127.9562
127.9140
127.6110
125.5912
124.9365
124.8994
124.8628
124.8252
122.3982
122.2412
3y
O
N
F3C
fl (ppm)


124.9365
124.8994
124.8628
124.8252
3y
f1 (ppm)