

Supporting Information

An I₂-catalyzed three-component consecutive reaction for the synthesis of 3-arylimidazo[1,2-*a*]-*N*-heterocycles

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Tables S1-S4 and Copies of NMR Spectra of the Synthesized Compounds

Tables S1-S4.....	S2
¹ H NMR and ¹³ C NMR spectra of compounds 3	S3
¹ H NMR and ¹³ C NMR spectra of compounds 5ab	S70

Table S1 Optimization of reaction conditions by screening the oxidants^a

Entry	Oxidant	Yield (%) ^b
1	K ₂ S ₂ O ₈	20
2	(NH ₄)S ₂ O ₈	Trace
3	Na ₂ S ₂ O ₈	13
4	Py • SO ₃	12
5	selectfluor	13
6	H ₂ O ₂	0
7	HOAc	0

^aReaction conditions: 2-aminopyridine (**1a**, 1 mmol), 1 -(*p*-tolyl)ethanone (**2b**, 1.2 mmol), DMSO (2 mL), oxidant (3 mmol), and I₂(10%) at 120 °C for 16 h; ^bIsolated yield.

Table S2 Optimization of reaction conditions by screening the amount of the oxidant^a

Entry	K ₂ S ₂ O ₈ (equiv.)	Yield (%) ^b
1	3	20
2	1	Trace
3	2	16
4	4	9
5	5	4
6	6	Trace

^aReaction conditions: 2-aminopyridine (**1a**, 1 mmol), 1 -(*p*-tolyl)ethanone (**2b**, 1.2 mmol), DMSO (2 mL), K₂S₂O₈ at the indicated amount, and I₂(10%) at 120 °C for 16 h; ^bIsolated yield.

Table S3 Optimization of reaction conditions by screening the solvents^a

Entry	Solvent	Yield (%) ^b
1	Xylene	0
2	1,4-dioxane	0
3	Pyridine	trace
4	DMSO	20

^aReaction conditions: 2-aminopyridine (**1a**, 1 mmol), 1 -(*p*-tolyl)ethanone (**2b**, 1.2 mmol), DMSO (2 mmol), K₂S₂O₈ (3 mmol), and I₂(10%) in solvent (2 mL) at 120 °C for 16 h.

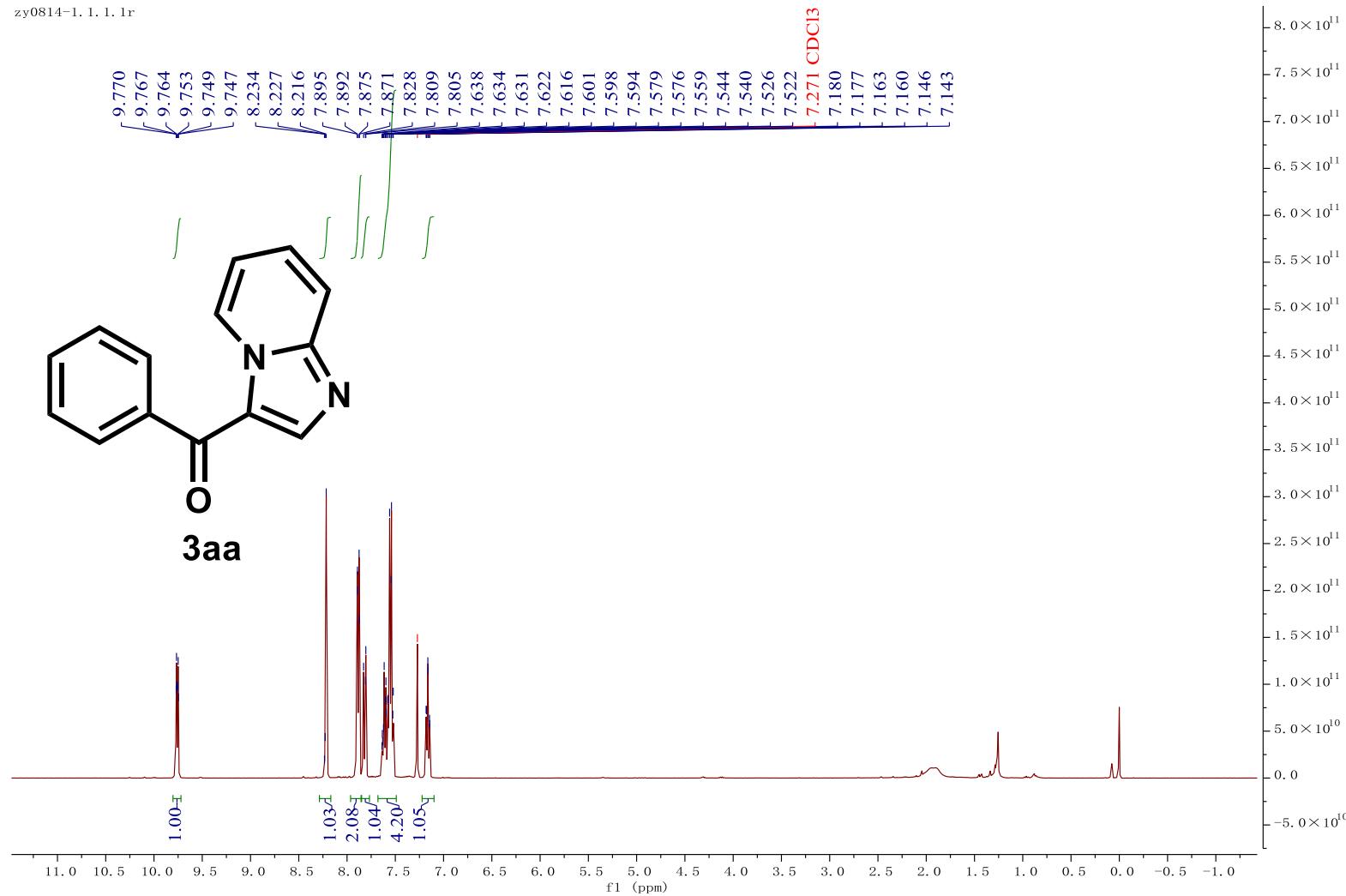
Table S4 Optimization of reaction condition by screening the additives^a

Entry	Additive	Yield (%) ^b
1	--	18
2	NaOAc	40
3	K ₂ CO ₃	32
4	NaHCO ₃	23
5	ET ₃ N	21
6	DBU	14

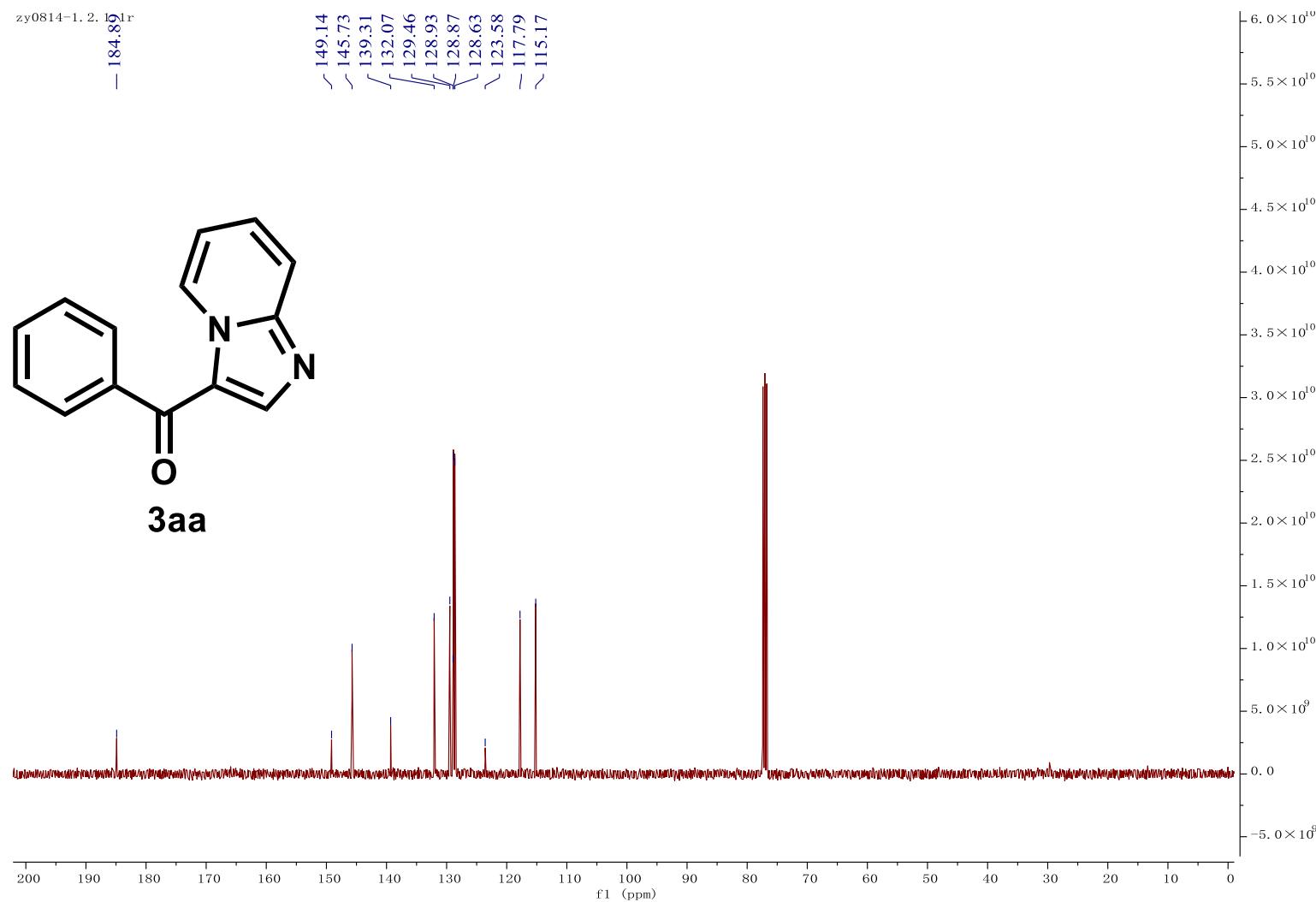
^aReaction conditions: 2-aminopyridine (**1a**, 1 mmol), 1 -(*p*-tolyl)ethanone (**2b**, 1.2 mmol), DMSO (2 mL), K₂S₂O₈ (3 mmol), additive (2 mmol) at 120 °C for 9 h then add I₂ (10%) for another 7 h; ^bIsolated yield.

¹H NMR of Compound 3aa (400 MHz, CDCl₃)

zy0814-1. 1. 1. 1r

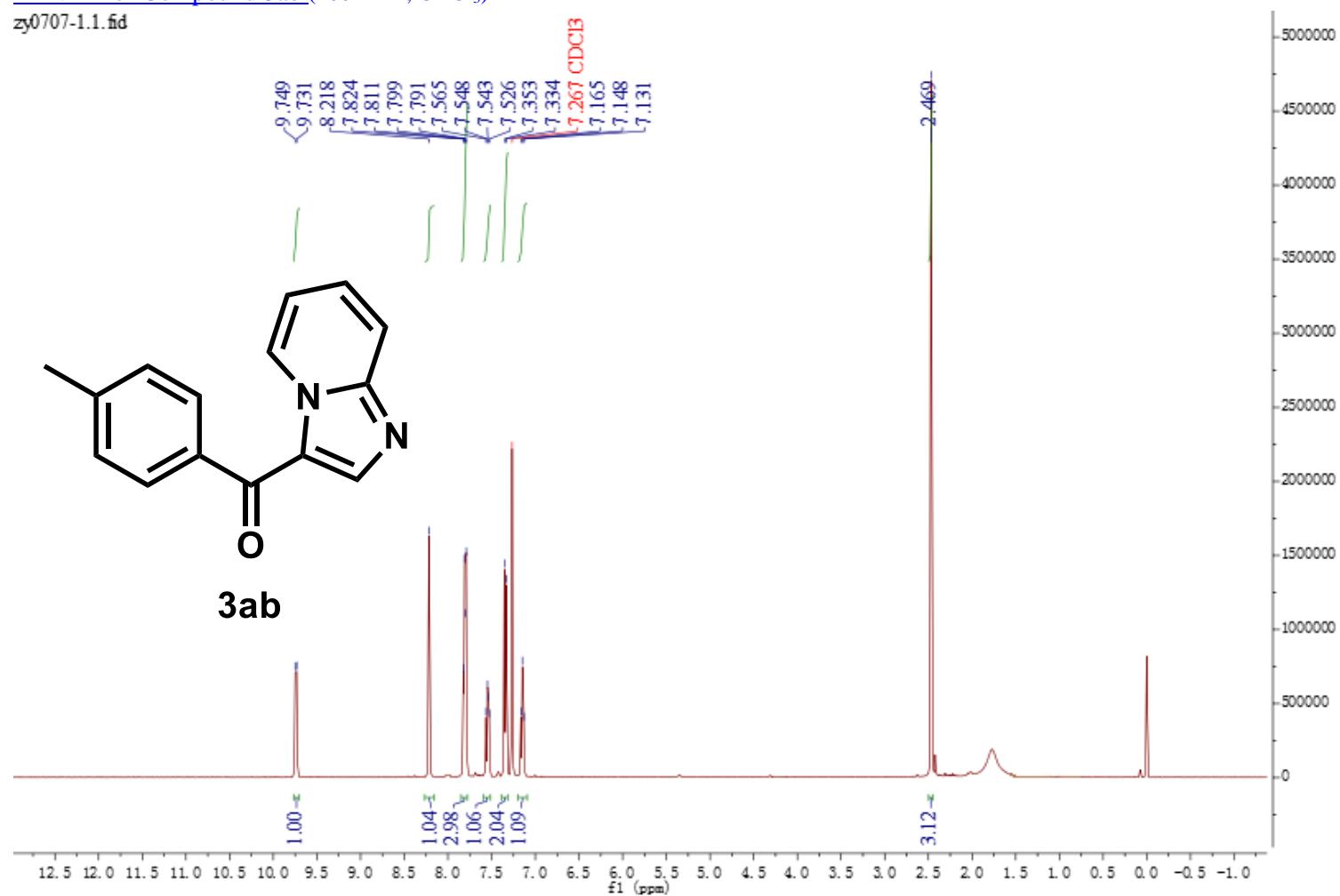


¹³C{H} NMR of Compound 3aa (101 MHz, CDCl₃)



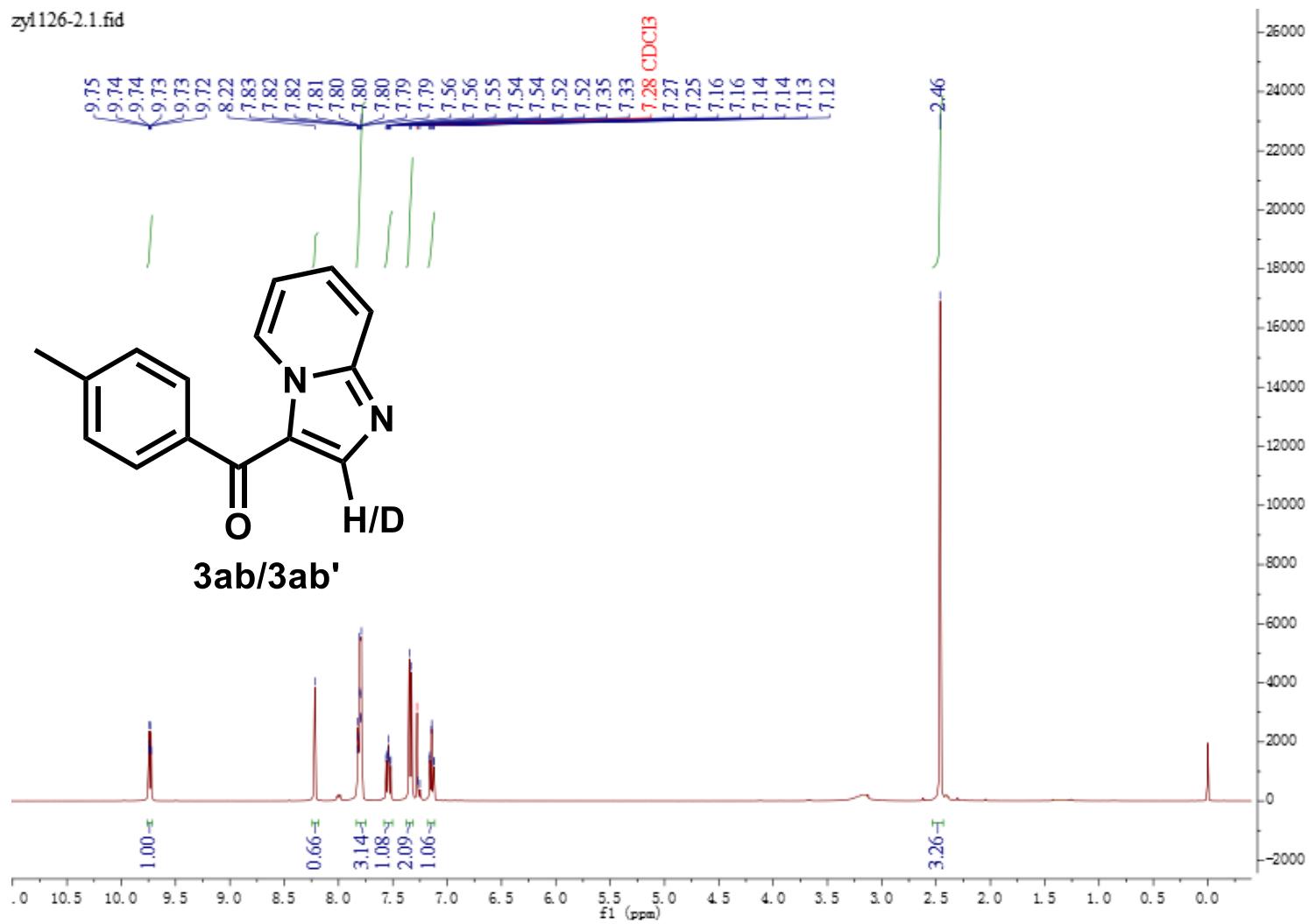
¹H NMR of Compound 3ab (400 MHz, CDCl₃)

zy0707-1.1.fid

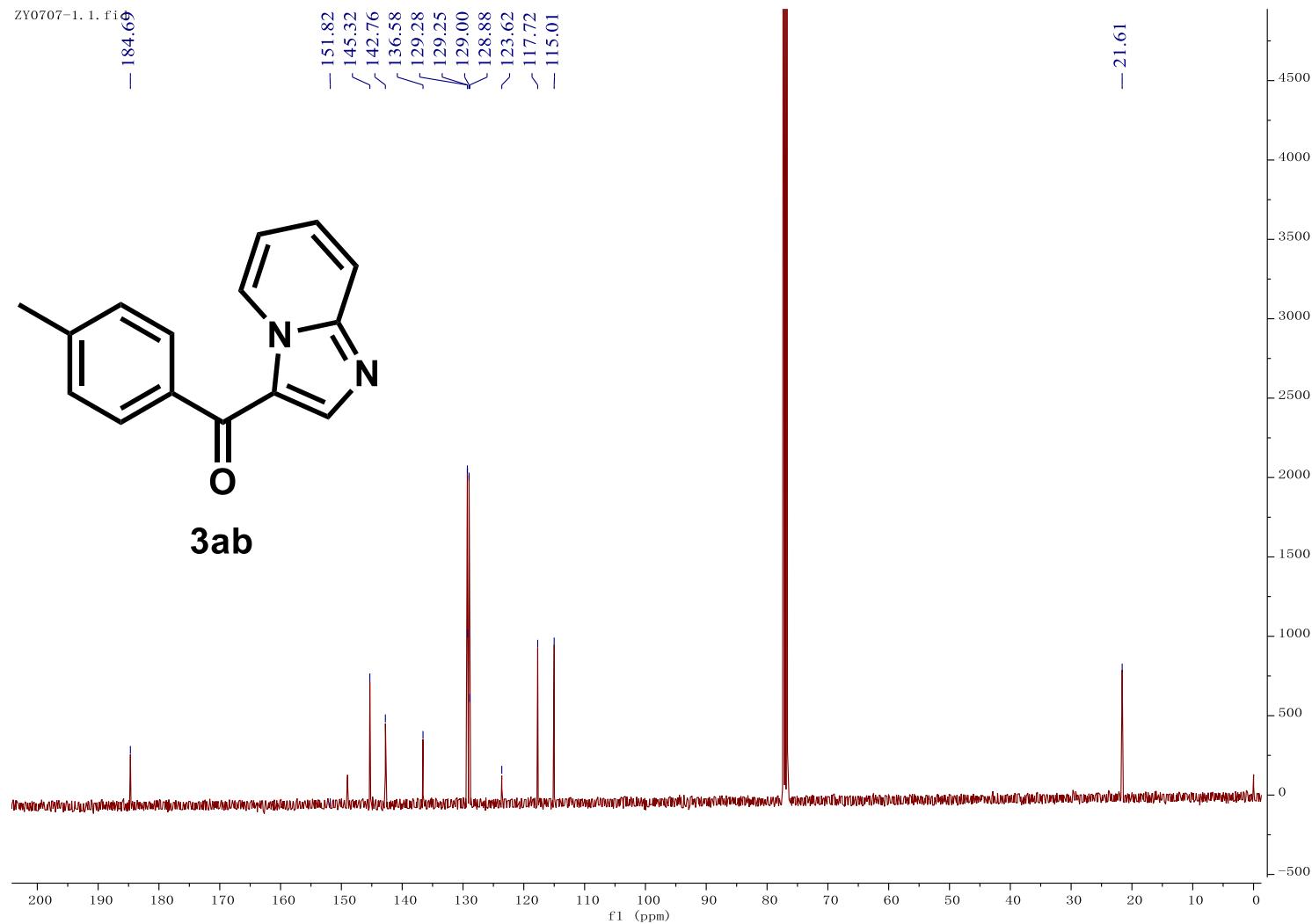


¹H NMR of Compound 3ab/3ab' (400 MHz, CDCl₃)

zy1126-2.1.fid

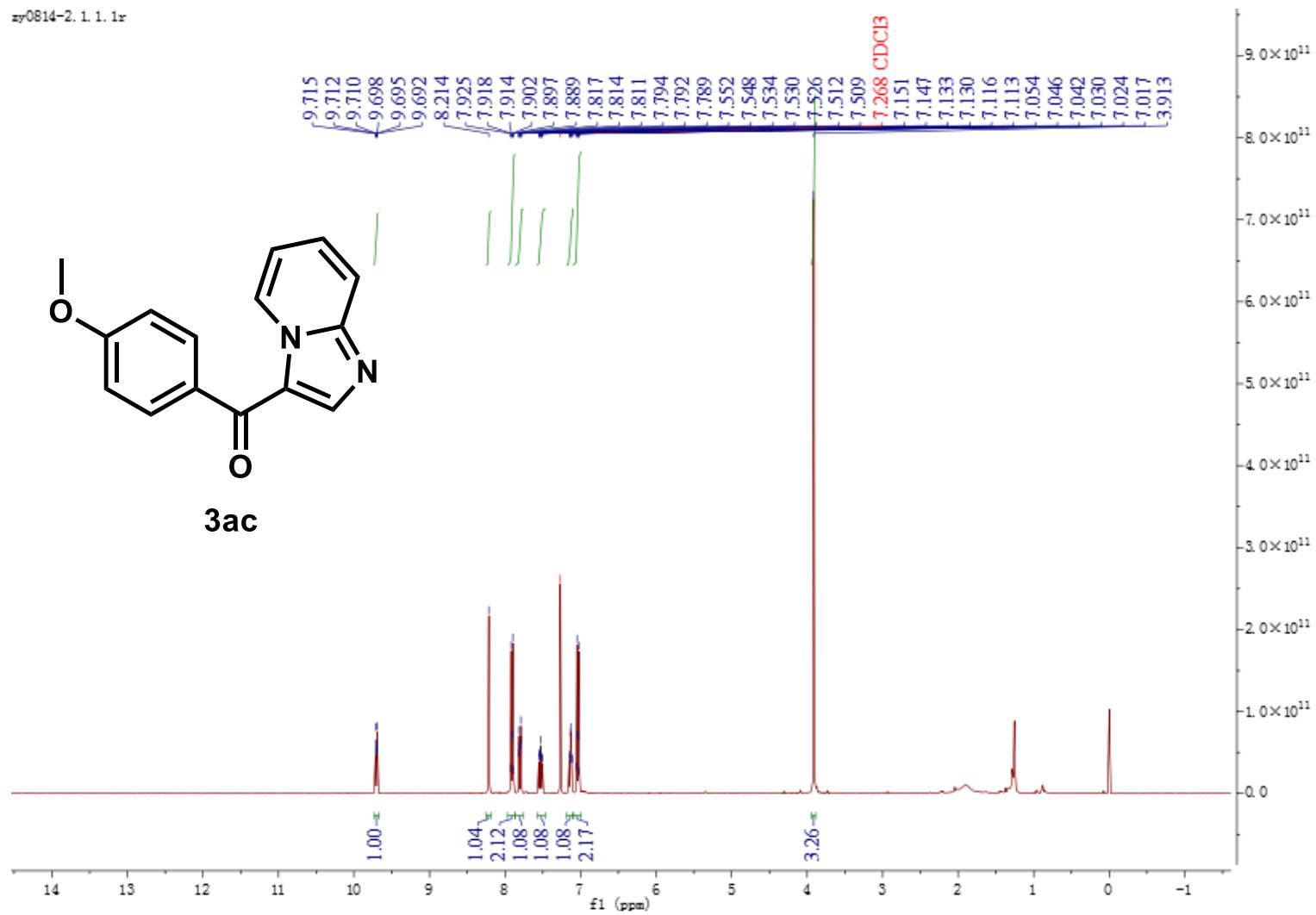


¹³C{H} NMR of Compound 3ab (101 MHz, CDCl₃)

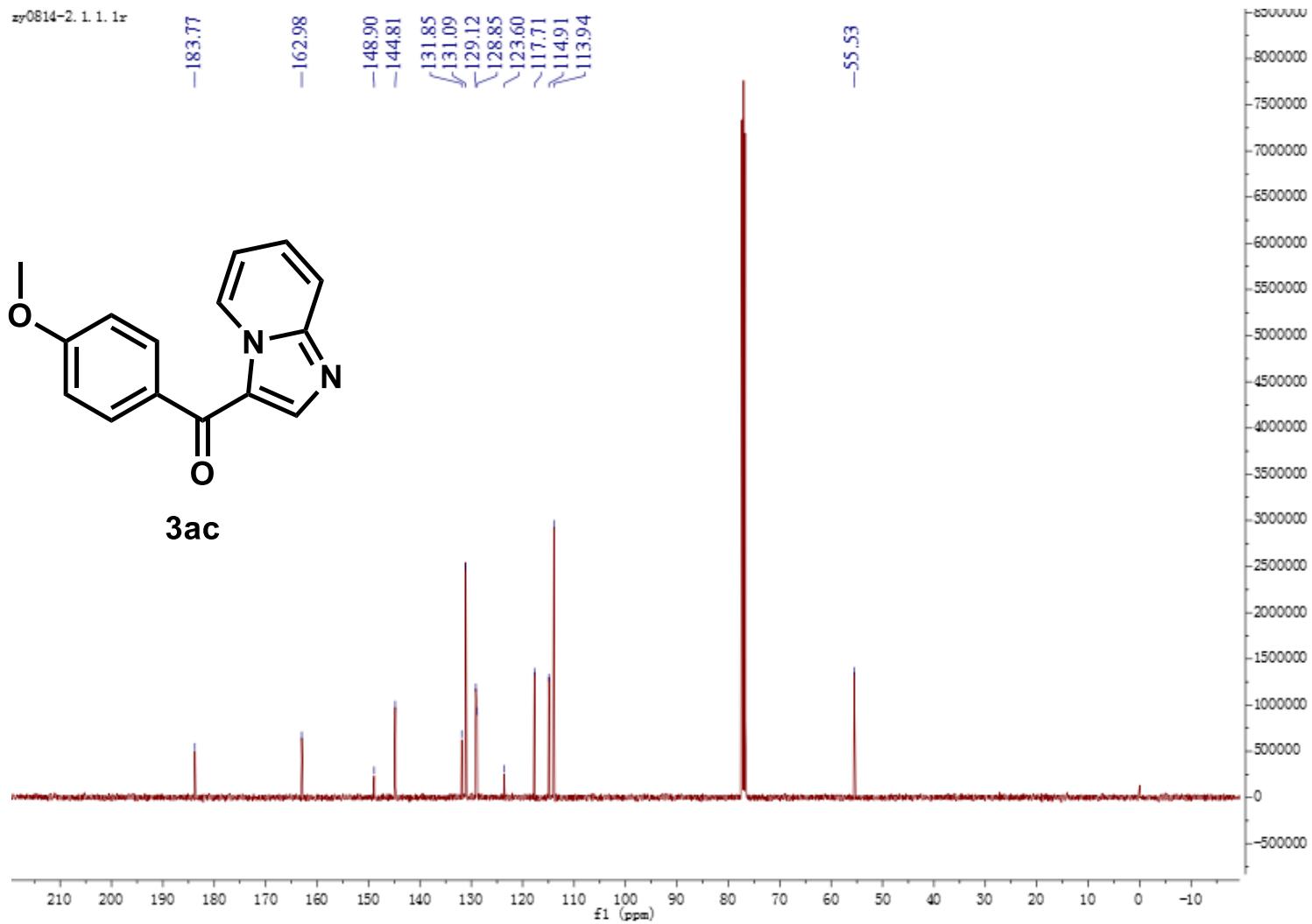


¹H NMR of Compound 3ac (400 MHz, CDCl₃)

zy0814-2. 1. 1. 1r

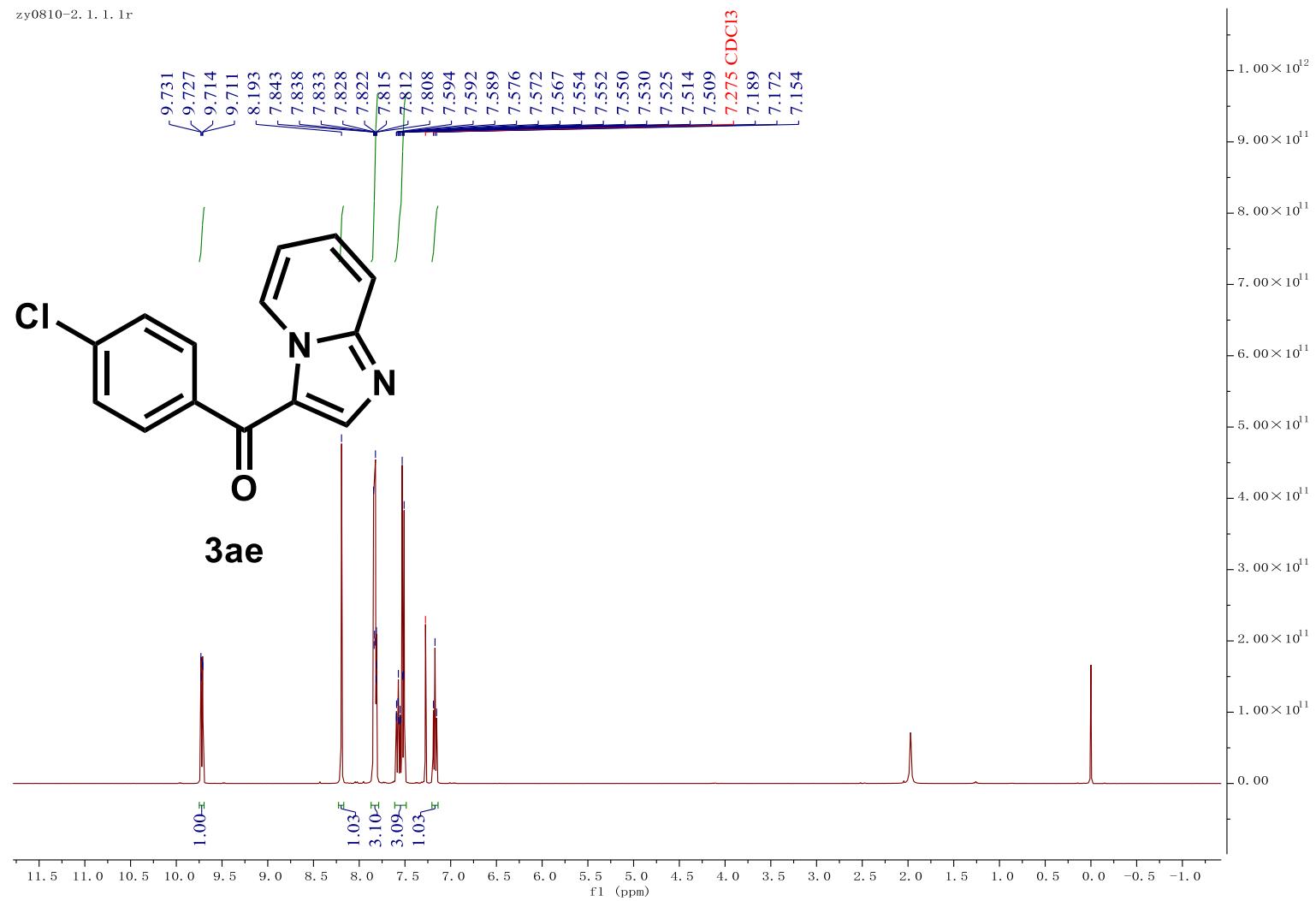


¹³C{H} NMR of Compound 3ac (101 MHz, CDCl₃)

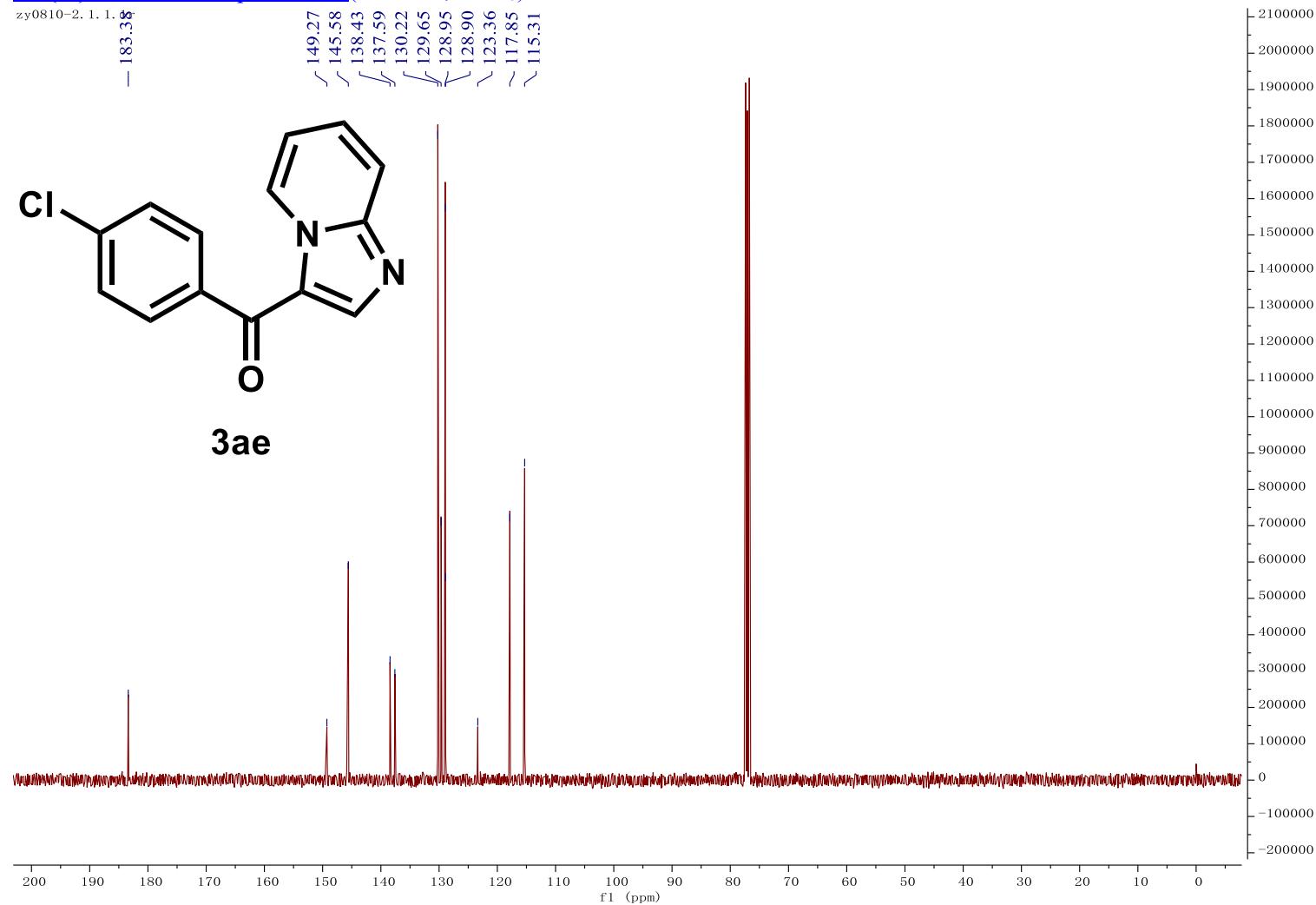


¹H NMR of Compound 3ae (400 MHz, CDCl₃)

zy0810-2. 1. 1. 1r

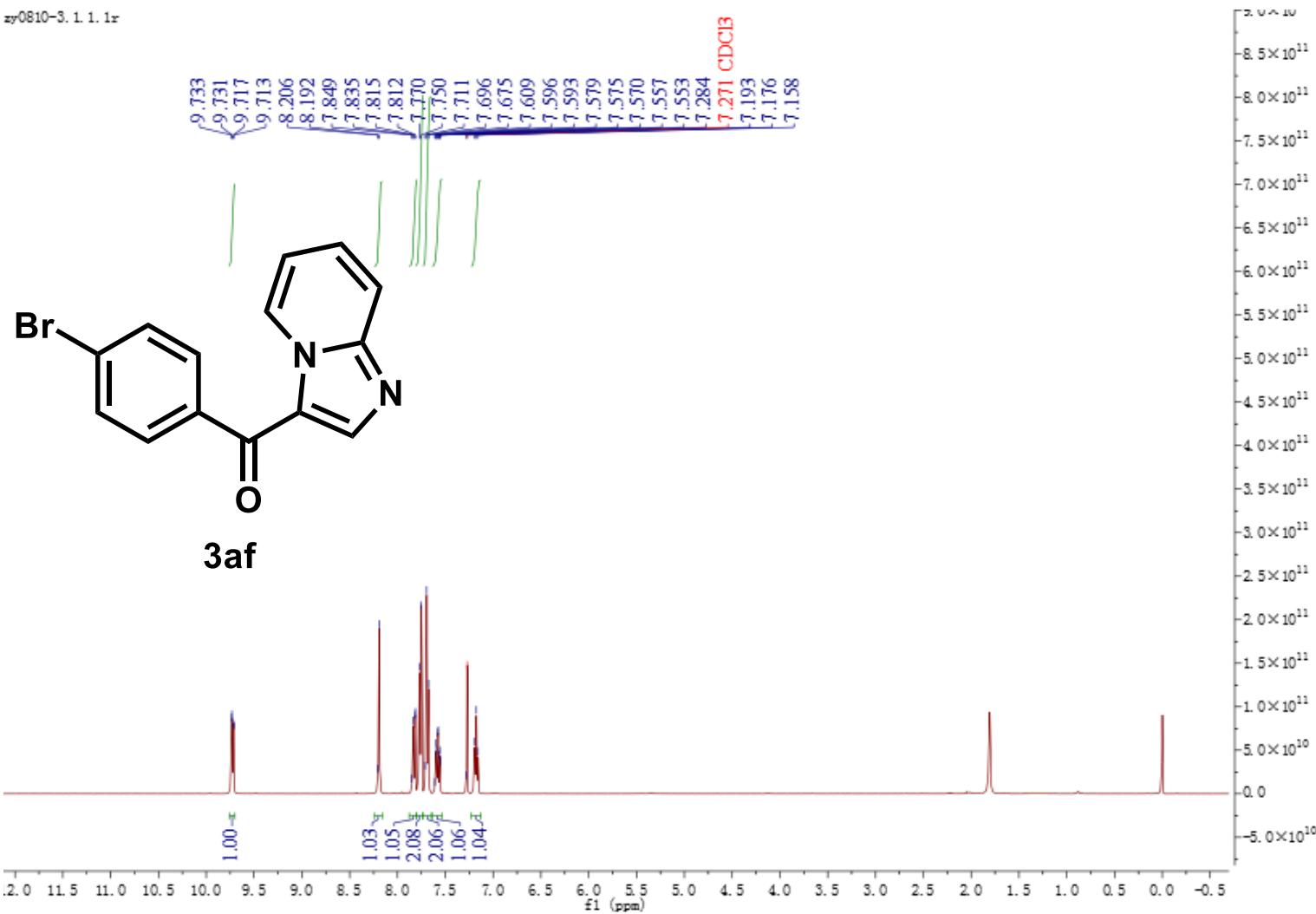


¹³C{H} NMR of Compound 3ae (101 MHz, CDCl₃)



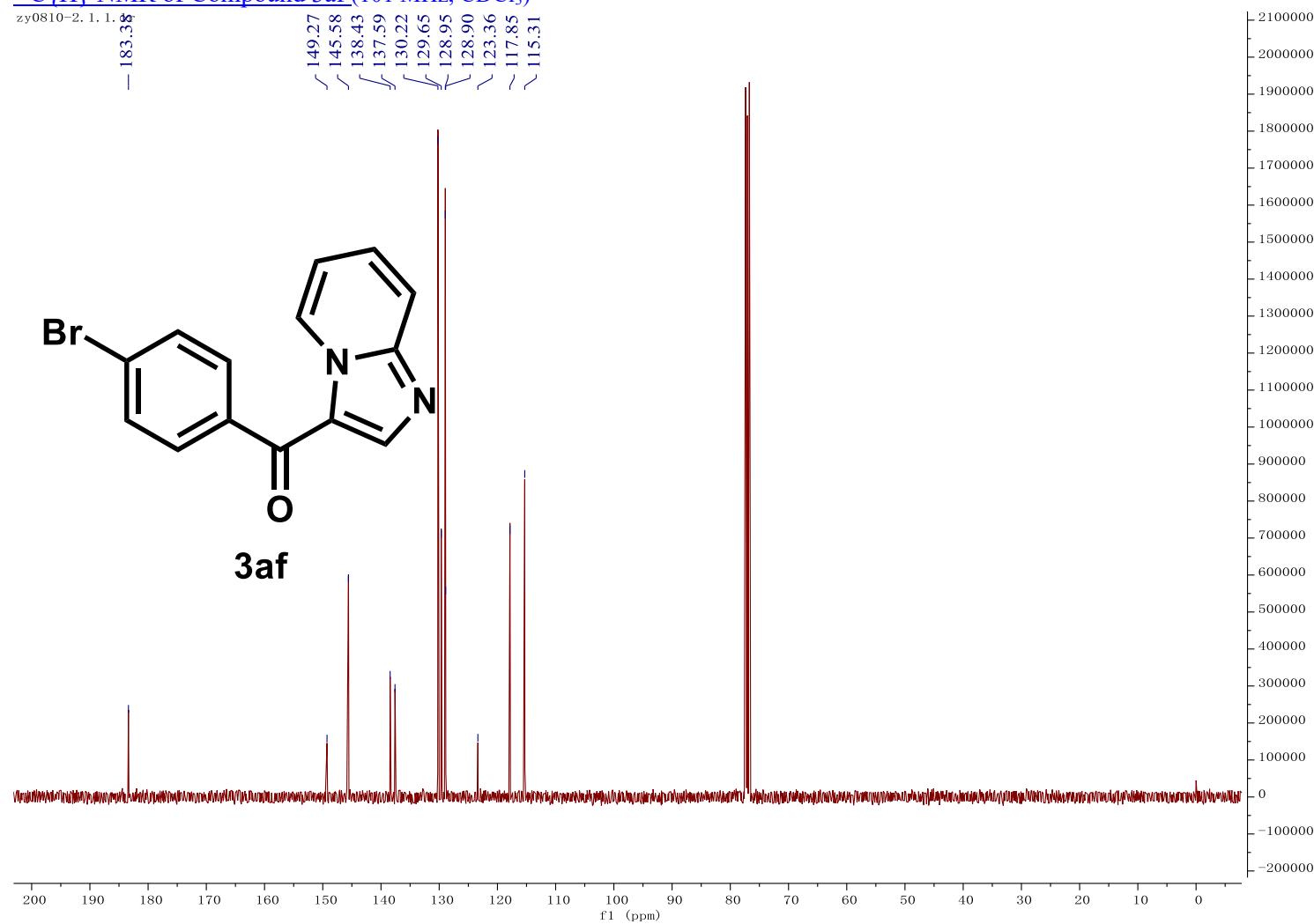
¹H NMR of Compound 3af (400 MHz, CDCl₃)

xy0810-3.1.1.1r



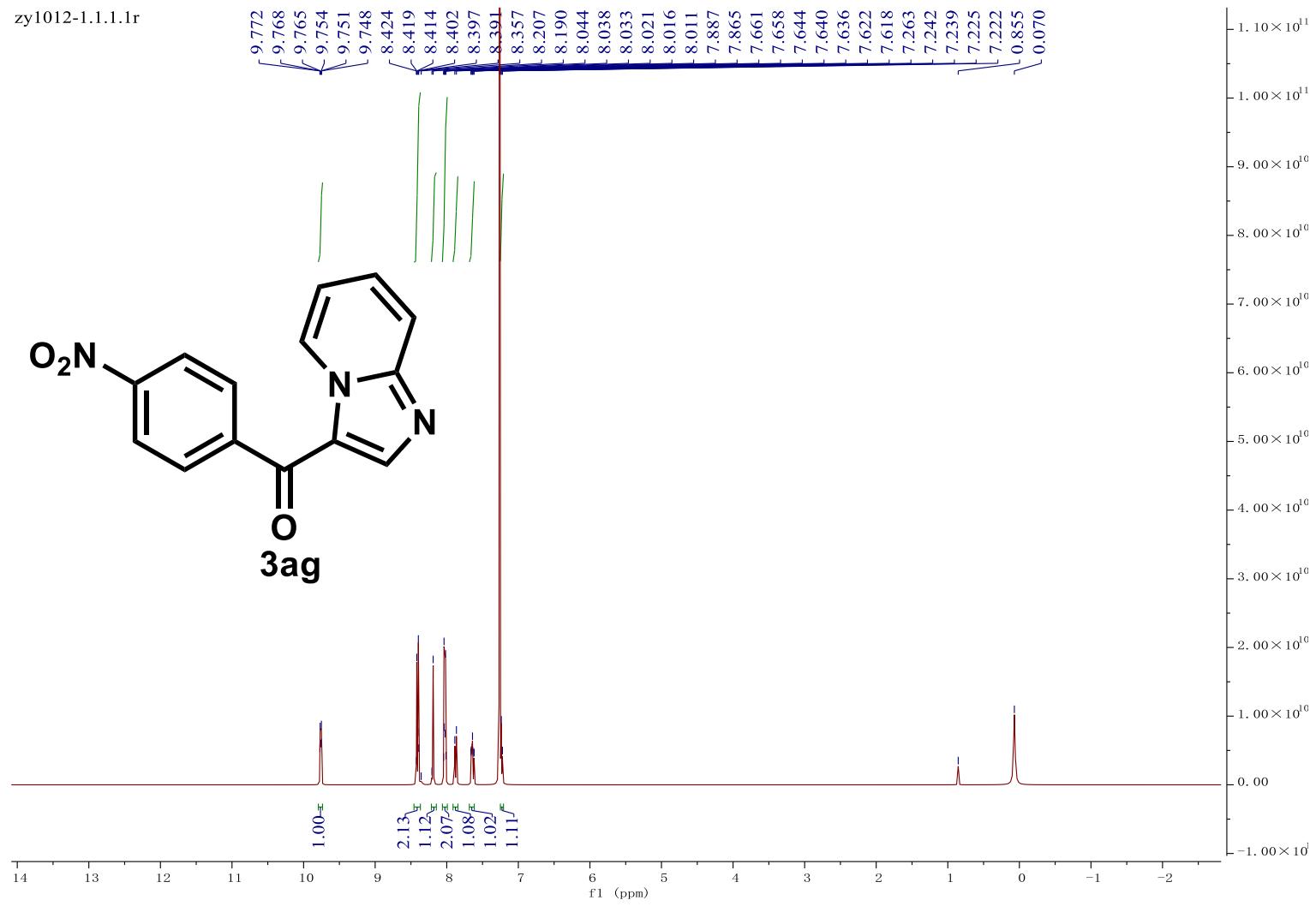
¹³C{H} NMR of Compound 3af (101 MHz, CDCl₃)

zy0810-2, 1, 1.48



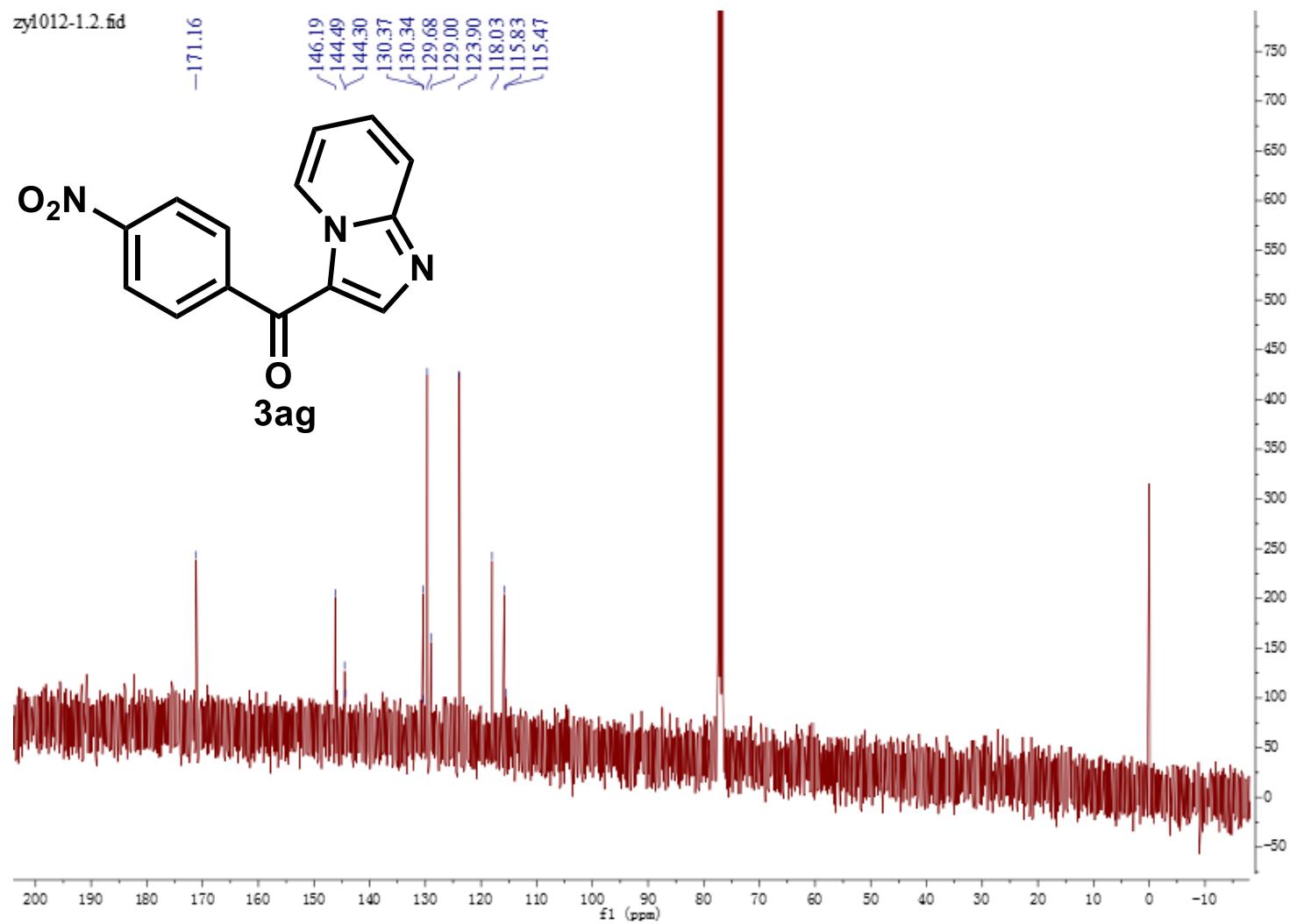
¹H NMR of Compound 3ag (400 MHz, CDCl₃)

zy1012-1.1.1.1r



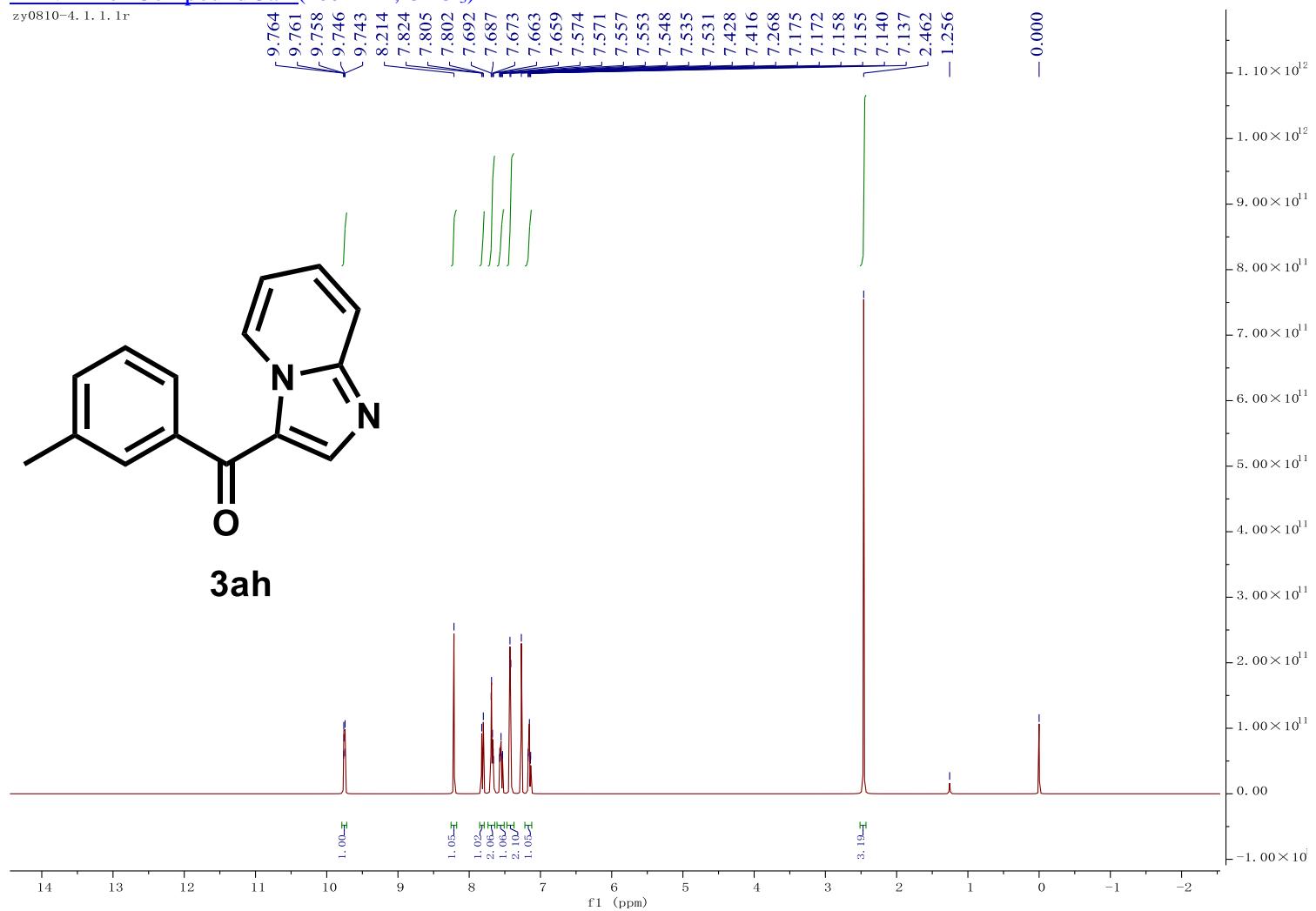
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zy1012-1.2.fid



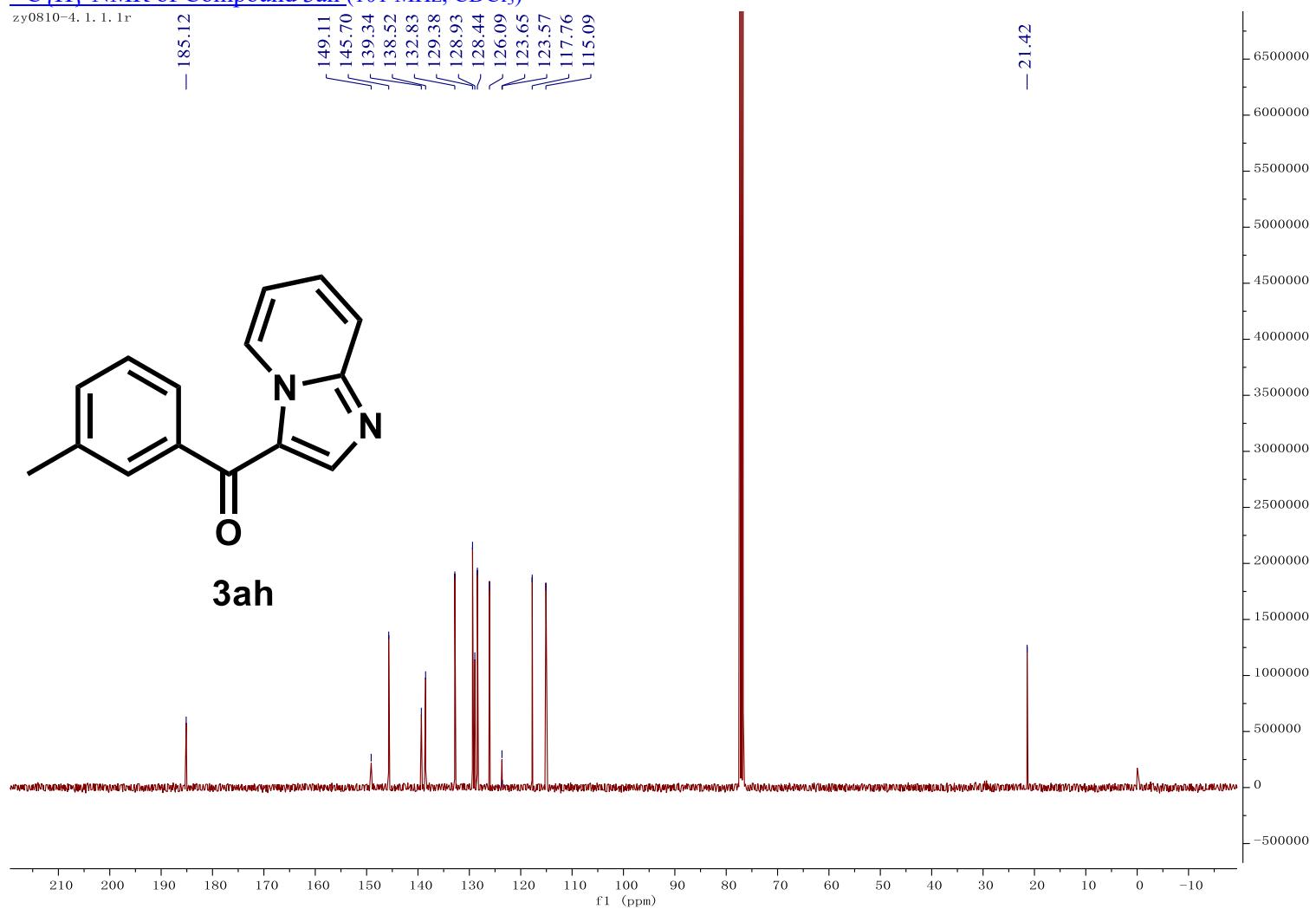
¹H NMR of Compound 3ah (400 MHz, CDCl₃)

zy0810-4. 1. 1. 1r



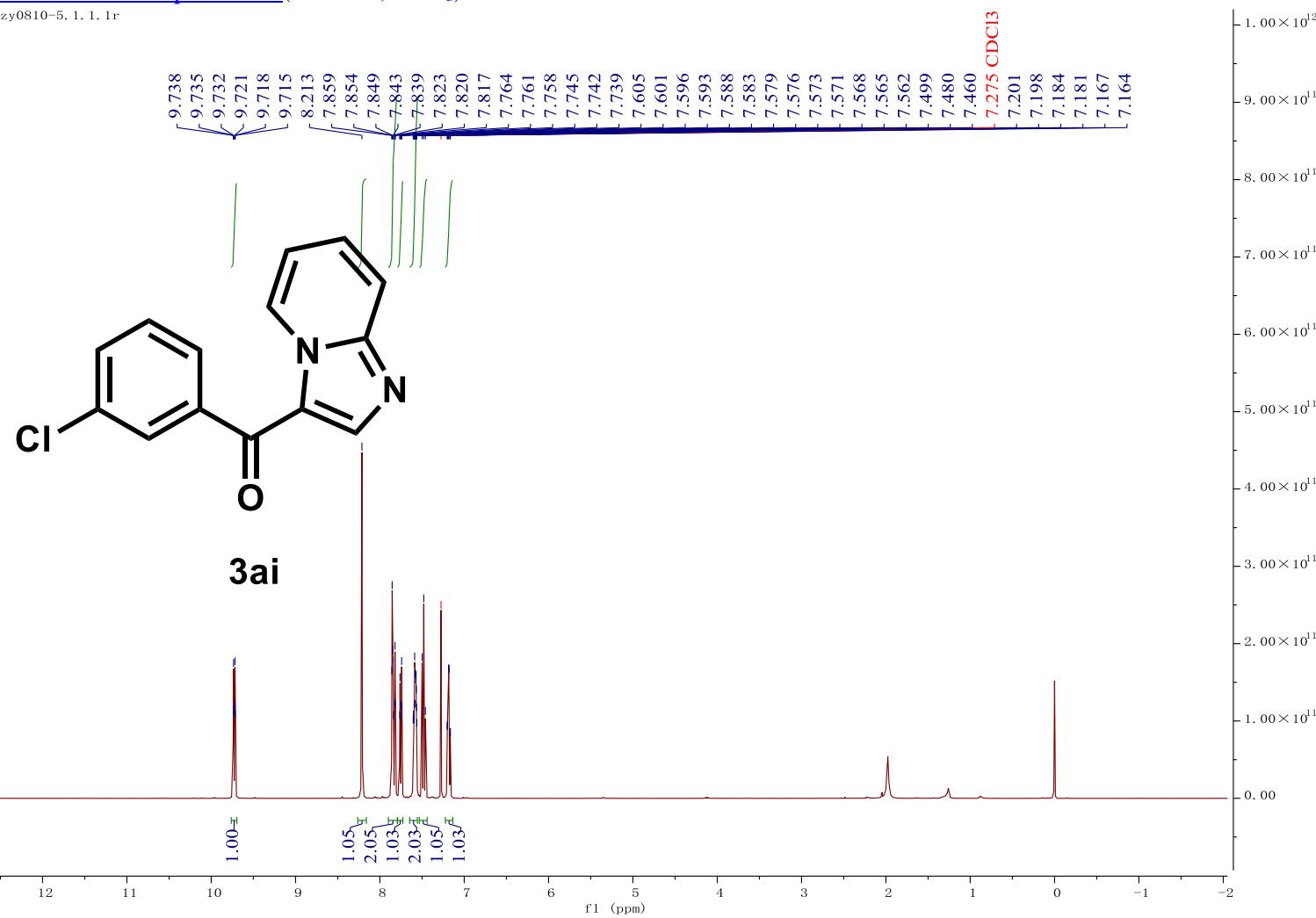
¹³C{H} NMR of Compound 3ah (101 MHz, CDCl₃)

zy0810-4. 1. 1. lr

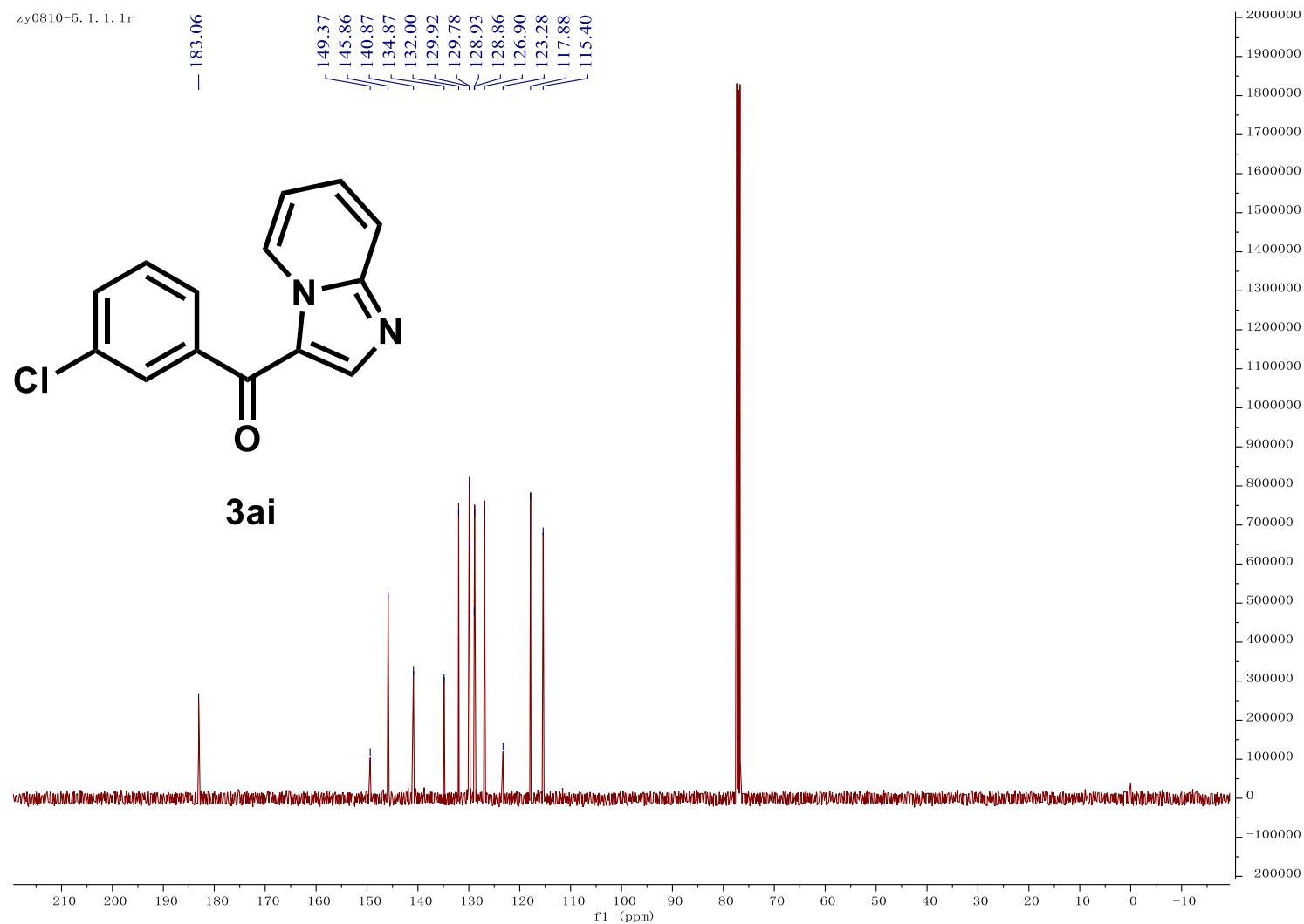


¹H NMR of Compound 3ai (400 MHz, CDCl₃)

zy0810-5. 1. 1. 1r

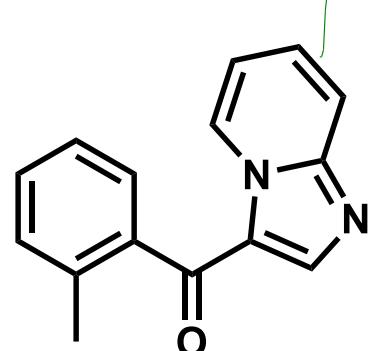


¹³C{H} NMR of Compound 3ai (101 MHz, CDCl₃)

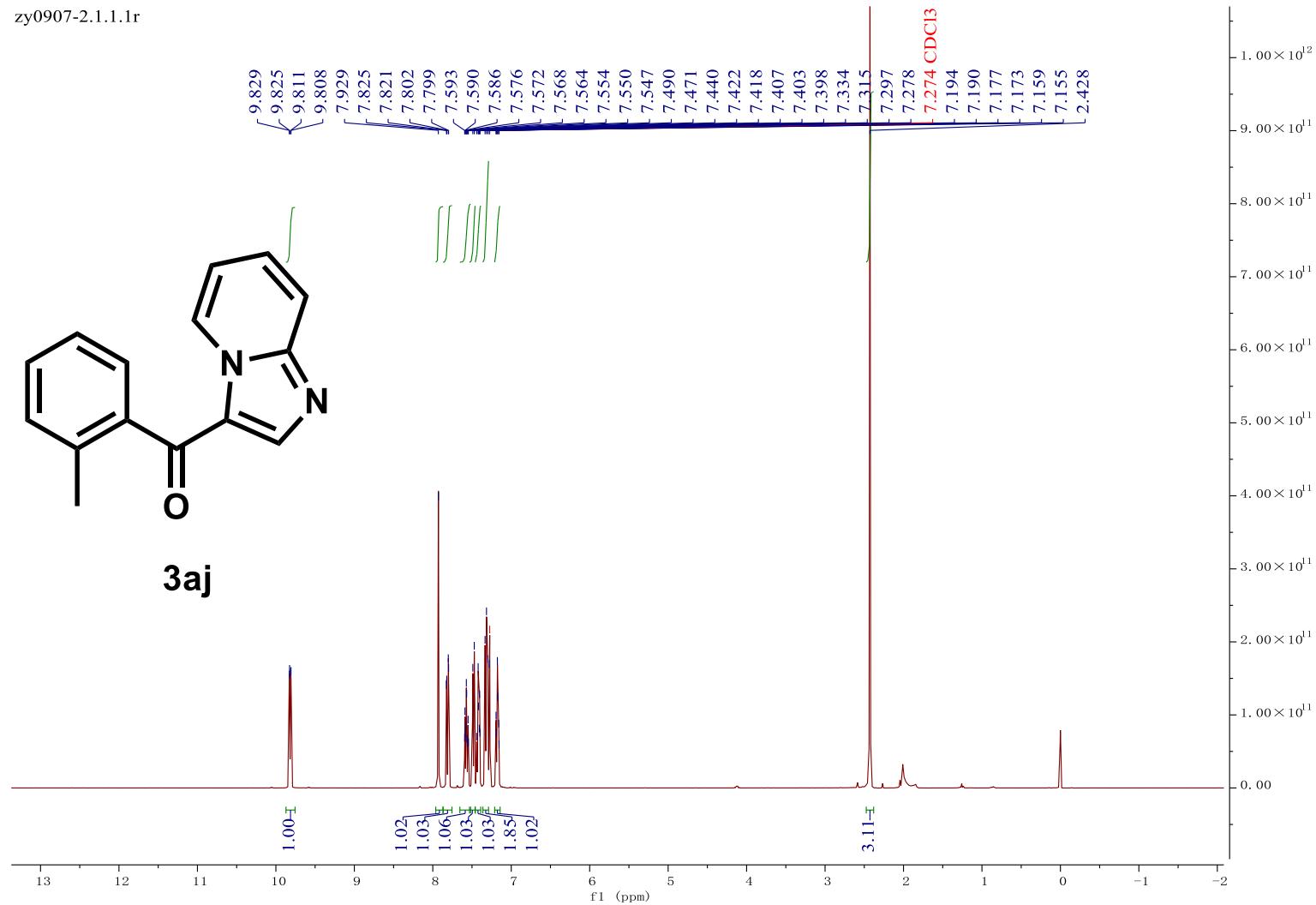


¹H NMR of Compound 3aj (400 MHz, CDCl₃)

zy0907-2.1.1.1r



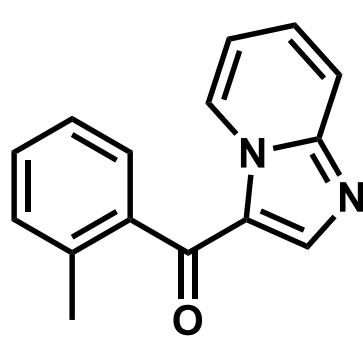
3aj



¹³C{H} NMR of Compound 3aj (101 MHz, CDCl₃)

zy0907-2.2.1.1r

- 186.88

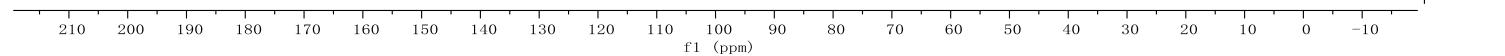


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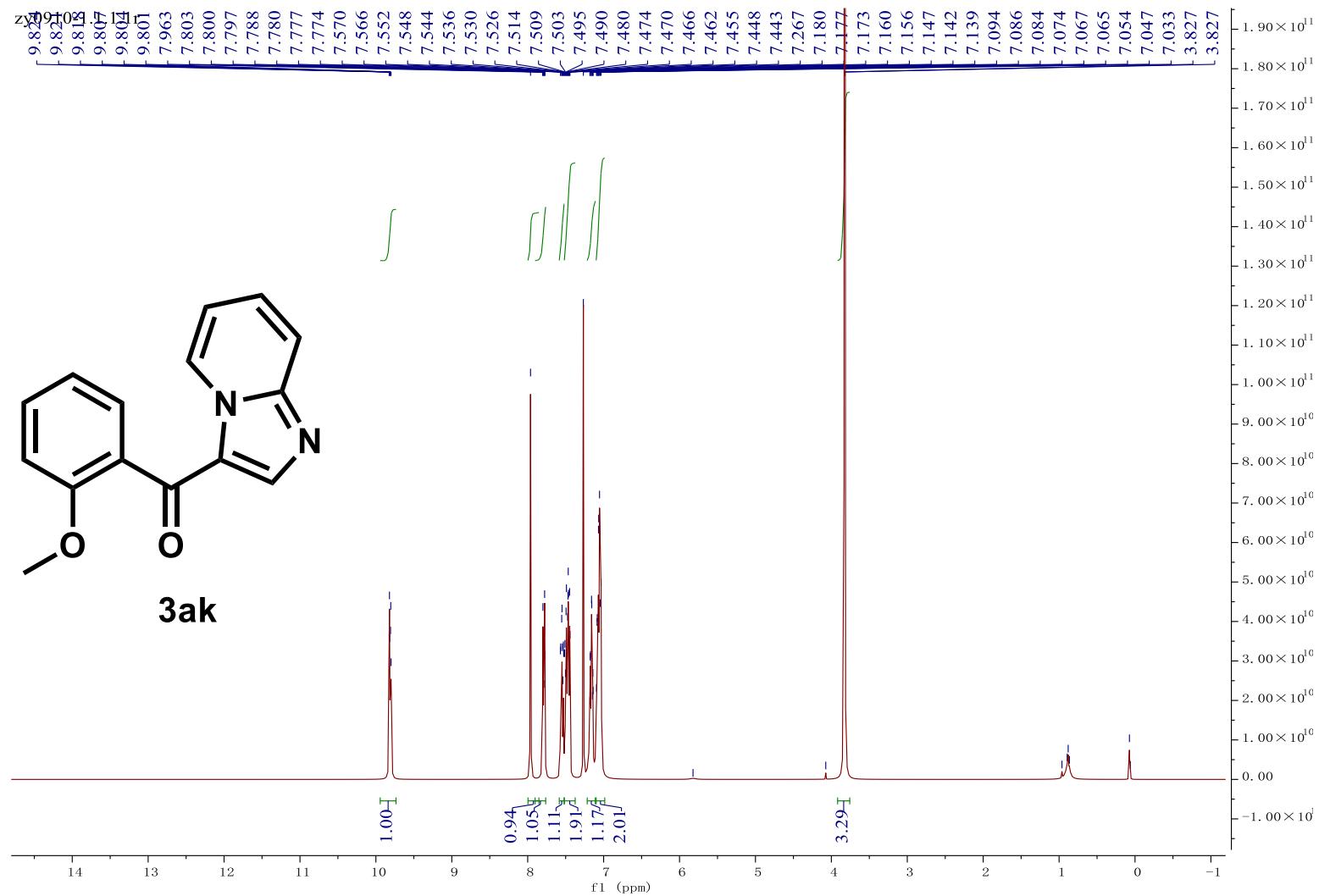
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146.47
138.98
136.52
131.17
130.29
129.57
128.96
128.25
125.34
124.49
117.84
115.26

- 19.64

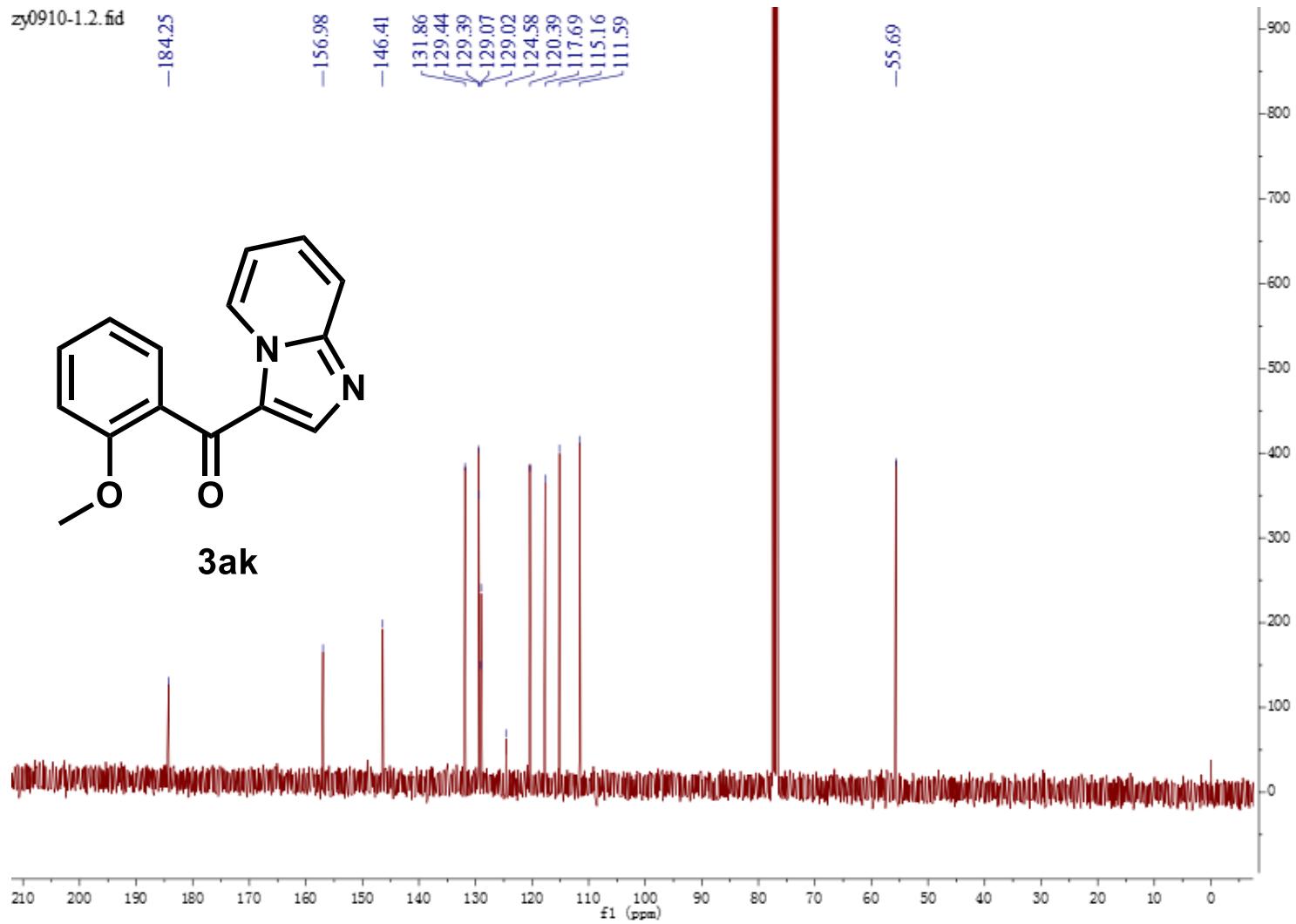
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1500000
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500000
0
-500000



¹H NMR of Compound 3ak (400 MHz, CDCl₃)

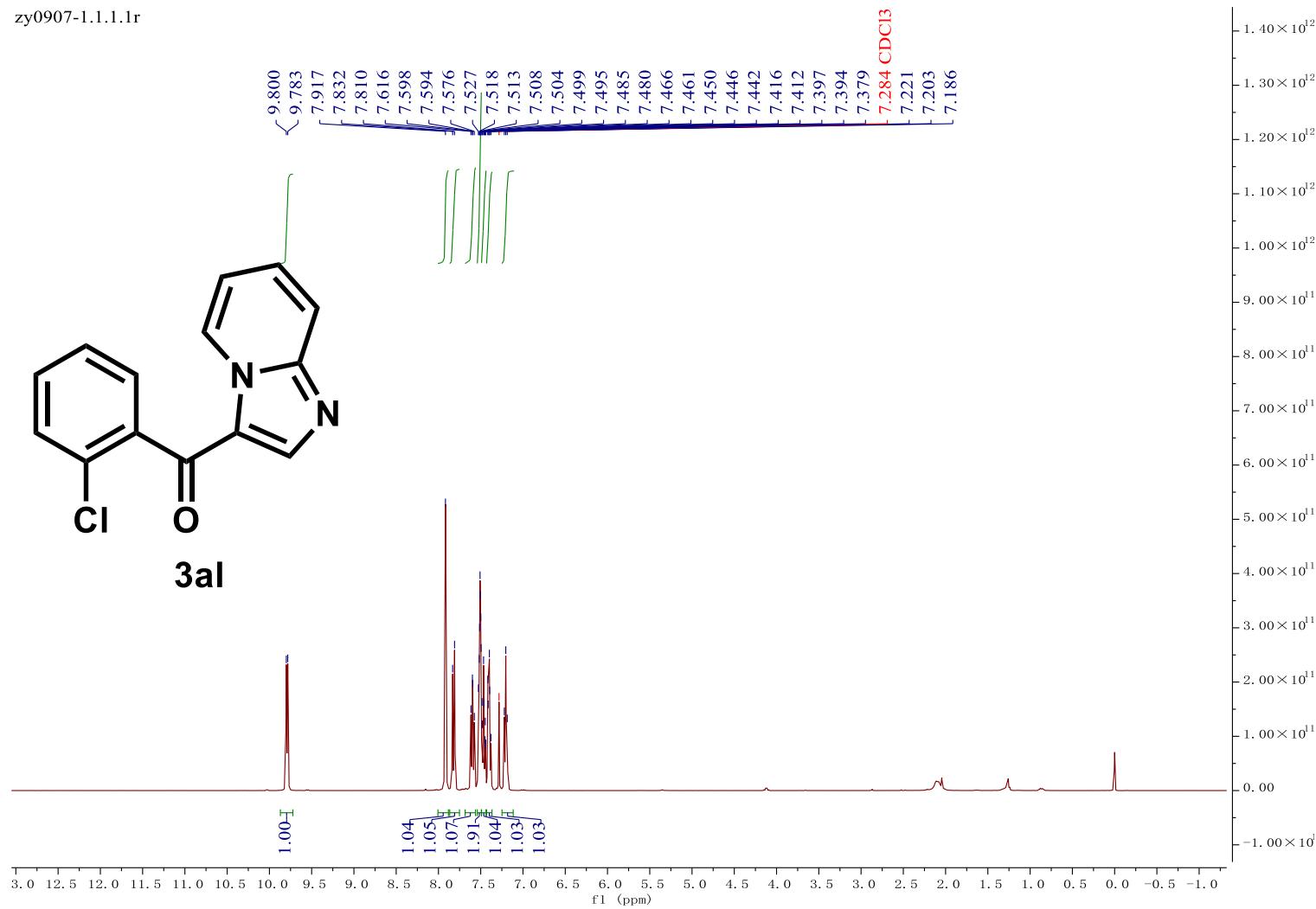


¹³C{H} NMR of Compound 3ak (101 MHz, CDCl₃)

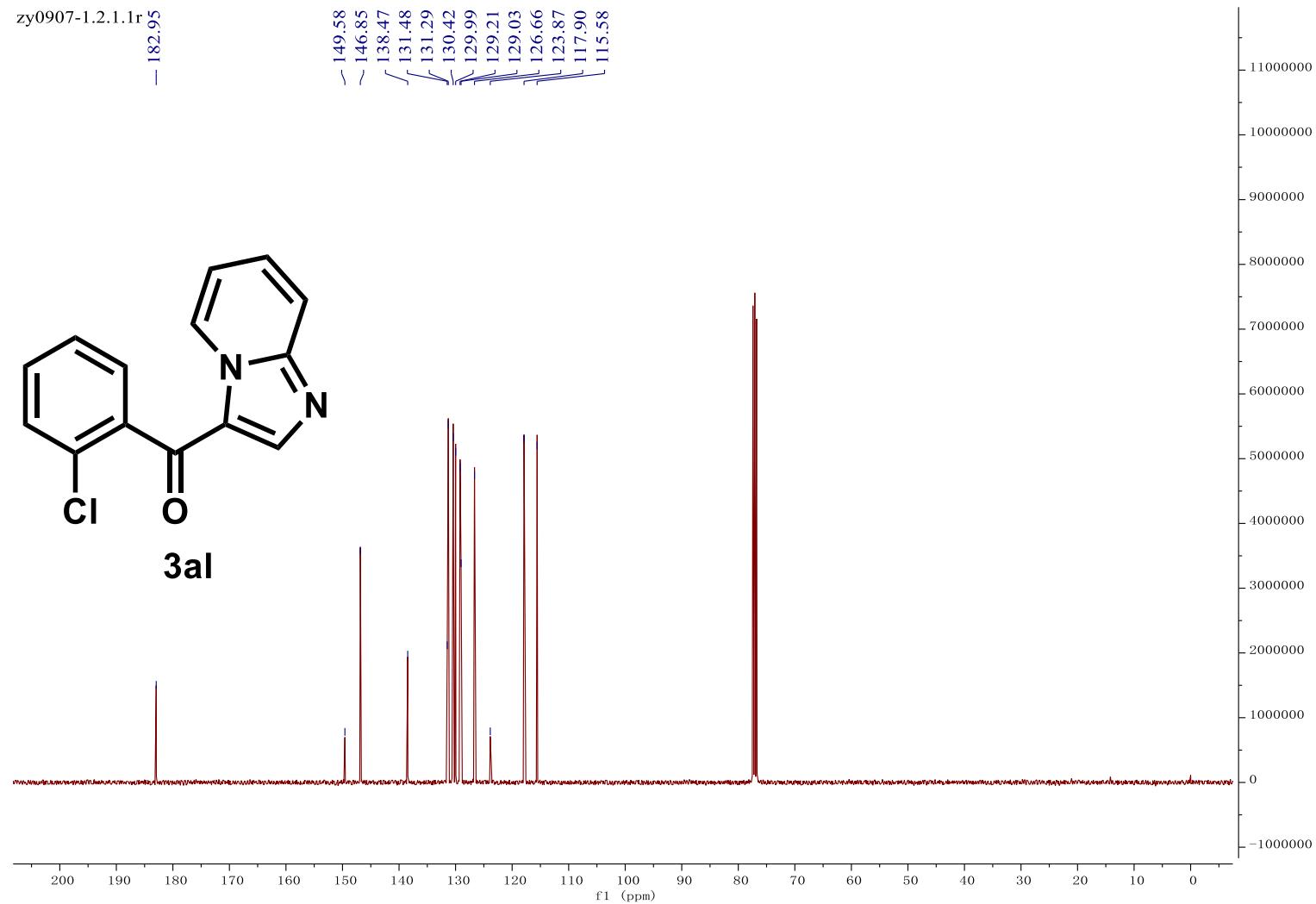


¹H NMR of Compound 3al (400 MHz, CDCl₃)

zy0907-1.1.1.1r

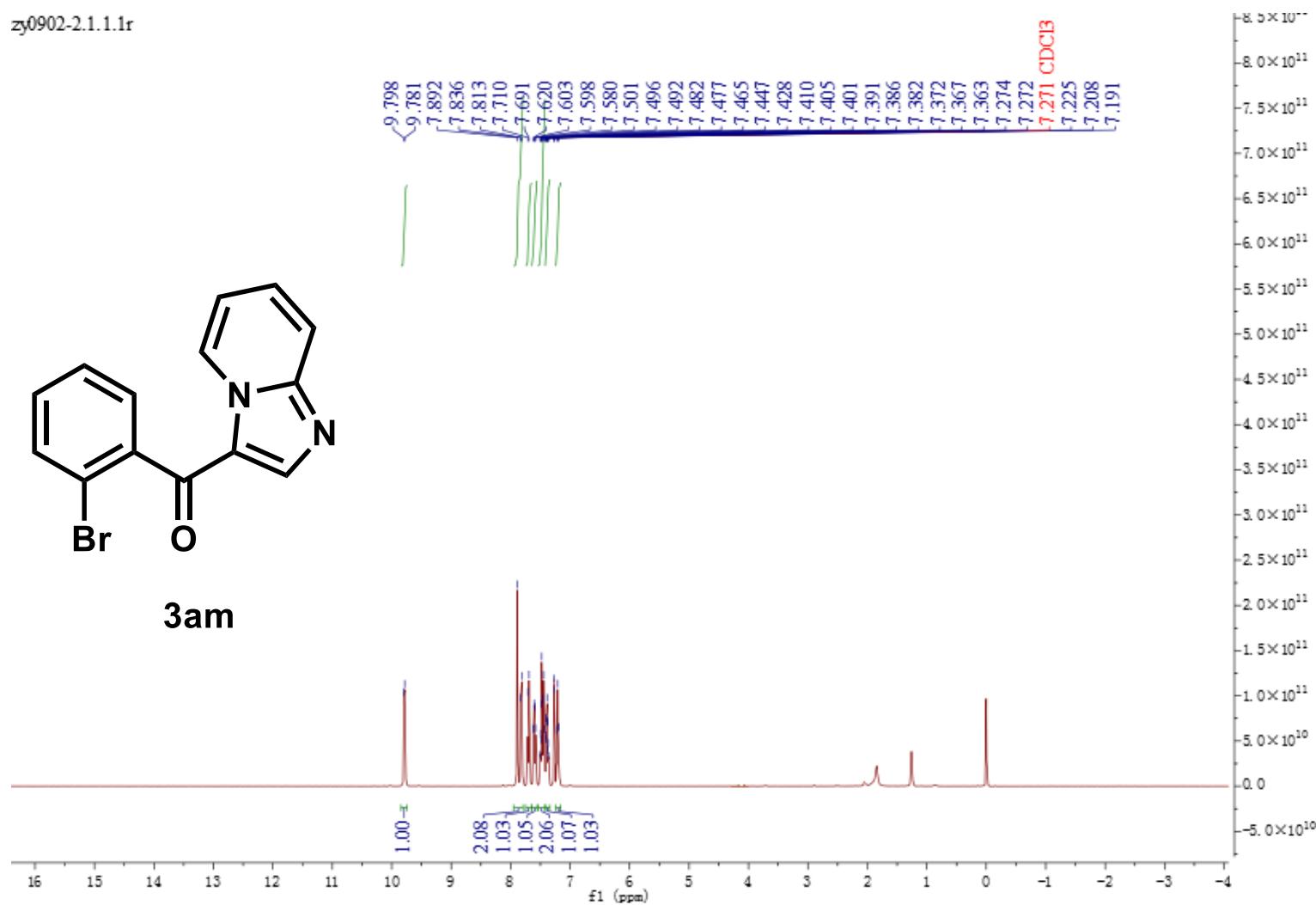


¹³C{H} NMR of Compound 3al (101 MHz, CDCl₃)



¹H NMR of Compound 3am (400 MHz, CDCl₃)

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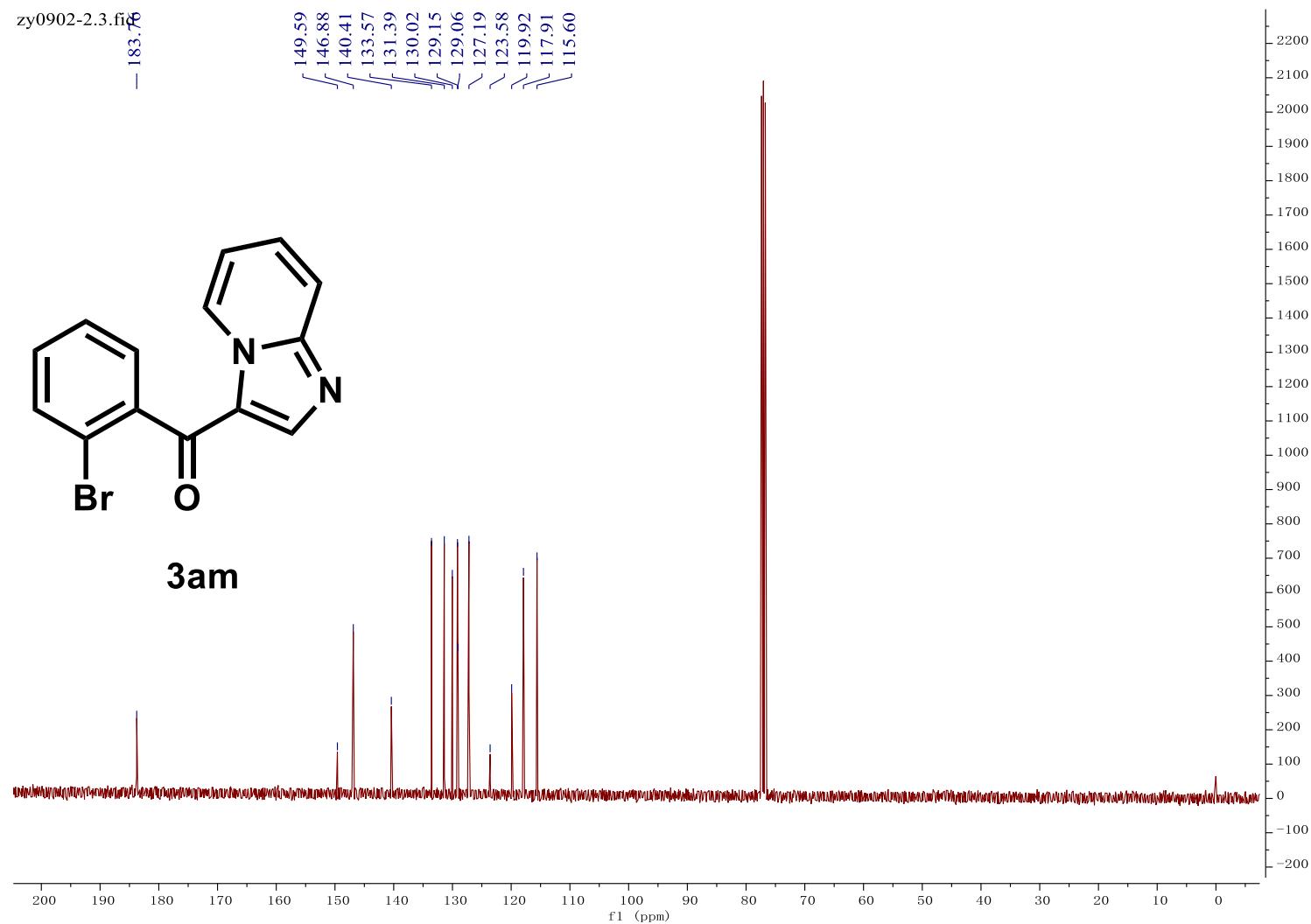
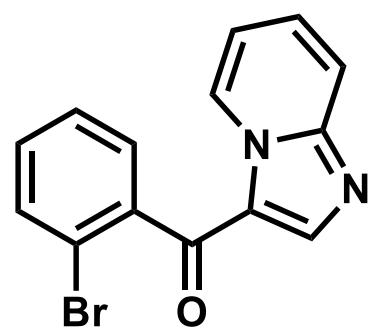


¹³C{H} NMR of Compound 3am (101 MHz, CDCl₃)

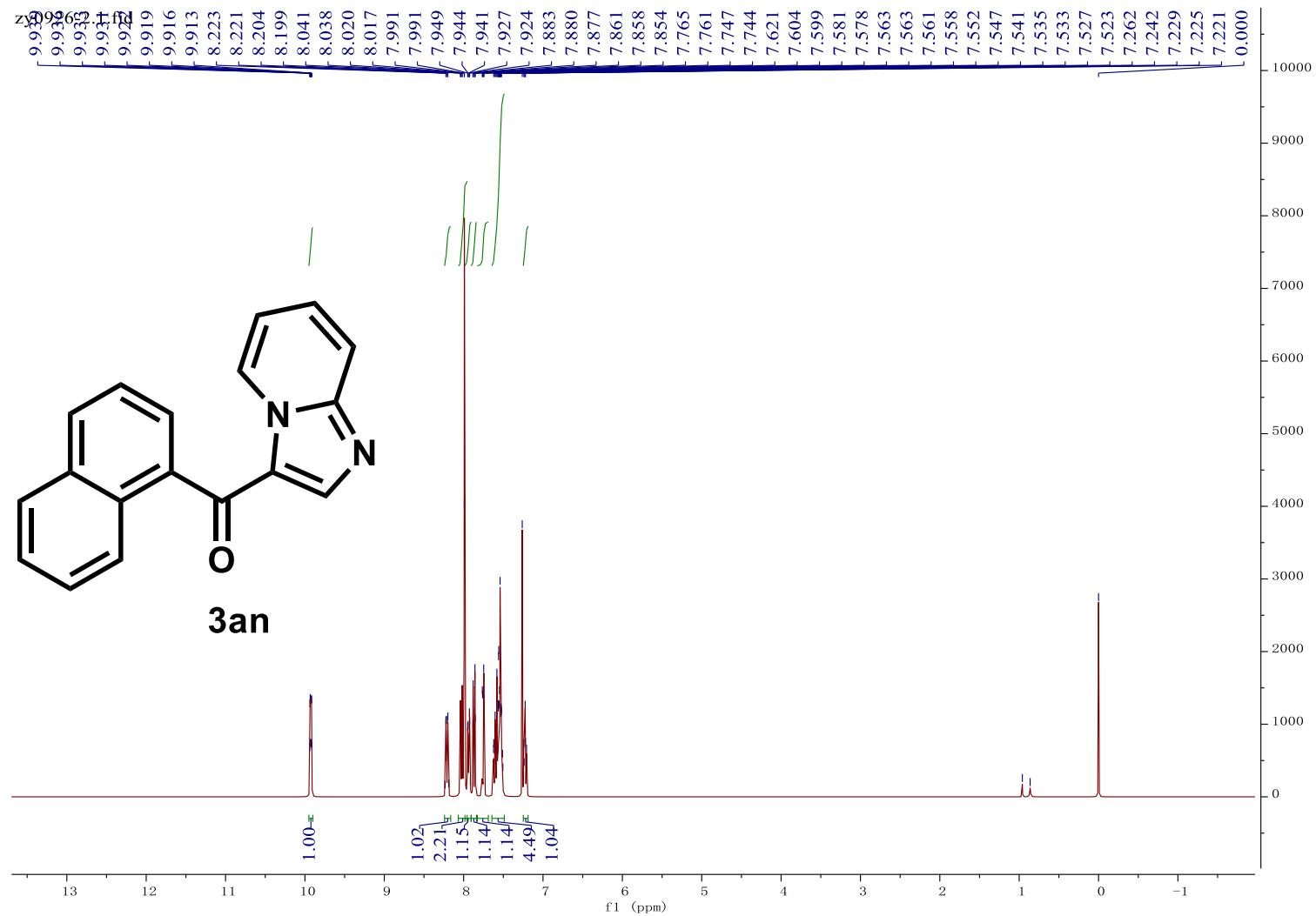
zy0902-2.3.firebaseio

- 183.78

149.59
146.88
140.41
133.57
131.39
130.02
129.15
129.06
127.19
123.58
119.92
117.91
115.60



¹H NMR of Compound 3an (400 MHz, CDCl₃)

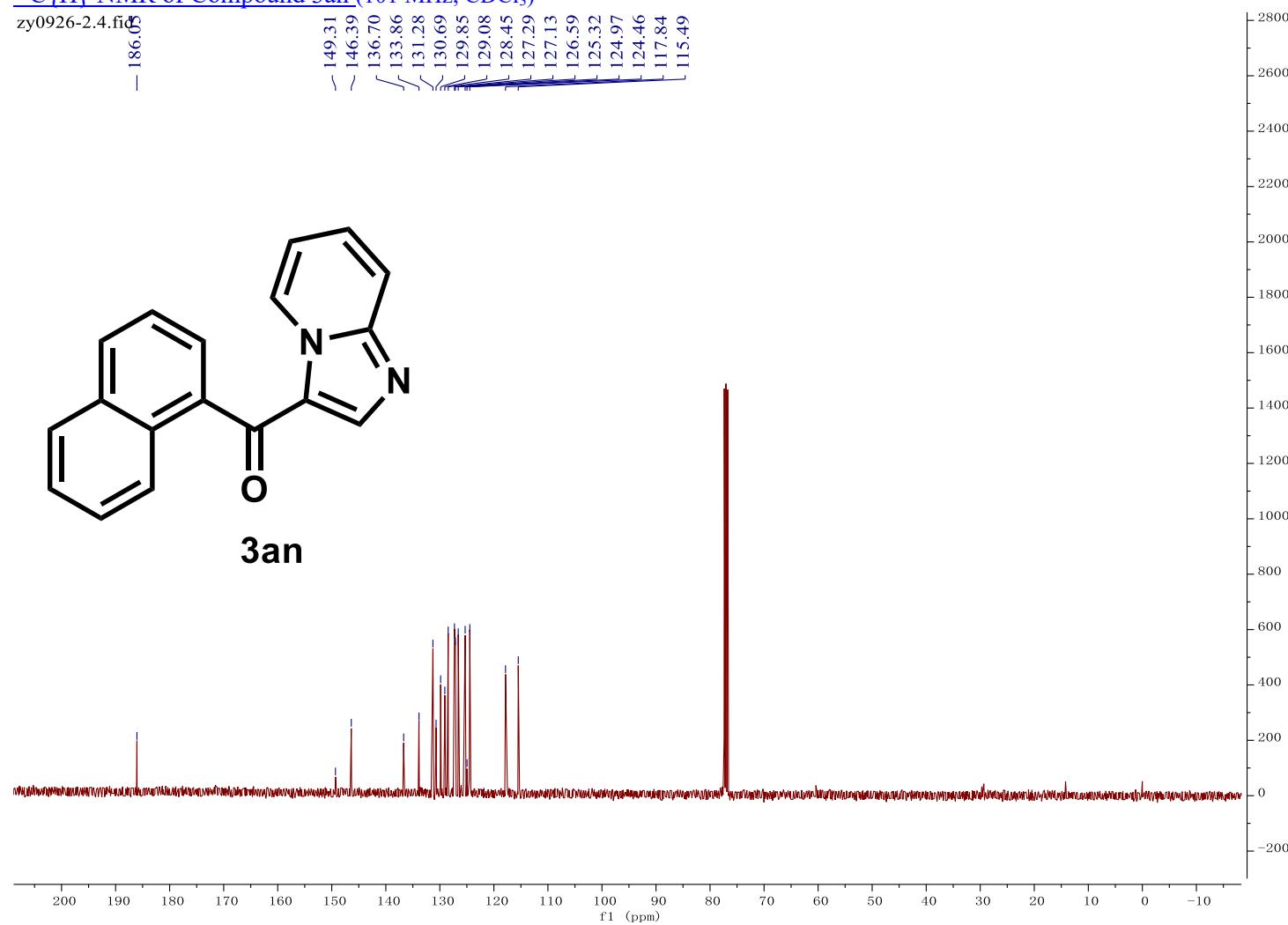
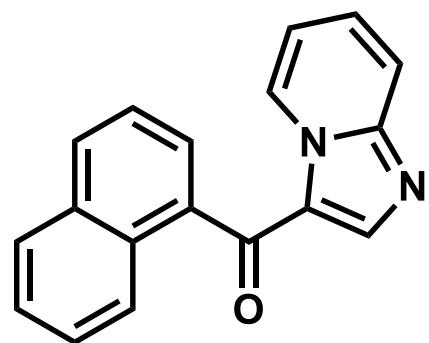


¹³C{H} NMR of Compound 3an (101 MHz, CDCl₃)

zy0926-2.4.fid

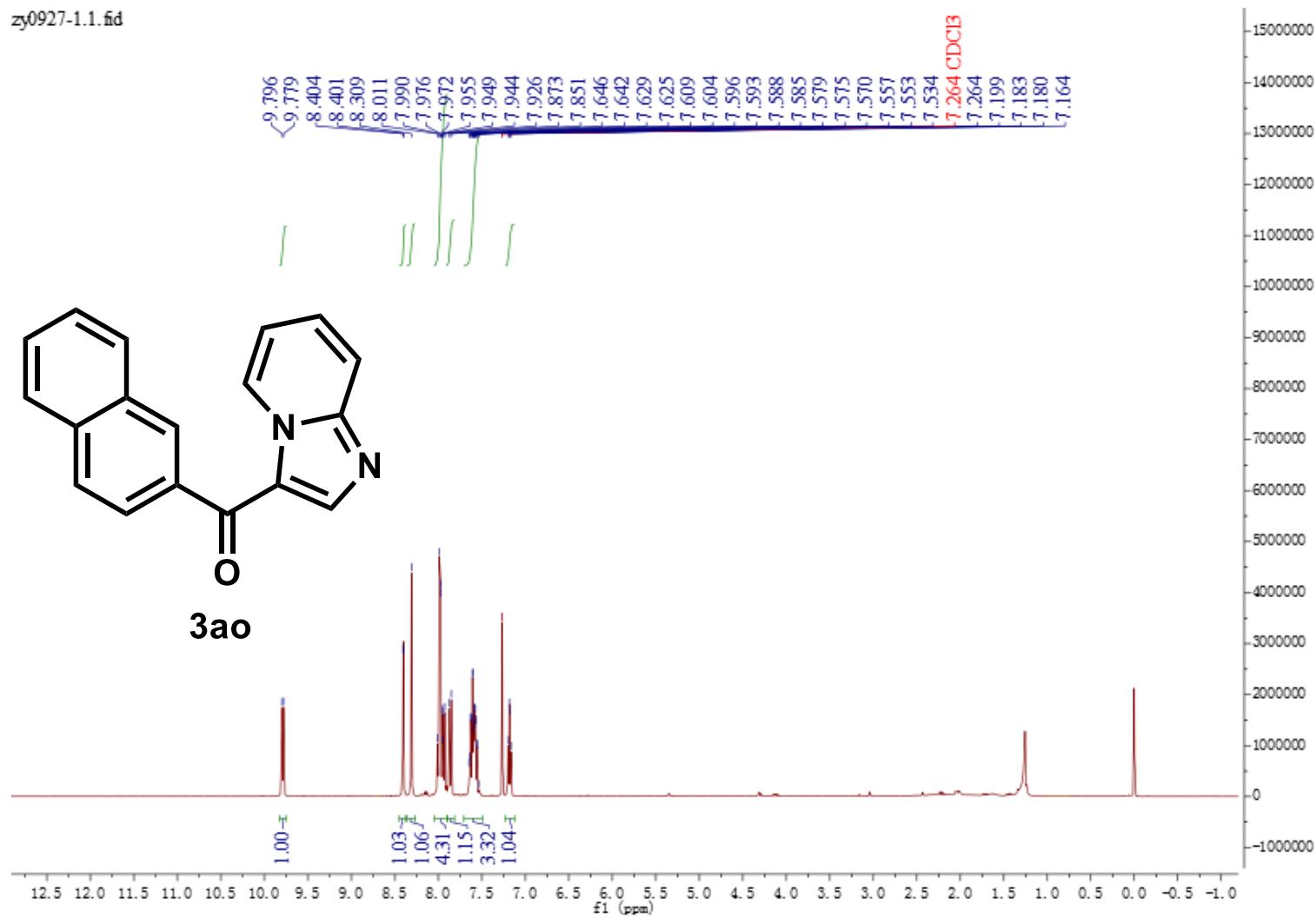
-186.0

149.31
146.39
136.70
133.86
131.28
130.69
129.85
129.08
128.45
127.29
127.13
126.59
125.32
124.97
124.46
117.84
115.49



¹H NMR of Compound 3ao (400 MHz, CDCl₃)

zy0927-1.1.fid

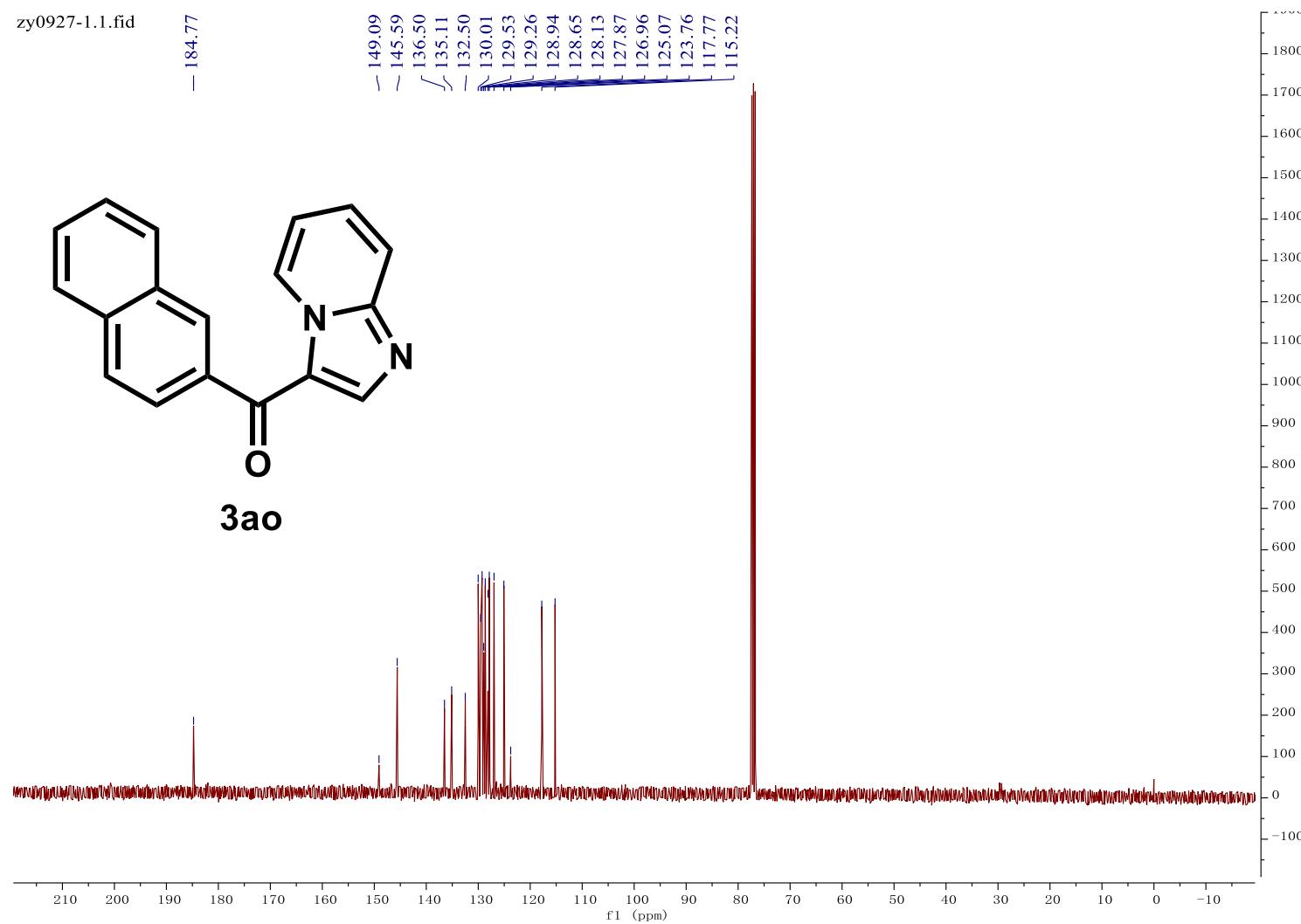
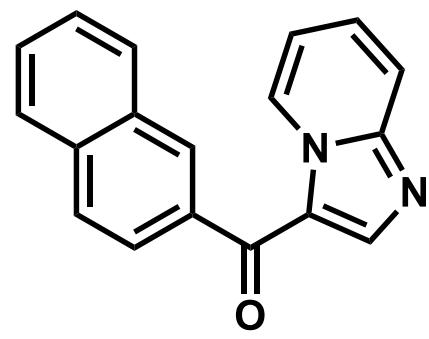


¹³C{H} NMR of Compound 3ao (101 MHz, CDCl₃)

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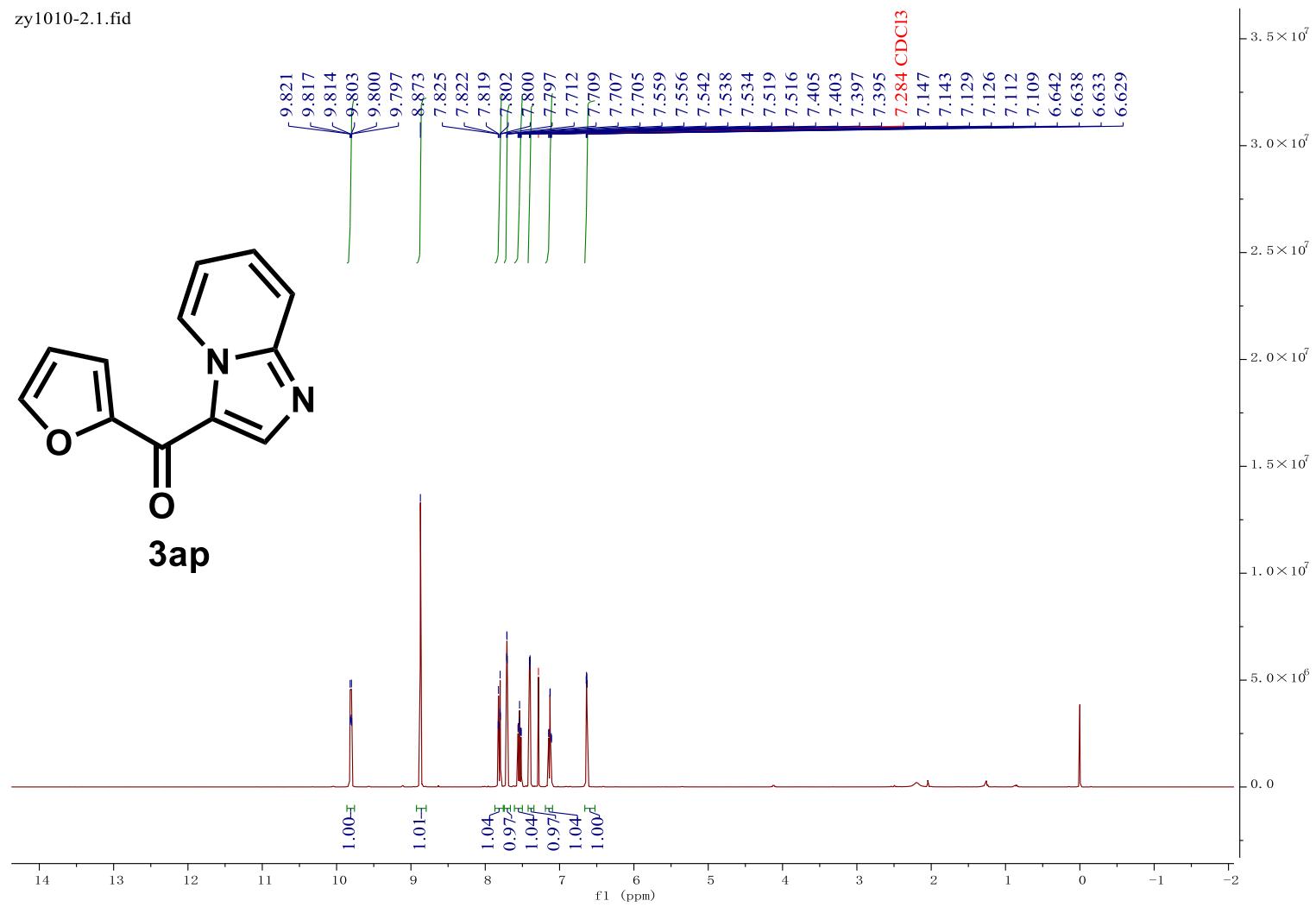
- 184.77

- 149.09
- 145.59
- 136.50
- 135.11
- 132.50
- 130.01
- 129.53
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- 128.65
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- 127.87
- 126.96
- 125.07
- 123.76
- 117.77
- 115.22

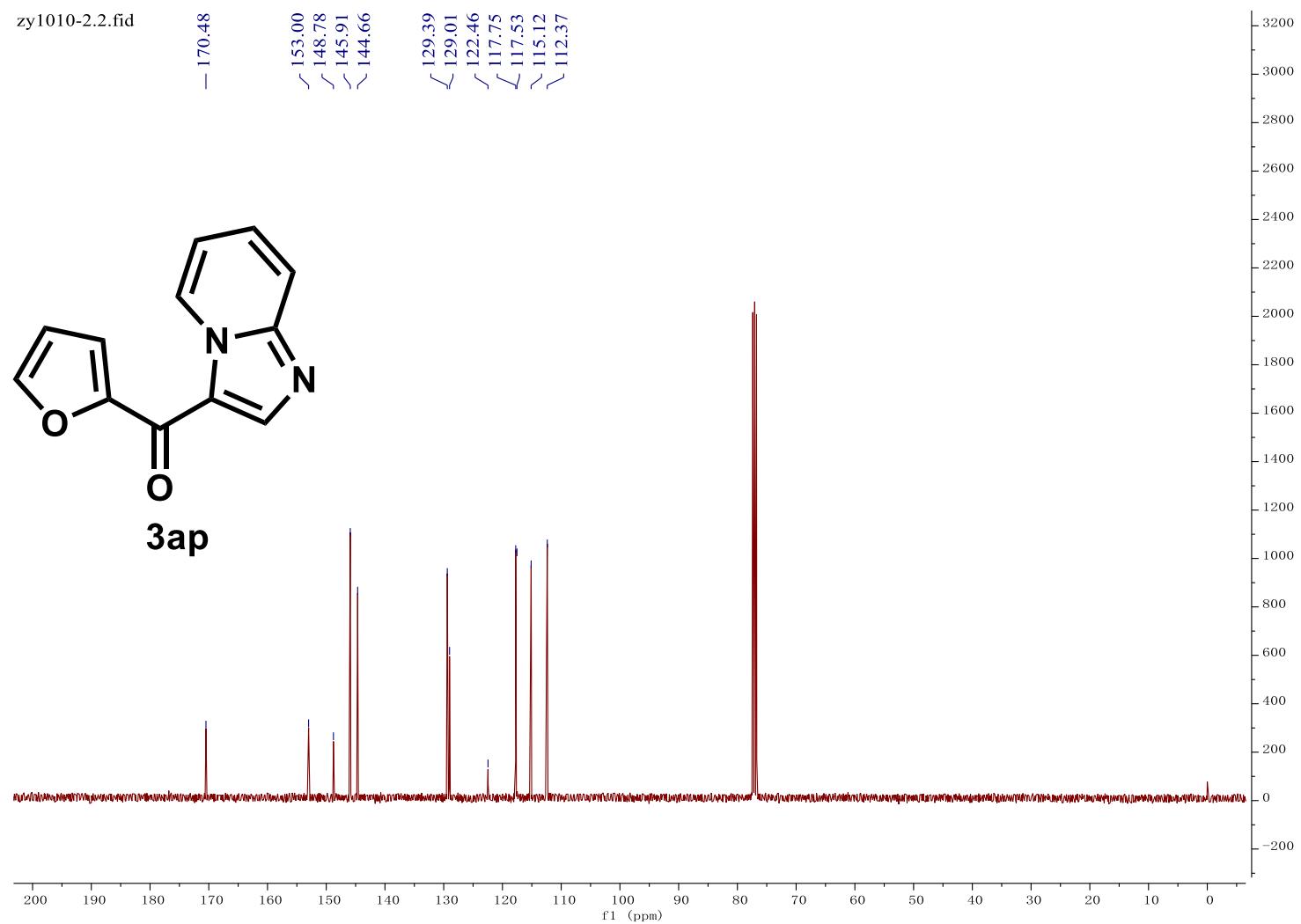


¹H NMR of Compound 3ap (400 MHz, CDCl₃)

zy1010-2.1.fid

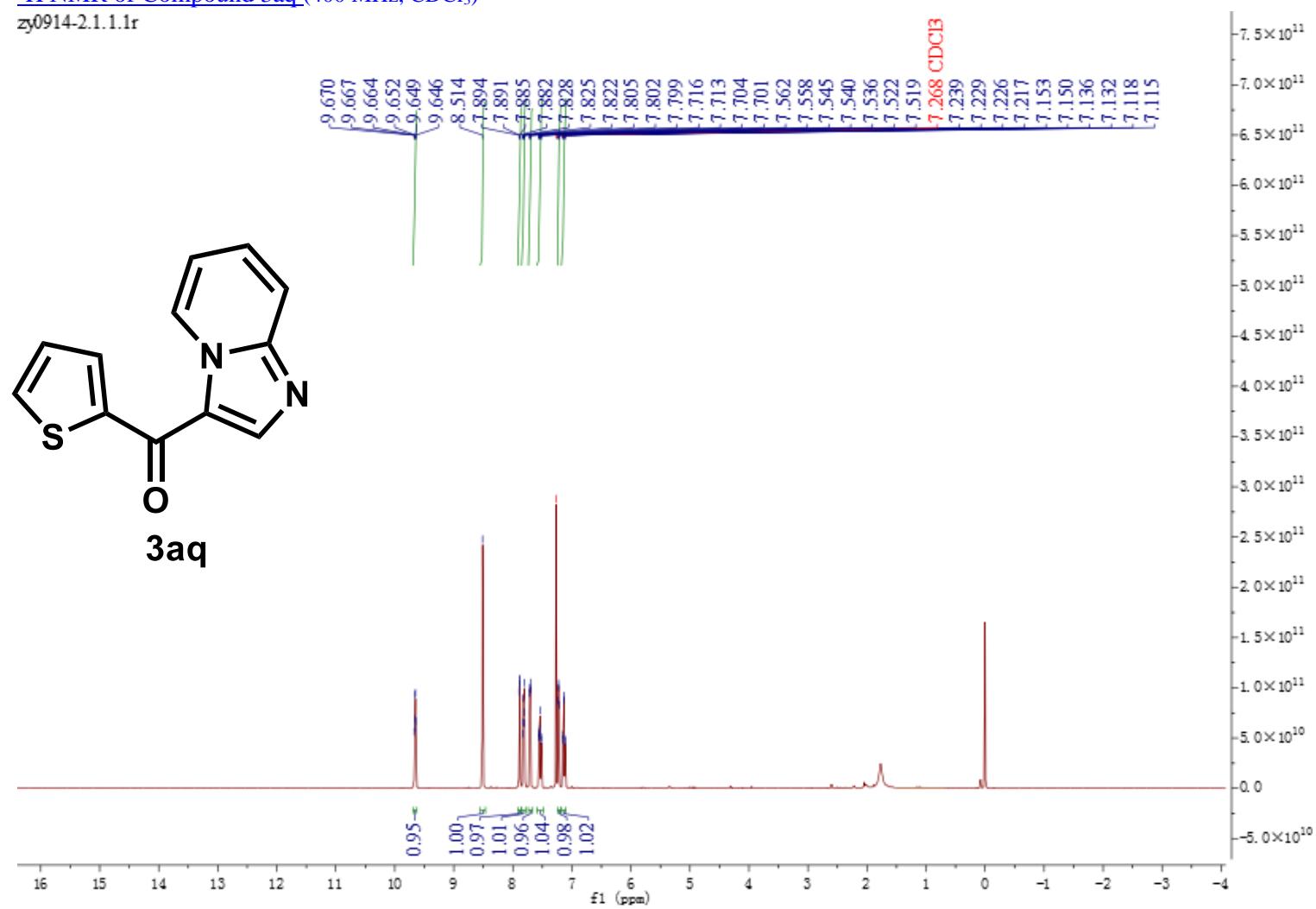


¹³C{H} NMR of Compound 3ao (101 MHz, CDCl₃)



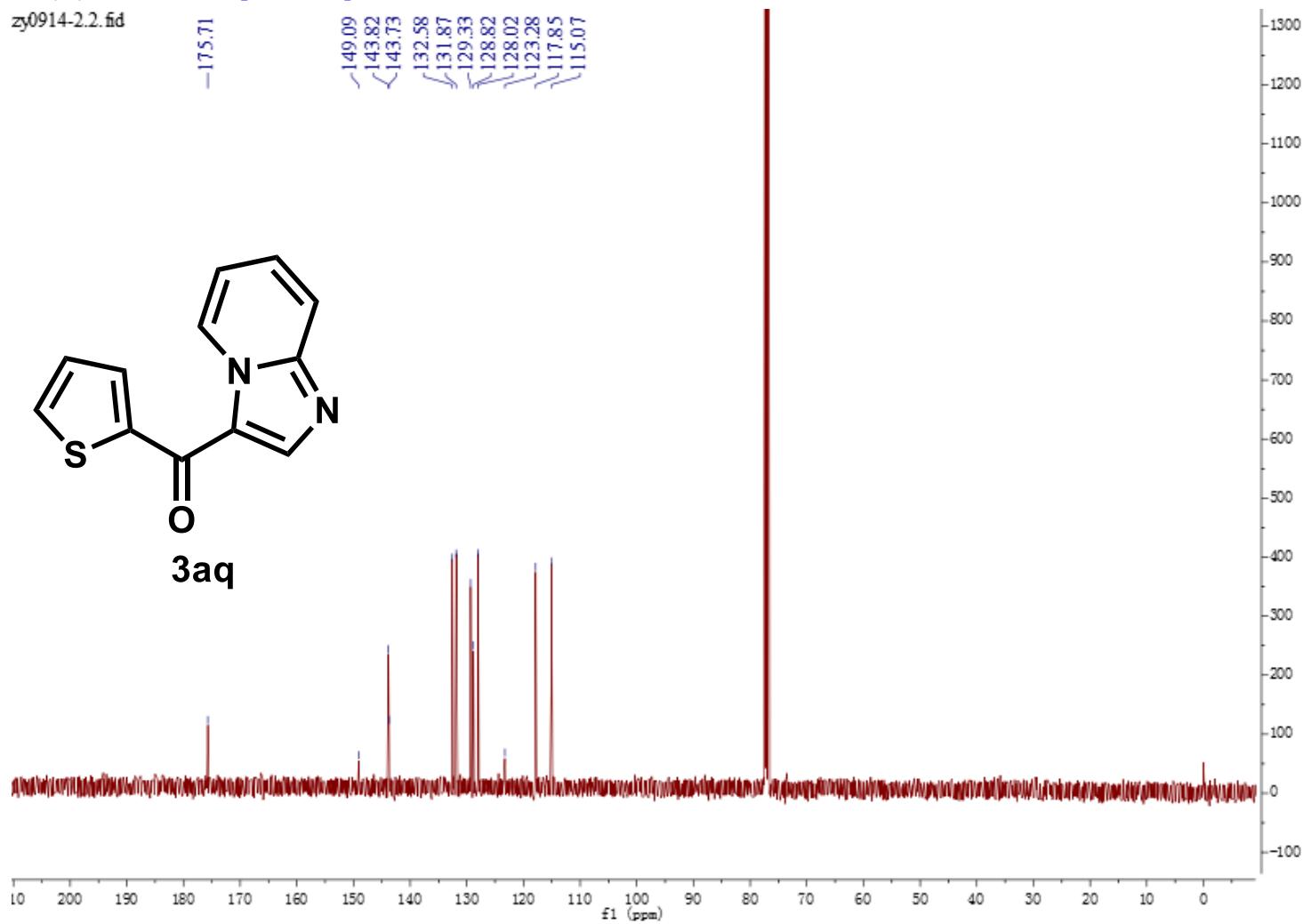
¹H NMR of Compound 3aq (400 MHz, CDCl₃)

zy0914-2.1.1.1r



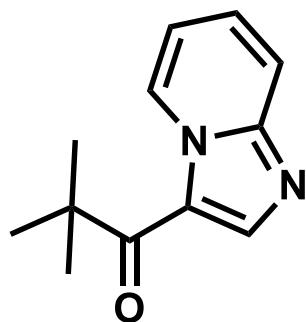
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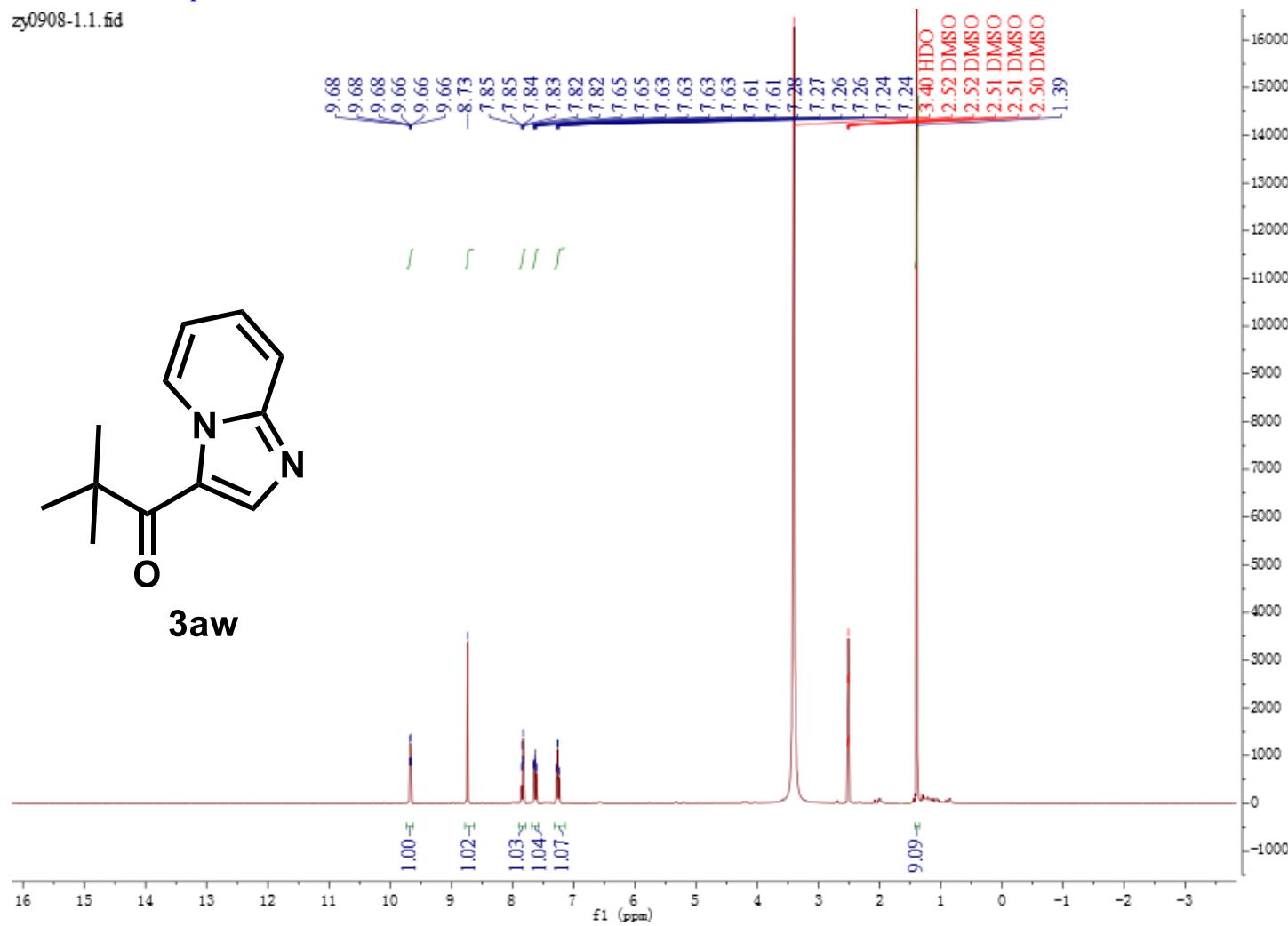


¹H NMR of Compound 3aw (400 MHz, DMSO-d₆)

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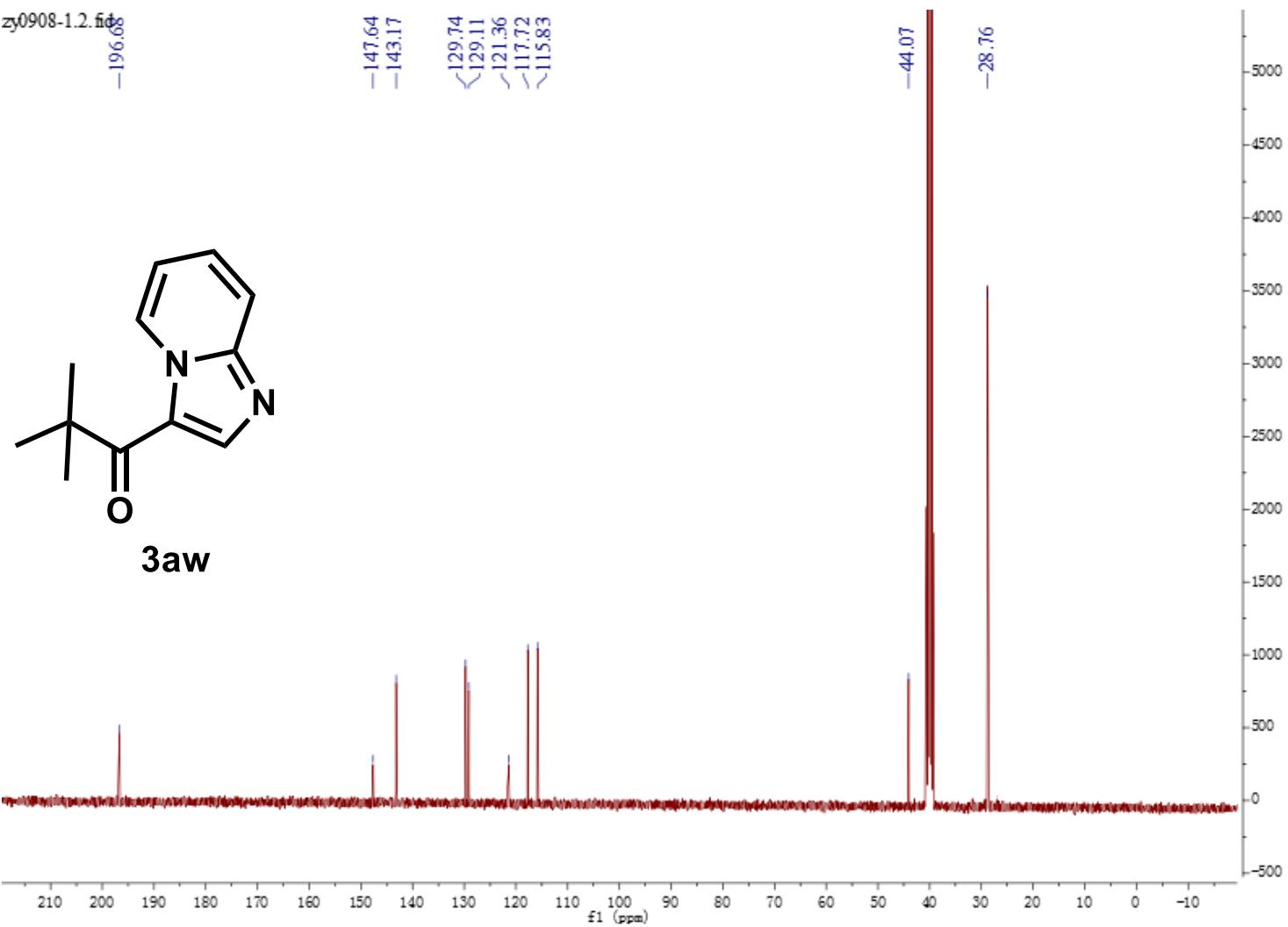


3aw



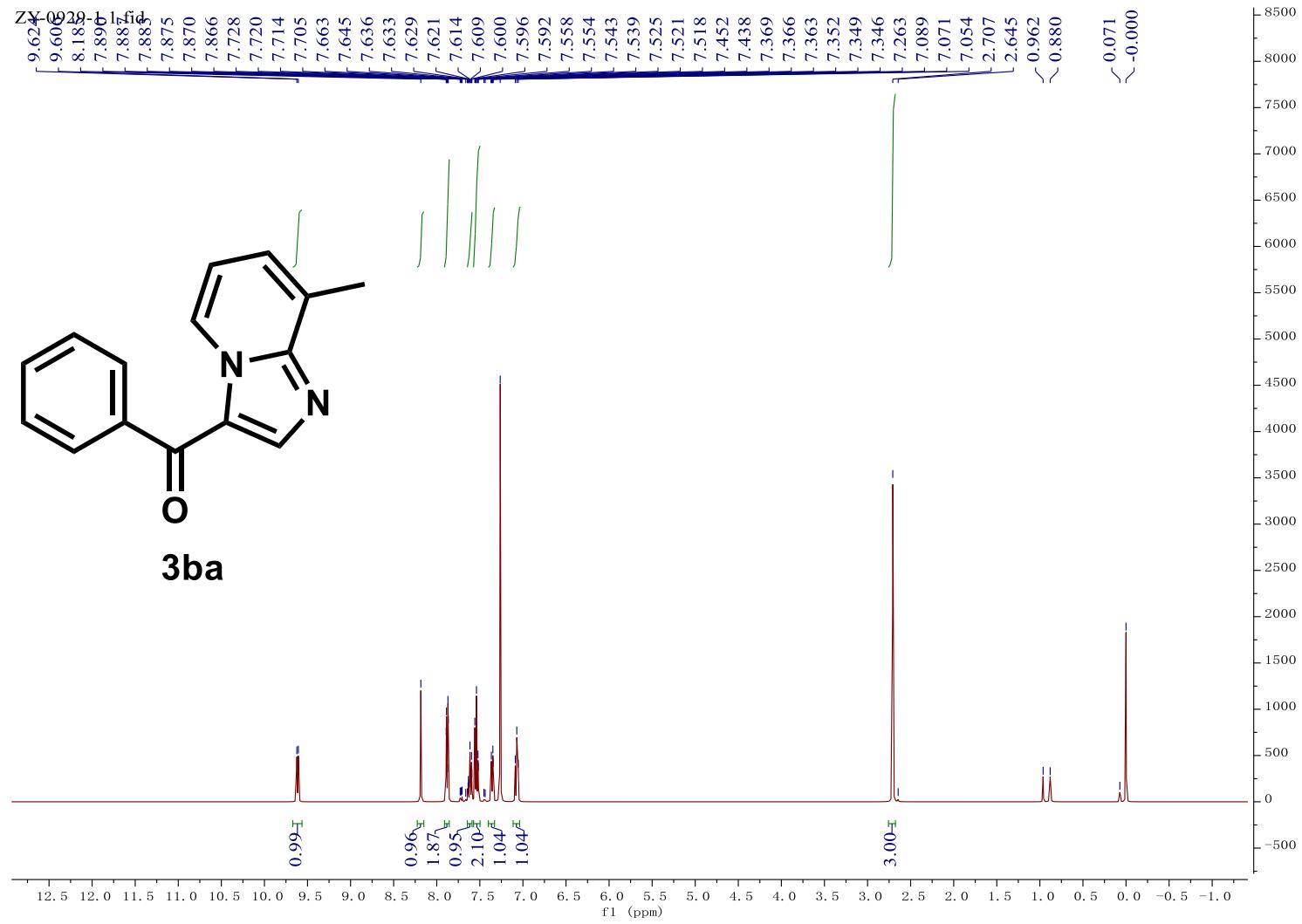
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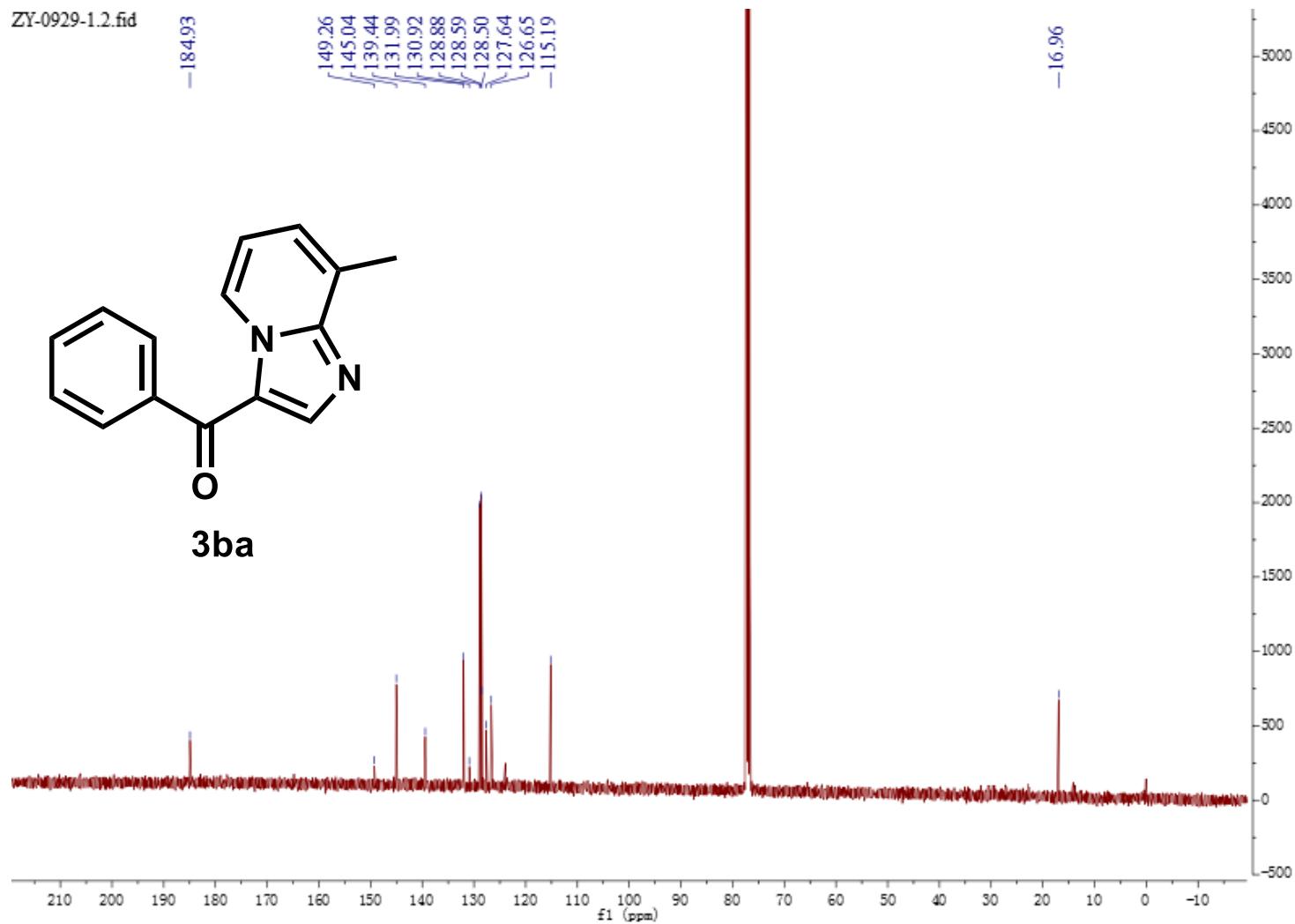
3aw

¹H NMR of Compound 3ba (400 MHz, CDCl₃)



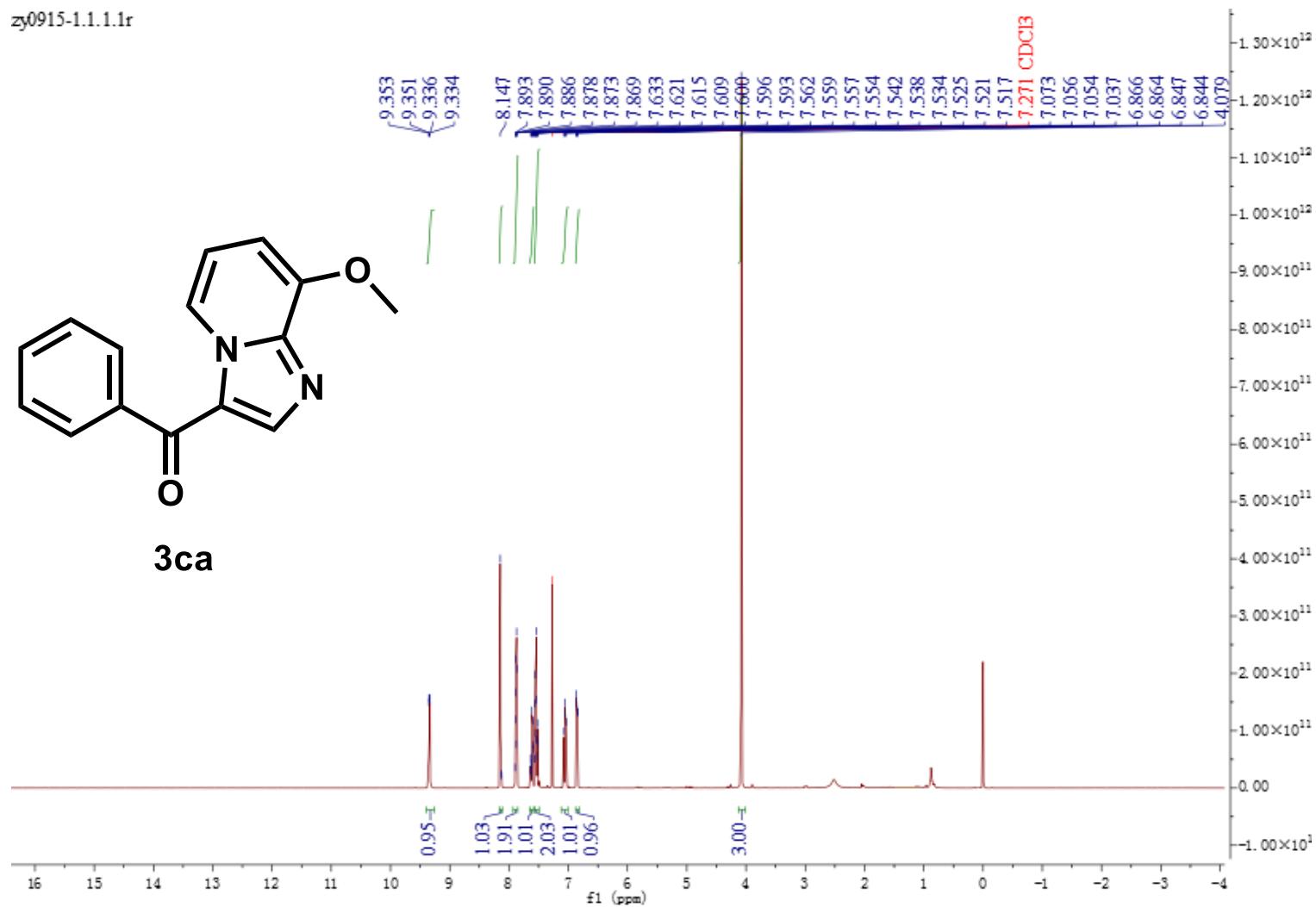
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ZY-0929-1.2.fid



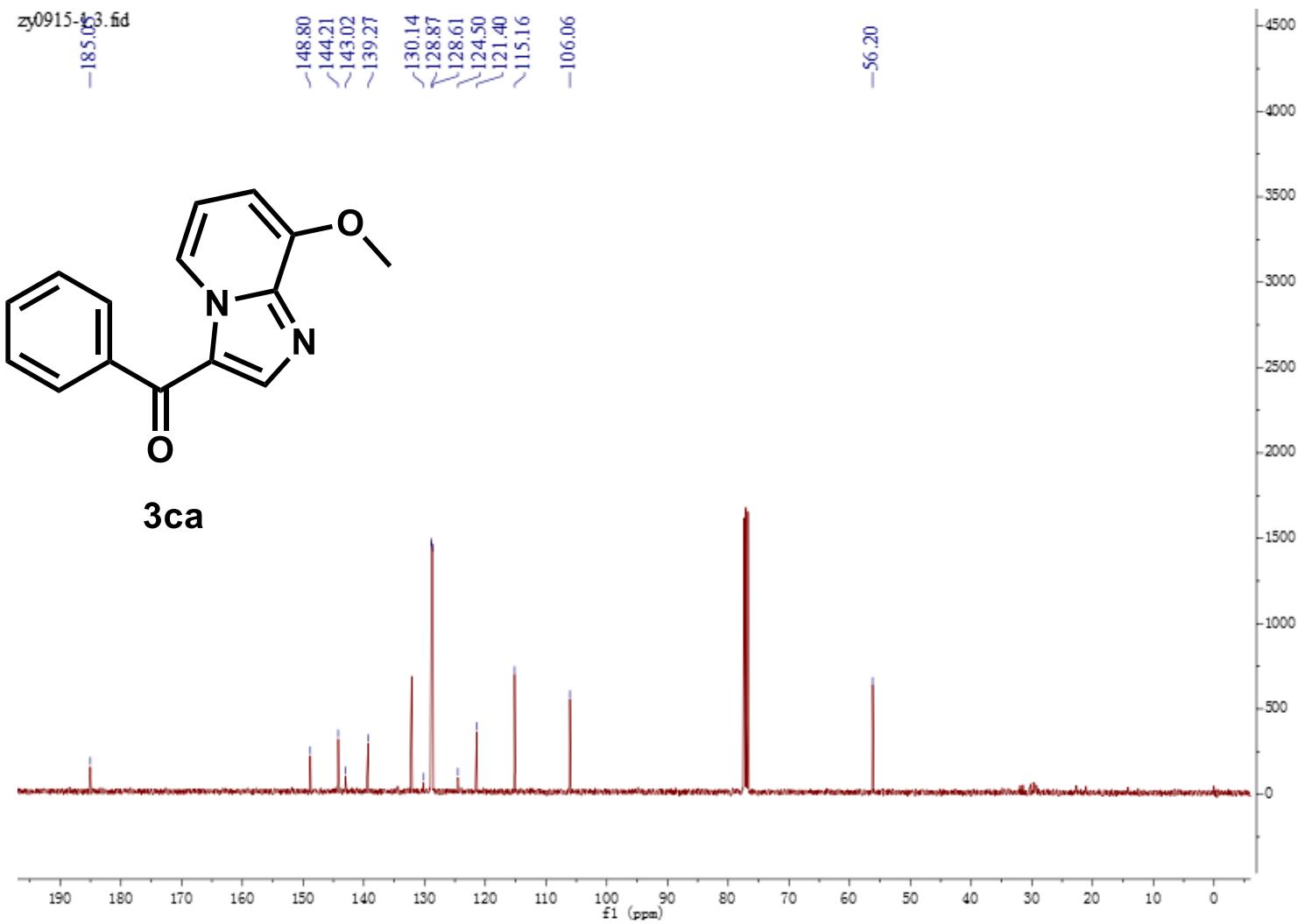
¹H NMR of Compound 3ca (400 MHz, CDCl₃)

zy0915-1.1.1.1r



¹³C{H} NMR of Compound 3ca (101 MHz, CDCl₃)

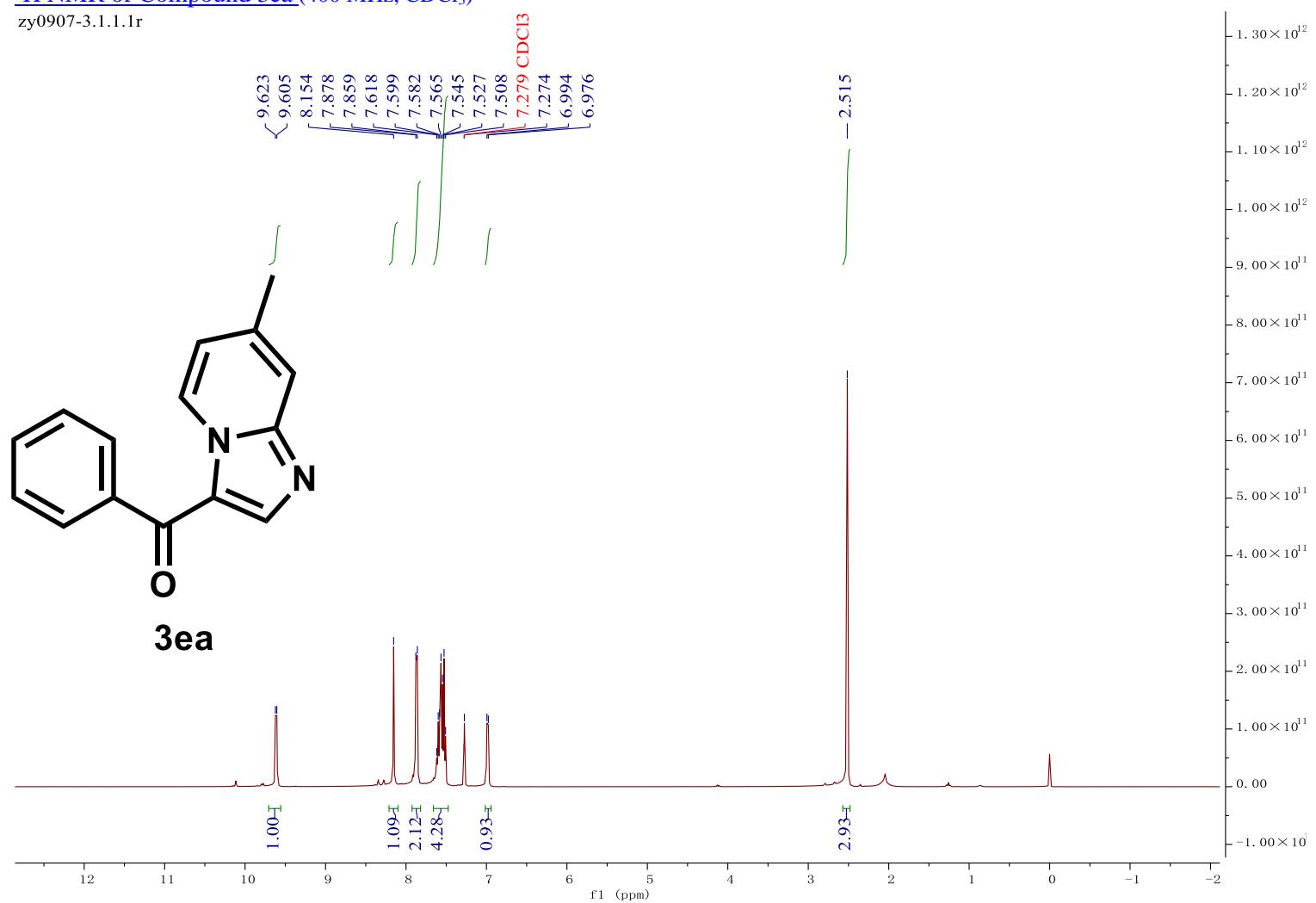
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3ca

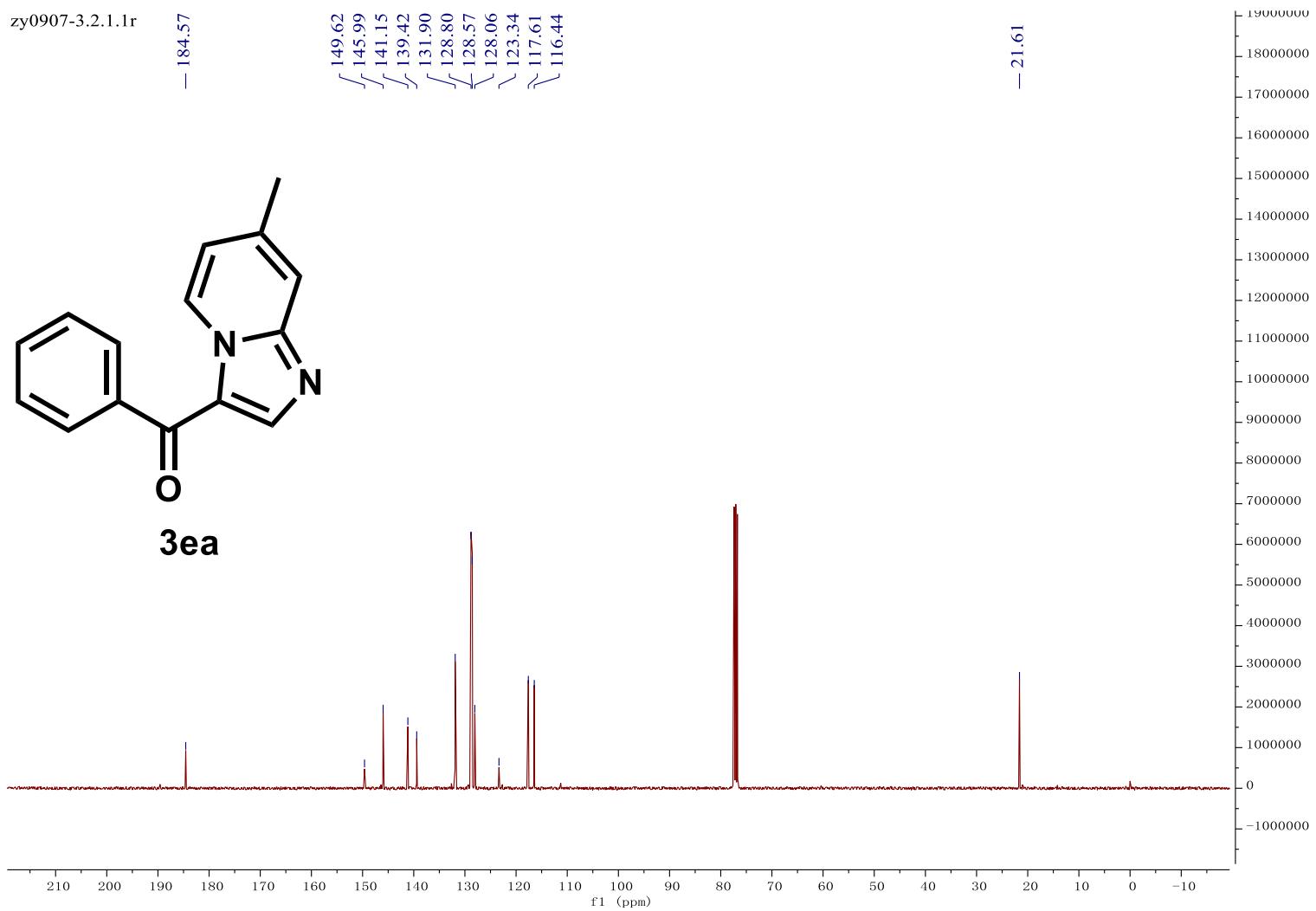
¹H NMR of Compound 3ea (400 MHz, CDCl₃)

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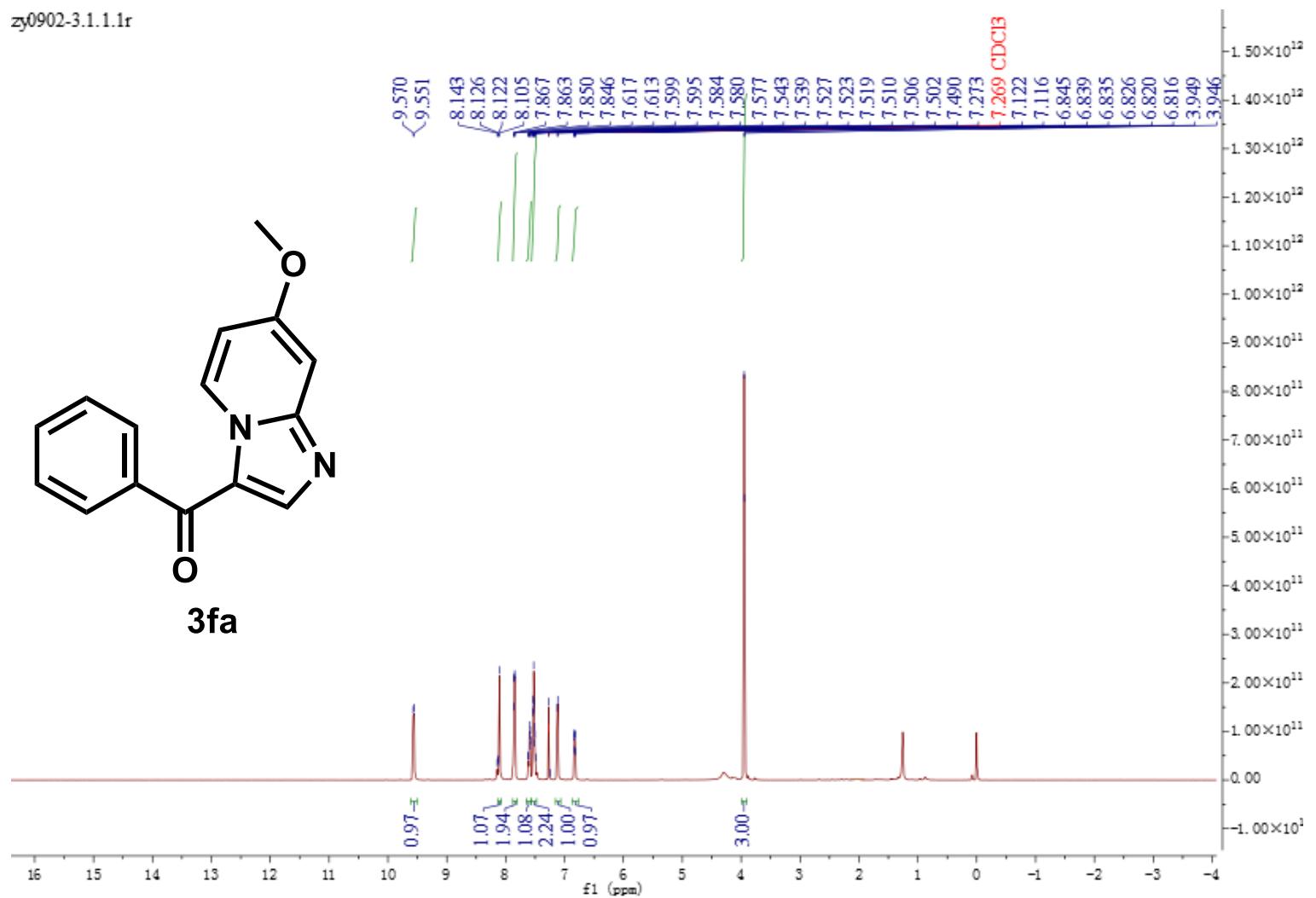
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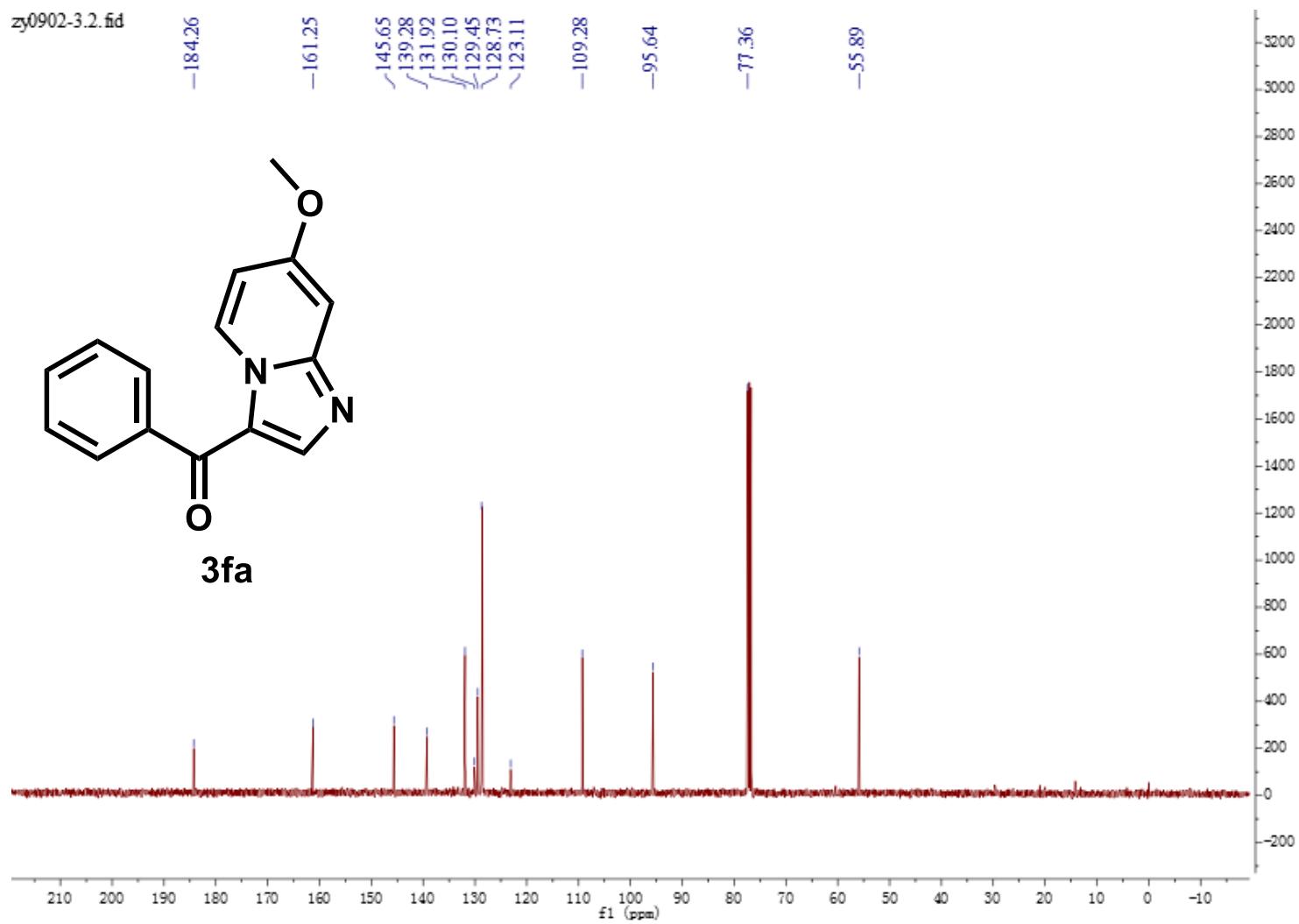
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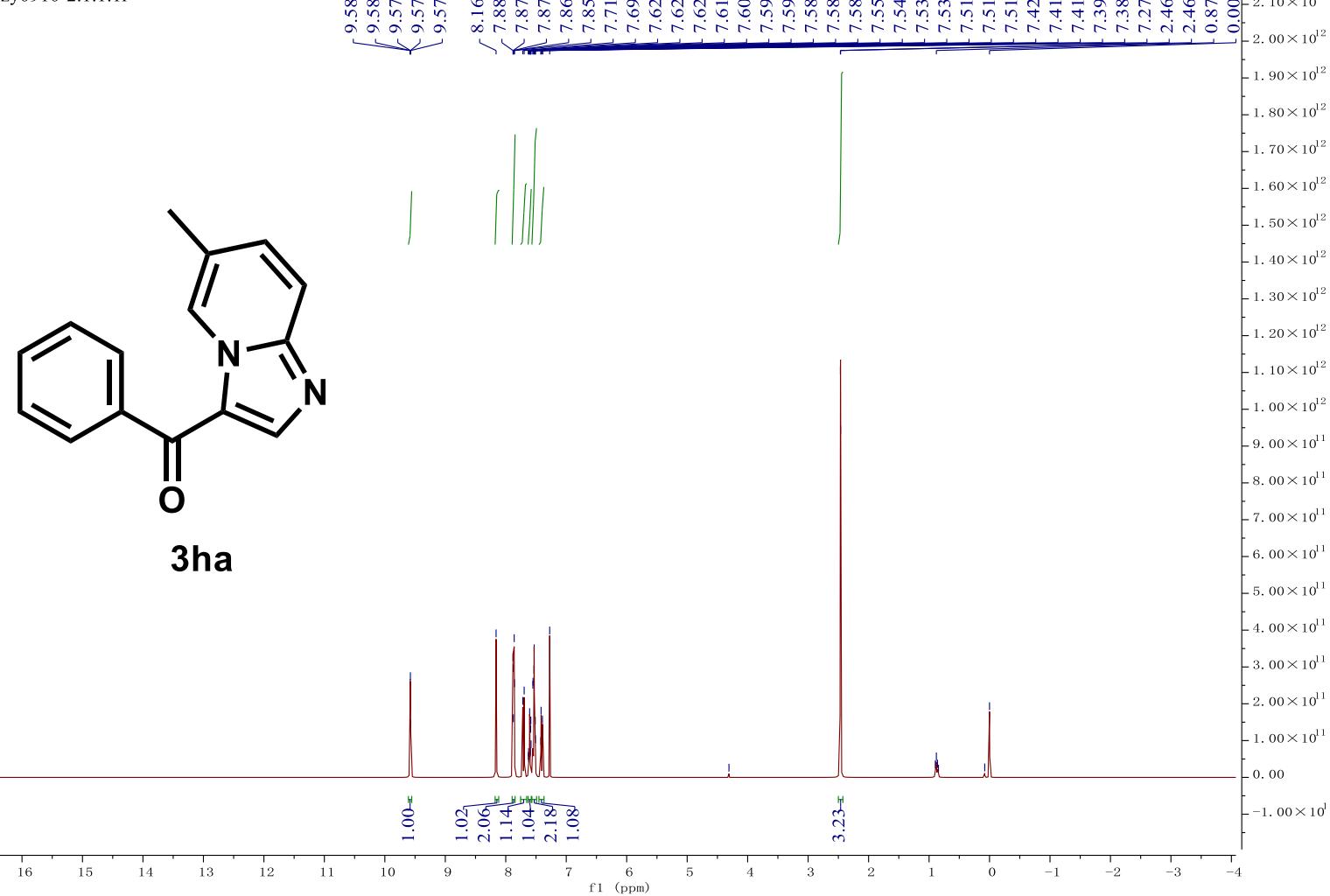
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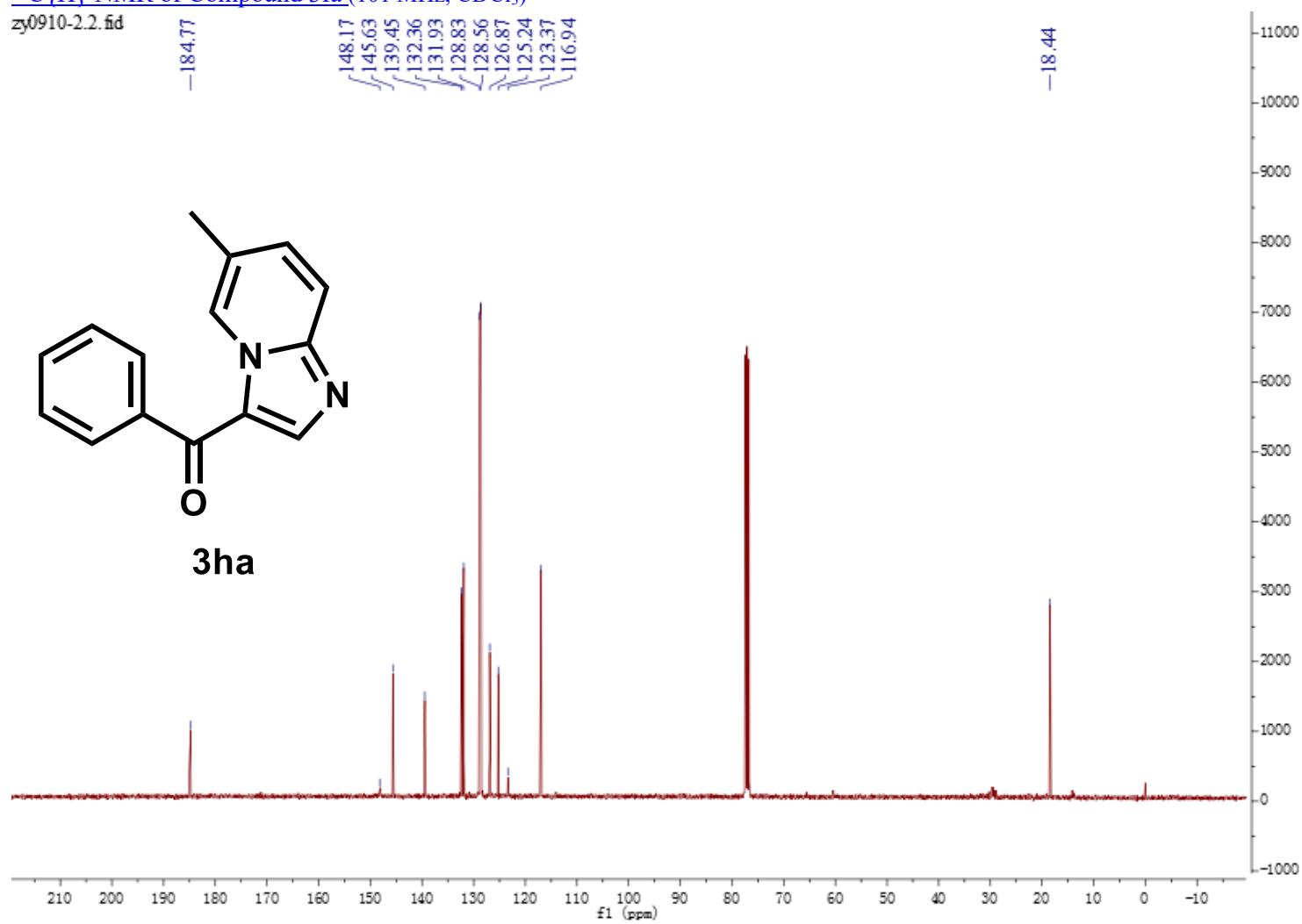
¹H NMR of Compound 3ha (400 MHz, CDCl₃)

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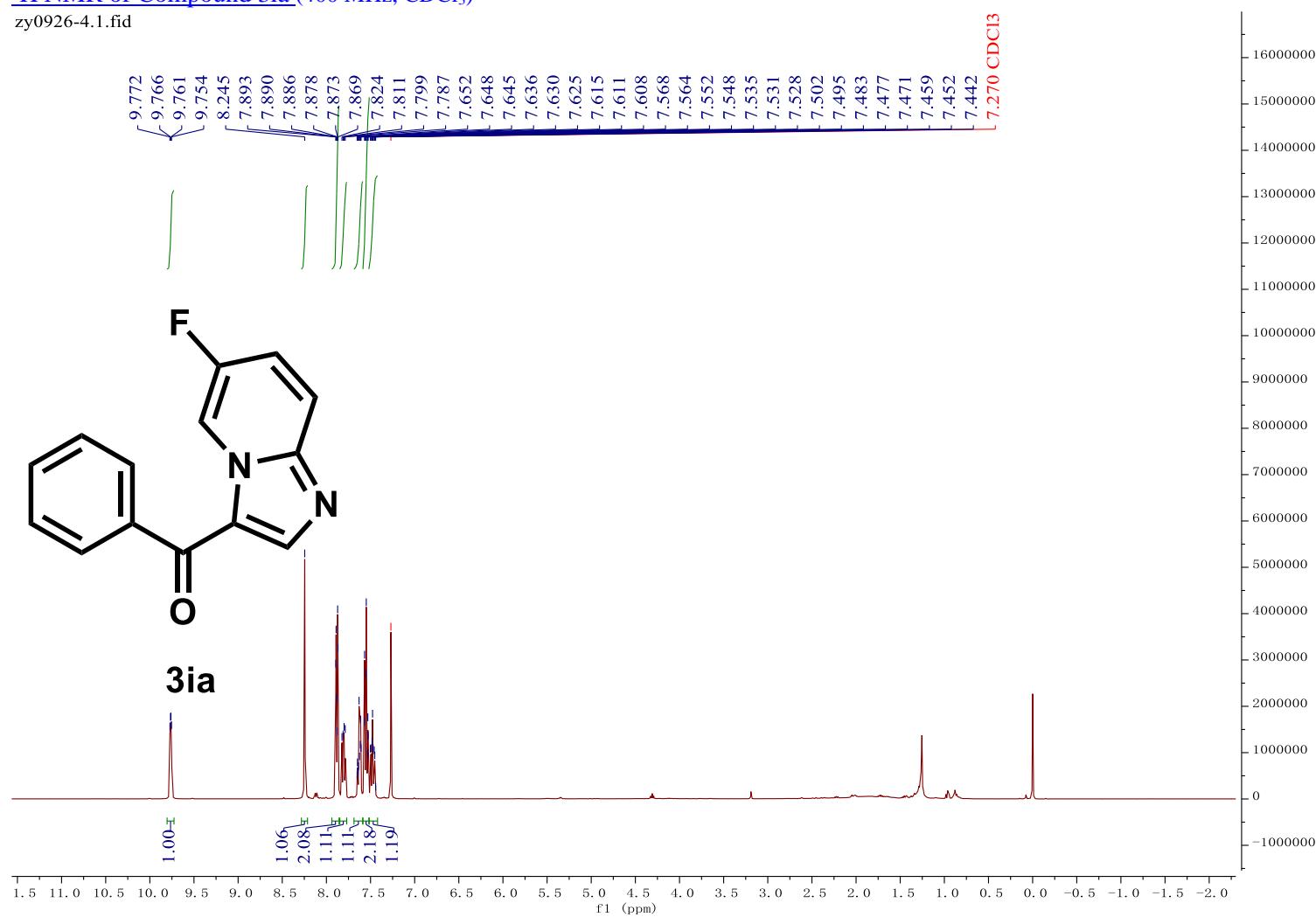
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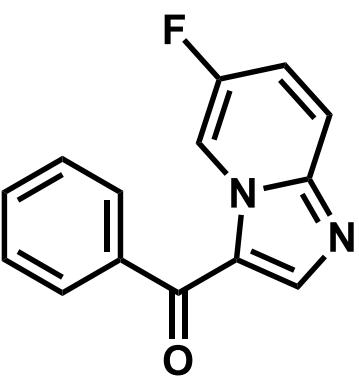
¹H NMR of Compound 3ia (400 MHz, CDCl₃)

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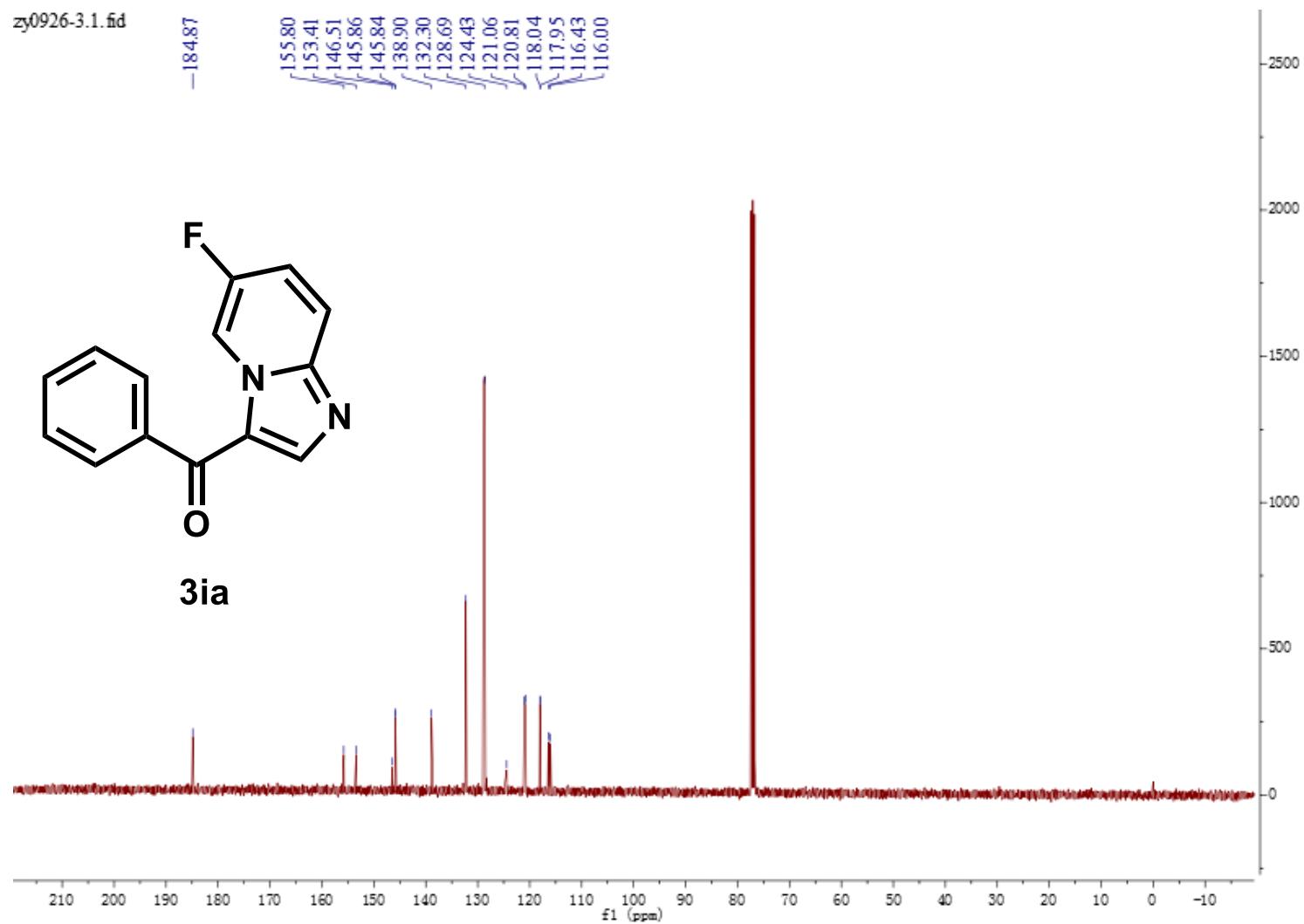


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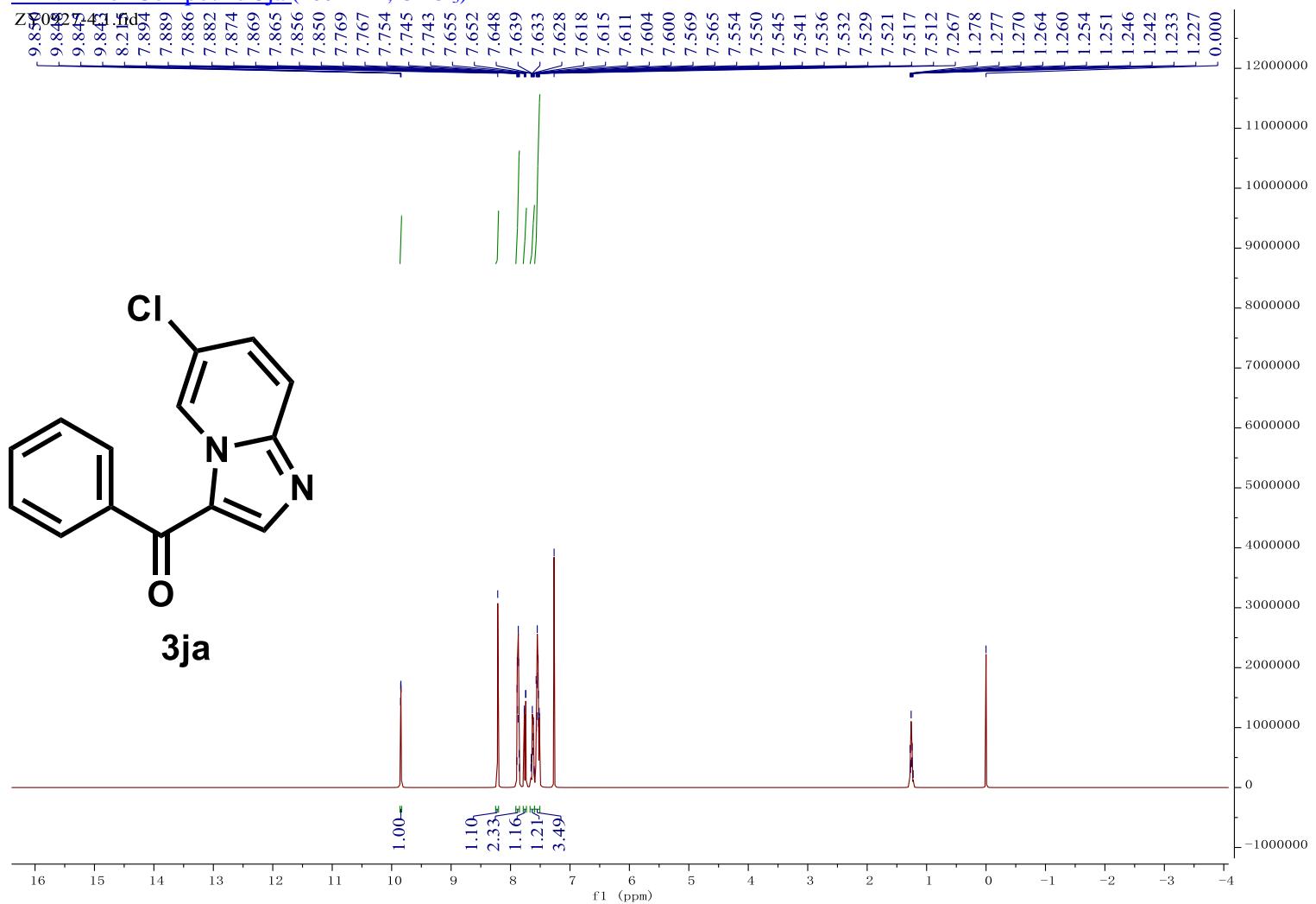
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3ia

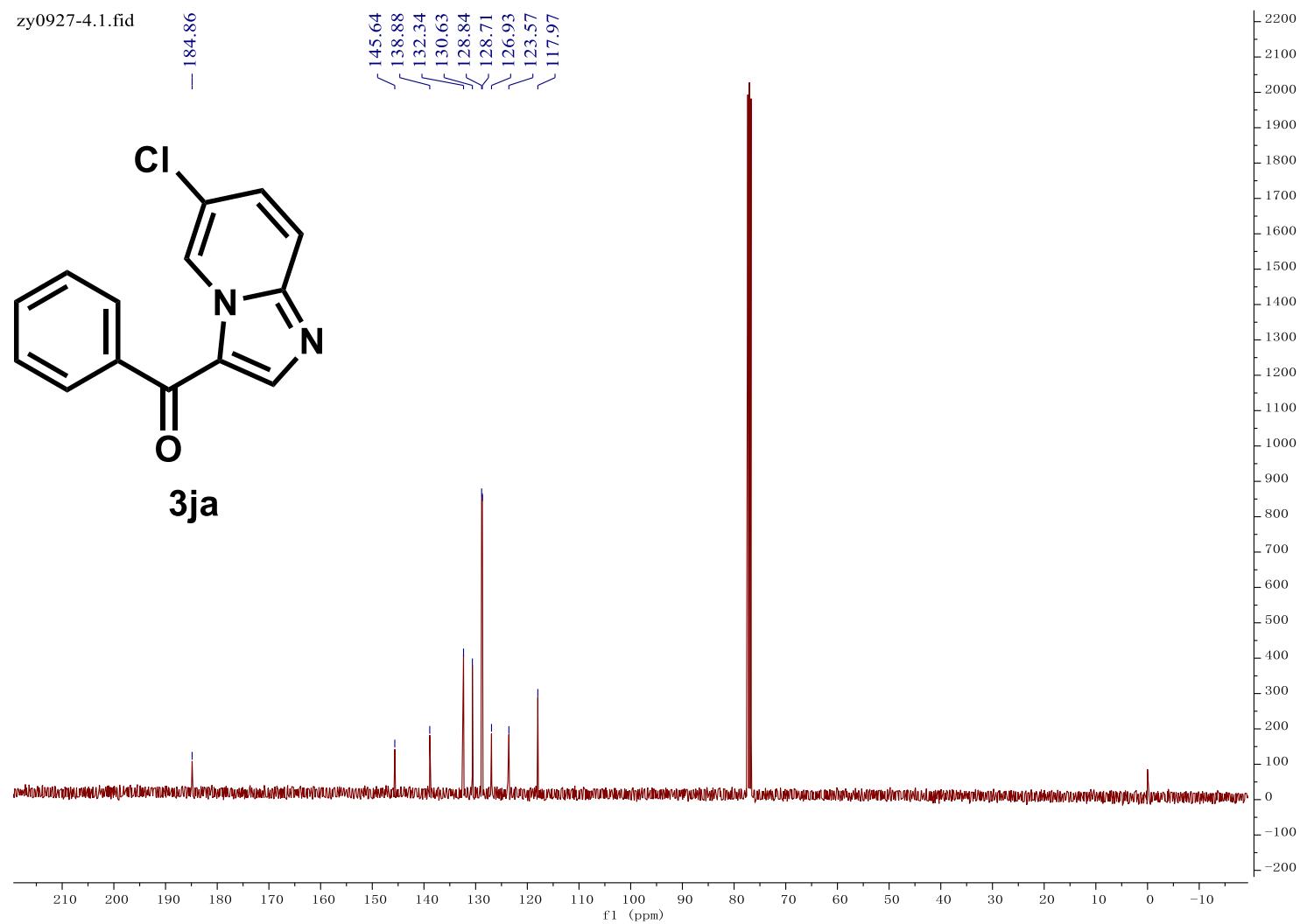


¹H NMR of Compound 3ja (400 MHz, CDCl₃)



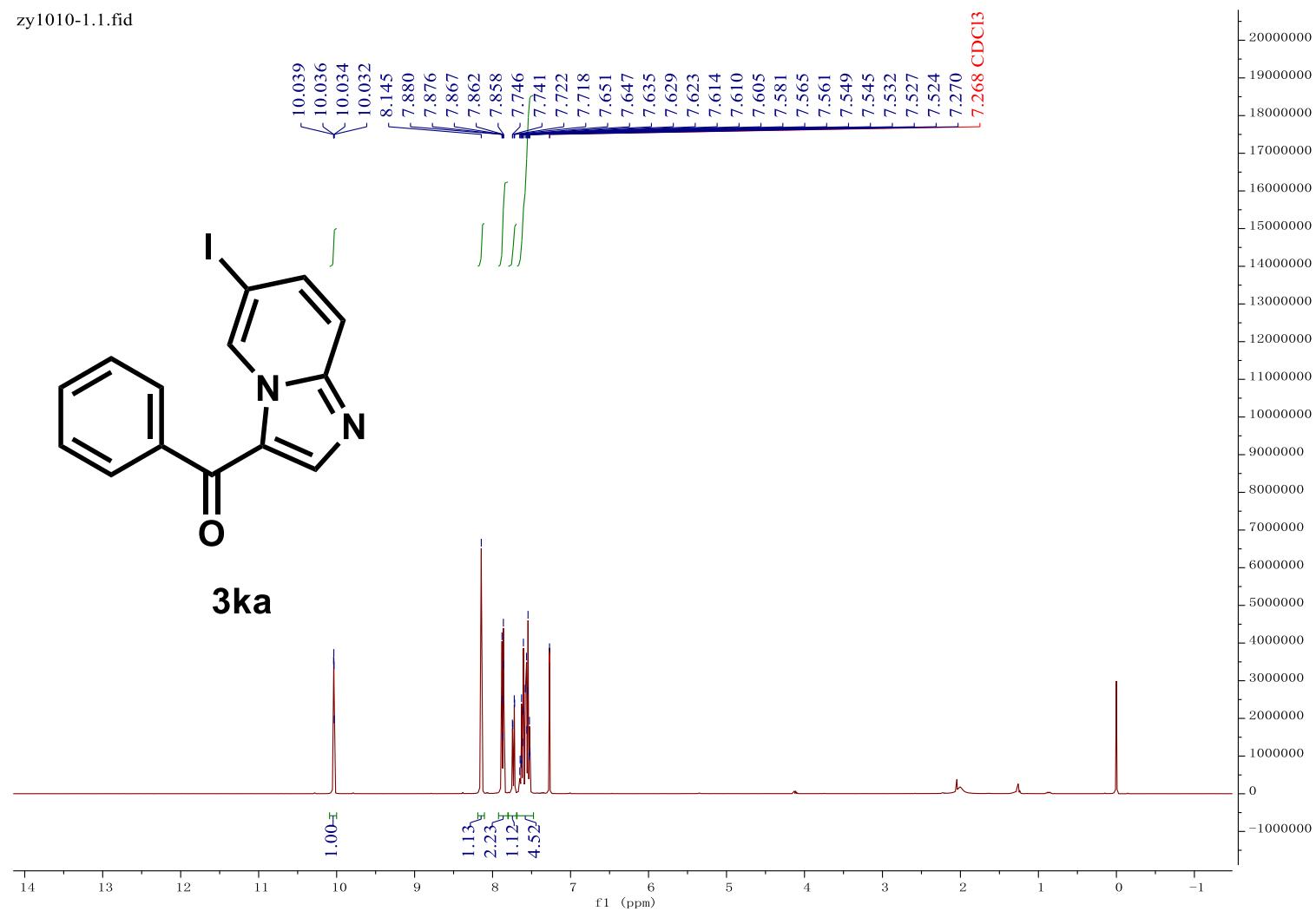
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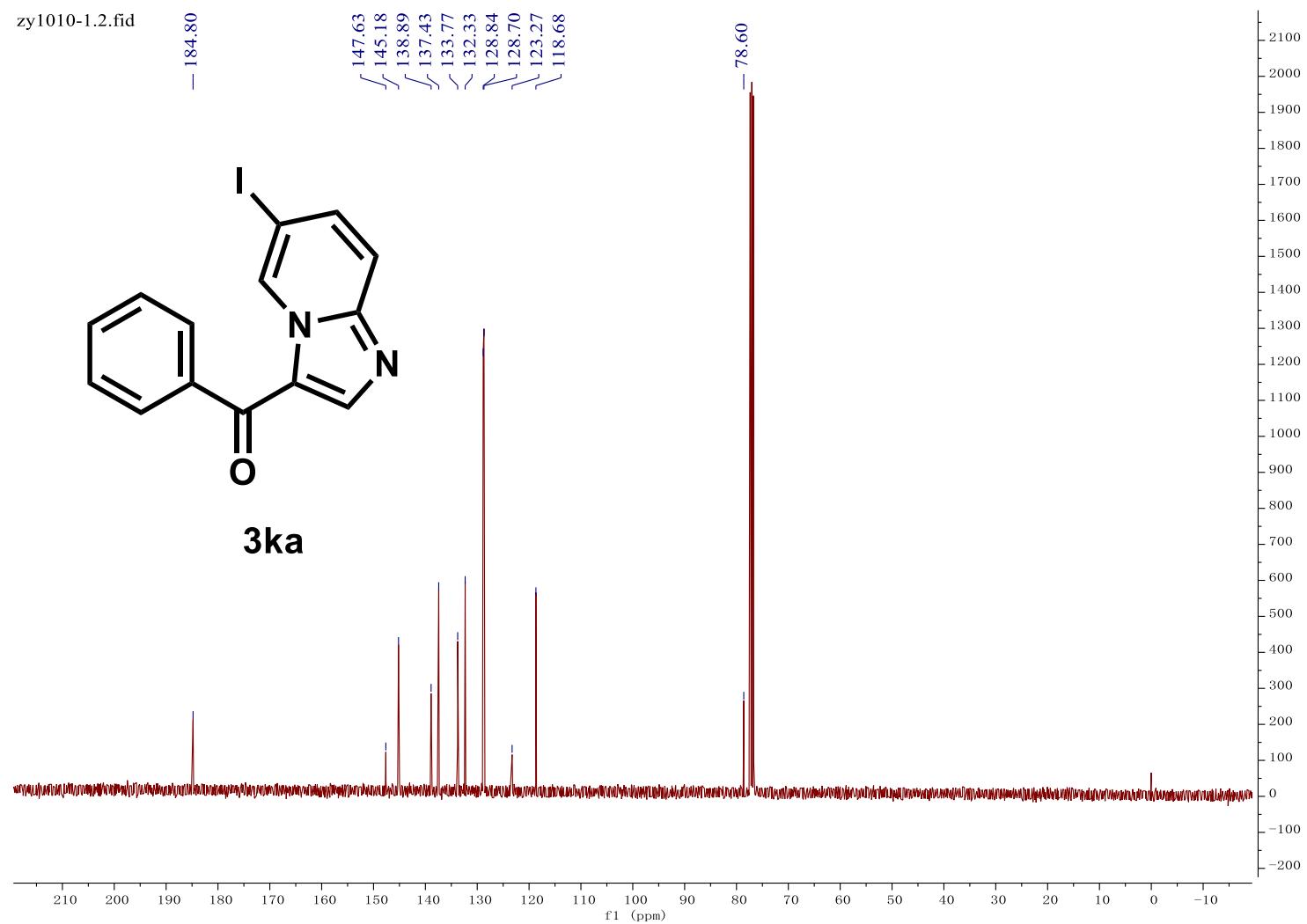


¹H NMR of Compound 3ka (400 MHz, CDCl₃)

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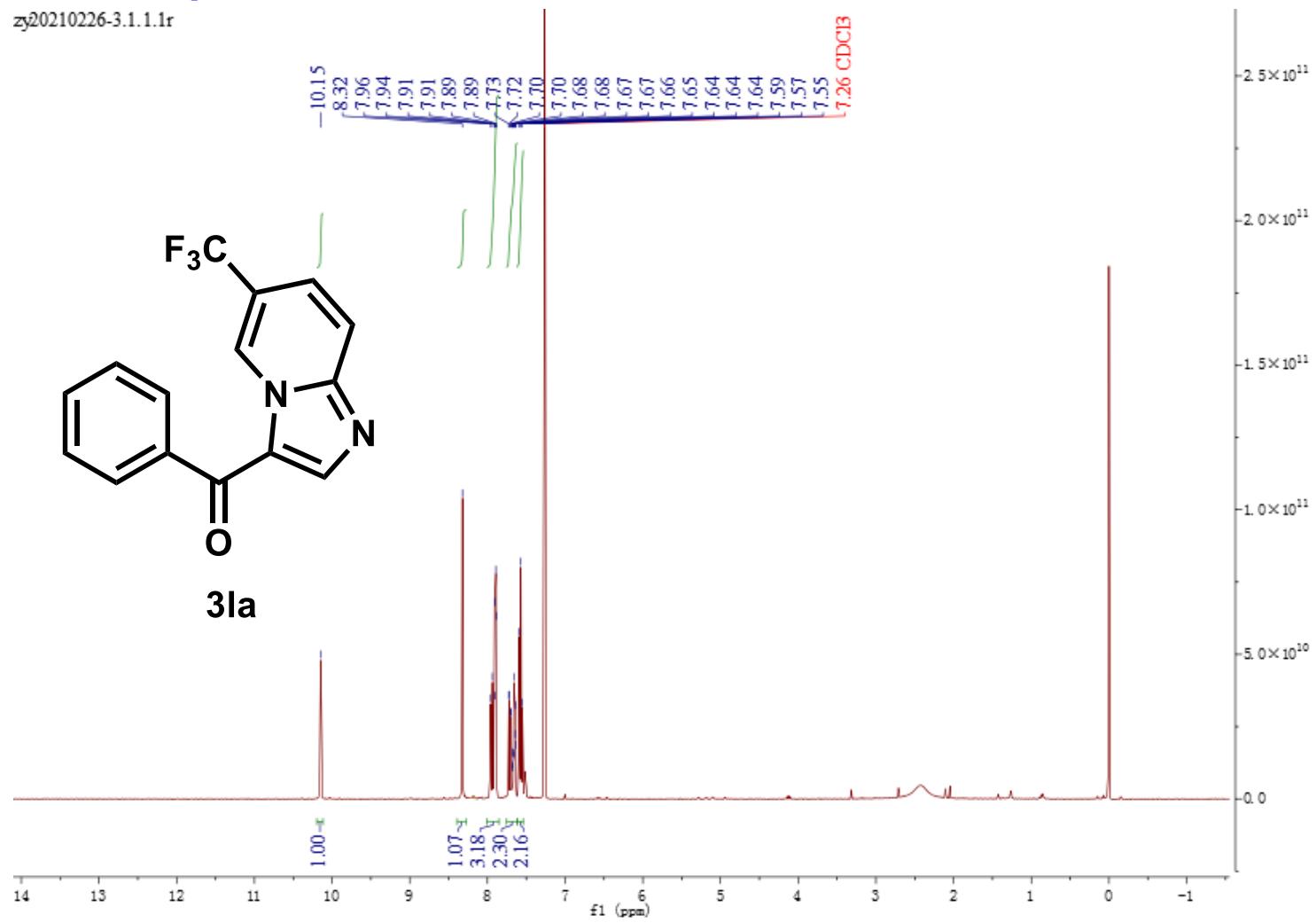


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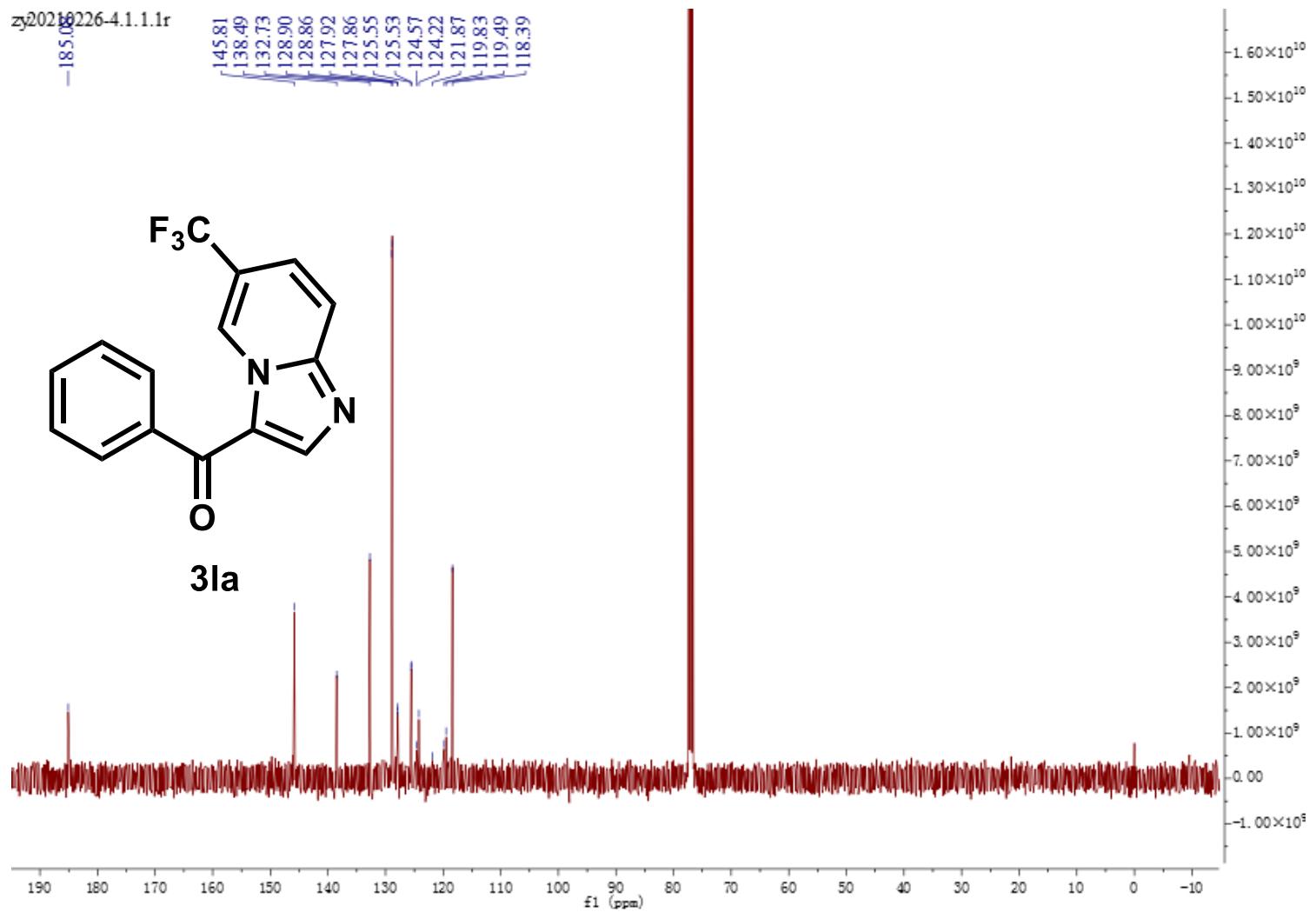


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zy20210226-3.1.1.1r

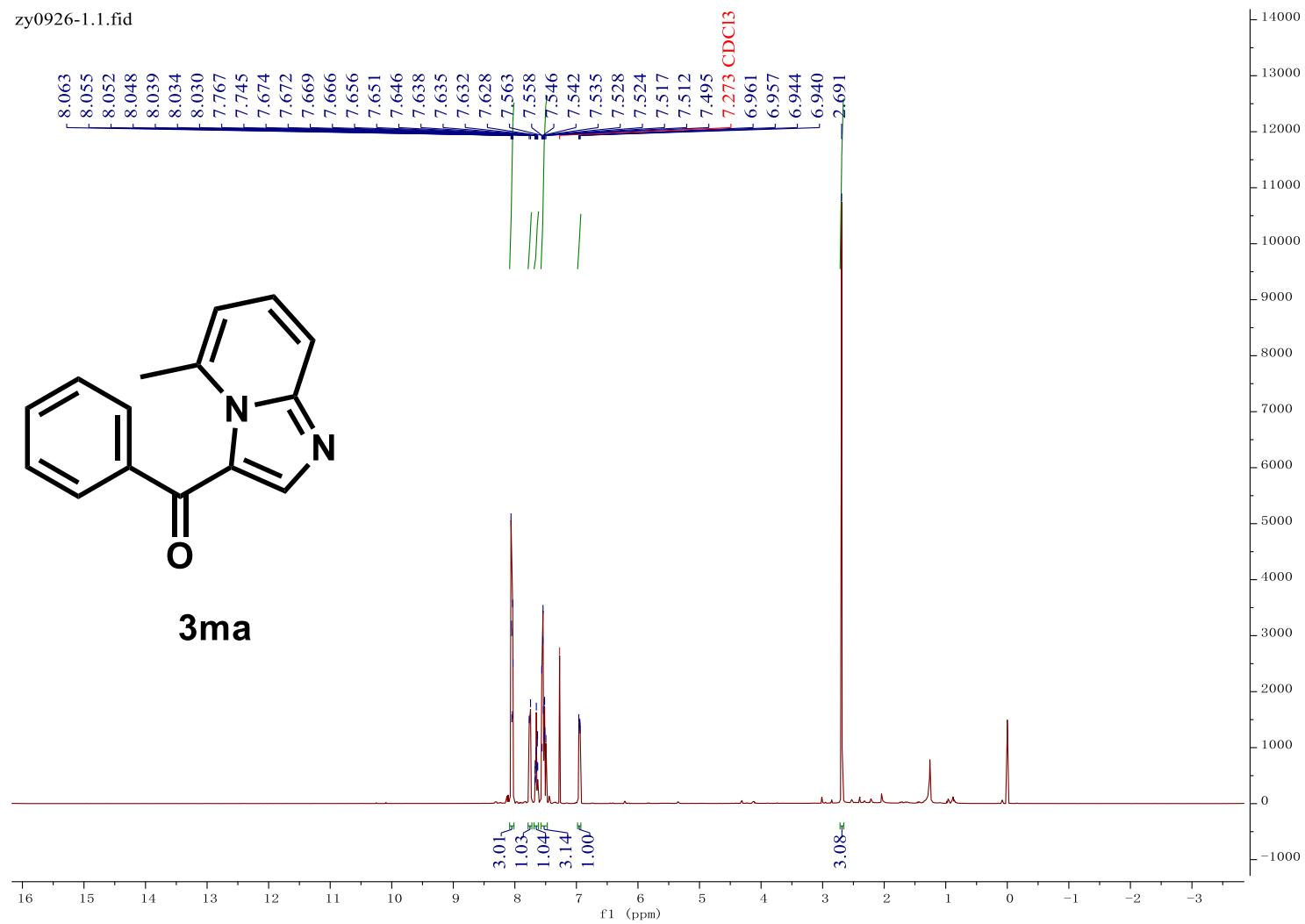


¹³C{H} NMR of Compound 3la (101 MHz, CDCl₃)



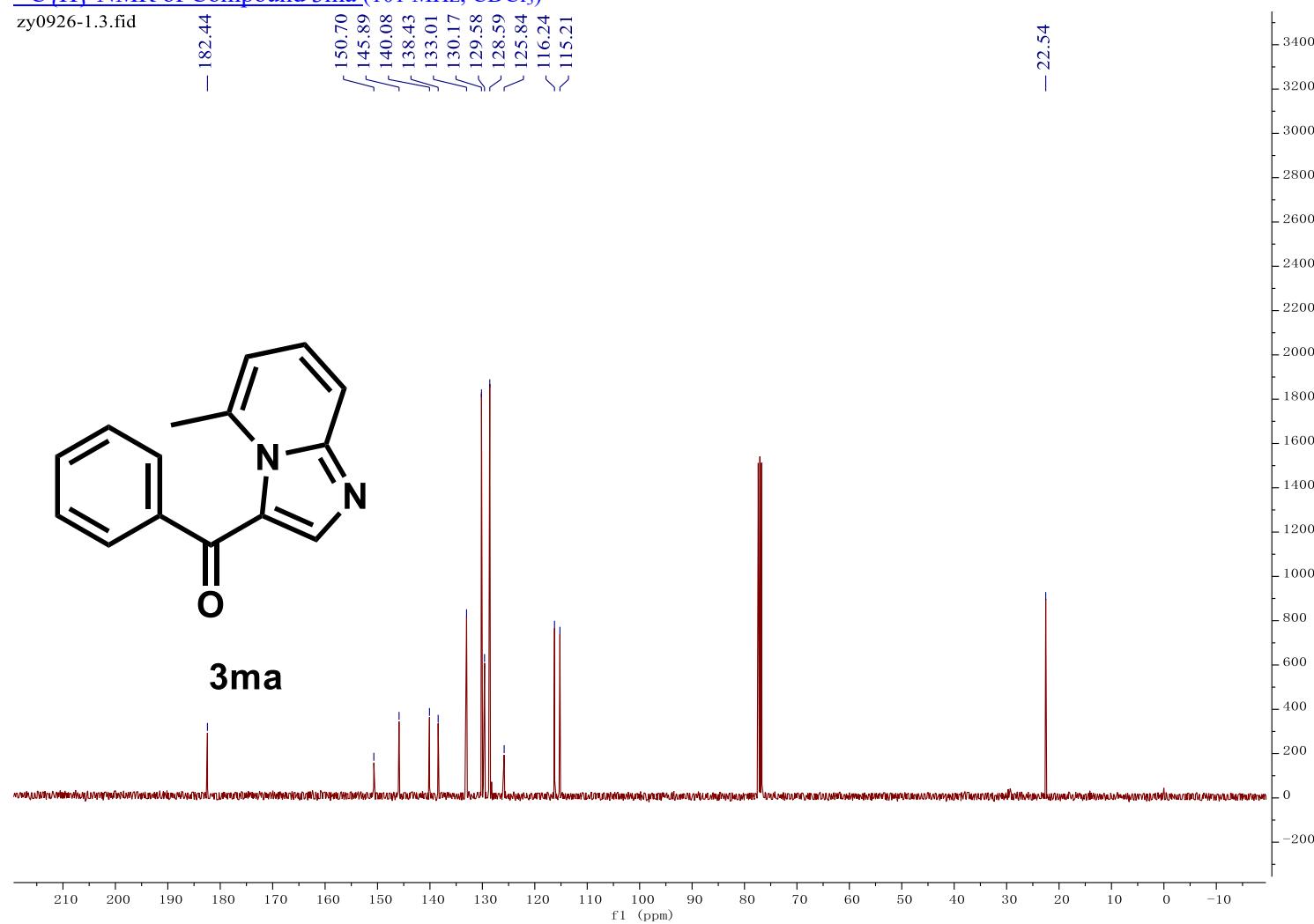
¹H NMR of Compound 3ma (400 MHz, CDCl₃)

zy0926-1.i.fid



¹³C{H} NMR of Compound 3ma (101 MHz, CDCl₃)

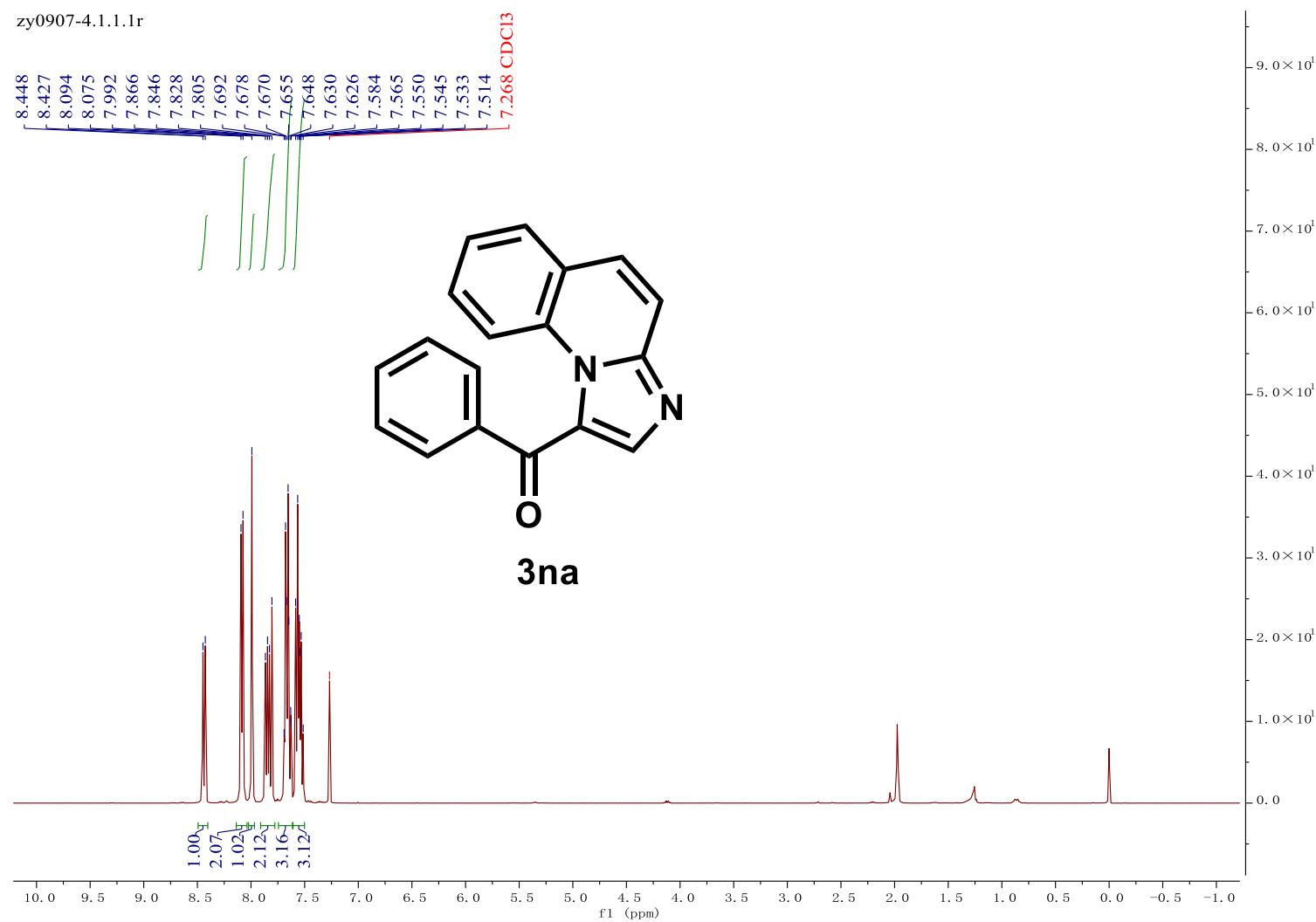
zy0926-1.3.fid



3ma

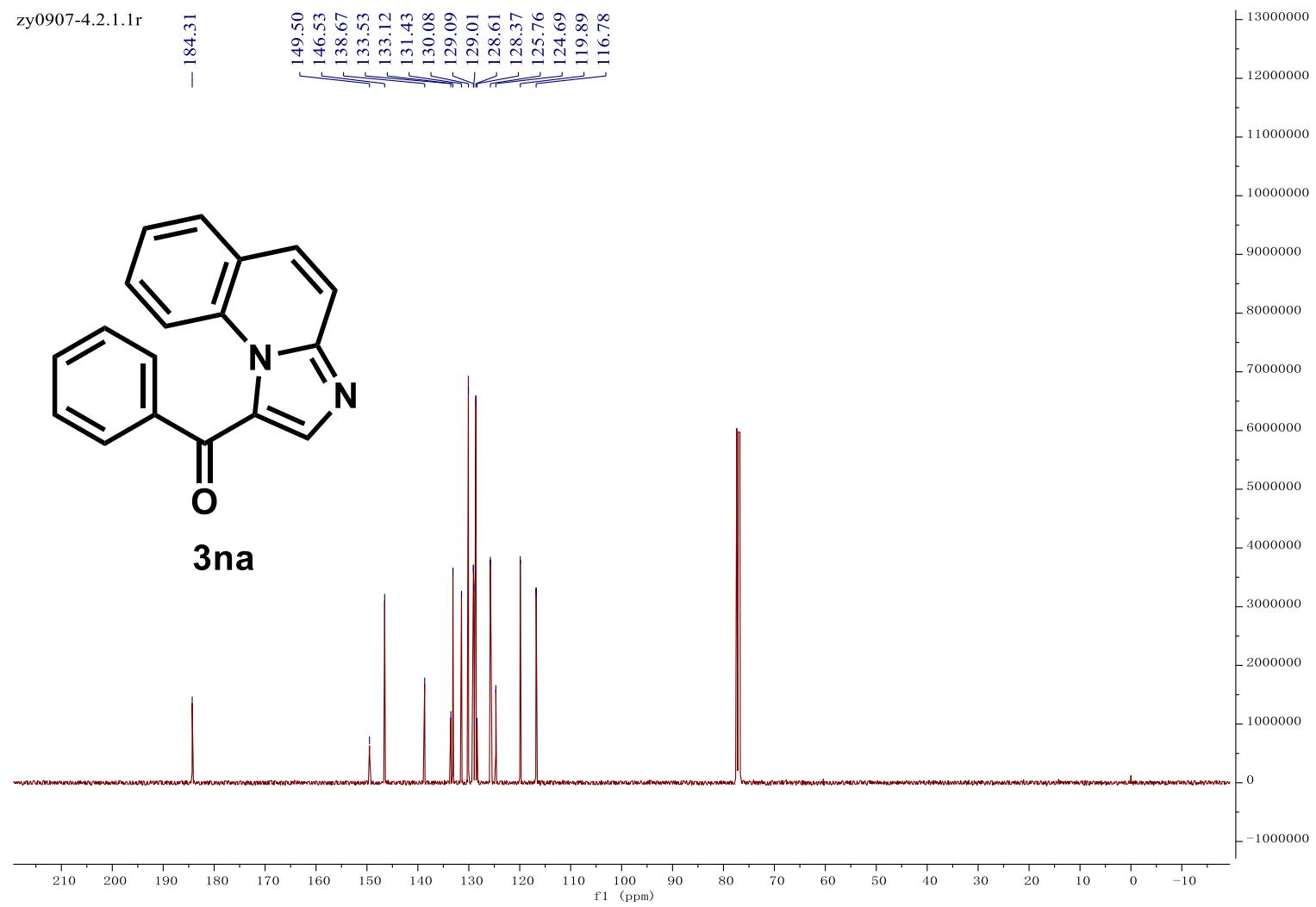
¹H NMR of Compound 3na (400 MHz, CDCl₃)

zy0907-4.1.1.1r



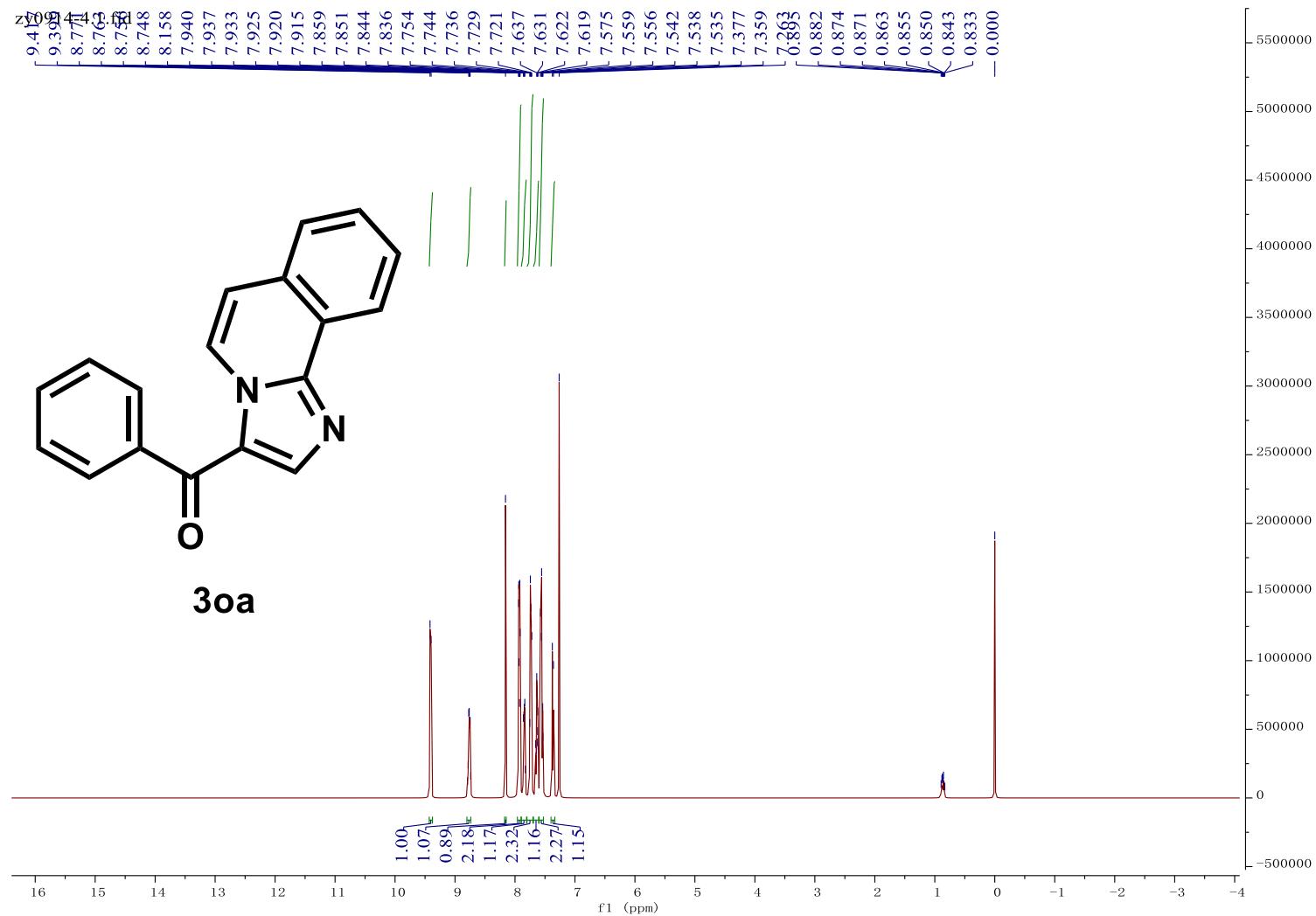
¹³C{H} NMR of Compound 3na (101 MHz, CDCl₃)

zy0907-4.2.1.1r

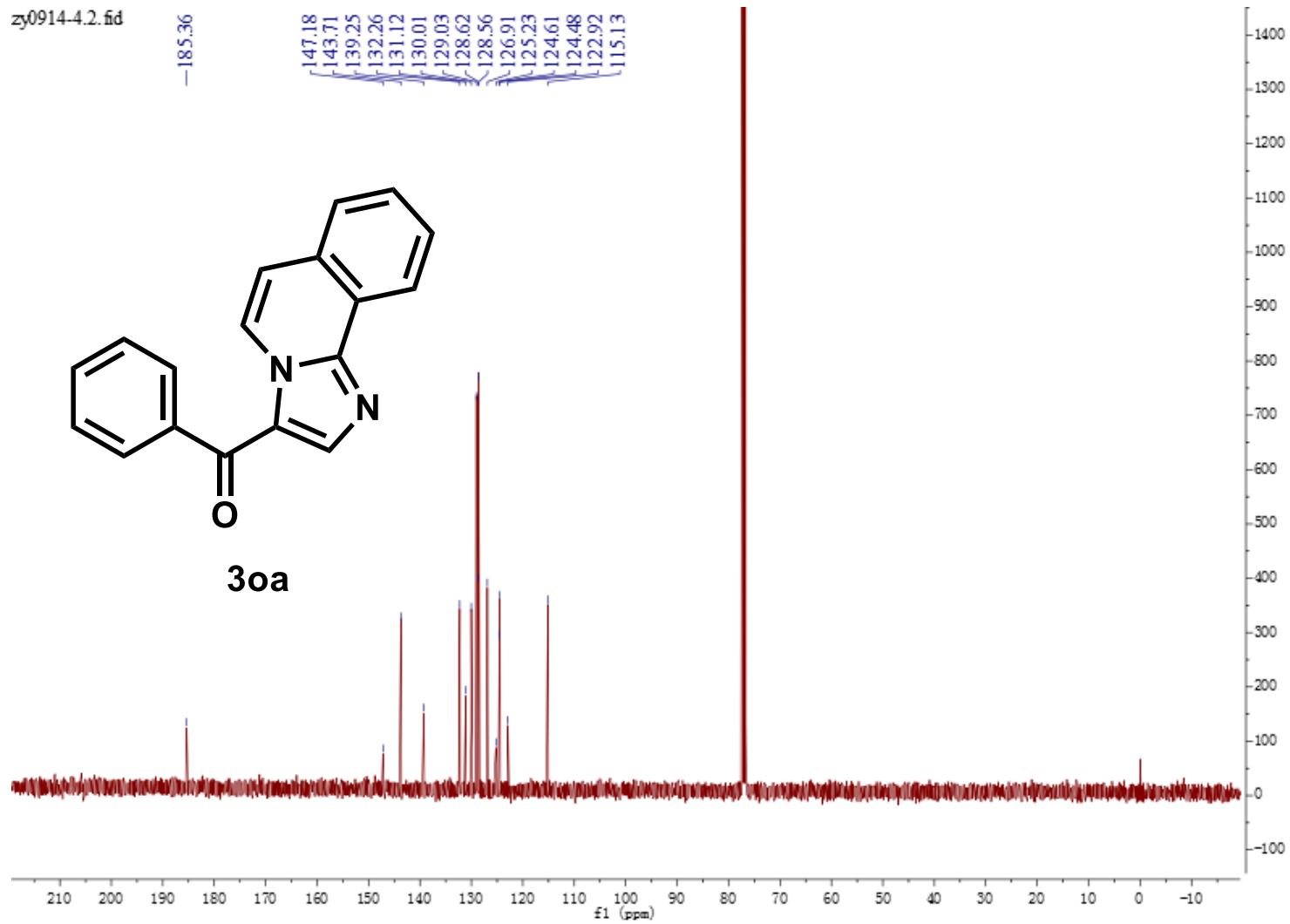


3na

¹H NMR of Compound 3oa (400 MHz, CDCl₃)

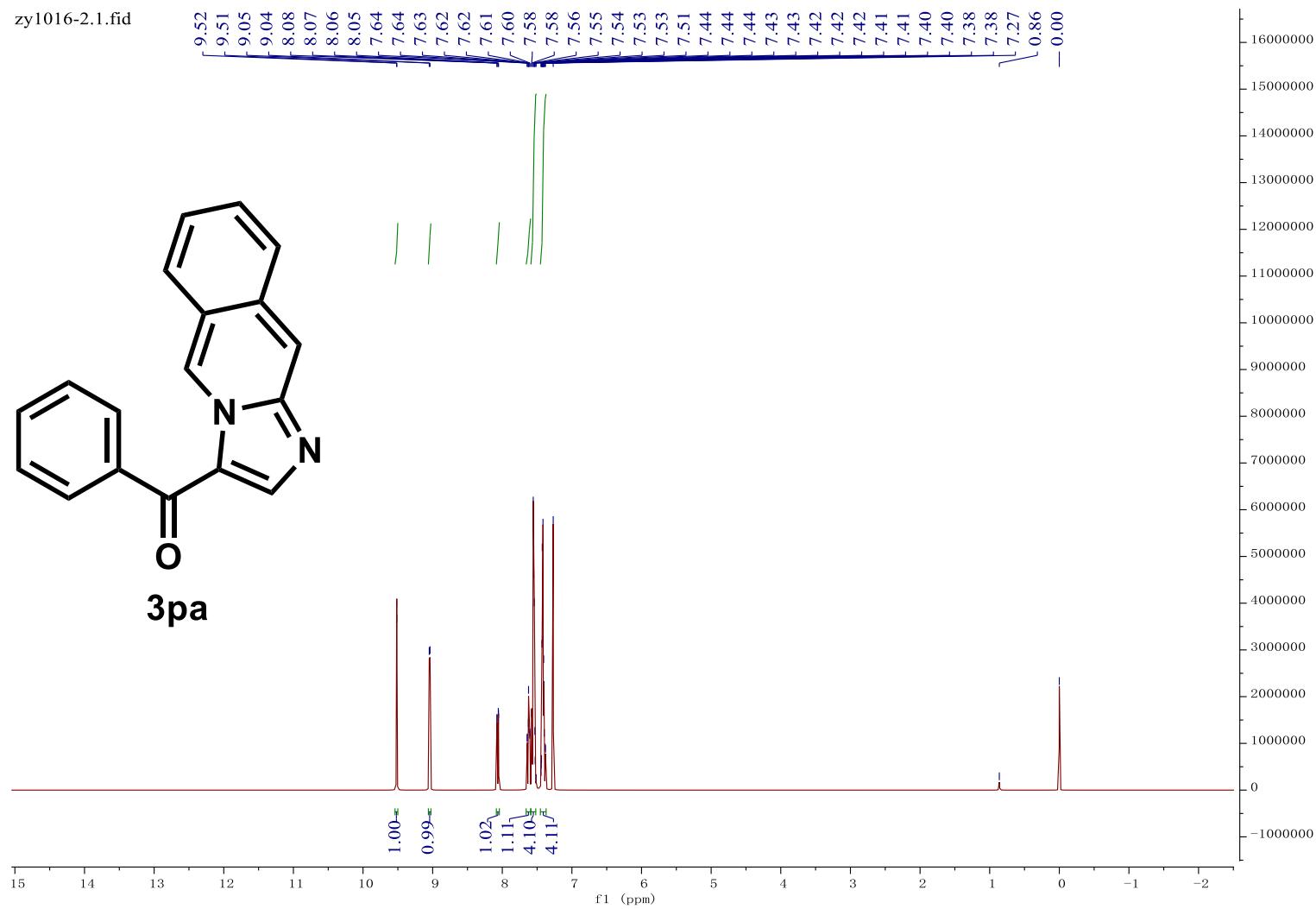


¹³C{H} NMR of Compound 3oa (101 MHz, CDCl₃)



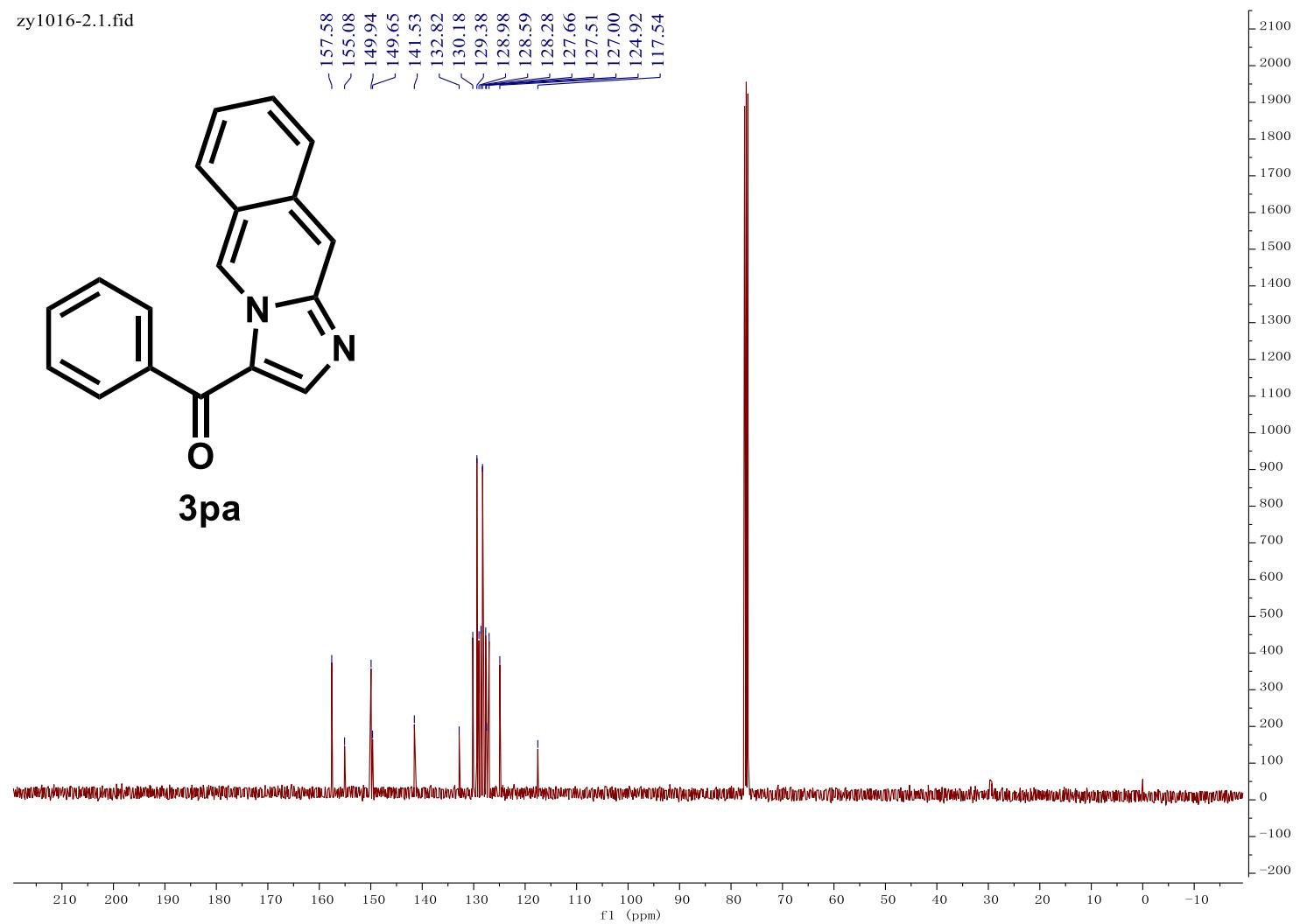
¹H NMR of Compound 3pa (400 MHz, CDCl₃)

zy1016-2.1.fid



¹³C{H} NMR of Compound 3pa (101 MHz, CDCl₃)

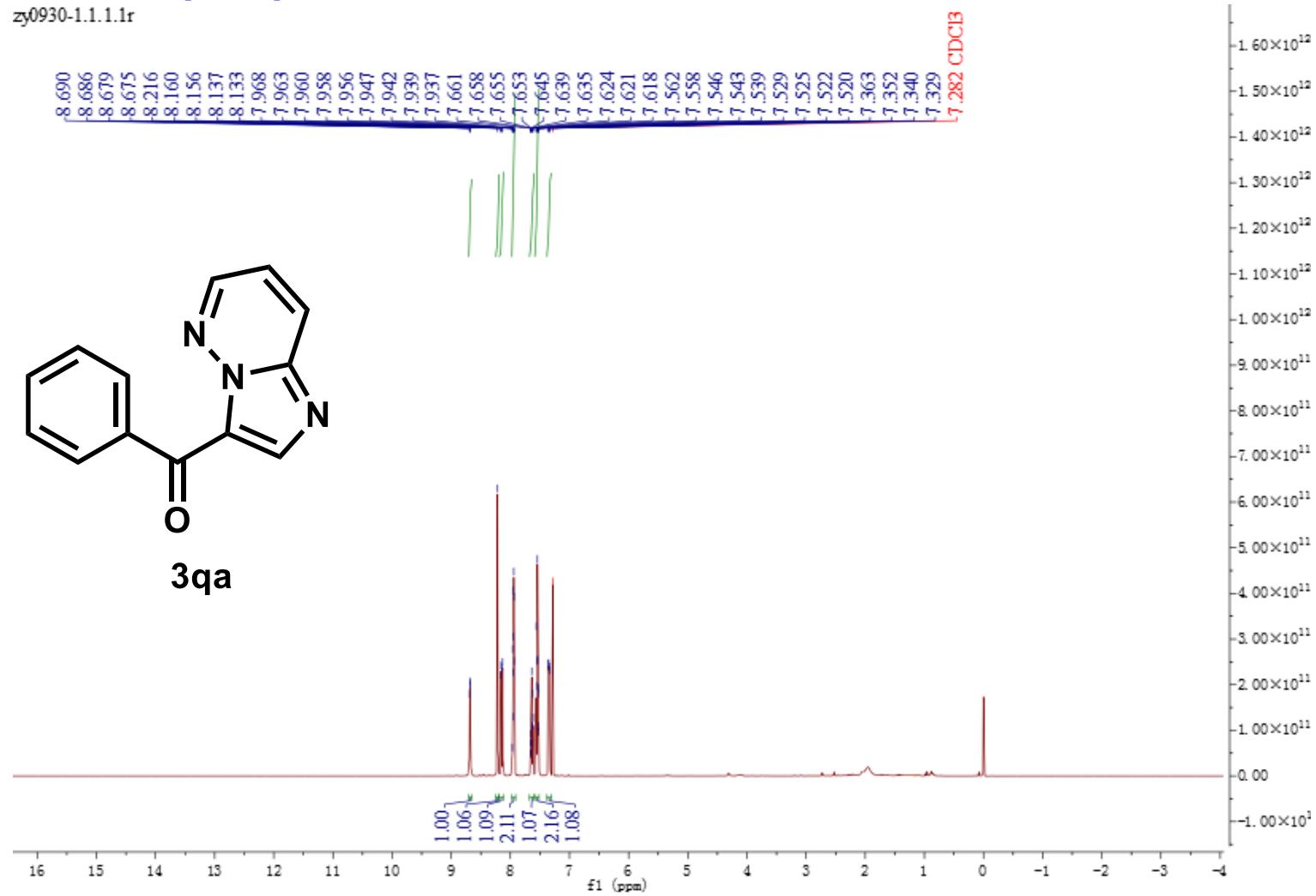
zy1016-2.1.fid



3pa

¹H NMR of Compound 3qa (400 MHz, CDCl₃)

zy0930-1.1.1.1r

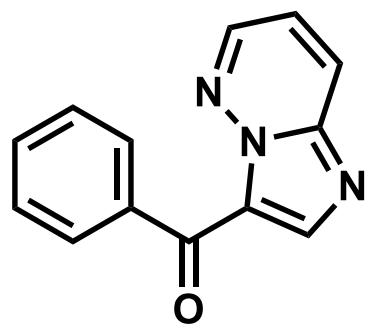


¹³C{H} NMR of Compound 3qa (101 MHz, CDCl₃)

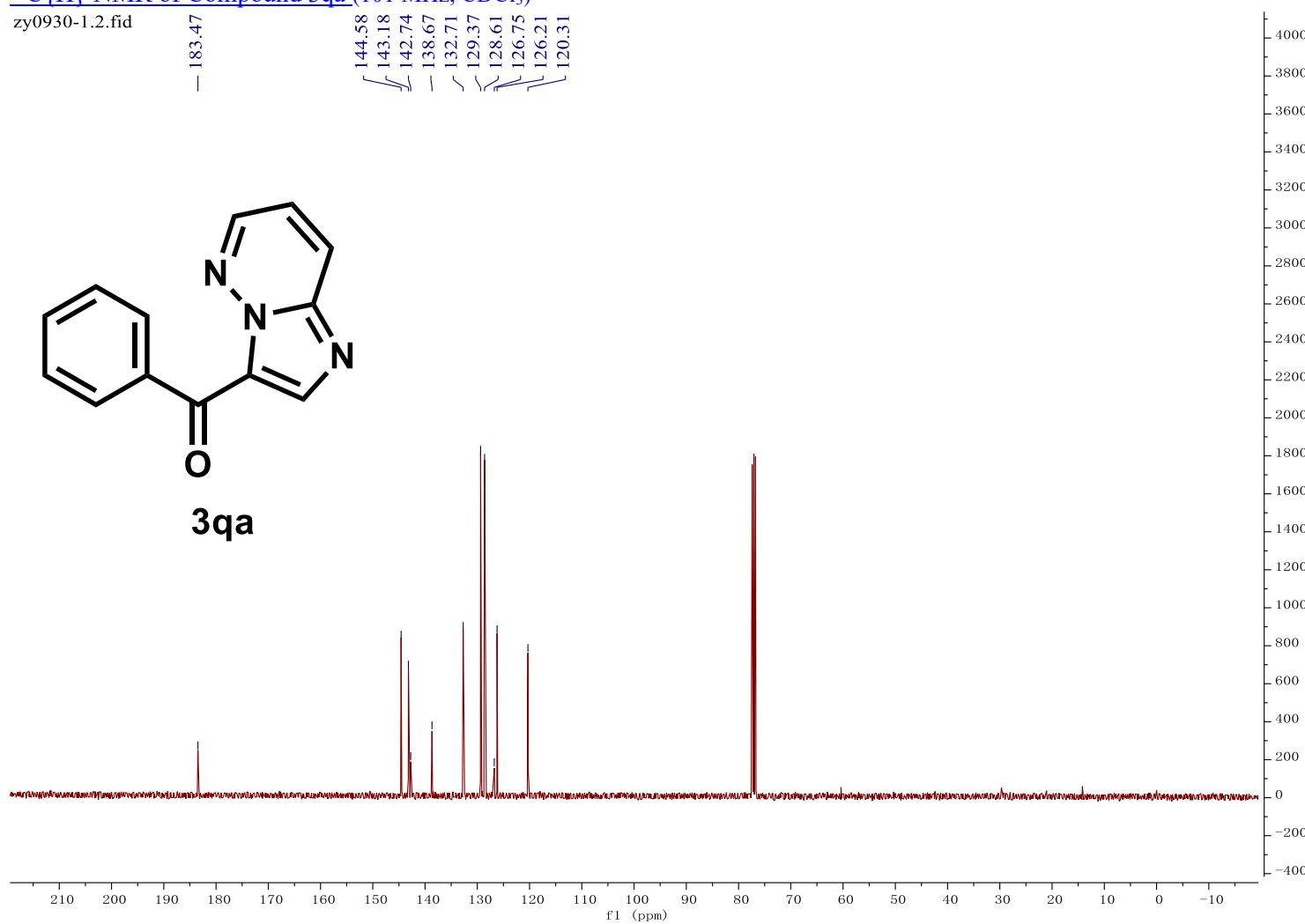
zy0930-1.2.fid

- 183.47

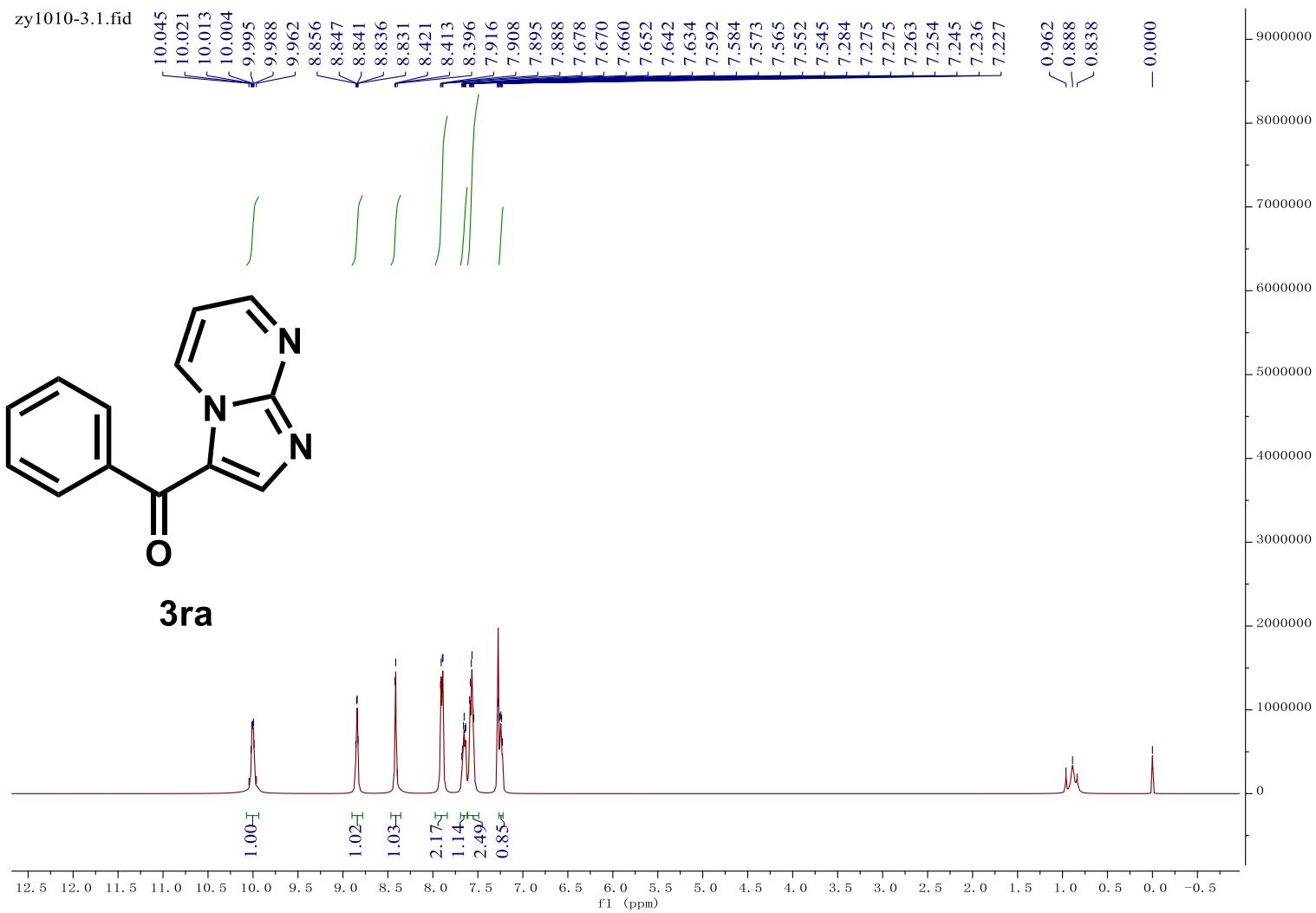
144.58
143.18
142.74
138.67
132.71
129.37
128.61
126.75
126.21
120.31



3qa

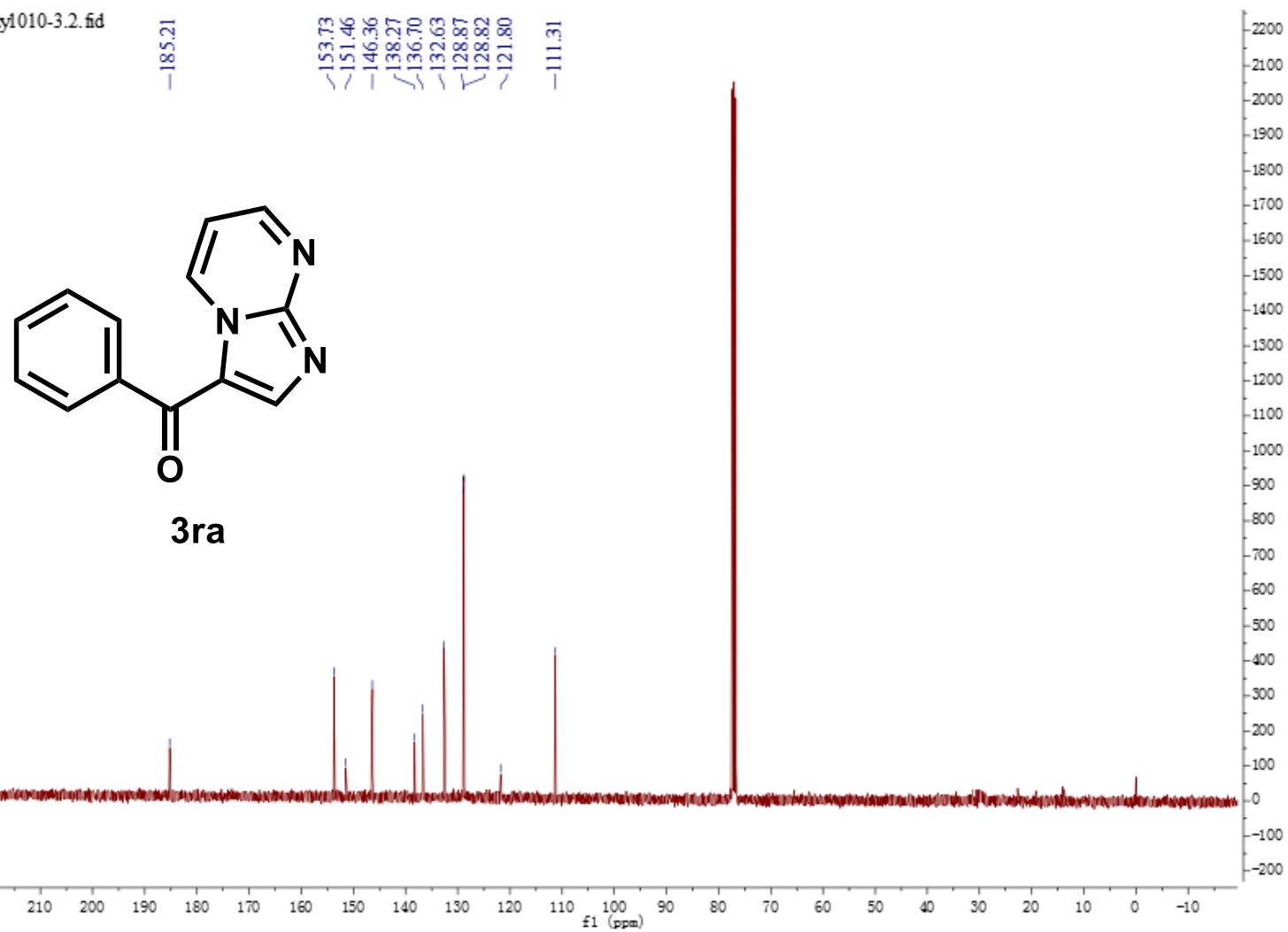


¹H NMR of Compound 3ra (400 MHz, CDCl₃)



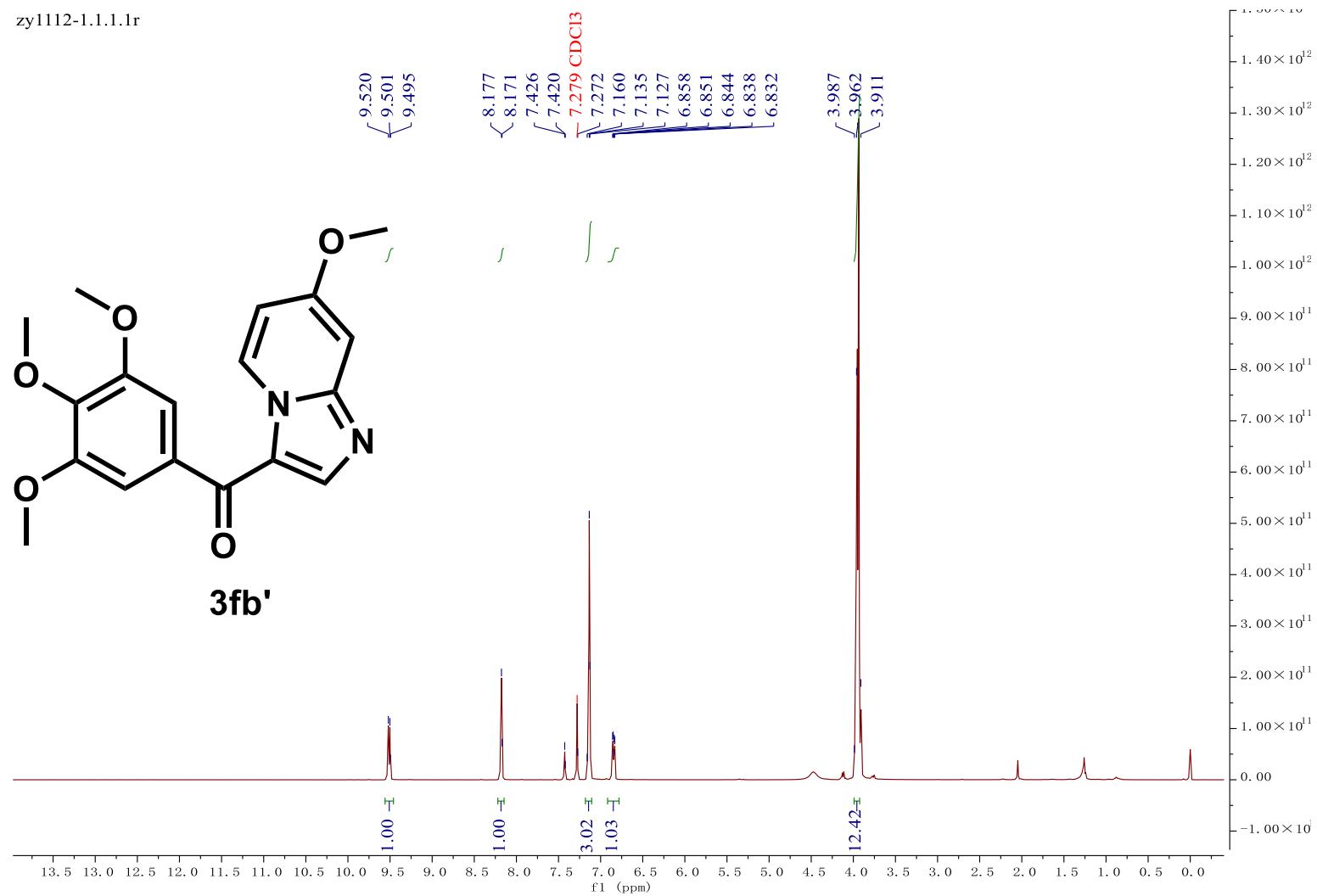
¹³C{H} NMR of Compound 3ra (101 MHz, CDCl₃)

zy1010-3.2.fid



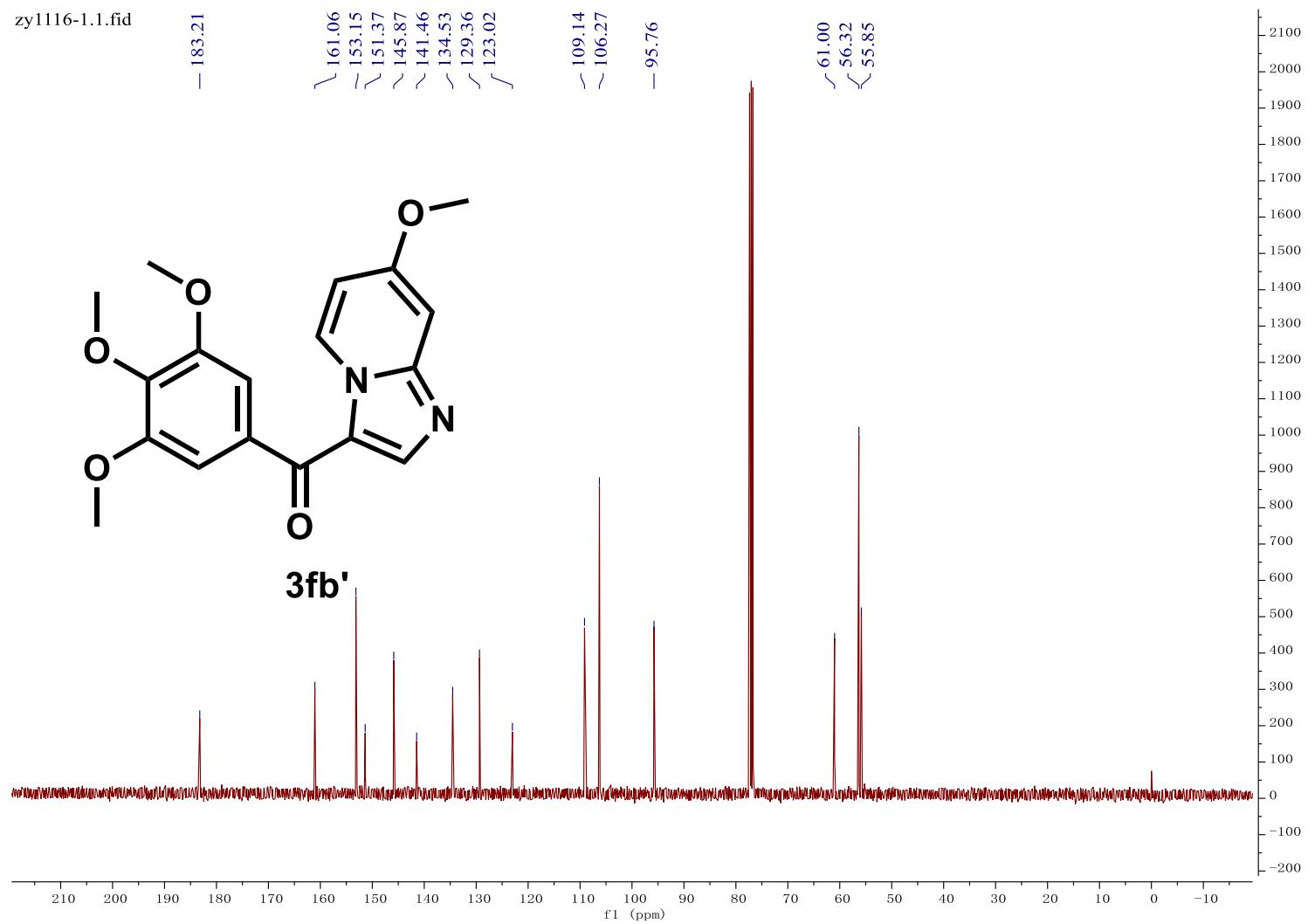
¹H NMR of Compound 3fb' (400 MHz, CDCl₃)

zy1112-1.1.1.1r



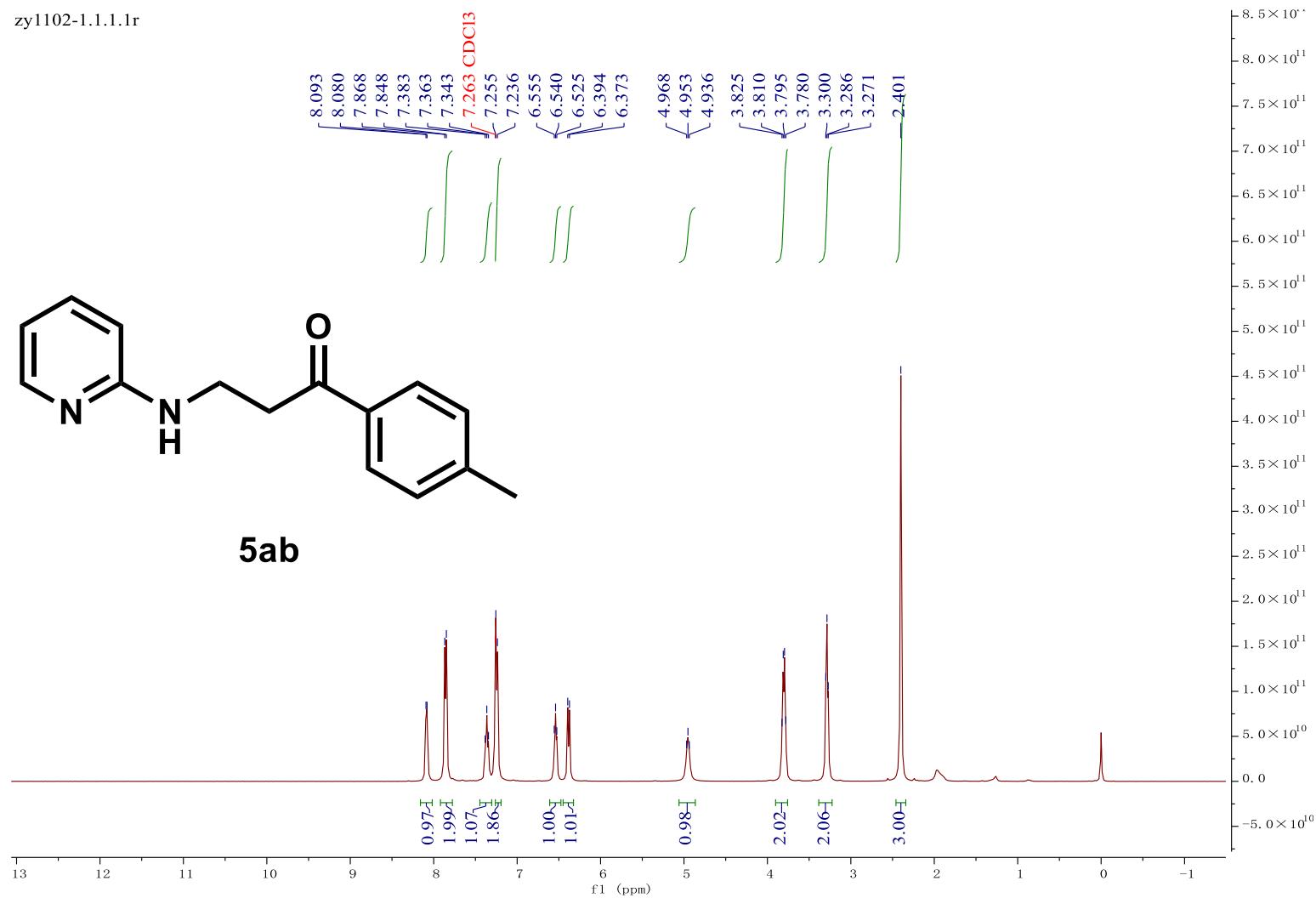
¹³C{H} NMR of Compound 3ew (101 MHz, CDCl₃)

zy1116-1.1.fid



¹H NMR of Compound 5ab (400 MHz, CDCl₃)

zy1102-1.1.1.1r



¹³C{H} NMR of Compound 5ab (101 MHz, CDCl₃)

