Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for

A Versatile Rhodium(III) Catalytic System for Direct Acyloxylation of Aryl and Alkenyl C-H Bonds with Carboxylic Acids

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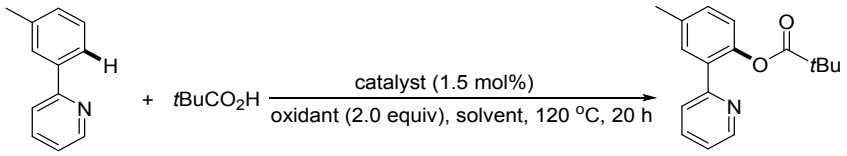
1. General information:

Unless otherwise noted, all experiments were carried out under nitrogen atmosphere, and all commercially available chemicals were used as received without further purification. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Model Advance DMX 400 Spectrometer (^{1}H 400 MHz and ^{13}C 100.6 MHz, respectively). Chemical shifts (δ) are given in ppm and are referenced to residual solvent peaks, and coupling constants (*J*) were reported in Hertz. 2-phenylpyridine (**1a-l**),[1] 2-phenoxypyridine (**3o**),[2a] *N*-phenylpyridin-2-amine (**3p**),[2b] 2-phenylpyrimidine (**3q**),[2c] 2-(1H-pyrrol-1-yl)pyrimidine (**3r**),[2d] 1-phenyl-1*H*-pyrazole (**3s**),[2d] 2-phenyl-4,5-dihydrooxazole (**3w**),[3] 9-isopropyl-6-phenyl-9*H*-purine (**5x-z**),[4] *N*-methyl-*N*-(1-phenylvinyl)acetamide (**9a**),[5] 2-(1-phenylvinyl)pyridine (**9b**),[6] (8*R*,9*S*,13*S*,14*S*)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthrene-3-carboxylic acid,[7] 2-(phenyl-d_5)pyridine (**[D_5]-1c**),[8] and $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$,[9] were prepared according to the previous reports.

2. Optimization of reaction conditions



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

Entry	Catalyst	Solvent	Oxidant	Yield(%)[b]
1	$[Cp^*RhCl_2]_2$	DCE	AgF	0
2	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	AgF	93
3	$RhCl_3.xH_2O$	DCE	AgF	NR
4	$Rh(acac)_3$	DCE	AgF	NR
5	$[Rh(cod)Cl]_2$	DCE	AgF	NR
6	$Rh(PPh_3)_3Cl$	DCE	AgF	NR
7	$Pd(OAc)_2$	DCE	AgF	NR
8	$[Ru(p\text{-cymen})Cl_2]_2$	DCE	AgF	NR
9	$[Cp^*IrCl_2]_2$	DCE	AgF	NR
10	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DME	AgF	30
11	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	toluene	AgF	18
12	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	MeOH	AgF	NR
13	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	EtOH	AgF	NR
14	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	*i*PrOH	AgF	NR
15	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	CH_3CN	AgF	NR
16	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DMF	AgF	NR
17	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	PhCl	AgF	NR
18	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	Ag_2O	68
19	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	Ag_2CO_3	48

20	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	Ag_2SO_4	NR
21	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$AgNO_3$	NR
22	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	AgOAc	NR
23	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$Cu(OAc)_2.H_2O$	NR
24	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$Cu(OAc)_2$	NR
25	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$K_2S_2O_8$	NR
26	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$(NH_4)_2S_2O_8$	NR
27	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	$PhI(OAc)_2$	NR
28	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	Oxone	NR
29	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	BQ	NR
30	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	O_2(1am)	NR
31[c]	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	AgF	60
32[d]	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	AgF	63
33[e]	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	AgF	84
34[f]	$[Cp^*RhCl_2]_2$ /$AgSbF_6$	DCE	AgF	91
35	none	DCE	AgF	NR
36	$[Cp^*Rh(CH_3CN)_3][SbF_6]_2$	DCE	none	NR

[a] Reaction Conditions: **1a** (0.3 mmol.), **2a** (0.6 mmol), [Rh] (1.5 mol%), oxidant (0.60 mmol), solvent (1.5 mL), 120 °C, 20 h. NR: no reaction. [b] Isolated yield. [c] $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (1.0 mol%) was employed. [d] Reaction temperature 110 °C. [e] Reaction temperature 130 °C. [f] $[Cp^*RhCl_2]_2$ (0.75 mol%) and $AgSbF_6$ (3.00 mol%) were employed.

3. The general procedure

(a) The general procedure for direct acyloxylation of C-H bonds

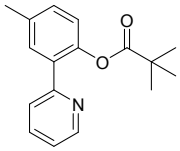
To an oven-dried pressure tube were sequentially added arylpyridine **1** (0.30 mmol), carboxylic acid **2** (0.60 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.79 mg, 0.0045 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 20 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure product.

(b) Experimental procedures for grammar-scale transformation reaction

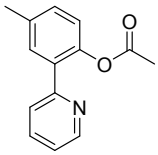
To an oven-dried pressure tube were sequentially added 2-(*m*-tolyl)pyridine **1a** (1.02 g, 6.0 mmol), pivalic acid **2a** (1.23 g, 12.0 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (75.87 mg, 0.090 mmol), AgF (1.52 g, 12.0 mmol) and 1,2-dichloroethane (30.0 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 24 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (50.0 mL) and extracted with CH_2Cl_2 (50.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum

evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give pure **3aa** (light yellow oil, 1.42 g, 88%).

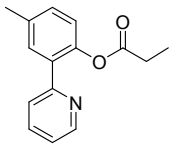
4. Characterization of products



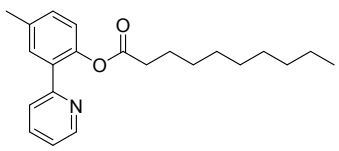
4-Methyl-2-(pyridin-2-yl)phenyl pivalate[10] **(3aa)**, yellow oil, 75.3 mg, yield: 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (dq, *J* = 4.9, 0.9 Hz, 1H), 7.70 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.53-7.43 (m, 2H), 7.34-7.13 (m, 2H), 7.00 (d, *J* = 8.2 Hz, 1H), 2.42 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.90, 155.91, 149.53, 146.12, 135.86, 135.72, 133.18, 131.17, 130.17, 124.13, 122.66, 122.07, 38.96, 27.09, 20.88; HRMS (ESI) calcd. for $C_{17}H_{20}NO_2$ $[M+H]^+$: 270.1489, found: 270.1483.



4-Methyl-2-(pyridin-2-yl)phenyl acetate [11]**(3ab)**, yellow oil, 58.1 mg, yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (dd, *J* = 4.9, 0.9 Hz, 1H), 7.73 (d, *J* = 1.9 Hz, 1H), 7.55-7.48 (m, 2H), 7.25-7.18 (m, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 2.40 (s, 3H), 2.16 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.62, 155.87, 149.59, 145.85, 136.17, 136.07, 132.71, 131.25, 130.31, 123.59, 122.89, 122.11, 20.96, 20.91; HRMS (ESI) calcd. for $C_{14}H_{14}NO_2$ $[M+H]^+$: 228.1019, found: 228.1016.

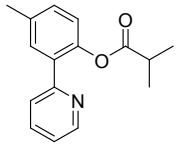


4-Methyl-2-(pyridin-2-yl)phenyl propionate (3ac), yellow oil, 58.3 mg, yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, *J* = 4.8, 0.9 Hz, 1H), 7.79-7.62 (m, 1H), 7.50 (d, *J* = 1.1 Hz, 2H), 7.21 (d, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.2 Hz, 1H), 2.45 (q, *J* = 7.6 Hz, 2H), 2.40 (s, 3H), 1.13 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.96, 155.91, 149.55, 145.88, 136.08, 135.92, 132.77, 131.21, 130.27, 123.72, 122.87, 122.06, 27.69, 20.90, 9.00; HRMS (ESI) calcd. for $C_{15}H_{16}NO_2$ $[M+H]^+$: 242.1176, found: 242.1172.

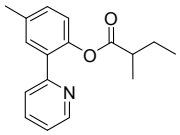


4-Methyl-2-(pyridin-2-yl)phenyl decanoate (3ad), yellow oil, 76.5 mg, yield: 75% ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (dt, *J* = 4.7, 1.4 Hz, 1H), 7.70 (td, *J* = 7.7, 1.9 Hz, 1H), 7.62-7.40 (m, 2H), 7.31-7.15 (m, 2H), 7.03 (d, *J* = 8.2 Hz, 1H), 2.44-2.35 (m, 5H),

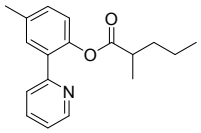
1.60 (t, J = 7.3 Hz, 2H), 1.33-1.22 (m, 12H), 0.88 (t, J = 7.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.25, 155.96, 149.52, 145.91, 136.04, 135.85, 132.87, 131.22, 130.23, 123.79, 122.88, 122.03, 34.29, 31.86, 29.38, 29.23, 29.06, 24.74, 22.65, 20.86, 14.08; HRMS (ESI) calcd. for $C_{22}H_{30}NO_2$ $[M+H]^+$: 340.2271, found: 340.2266.



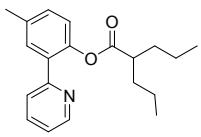
4-Methyl-2-(pyridin-2-yl)phenyl isobutyrate (3ae), yellow oil, 66.8 mg, yield: 87% ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (dd, J = 4.9, 0.9 Hz, 1H), 7.70 (td, J = 7.7, 1.9 Hz, 1H), 7.54-7.43 (m, 2H), 7.25-7.16 (m, 2H), 7.01 (d, J = 8.2 Hz, 1H), 2.68 (p, J = 7.0 Hz, 1H), 2.40 (s, 3H), 1.16 (d, J = 7.0 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.51, 155.92, 149.53, 145.88, 136.00, 135.86, 133.00, 131.21, 130.23, 123.97, 122.77, 122.09, 34.12, 20.90, 18.83; HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1332, found: 256.1328.



4-Methyl-2-(pyridin-2-yl)phenyl 2-methylbutanoate (3af), yellow oil，63.1 mg, yield: 78%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (dd, J = 4.9, 0.9 Hz, 1H), 7.69 (td, J = 7.7, 1.8 Hz, 1H), 7.54-7.40 (m, 2H), 7.24-7.16 (m, 2H), 7.01 (d, J = 8.2 Hz, 1H), 2.49 (q, J = 7.0 Hz, 1H), 2.39 (s, 3H), 1.72-1.65 (m, 1H), 1.52-1.42 (m, 1H), 1.13 (d, J = 7.0 Hz, 3H), 0.85 (t, J = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.02, 155.90, 149.46, 145.90, 136.04, 135.80, 133.03, 131.23, 130.22, 124.09, 122.79, 122.10, 41.12, 26.50, 20.87, 16.47, 11.51; HRMS (ESI) calcd. for $C_{17}H_{20}NO_2$ $[M+H]^+$: 270.1489, found: 270.1485.

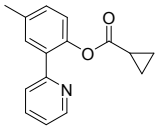


4-Methyl-2-(pyridin-2-yl)phenyl 2-methylpentanoate (3ag), yellow oil, 58.7 mg, yield: 69%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (ddd, J = 4.9, 1.8, 1.0 Hz, 1H), 7.69 (td, J = 7.7, 1.9 Hz, 1H), 7.54-7.42 (m, 2H), 7.26-7.18 (m, 2H), 7.00 (d, J = 8.2 Hz, 1H), 2.57 (q, J = 7.0 Hz, 1H), 2.39 (s, 3H), 1.73-1.58 (m, 1H), 1.44-1.33 (m, 1H), 1.28 – 1.20 (m, 2H), 1.12 (d, J = 7.0 Hz, 3H), 0.86 (t, J = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.17, 155.96, 149.49, 145.91, 135.97, 135.78, 133.10, 131.22, 130.18, 124.08, 122.78, 122.05, 39.39, 35.65, 20.86, 20.30, 16.88, 13.95; HRMS (ESI) calcd. for $C_{18}H_{22}NO_2$ $[M+H]^+$: 284.1645, found: 284.1644.

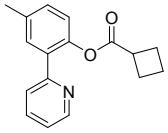


4-Methyl-2-(pyridin-2-yl)phenyl 2-propylpentanoate (3ah), yellow oil, 66.4 mg,

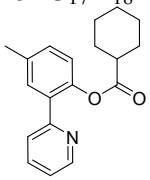
yield: 71%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73-8.66 (m, 1H), 7.69 (td, *J* = 7.7, 1.8 Hz, 1H), 7.58-7.48 (m, 1H), 7.45 (d, *J* = 2.4 Hz, 1H), 7.25-7.19 (m, 2H), 7.00 (d, *J* = 8.2 Hz, 1H), 2.52-2.44 (m, 1H), 2.39 (s, 3H), 1.61-1.55 (m, 2H), 1.43-1.37 (m, 2H), 1.24-1.14 (m, 4H), 0.84 (t, *J* = 7.3 Hz, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.76, 156.01, 149.49, 145.86, 135.94, 135.73, 133.23, 131.27, 130.13, 124.29, 122.81, 122.02, 45.25, 34.35, 20.86, 20.51, 14.03; HRMS (ESI) calcd. for $C_{20}H_{26}NO_2$ $[M+H]^+$: 312.1958, found: 312.1944.



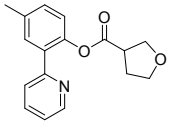
4-Methyl-2-(pyridin-2-yl)phenyl cyclopropanecarboxylate (3ai), yellow oil，68.5 mg, yield: 90%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.71 (td, *J* = 7.7, 1.9 Hz, 1H), 7.59-7.43 (m, 2H), 7.25-7.16 (m, 2H), 7.05 (d, *J* = 8.2 Hz, 1H), 2.40 (s, 3H), 1.79-1.69 (m, 1H), 1.07-0.96 (m, 2H), 0.94-0.82 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.33, 155.86, 149.54, 145.90, 136.02, 135.85, 132.82, 131.18, 130.22, 123.78, 122.82, 122.01, 20.88, 13.04, 8.76; HRMS (ESI) calcd. for $C_{16}H_{16}NO_2$ $[M+H]^+$: 254.1176, found: 254.1173.



4-Methyl-2-(pyridin-2-yl)phenyl cyclobutanecarboxylate (3aj), yellow oil, 65.9 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.73 (td, *J* = 7.7, 1.8 Hz, 1H), 7.54-7.47 (m, 2H), 7.28-7.21 (m, 2H), 7.05 (d, *J* = 8.2 Hz, 1H), 3.28 (td, *J* = 8.5, 1.1 Hz, 1H), 2.42 (s, 3H), 2.24-2.15 (m, 4H), 2.01-1.94 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.36, 152.77, 149.26, 147.44, 146.96, 135.82, 130.87, 128.78, 127.76, 125.38, 122.39, 120.19, 37.81, 29.71, 24.97, 18.39; HRMS (ESI) calcd. for $C_{17}H_{18}NO_2$ $[M+H]^+$: 268.1332, found: 268.1326.

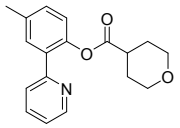


4-Methyl-2-(pyridin-2-yl)phenyl cyclohexanecarboxylate (3ak), yellow oil, 78.1 mg, yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78-8.67 (m, 1H), 7.73 (td, *J* = 7.7, 1.8 Hz, 1H), 7.55-7.45 (m, 2H), 7.27-7.21 (m, 2H), 7.02 (d, *J* = 8.2 Hz, 1H), 2.41 (s, 3H), 1.95-1.89 (m, 2H), 1.75 (dd, *J* = 8.5, 3.1 Hz, 2H), 1.66 (s, 1H), 1.46-1.41 (m, 2H), 1.32-1.22 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.52, 155.77, 149.37, 145.89, 137.67,36.20, 135.80, 131.24, 130.29, 124.10, 122.79, 122.19, 43.18, 28.79, 25.66, 25.32, 20.88; HRMS (ESI) calcd. for $C_{19}H_{22}NO_2$ $[M+H]^+$: 296.1645, found: 296.1637.

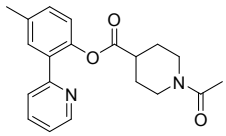


4-Methyl-2-(pyridin-2-yl)phenyl tetrahydrofuran-2-carboxylate (3al), yellow oil，

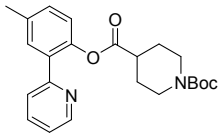
68.1 mg; yield: 80%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71 (dd, *J* = 4.9, 0.9 Hz, 1H), 7.74 (td, *J* = 7.7, 1.8 Hz, 1H), 7.48 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.44 (d, *J* = 2.2 Hz, 1H), 7.27 (s, 1H), 7.24-7.18 (m, 1H), 7.04 (d, *J* = 8.2 Hz, 1H), 3.99-3.95 (m, 2H), 3.84 (d, *J* = 9.1 Hz, 2H), 3.21 (ddt, *J* = 9.1, 8.0, 6.2 Hz, 1H), 2.40 (s, 3H), 2.17-2.10 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.24, 155.76, 149.22, 145.66, 137.67, 136.58, 132.53, 131.29, 130.43, 123.99, 122.69, 122.39, 70.05, 68.20, 43.81, 29.42, 20.87; HRMS (ESI) calcd. for $C_{17}H_{18}NO_3$ $[M+H]^+$: 284.1281, found: 284.1275.



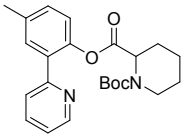
4-Methyl-2-(pyridin-2-yl)phenyl tetrahydro-2H-pyran-4-carboxylate (3am)，yellow oil, 77.8 mg, yield: 87%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.0 Hz, 1H), 7.73 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49-7.42 (m, 2H), 7.31-7.18 (m, 2H), 7.02 (d, *J* = 8.2 Hz, 1H), 3.93 (s, 2H), 3.43-3.40 (m, 2H), 2.70-2.62 (m, 1H), 2.39 (s, 3H), 1.81 (d, *J* = 2.7 Hz, 2H), 1.75-1.68 (m, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.83, 155.81, 149.26, 145.71, 136.38, 136.01, 132.70, 131.27, 130.35, 124.00, 122.70, 122.30, 66.91, 40.07, 28.42, 20.86; HRMS (ESI) calcd. for $C_{18}H_{20}NO_3$ $[M+H]^+$: 298.1438, found: 298.1431.



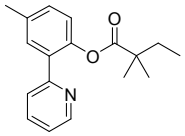
4-Methyl-2-(pyridin-2-yl)phenyl-1-acetylpiperidine-3-carboxylate (3an), yellow oil，82.3 mg, yield: 81%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (dd, *J* = 4.9, 1.5 Hz, 1H), 7.72 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49-7.40 (m, 2H), 7.23 (ddd, *J* = 9.9, 7.9, 2.4 Hz, 2H), 7.00 (d, *J* = 8.2 Hz, 1H), 4.34-4.28 (m, 1H), 3.73 (d, *J* = 13.7 Hz, 1H), 3.16-3.08 (m, 1H), 2.81 (t, *J* = 2.7 Hz, 1H), 2.69-2.62 (m, 1H), 2.39 (s, 3H), 2.08 (s, 3H), 1.91 (dd, *J* = 9.4, 4.2 Hz, 2H), 1.70-1.58 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.64, 169.00, 155.88, 149.33, 145.55, 136.36, 136.15, 132.80, 131.28, 130.34, 123.87, 122.68, 122.32, 45.42, 40.66, 28.10, 21.38, 20.88; HRMS (ESI) calcd. for $C_{20}H_{23}N_2O_3$ $[M+H]^+$: 339.1703, found: 339.1764.



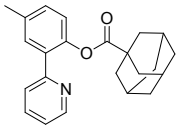
1-(*tert*-Butyl) 4-(4-methyl-2-(pyridin-2-yl)phenyl) Piperidine-1,4-dicarboxylate (3ao)，yellow oil, 101.2 mg, yield: 85%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74-8.63 (m, 1H), 7.72 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49-7.41 (m, 2H), 7.27-7.19 (m, 2H), 7.00 (d, *J* = 8.2 Hz, 1H), 3.97 (s, 2H), 2.84 (d, *J* = 11.9 Hz, 2H), 2.64-2.54 (m, 1H), 2.39 (s, 3H), 1.88 – 1.82 (m, 2H), 1.64-1.57 (m, 2H), 1.45 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.97, 155.89, 154.66, 149.36, 145.67, 136.27, 136.03, 132.83, 131.26, 130.31, 123.90, 122.71, 122.25, 79.65, 62.13, 41.09, 28.43, 27.77, 20.86; HRMS (ESI) calcd. for $C_{23}H_{29}N_2O_4$ $[M+H]^+$: 397.2122, found: 397.2121.



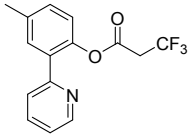
1-(*tert*-Butyl) 2-(4-methyl-2-(pyridin-2-yl)phenyl) piperidine-1,2-dicarboxylate (3ap), yellow oil, 92.9 mg, yield: 78%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.8 Hz, 1H), 7.79-7.66 (m, 1H), 7.56-7.43 (m, 2H), 7.23 (dd, *J* = 7.6, 4.7 Hz, 2H), 7.03 (dd, *J* = 29.2, 8.3 Hz, 1H), 4.01-3.80 (m, 1H), 2.88 (d, *J* = 112.3 Hz, 1H), 2.40 (s, 3H), 2.24 – 2.10 (m, 1H), 1.66 (ddd, *J* = 13.7, 6.2, 3.6 Hz, 1H), 1.60-1.51 (m, 2H), 1.44 (s, 9H), 1.38 (d, *J* = 16.9 Hz, 2H), 1.07 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.88, 155.79, 155,61, 149.59, 145.77, 136.22, 133.01, 131.43, 131.28, 130.21, 124.16, 122.83, 122.14, 80.00, 54.87, 42.05, 28.35, 26.56, 24.79, 20.85, 20.66; HRMS (ESI) calcd. for $C_{23}H_{29}N_2O_4$ $[M+H]^+$: 397.2122, found: 397.2118.



4-Methyl-2-(pyridin-2-yl)phenyl 2,2-dimethylbutanoate (3aq), yellow oil, 61.3 mg, yield: 72%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (ddd, *J* = 4.8, 1.8, 1.0 Hz, 1H), 7.68 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.50-7.42 (m, 2H), 7.22 (d, *J* = 1.1 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 1H), 2.39 (s, 3H), 1.59 (d, *J* = 7.5 Hz, 2H), 1.15 (s, 6H), 0.78 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.33, 155.97, 149.50, 146.14, 135.83, 135.64, 133.27, 131.20, 130.12, 124.25, 122.71, 122.05, 42.83, 33.14, 24.57, 20.85, 9.09; HRMS (ESI) calcd. for $C_{18}H_{22}NO_2$ $[M+H]^+$: 284.1645, found: 284.1641.

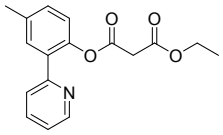


4-Methyl-2-(pyridin-2-yl)phenyl adamantane-1-carboxylate (3ar), yellow oil, 83.2 mg, yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.7 Hz, 1H), 7.71 (t, *J* = 7.7 Hz, 1H), 7.49 (d, *J* = 6.8 Hz, 2H), 7.25-7.16 (m, 2H), 6.98 (d, *J* = 8.2 Hz, 1H), 2.41 (s, 3H), 2.03 (s, 3H), 1.91 (s, 6H), 1.72 (q, *J* = 12.5 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.09, 155.81, 149.50, 146.08, 135.90, 135.69, 133.13, 131.17, 130.21, 124.21, 122.76, 122.11, 40.90, 38.66, 36.40, 27.85, 20.89; HRMS (ESI) calcd. for $C_{23}H_{26}NO_2$ $[M+H]^+$: 348.1958, found: 348.1954.

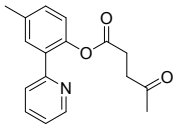


4-Methyl-2-(pyridin-2-yl)phenyl 3,3,3-trifluoropropanoate (3as), yellow oil, 53.2 mg, yield: 60%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.77 (td, *J* = 7.7, 1.9 Hz, 1H), 7.54-7.41 (m, 2H), 7.30-7.21 (m, 2H), 7.07 (s, 1H), 3.31 (q, *J* = 10.0 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.84, 155.57, 149.48, 145.10, 136.78, 136.49, 132.42, 131.31, 130.43, 123.52, 122.70, 122.33, 39.63,

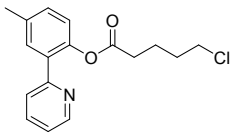
20.94; HRMS (ESI) calcd. for $C_{15}H_{13}F_3NO_2$ $[M+H]^+$: 296.0893, found: 296.0891.



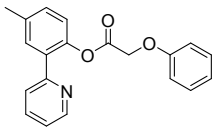
Ethyl (4-methyl-2-(pyridin-2-yl)phenyl) malonate (3at), yellow oil, 53.3 mg, yield: 41.4%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.76 (td, *J* = 7.7, 1.8 Hz, 1H), 7.49 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.32-7.25 (m, 3H), 7.25-7.15 (m, 1H), 4.07 (q, *J* = 7.1 Hz, 2H), 3.79 (s, 2H), 2.41 (s, 3H), 1.17 (d, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.08, 159.57, 148.96, 140.28, 136.97, 136.34, 131.19, 130.60, 129.43, 129.25, 123.95, 121.71, 60.52, 38.91, 21.08, 14.17; HRMS (ESI) calcd. for $C_{17}H_{18}NO_4$ $[M+H]^+$: 300.1230, found: 300.1234.



4-Methyl-2-(pyridin-2-yl)phenyl 4-oxopentanoate (3au), yellow oil, 64.7 mg, yield: 76%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.77 (td, *J* = 7.8, 1.8 Hz, 1H), 7.57-7.44 (m, 2H), 7.32-7.17 (m, 2H), 7.05 (d, *J* = 8.2 Hz, 1H), 2.75-2.69 (m, 4H), 2.39 (s, 3H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 206.90, 177.94, 157.85, 157.57, 145.85, 137.72, 132.31, 127.74, 126.27, 121.40, 118.98, 118.32, 37.71, 29.80, 27.77, 20.73; HRMS (ESI) calcd. for $C_{17}H_{18}NO_3$ $[M+H]^+$: 284.1281, found: 284.1275.

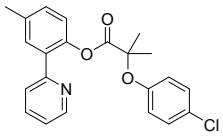


4-Methyl-2-(pyridin-2-yl)phenyl 5-chloropentanoate (3av), yellow oil, 53.3 mg, yield: 56 %; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.72 (td, *J* = 7.7, 1.9 Hz, 1H), 7.52-7.46 (m, 2H), 7.28-7.20 (m, 2H), 7.03 (d, *J* = 8.2 Hz, 1H), 4.05 (t, *J* = 6.3 Hz, 2H), 2.40 (s, 3H), 2.37-2.30 (m, 2H), 1.70-1.65 (m, 2H), 1.61 (dt, *J* = 6.8, 1.9 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 173.15, 155.99, 149.49, 145.76, 136.21, 136.05, 132.76, 131.26, 130.32, 123.75, 122.84, 122.13, 44.44, 31.85, 27.96, 22.25, 21.24; HRMS (ESI) calcd. for $C_{17}H_{19}ClNO_2$ $[M+H]^+$: 304.1099, found: 304.1086.

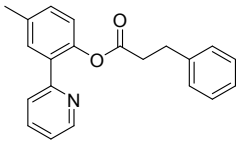


4-Methyl-2-(pyridin-2-yl)phenyl 2-phenoxyacetate (3aw), yellow oil，49.2 mg, yield: 52%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.50 (dd, *J* = 5.0, 0.9 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.59 (d, *J* = 2.1 Hz, 1H), 7.34-7.28 (m, 2H), 7.22 (ddd, *J* = 7.5, 5.0, 1.1 Hz, 1H), 7.12 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.04-6.99 (m, 1H), 6.93 (t, *J* = 8.3 Hz, 3H), 4.68 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.89,

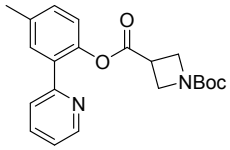
157.62, 157.43, 145.85, 137.73, 132.37, 129.69, 127.76, 126.29, 122.08, 121.39, 119.02, 118.38, 114.67, 64.88, 20.76; HRMS (ESI) calcd. for $C_{20}H_{18}NO_3$ $[M+H]^+$: 320.1281, found: 320.1256.



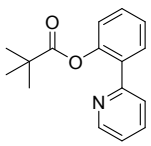
4-Methyl-2-(pyridin-2-yl)phenyl 2-(4-chlorophenoxy)-2-methylpropanoate (3ax), yellow oil, 61.8 mg, yield: 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (dt, *J* = 5.2, 1.3 Hz, 1H), 7.94 (d, *J* = 8.3 Hz, 1H), 7.84 (td, *J* = 7.9, 1.8 Hz, 1H), 7.62 (d, *J* = 2.1 Hz, 1H), 7.28 (s, 1H), 7.22 (d, *J* = 2.2 Hz, 2H), 6.98 – 6.94 (m, 1H), 6.90 (s, 2H), 6.73 (d, *J* = 2.2 Hz, 1H), 2.36 (s, 3H), 1.62 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.95, 153.72, 153.53, 152.00, 149.39, 147.14, 146.74, 135.90, 131.25, 129.12, 128.97, 127.98, 127.47, 125.78, 122.36, 120.86, 79.83, 25.27, 16.39; HRMS (ESI) calcd. for $C_{22}H_{21}ClNO_3$ $[M+H]^+$: 382.1204, found: 382.1217.



4-Methyl-2-(pyridin-2-yl)phenyl 3-phenylpropanoate (3ay)，yellow oil, 81.8 mg, yield: 86%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (m, 1H), 7.69 (t, *J* = 8.0 Hz, 1H), 7.49 (m, 2H), 7.32 (m, 2H), 7.23(m, 5H), 7.01 (d, *J* = 8.2 Hz, 1H), 2.96 (t, *J* = 7.9, Hz, 2H), 2.78 (t, *J* = 7.48 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.54 155.59, 149.24, 145.72, 140.26, 136.54, 136.11, 132.38, 131.30, 128.57, 128.40, 128.32, 126.38, 126.29, 122.84, 35.86, 30.68, 20.93; HRMS (ESI) calcd. for $C_{21}H_{20}NO_2$ $[M+H]^+$: 318.3884, found: 318.3421.

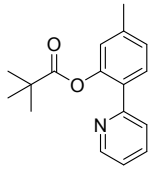


1-*tert*-Butyl 3-(4-methyl-2-(pyridin-2-yl)phenyl) azetidine-1,3-dicarboxylate (3az)，yellow oil, 87.2 mg, yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (m, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.85 (td, *J* = 7.7, 1.8 Hz, 1H), 7.62 (s, 1H), 7.26 (m, 1H), 7.15 (m, 1H), 6.95 (d, *J* = 8.2 Hz, 1H), 4.15 (d, *J* = 7.4 Hz, 4H), 3.40 (m, 1H), 2.36 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.79, 157.92, 157.64, 156.17, 145.89, 137.70, 132.34, 127.73, 126.28, 121.39, 118.99, 118.37, 80.13, 51.60, 31.92, 28.35, 20.76; HRMS (ESI) calcd. for $C_{21}H_{25}N_2O_4$ $[M+H]^+$: 369.4336, found: 369.3812.

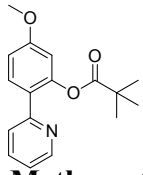


2-(Pyridin-2-yl)Phenyl pivalate (3ba)[10]**,** yellow oil, 69.12 mg, yield: 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73-8.65 (m, 1H), 7.74-7.64 (m, 2H), 7.51 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.43 (dd, *J* = 7.9, 1.9 Hz, 1H), 7.39-7.32 (m, 1H), 7.31-7.22 (m, 1H), 7.17-7.10

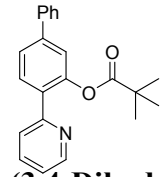
(m, 1H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.71, 155.87, 149.50, 148.38, 135.99, 130.76, 129.57, 126.08, 124.12, 122.99, 122.17, 120.15, 38.98, 27.07; HRMS (ESI) calcd. for $C_{16}H_{18}NO_2$ $[M+H]^+$: 256.1332, found: 256.1330.



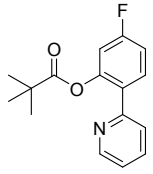
5-Methyl-2-(pyridin-2-yl)phenyl pivalate (3ca), yellow oil, 71.2 mg, yield: 88%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.68 (td, *J* = 7.7, 1.8 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.46 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.21 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 7.14 (ddd, *J* = 7.8, 1.7, 0.8 Hz, 1H), 6.91 (dd, *J* = 1.7, 0.8 Hz, 1H), 2.40 (s, 3H), 1.21 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.82, 155.93, 149.46, 148.21, 139.96, 135.89, 130.75, 130.50, 126.94, 124.01, 123.43, 121.91, 38.99, 27.10, 21.14; HRMS (ESI) calcd. for $C_{17}H_{20}NO_2$ $[M+H]^+$: 270.1489, found: 270.1481.



5-Methoxy-2-(pyridin-2-yl)phenyl pivalate (3da), yellow oil, 76.3 mg, yield: 89% ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.74-7.67 (m, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.52-7.41 (m, 1H), 7.21 (ddd, *J* = 7.6, 4.9, 1.2 Hz, 1H), 6.91 (dd, *J* = 8.6, 2.6 Hz, 1H), 6.70-6.58 (m, 1H), 3.87 (s, 3H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.61, 160.57, 155.72, 149.45, 135.94, 131.45, 126.24, 123.88, 121.71, 112.17, 108.44, 106.34, 55.58, 39.03, 27.10; HRMS (ESI) calcd. for $C_{17}H_{20}NO_3$ $[M+H]^+$: 286.1438, found: 286.1435.

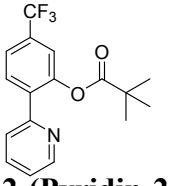


4-(3,4-Dihydropyridin-2-yl)-[1,1'-biphenyl]-3-yl pivalate (3ea), yellow oil, 83.6 mg, yield: 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ8.70 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.78-7.69 (m, 2H), 7.66-7.60 (m, 2H), 7.57 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.54 (dt, *J* = 7.8, 1.0 Hz, 1H), 7.45 (dd, *J* = 8.4, 7.0 Hz, 2H), 7.38 (d, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 1.8 Hz, 1H), 7.29-7.21 (m, 1H), 1.24 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.69, 155.65, 149.60, 148.72, 142.87, 139.82, 136.00, 132.38, 131.13, 128.82, 127.81, 127.21, 127.22, 124.77, 124.07, 122.16, 121.67, 39.06, 27.13; HRMS (ESI) calcd. for C22H22NO2 $[M+H]^+$: 332.1645, found: 332.1634.

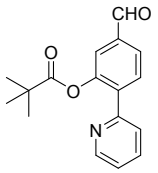


5-Fluoro-2-(pyridin-2-yl)phenyl pivalate (3fa), yellow oil, 56.7 mg, yield: 69%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.74 (td, *J* = 7.7, 1.8 Hz, 1H), 7.66 (dd, *J* = 8.6, 6.4 Hz, 1H), 7.48 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.28-7.22 (m,

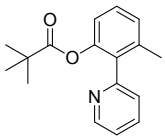
1H), 7.09 (ddd, *J* = 8.6, 7.9, 2.5 Hz, 1H), 6.90 (dd, *J* = 9.1, 2.5 Hz, 1H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.34, 149.59, 136.08, 131.80, 131.81, 129.94, 124.06, 122.25, 113.40, 113.19, 110.89, 110.65, 39.05, 27.02; HRMS (ESI) calcd. for $C_{16}H_{17}FNO_2$ $[M+H]^+$: 274.1238, found: 274.1232.



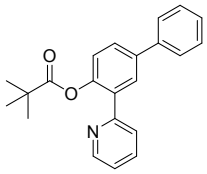
2-(Pyridin-2-yl)-5-(trifluoromethyl)phenyl pivalate (3ga), yellow oil, 53.4 mg, yield: 55%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73-8.70 (m, 1H), 7.79 (dd, *J* = 8.1, 1.0 Hz, 1H), 7.74 (dd, *J* = 7.7, 1.8 Hz, 1H), 7.60 (ddd, *J* = 8.0, 1.7, 0.8 Hz, 1H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 1.7 Hz, 1H), 7.26 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.29, 154.57, 149.77, 148.53, 137.15, 136.20, 135.90, 131.47, 125.38, 124.13, 122.83, 120.53, 117.60, 39.06, 27.00; HRMS (ESI) calcd. for $C_{17}H_{17}F_3NO_2$ $[M+H]^+$: 324.1206, found: 324.1198.



5-Formyl-2-(pyridin-2-yl)phenyl pivalate (3ha), yellow oil, 50.3 mg, yield: 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.75 (dd, *J* = 4.1, 2.7 Hz, 1H), 7.88 (s, 2H), 7.84-7.72 (m, 1H), 7.67 (d, *J* = 1.2 Hz, 1H), 7.56 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.39-7.28 (m, 1H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 191.00, 176.48, 154.55, 149.81, 149 .05, 139.35, 137.32, 136.22, 131.68, 127.31, 124.25, 124.01, 122.96, 39.08, 27.03; HRMS (ESI) calcd. for$C_{17}H_{18}NO_3$ $[M+H]^+$: 284.1281, found: 284.1276.

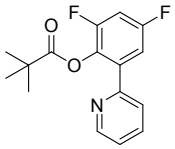


2-(3,4-Dihydropyridin-2-yl)-3-methylphenyl pivalate (3ia), yellow oil, 61.5 mg, yield: 76%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74-8.66 (m, 1H), 7.71 (td, *J* = 7.7, 1.8 Hz, 1H), 7.30 (t, *J* = 7.9 Hz, 1H), 7.27-7.19 (m, 2H), 7.16 (dt, *J* = 7.6, 1.0 Hz, 1H), 6.95 (dt, *J* = 8.2, 1.0 Hz, 1H), 2.12 (s, 3H), 0.98 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.73, 156.10, 149.48, 148.66, 137.98, 135.93, 133.83, 128.76, 127.55, 124.97, 122.07, 119.84, 38.77, 26.78, 19.75; HRMS (ESI) calcd. for $C_{17}H_{20}NO_2$ $[M+H]^+$: 270.1489, found: 270.1481.

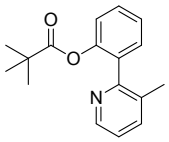


3-(Pyridin-2-yl)-[1,1'-biphenyl]-4-yl pivalate (3ja), yellow oil, 89.6 mg, yield: 90%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.87 (d, *J* = 2.3 Hz, 1H), 7.72 (td, *J* = 7.7, 1.9 Hz, 1H), 7.63 (ddd, *J* = 8.2, 3.7, 1.8 Hz, 3H), 7.57-7.48 (m,

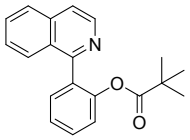
1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 7.4 Hz, 1H), 7.30-7.23 (m, 1H), 7.19 (d, *J* = 8.4 Hz, 1H), 1.22 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.79, 155.83, 149.56, 147.81, 140.21, 139.23, 136.03, 133.85, 129.56, 128.76, 128.19, 127.41, 127.21, 124.19, 123.36, 122.28, 39.05, 27.10; HRMS (ESI) calcd. for $C_{22}H_{22}NO_2$ $[M+H]^+$: 332.1645, found: 332.1640.



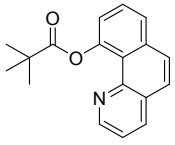
2-(3,4-Dihydropyridin-2-yl)-4,6-difluorophenyl pivalate (3ka), yellow oil, 37.6 mg, yield: 43%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.79-7.68 (m, 1H), 7.50 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.29-7.25 (m, 2H), 6.97 (ddd, *J* = 9.7, 8.0, 3.0 Hz, 1H), 1.26 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.70, 158.86, 153.53, 149.84, 146.10, 138.24, 136.39, 136.21, 123.96, 123.03, 112.47, 104.91, 39.09, 27.02; HRMS (ESI) calcd. for $C_{16}H_{16}F_2NO_2$ $[M+H]^+$: 292.1144, found: 292.1137.



2-(3-Methyl-3,4-dihydropyridin-2-yl)phenyl pivalate (3la), yellow oil, 65.6 mg, yield: 81%; ^{1}H NMR (600 MHz, $CDCl_3$ δ 8.54-8.44 (m, 1H), 7.55 (ddd, *J* = 7.7, 1.7, 0.9 Hz, 1H), 7.42 (ddd, *J* = 8.1, 7.1, 2.0 Hz, 1H), 7.34-7.29 (m, 2H), 7.22-7.10 (m, 2H), 2.18 (s, 3H), 1.00 (s, 9H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 176.29, 155.74, 148.37, 146.52, 137.63, 133.73, 132.48, 130.01, 129.14, 125.71, 122.76, 122.50, 38.81, 26.77, 19.03; HRMS (ESI) calcd. for $C_{17}H_{20}NO_2$ $[M+H]^+$: 270.1489, found: 270.1484.

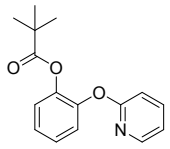


2-(Isoquinolin-1-yl)phenyl pivalate (3ma), yellow oil, 80.7 mg, yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 5.7 Hz, 1H), 7.88 (dt, *J* = 8.2, 1.0 Hz, 1H), 7.78 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.74-7.66 (m, 2H), 7.62-7.51 (m, 3H), 7.43 (dd, *J* = 7.5, 1.2 Hz, 1H), 7.33-7.18 (m, 1H), 0.76 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.13, 157.50, 148.79, 142.14, 136.14, 132.36, 130.97, 130.16, 129.66, 127.57, 127.26, 126.66, 125.80, 122.88, 120.21, 38.65, 26.44; HRMS (ESI) calcd. for $C_{20}H_{20}NO_2$ $[M+H]^+$: 306.1489, found: 306.1493.

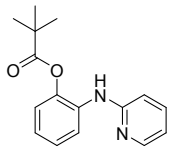


Benzo[*h*]quinolin-10-yl pivalate (3na) [12], yellow oil, 76.4 mg, yield: 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (dd, *J* = 4.4, 1.8 Hz, 1H), 8.16 (dd, *J* = 8.0, 1.8 Hz, 1H), 7.85 (dd, *J* = 8.5, 2.8 Hz, 2H), 7.73-7.65 (m, 2H), 7.52 (dd, *J* = 8.0, 4.3 Hz, 1H), 7.35 (dd, *J* = 7.6, 1.2 Hz, 1H), 1.60 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 177.75, 147.76, 136.01,

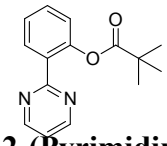
135.57, 128.01, 127.30, 126.55, 126.29, 122.10, 121.51, 39.43, 27.57; HRMS (ESI) calcd. for $C_{18}H_{18}NO_2$ [M+H]+: 280.1332, found: 280.1335.



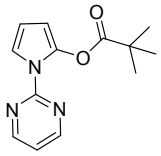
2-Phenoxyphenyl pivalate (3oa), yellow oil，57.1 mg, yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (ddd, *J* = 5.0, 2.0, 0.8 Hz, 1H), 7.68 (ddd, *J* = 8.3, 7.2, 2.0 Hz, 1H), 7.33-7.24 (m, 3H), 7.24-7.18 (m, 1H), 7.00 – 6.96 (m, 1H), 6.96-6.87 (m, 1H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.05, 163.11, 147.56, 144.95, 143.22, 139.34, 126.67, 125.74, 123.67, 123.39, 118.40, 110.64, 38.97, 26.86; HRMS (ESI) calcd. for $C_{16}H_{18}NO_3$[M+H]$^+$: 272.1281, found: 272.1287.



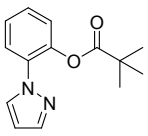
2-(Pyridin-2-ylamino)phenyl pivalate (3pa), yellow. oil, 60.1 mg, yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (ddd, *J* = 5.0, 1.9, 0.9 Hz, 1H), 7.72-7.65 (m, 1H), 7.49 (ddd, *J* = 8.4, 7.2, 1.9 Hz, 1H), 7.31-7.21 (m, 1H), 7.18-7.11 (m, 2H), 6.79-6.66 (m, 2H), 6.44 (s, 1H)., 2.49 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.50, 156.07, 148.19, 143.47, 137.74, 132.54, 126.43, 124.32, 123.51, 122.86, 115.12, 108.24, 39.23, 27.10; HRMS (ESI) calcd. for $C_{16}H_{19}N_2O_2$ [M+H]$^+$: 271.1441, found: 271.1428.



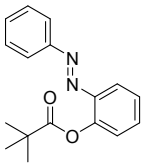
2-(Pyrimidin-2-yl)phenyl pivalate (3qa), yellow oil, 53.9 mg, yield: 70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 4.9 Hz, 2H), 8.16 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.51 (ddd, *J* = 8.1, 7.4, 1.8 Hz, 1H), 7.40 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.23 (t, *J* = 4.9 Hz, 1H), 7.13 (dd, *J* = 8.0, 1.2 Hz, 1H), 1.36 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.93, 164.25, 156.93, 149.58, 131.53, 131.13, 126.03, 123.71, 119.03, 39.11, 27.29; HRMS (ESI) calcd. for $C_{15}H_{17}N_2O_2$ [M+H]$^+$: 257.1285, found: 257.1284.



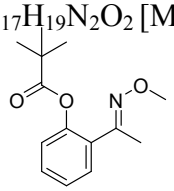
1-(Pyrimidin-2-yl)-1H-pyrrol-2-yl pivalate (3ra), yellow oil, 31.7 mg, yield: 43%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 4.8 Hz, 2H), 7.26 (s, 1H), 7.13 (dd, *J* = 6.0, 1.9 Hz, 1H), 6.66 (t, *J* = 4.8 Hz, 1H), 6.28 (d, *J* = 6.0 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.98, 158.33, 143.09, 129.77, 117.06, 82.28, 39.70, 27.09; HRMS (ESI) calcd. for $C_{13}H_{16}N_3O_2$ [M+H]$^+$: 246.1237, found: 246.1233.



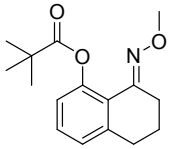
2-(1*H*-Pyrazol-1-yl)phenyl pivalate (3sa), yellow oil, 38.2 mg, yield: 52%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (ddd, *J* = 10.9, 2.1, 0.6 Hz, 2H), 7.61 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.48-7.32 (m, 2H), 7.20 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.44 (dd, *J* = 2.4, 1.8 Hz, 1H), 1.25 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.41, 144.30, 140.79, 133.44, 130.70, 128.70, 126.52, 126.47, 123.78, 106.58, 39.03, 27.05; HRMS (ESI) calcd. for $C_{14}H_{17}N_2O_2$ $[M+H]^+$: 245.1285, found: 245.1279.



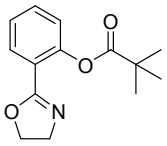
(*E*)-2-(Phenyldiazenyl)phenyl pivalate (3ta), orange oil, 61.7 mg, yield: 84%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92-7.86 (m, 2H), 7.82 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.56-7.48 (m, 4H), 7.36 (ddd, *J* = 8.1, 7.4, 1.4 Hz, 1H), 7.24 (dd, *J* = 8.1, 1.4 Hz, 1H), 1.45 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.94, 152.83, 149.46, 144.38, 131.94, 131.22, 129.01, 126.33, 123.43, 123.05, 117.13, 39.21, 27.35; HRMS (ESI) calcd. for $C_{17}H_{19}N_2O_2$ $[M+H]^+$: 283.1441, found: 283.1438.



2-(1-(Methoxyimino)ethyl)phenyl pivalate (3ua), yellow oil, 60.3 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.34 (m, 2H), 7.29-7.22 (m, 1H), 7.11-7.03 (m, 1H), 3.98 (s, 3H), 2.16 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.69, 153.67, 148.38, 130.88, 129.62, 129.42, 125.82, 122.87, 61.84, 39.06, 27.14, 15.80; HRMS (ESI) calcd. for $C_{14}H_{20}NO_3$$[M+H]^+$: 250.1438, found: 250.1437.

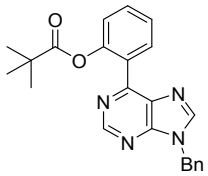


8-(Methoxyimino)-5,6,7,8-tetrahydronaphthalen-1-yl pivalate (3va), yellow oil, 65.4 mg, yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 (t, *J* = 7.8 Hz, 1H), 7.10 – 7.03 (m, 1H), 6.88-6.82 (m, 1H), 3.98 (s, 3H), 2.76 (t, *J* = 6.8 Hz, 2H), 2.73-2.67 (m, 2H), 1.85-1.74 (m, 2H), 1.41 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.93, 153.17, 148.26, 142.98, 128.97, 125.86, 124.14, 121.70, 61.95, 38.97, 30.63, 27.24, 25.10, 21.08; HRMS (ESI) calcd. for $C_{16}H_{22}NO_3$ $[M+H]^+$: 276.1594, found: 276.1590.

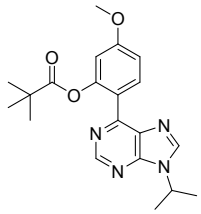


2-(4,5-Dihydrooxazol-2-yl)phenyl pivalate (3wa), yellow oil, 40.1 mg, yield: 54%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (m, 1H), 7.78 (dd, *J* = 9.9, 1.7 Hz, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.44 (d, *J* = 1.8 Hz, 1H), 4.59 (t, *J* = 5.2 Hz, 2H), 3.90 (t, *J* = 5.3 Hz, 2H), 1.27 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.68, 134.19, 133.33, 131.62, 129.71, 126.94, 63.86, 54.69, 39.80, 27.19; HRMS (ESI) calcd. for $C_{14}H_{18}NO_3$ $[M+H]^+$:

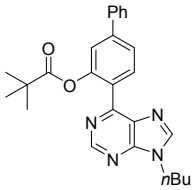
248.1281, found: 248.1276.



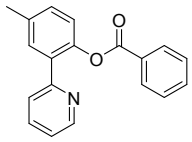
2-(9-Benzyl-9*H*-purin-6-yl)phenyl pivalate (3xa), yellow oil, 84.9 mg, yield: 77%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.10 (d, *J* = 1.3 Hz, 2H), 7.54 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.40-7.33 (m, 6H), 7.25-7.22 (m, 1H), 5.51 (s, 2H), 1.17 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.07, 152.39, 149.09, 144.54, 135.10, 132.06, 131.11, 129.19, 128.67, 128.37, 127.86, 125.87, 123.57, 47.36, 38.99, 27.01; HRMS (ESI) calcd. for $C_{23}H_{23}N_4O_2$ $[M+H]^+$: 387.1816, found: 387.1811.



2-(9-Isopropyl-9*H*-purin-6-yl)-5-methoxyphenyl pivalate (3ya), yellow oil, 81.7 mg, yield: 74%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (s, 1H), 8.22 (s, 1H), 8.15 (s, 1H), 6.98 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.74 (d, *J* = 2.6 Hz, 1H), 5.04-4.87 (m, 1H), 3.89(s, 3H), 1.68 (d, *J* = 6.8 Hz, 6H), 1.24 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.54, 161.80, 154.71, 151.73, 151.52, 150.49, 141.91, 133.38, 131.82, 121.01, 111.92, 109.25, 55.64, 47.23, 39.06, 27.11, 22.63; HRMS (ESI) calcd. for $C_{20}H_{25}N_4O_3$ $[M+H]^+$: 369.1921, found: 369.1912.

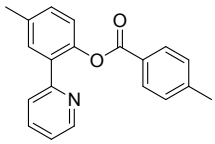


4-(9-Butyl-9*H*-purin-6-yl)-[1,1'-biphenyl]-3-yl pivalate (3za), yellow oil, 91.4 mg, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (s, 1H), 8.29 (d, *J* = 2.3 Hz, 1H), 8.12 (s, 1H), 7.76 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.67 (d, *J* = 7.3 Hz, 2H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.35 (dd, *J* = 19.8, 7.9 Hz, 2H), 4.35 (t, *J* = 7.2 Hz, 2H), 1.96 (dd, *J* = 8.7, 6.4 Hz, 2H), 1.49-1.37 (m, 2H), 1.19 (s, 9H), 1.01 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.57, 154.86, 152.15, 148.47, 144.74, 138.93, 131.99, 130.78, 129.61, 128.76, 127.44, 127.28, 123.85, 43.76, 39.03, 31.98, 27.01, 19.92, 13.52; HRMS (ESI) calcd. for $C_{26}H_{29}N_4O_2$ $[M+H]^+$: 429.2285, found: 429.2280.

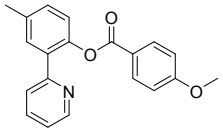


4-Methyl-2-(pyridin-2-yl)phenyl benzoate (5aa) [8], yellow oil, 79.4 mg, yield: 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 5.0 Hz, 1H), 8.13-8.04 (m, 2H), 7.63 – 7.53 (m, 4H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.31-7.24 (m, 1H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.18 –

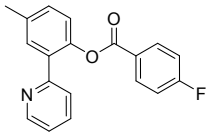
7.13 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.32, 155.55, 149.54, 146.04, 136.21, 136.10, 133.42, 132.75, 130.40, 130.16, 129.97, 129.54, 128.48, 123.82, 123.00, 122.14, 20.95; HRMS (ESI) calcd. for $C_{19}H_{16}NO_2$ $[M+H]^+$: 290.1176, found: 290.1170.



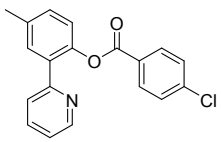
2-(Pyridin-2-yl)phenyl 4-methylbenzoate (5ab), yellow oil, 81.1 mg, yield: 89%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (ddd, *J* = 4.9, 1.9, 0.9 Hz, 1H), 7.76-7.63 (m, 2H), 7.63-7.47 (m, 2H), 7.33-7.26 (m, 1H), 7.22 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.78 (s, 2H), 6.48 (d, *J* = 15.9 Hz, 1H), 3.90 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.58, 155.75, 153.45, 149.62, 146.49, 145.85, 136.22, 132.85, 131.33, 130.36, 129.61, 123.71, 122.89, 122.09, 116.27, 105.42, 20.94; HRMS (ESI) calcd. for $C_{20}H_{18}NO_2$ $[M+H]^+$: 304.1332, found: 304.1330.



4-Methyl-2-(pyridin-2-yl)phenyl 4-methoxybenzoate (5ac), yellow oil, 89.2 mg, yield: 93%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (ddd, *J* = 4.9, 1.8, 1.0 Hz, 1H), 8.06 (d, *J* = 8.9 Hz, 2H), 7.62 (dt, *J* = 4.5, 1.9 Hz, 2H), 7.58-7.53 (m, 1H), 7.33-7.27 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.94 (s, 2H), 3.89 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.68, 164.32, 159.21, 155.53, 149.38, 145.92, 135.94, 134.03, 132.01, 131.12, 130.15, 123.86, 123.06, 121.93, 119.94, 111.90, 55.76, 20.79; HRMS (ESI) calcd. for $C_{20}H_{18}NO_3$ $[M+H]^+$: 320.1281, found: 320.1283.

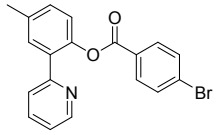


4-Methyl-2-(pyridin-2-yl)phenyl 4-fluorobenzoate (5ad), yellow oil, 75.76 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (dd, *J* = 4.9, 0.8 Hz, 1H), 8.12 (dd, *J* = 8.9, 5.4 Hz, 2H), 7.64 (d, *J* = 1.8 Hz, 2H), 7.58-7.48 (m, 1H), 7.35-7.27 (m, 1H), 7.22-7.05 (m, 4H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.29, 164.76, 164.40, 155.63, 149.61, 145.91, 136.14, 132.81, 131.34, 130.39, 125.80, 123.64, 122.97, 122.12, 115.80, 115.58, 20.96; HRMS (ESI) calcd. for $C_{19}H_{15}FNO_2$ $[M+H]^+$: 308.1081, found: 308.1075.

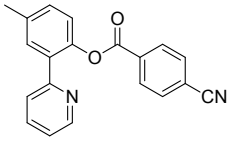


4-Methyl-2-(pyridin-2-yl)phenyl 4-chlorobenzoate (5ae), yellow oil, 82.62 mg, yield: 85%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73-8.54 (m, 1H), 8.03 (d, *J* = 8.3 Hz, 2H), 7.66-7.58 (m, 2H), 7.52 (s, 1H), 7.43 (d, *J* = 8.3 Hz, 2H), 7.29 (dd, *J* = 8.3, 2.0 Hz, 1H),

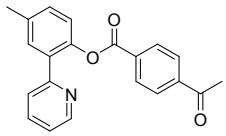
7.23-7.09 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.52, 155.59, 149.59, 145.88, 139.90, 136.26, 136.19, 132.77, 131.53, 131.34, 130.40, 128.86, 128.02, 123.61, 122.95, 122.15, 20.97; HRMS (ESI) calcd. for $C_{19}H_{15}ClNO_2$ $[M+H]^+$: 324.0786, found: 324.0783.



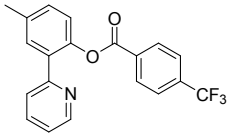
4-Methyl-2-(pyridin-2-yl)phenyl 4-bromobenzoate (5af), white solid, mp: 150.5-153.5 °C , 96.0 mg, yield: 87%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.97-7.88 (m, 2H), 7.64-7.55 (m, 4H), 7.51 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.27 (ddd, *J* = 8.1, 2.2, 0.9 Hz, 1H), 7.22-7.07 (m, 2H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.67, 155.60, 149.61, 145.86, 136.29, 136.17, 132.76 , 131.85 , 131.65, 131.34, 130.40, 128.63, 128.48, 123.59, 122.93, 122.14, 20.98; HRMS (ESI) calcd. for $C_{19}H_{15}BrNO_2$ $[M+H]^+$: 368.0281, found: 368.0275.



4-Methyl-2-(pyridin-2-yl)phenyl 4-cyanobenzoate (5ag), white solid, mp: 129.5-131.5 °C, 66.15 mg, yield: 70%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 8.25-8.10 (m, 2H), 7.83-7.70 (m, 2H), 7.64 (td, *J* = 7.7, 1.8 Hz, 1H), 7.55 (d, *J* = 2.1 Hz, 1H), 7.51 (dt, *J* = 8.0, 1.1 Hz, 1H), 7.29 (ddd, *J* = 8.2, 2.2, 0.8 Hz, 1H), 7.22 – 7.13 (m, 2H), 2.44 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 163.84, 155.66, 149.50, 145.72, 136.57, 136.27, 133.55, 132.60, 132.27, 131.35, 130.58, 130.46, 123.45, 122.82, 122.20, 117.87, 116.75, 20.96; HRMS (ESI) calcd. for $C_{20}H_{15}N_2O_2$ $[M+H]^+$: 315.1128, found: 315.1121.

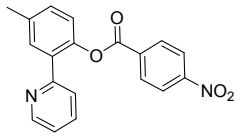


4-Methyl-2-(pyridin-2-yl)phenyl 4-acetylbenzoate (5ah), yellow oil, 78.2 mg, yield: 81%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.56 (ddd, *J* = 4.8, 1.9, 0.9 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 2H), 8.01 (d, *J* = 8.6 Hz, 2H), 7.63 (d, *J* = 1.8 Hz, 1H), 7.58 (dd, *J* = 2.1, 0.9 Hz, 1H), 7.56-7.50 (m, 1H), 7.30-7.27 (m, 1H), 7.20 (d, *J* = 8.2 Hz, 1H), 7.15 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 2.65 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 197.43, 164.52, 155.65, 149.58, 145.89, 140.56, 136.36, 136.15, 133.41, 132.73, 131.34, 130.40, 128.24, 123.57, 122.88, 122.13, 26.88, 20.96; HRMS (ESI) calcd. for $C_{21}H_{18}NO_3$ $[M+H]^+$: 332.1281, found: 332.1276.

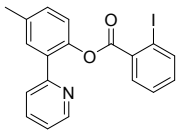


4-Methyl-2-(pyridin-2-yl)phenyl 4-(trifluoromethyl)benzoate (5ai), yellow oil, 78.4

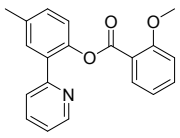
mg, yield: 73%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.56 (dt, *J* = 4.8, 1.3 Hz, 1H), 8.19 (d, *J* = 8.1 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 2H), 7.62 (td, *J* = 7.7, 1.8 Hz, 1H), 7.57 (d, *J* = 2.1 Hz, 1H), 7.52 (dt, *J* = 7.9, 1.1 Hz, 1H), 7.35-7.25 (m, 1H), 7.22-7.16 (m, 1H), 7.16-7.08 (m, 1H), 2.44 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.19, 155.67, 149.58, 136.43, 136.20, 134.90, 134.68, 132.93, 132.74, 131.36, 130.52, 130.42, 125.50, 123.51, 122.87, 122.16, 20.94; HRMS (ESI) calcd. for $C_{20}H_{15}F_3NO_2[M+H]^+$: 358.1049, found: 358.1045.



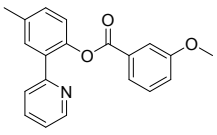
4-Methyl-2-(pyridin-2-yl)phenyl 4-nitrobenzoate (5aj), white solid, mp: 140.5-142.5 °C，79.4 mg, yield: 79%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60-8.46 (m, 1H), 8.34-8.18 (m, 4H), 7.67 (td, *J* = 7.7, 1.8 Hz, 1H), 7.61-7.46 (m, 2H), 7.34-7.27 (m, 1H), 7.24-7.14 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.61, 155.58, 150.72, 149.40, 145.66, 136.67, 136.47, 135.05, 132.45, 131.38, 131.24, 130.55, 123.61, 123.54, 122.80, 122.32, 20.99; HRMS (ESI) calcd. for $C_{19}H_{15}N_2O_4$ $[M+H]^+$: 335.1026, found: 335.1019.



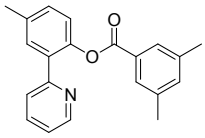
4-Methyl-2-(pyridin-2-yl)phenyl 2-iodobenzoate (5ak), yellow oil, 99.8 mg, yield: 80%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68-8.65 (m, 1H), 8.02 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.68 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.57 (dd, *J* = 5.0, 2.9 Hz, 2H), 7.41 (td, *J* = 7.6, 1.2 Hz, 1H), 7.30 (dd, *J* = 2.2, 0.7 Hz, 1H), 7.28-7.22 (m, 2H), 7.17 (dd, *J* = 7.6, 1.8 Hz, 1H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.07, 155.75, 149.56, 145.82, 141.45, 136.35, 134.27, 132.99, 130.43, 130.16, 128.49, 127.90, 123.79, 122.94, 122.25, 94.65, 20.98; HRMS (ESI) calcd. for $C_{19}H_{15}INO_2$ $[M+H]^+$: 416.0142, found: 416.0133.



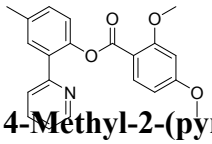
2-(Pyridin-2-yl)phenyl 2-methoxybenzoate (5al), yellow oil, 78.3 mg, yield: 83%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71-8.59 (m, 1H), 7.90-7.81 (m, 1H), 7.66-7.56 (m, 3H), 7.51-7.48 (m, 1H), 7.27 (dd, *J* = 6.2, 0.9 Hz, 1H), 7.23-7.15 (m, 2H), 6.98 (d, *J* = 7.9 Hz, 2H), 3.85 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.83, 164.46, 159.71, 155.67, 149.51, 146.06, 136.08, 134.18, 133.77, 132.91, 132.16, 131.74, 131.26, 130.29, 124.01, 123.20, 122.08, 120.09, 112.07, 55.91, 20.94; HRMS (ESI) calcd. for $C_{20}H_{18}NO_3$ $[M+H]^+$: 320.1281, found: 320.1278.



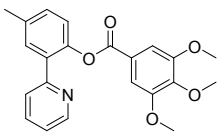
4-Methyl-2-(pyridin-2-yl)phenyl 3-methoxybenzoate (5am), yellow oil, 78.7 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.8 Hz, 1H), 7.75-7.66 (m, 1H), 7.66-7.52 (m, 4H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.29 (d, *J* = 3.1 Hz, 1H), 7.22-7.10 (m, 3H), 3.85 (s, 3H), 2.46 (s, 3H) ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.23, 159.58, 155.60, 149.63, 146.01, 136.13, 132.83, 131.34, 130.81, 130.36, 129.50, 123.75, 122.94, 122.59, 122.09, 120.12, 114.37, 55.48, 20.96; HRMS (ESI) calcd. for $C_{20}H_{18}NO_3$ $[M+H]^+$: 320.1281, found: 320.1286.



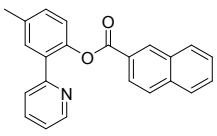
4-Methyl-2-(pyridin-2-yl)phenyl 3,5-dimethylbenzoate (5an), yellow oil, 83.3 mg, yield: 87%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 (ddd, *J* = 4.9, 1.8, 1.0 Hz, 1H), 7.74-7.65 (m, 2H), 7.62-7.48 (m, 3H), 7.31-7.23 (m, 1H), 7.20 (d, *J* = 1.8 Hz, 1H), 7.18-7.10 (m, 2H), 2.43 (s, 3H), 2.34 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.63, 155.67, 149.59, 146.16, 138.15, 136.10, 135.99, 135.11, 132.90, 131.34, 130.35, 129.41, 127.89, 123.80, 122.98, 122.06, 21.14, 20.94; HRMS (ESI) calcd. for $C_{21}H_{20}NO_2$ $[M+H]^+$: 318.1489 found: 318.1482.



4-Methyl-2-(pyridin-2-yl)phenyl 2,4-dimethoxybenzoate (5ao), yellow oil, 94.5 mg, yield: 90%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69-8.60 (m, 1H), 7.90 (d, *J* = 9.3 Hz, 1H), 7.60 (ddd, *J* = 5.1, 2.6, 1.5 Hz, 3H), 7.26-7.22 (m, 1H), 7.16 (d, *J* = 8.2 Hz, 2H), 6.47 (dd, *J* = 4.6, 2.4 Hz, 2H), 3.84 (s, 6H), 2.41 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.80, 163.76, 162.07, 155.78, 149.52, 146.19, 135.90, 135.62, 134.50, 132.93, 131.17, 130.18, 124.02, 123.34, 121.92, 111.34, 104.70, 98.95, 55.91, 55.51, 20.91; HRMS (ESI) calcd. for $C_{21}H_{20}NO_4$ $[M+H]^+$: 350.1387, found: 350.1381.

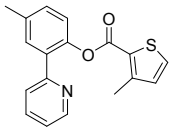


4-Methyl-2-(pyridin-2-yl)phenyl 3,4,5-trimethoxybenzoate (5ap), yellow oil, 104.8 mg, yield: 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68-8.52 (m, 1H), 7.62 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.57 (dd, *J* = 2.2, 0.8 Hz, 1H), 7.56-7.50 (m, 1H), 7.32 (s, 2H), 7.29-7.25 (m, 1H), 7.21-7.14 (m, 2H), 3.91 (s, 3H), 3.86 (s, 6H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.89, 155.69, 152.92, 149.58, 145.99, 142.52, 136.19, 132.78, 131.29, 130.36, 124.41, 123.73, 122.93, 122.10, 107.29, 60.90, 56.22, 20.93; HRMS (ESI) calcd. for $C_{22}H_{22}NO_5$ $[M+H]^+$: 380.1492, found: 380.1489.

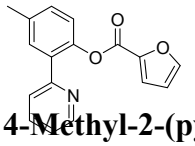


4-Methyl-2-(pyridin-2-yl)phenyl 2-naphthoate (5aq), yellow oil, 81.6 mg, yield:

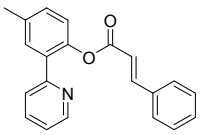
80%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (d, *J* = 1.6 Hz, 1H), 8.67 (d, *J* = 4.8 Hz, 1H), 8.12 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.96 (d, *J* = 1.3 Hz, 1H), 7.91 (d, *J* = 8.4 Hz, 2H), 7.70-7.52 (m, 5H), 7.40 – 7.31 (m, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.21-7.09 (m, 1H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.52, 155.60, 149.51, 146.16, 136.35, 136.17, 135.76, 132.77, 132.47, 131.97, 131.42, 130.50, 129.49, 128.59, 128.31, 127.81, 126.79, 126.72, 125.51, 123.88, 123.06, 122.20, 21.00; HRMS (ESI) calcd. for $C_{23}H_{18}NO_2$ $[M+H]^+$: 340.1332, found: 340.1320.



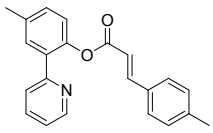
4-Methyl-2-(pyridin-2-yl)phenyl 3-methylthiophene-2-carboxylate (5ar), yellow oil, 81.8 mg, yield: 88%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68-8.59 (m, 1H), 7.70-7.58 (m, 3H), 7.44 (d, *J* = 5.0 Hz, 1H), 7.26 (d, *J* = 3.7 Hz, 1H), 7.20-7.13 (m, 2H), 6.93 (d, *J* = 5.0 Hz, 1H), 2.50 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 161.02, 155.44, 149.63, 147.90, 145.58, 136.00, 132.84, 131.75, 131.28, 130.98, 130.18, 125.59, 124.07, 123.14, 122.01, 20.93, 15.94; HRMS (ESI) calcd. for $C_{18}H_{16}NO_2S$ $[M+H]^+$: 310.0896, found: 310.0893.



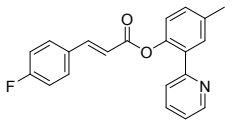
4-Methyl-2-(pyridin-2-yl)phenyl furan-2-carboxylate (5as), yellow oil, 76.4 mg, yield: 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (ddd, *J* = 4.9, 1.8, 1.0 Hz, 1H), 7.72-7.52 (m, 4H), 7.32-7.24 (m, 2H), 7.24-7.10 (m, 2H), 6.56 (dd, *J* = 3.5, 1.7 Hz, 1H), 2.45 (d, *J* = 0.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.01, 155.29, 149.53, 147.07, 145.20, 144.02, 136.37, 136.22, 132.66, 131.43, 130.40, 123.90, 122.86, 122.19, 119.31, 112.08, 20.96; HRMS (ESI) calcd. for $C_{17}H_{14}NO_3$ $[M+H]^+$: 280.0968, found: 280.0960.



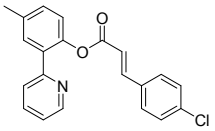
4-Methyl-2-(pyridin-2-yl)phenyl cinnamate (7aa), yellow oil, 85.32 mg, yield: 91%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (dd, *J* = 4.9, 1.6 Hz, 1H), 7.79 (d, *J* = 16.0 Hz, 1H), 7.70 (td, *J* = 7.7, 1.8 Hz, 1H), 7.64-7.49 (m, 4H), 7.43 (dd, *J* = 4.9, 1.9 Hz, 3H), 7.30-7.26 (m, 1H), 7.24-7.18 (m, 1H), 7.16 (d, *J* = 8.2 Hz, 1H), 6.58 (d, *J* = 16.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.59, 155.70, 149.65, 146.57, 145.84, 136.21, 136.09, 134.14, 132.84, 131.33, 130.70, 130.36, 128.98, 128.30, 123.77, 122.90, 122.13, 117.08, 20.97; HRMS (ESI) calcd. for $C_{21}H_{18}NO_2$ $[M+H]^+$: 316.1332, found: 316.1333.



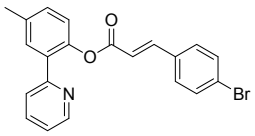
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(p-tolyl)acrylate (7ab), yellow oil, 88.1 mg, yield: 89%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.8, 1.8, 0.9 Hz, 1H), 7.73 (d, *J* = 16.0 Hz, 1H), 7.66 (td, *J* = 7.7, 1.8 Hz, 1H), 7.59-7.50 (m, 2H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.28-7.22 (m, 1H), 7.20-7.15 (m, 3H), 7.12 (d, *J* = 8.1 Hz, 1H), 6.49 (d, *J* = 16.0 Hz, 1H), 2.42 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.74, 155.74, 149.65, 146.55, 145.94, 141.19, 136.12, 135.97, 132.88, 131.47, 131.31, 130.31, 129.70, 128.29, 123.77, 122.93, 122.06, 116.02, 21.52, 20.95; HRMS (ESI) calcd. for $C_{22}H_{20}NO_2$ $[M+H]^+$: 330.1489, found: 330.1487.



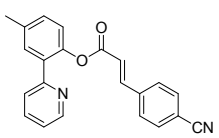
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(4-fluorophenyl)acrylate (7ac), yellow oil, 85.4 mg, yield: 80%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.72-7.62 (m, 2H), 7.59-7.47 (m, 4H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.28-7.19 (m, 2H), 7.12 (d, *J* = 8.2 Hz, 1H), 6.55 (d, *J* = 16.0 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.46, 162.74, 155.65, 149.51, 145.23, 136.36, 132.68, 131.36, 130.42, 130.11, 123.83, 122.86, 122.20, 116.79, 116.21, 115.99, 20.95; HRMS (ESI) calcd. for $C_{21}H_{17}FNO_2$ $[M+H]^+$: 334.1238, found: 334.1238.



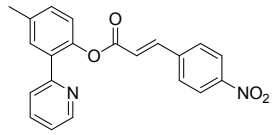
4-Methyl-2-(pyridin-2-yl)phenyl (E)-3-(4-chlorophenyl)acrylate (7ad), yellow oil, 80.8 mg, yield: 77%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.66 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.71-7.64 (m, 2H), 7.60-7.53 (m, 2H), 7.46-7.42 (m, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.27-7.22 (m, 1H), 7.22-7.16 (m, 1H), 7.12 (d, *J* = 8.2 Hz, 1H), 6.51 (d, *J* = 16.0 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.30, 155.75, 149.63, 145.81, 145.00, 136.61, 136.18, 136.13, 132.82, 132.66, 131.34, 130.35, 129.42, 129.25, 123.71, 122.85, 122.11, 117.72, 20.95; HRMS (ESI) calcd. for $C_{21}H_{17}ClNO_2$ $[M+H]^+$: 350.0942, found: 350.0938.



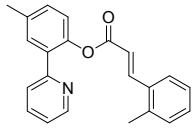
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(4-bromophenyl)acrylate (7ae), yellow oil, 92.2 mg, yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.76-7.66 (m, 2H), 7.63-7.49 (m, 4H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.29-7.27 (m, 1H), 7.24-7.19 (m, 1H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.55 (d, *J* = 16.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.33, 149.61, 145.75, 145.13, 136.28, 133.05, 132.22, 131.34, 130.38, 129.63, 123.73, 122.83, 122.14, 117.78, 20.96; HRMS (ESI) calcd. for $C_{21}H_{17}BrNO_2$ $[M+H]^+$: 394.0437, found: 394.0439.



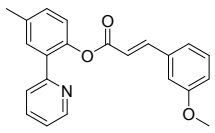
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(4-cyanophenyl)acrylate (7af)，white solid, mp: 165.5-166.5°C, 79.8 mg, yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.77-7.67 (m, 4H), 7.62 (d, *J* = 8.3 Hz, 2H), 7.58-7.50 (m, 2H), 7.31-7.26 (m, 1H), 7.26-7.18 (m, 1H), 7.13 (s, 1H), 6.64 (d, *J* = 16.0 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.77, 155.73, 149.61, 145.64, 143.92, 138.36, 136.33, 136.27, 132.69, 131.37, 130.40, 128.58, 123.63, 122.77, 122.18, 120.73, 118.31, 113.67, 20.96; HRMS (ESI) calcd. for $C_{22}H_{17}N_2O_2$ $[M+H]^+$: 341.1285, found: 341.1276.



4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(4-nitrophenyl)acrylate (7ag), yellow solid, mp: 170.5-172.5 °C, 83.3 mg, yield: 77%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.28 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 16.0 Hz, 1H), 7.77-7.65 (m, 3H), 7.57 (d, *J* = 2.1 Hz, 2H), 7.34-7.25 (m, 2H), 7.26-7.20 (m, 1H), 7.15 (d, *J* = 8.2 Hz, 1H), 6.69 (d, *J* = 16.0 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.67, 149.59, 148.67, 145.61, 143.35, 140.19, 136.29, 131.38, 130.42, 128.84, 124.21, 123.65, 122.74, 122.19, 121.46; HRMS (ESI) calcd. for $C_{21}H_{17}N_2O_4$ $[M+H]^+$: 361.1183, found: 361.1178.

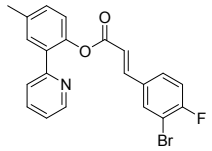


4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(o-tolyl)acrylate (7ah), yellow oil, 86.1 mg, yield: 87%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.70 (ddd, *J* = 4.9, 1.9, 0.9 Hz, 1H), 8.04 (d, *J* = 15.9 Hz, 1H), 7.68 (td, *J* = 7.7, 1.9 Hz, 1H), 7.62-7.51 (m, 3H), 7.28 (d, *J* = 1.4 Hz, 1H), 7.25 (t, *J* = 2.0 Hz, 1H), 7.20 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 3H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.46 (d, *J* = 15.9 Hz, 1H), 2.42 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.51, 155.71, 149.55, 145.94, 144.14, 137.91, 136.27, 136.00, 133.12, 132.69, 131.35, 130.90, 130.78, 130.41, 130.37, 126.54, 126.42, 123.90, 122.94, 122.15, 118.16, 20.95 , 19.80; HRMS (ESI) calcd. for $C_{22}H_{20}NO_2$ $[M+H]^+$: 330.1489, found: 330.1482.

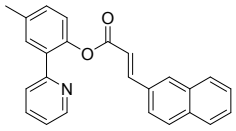


4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(3-methoxyphenyl)acrylate (7ai), yellow oil, 91.3 mg, yield: 88%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (ddd, *J* = 4.9, 1.8, 1.0 Hz, 1H), 7.80-7.68 (m, 2H), 7.64-7.53 (m, 2H), 7.39-7.27 (m, 2H), 7.23 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 7.20-7.10 (m, 2H), 7.07 (dd, *J* = 2.6, 1.5 Hz, 1H), 6.98 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 6.56 (d, *J* = 16.0 Hz, 1H), 3.85 (s, 3H), 2.45 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.52, 159.91, 155.63, 149.54, 146.49, 145.83, 136.36, 136.09, 135.48, 132.70, 131.35, 130.42, 129.98, 123.85, 122.89, 122.20, 121.00, 117.36, 116.58,

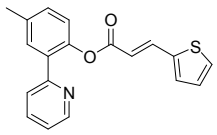
113.06, 55.33, 20.97; HRMS (ESI) calcd. for $C_{22}H_{20}NO_3[M+H]^+$: 346.1438, found: 346.1439.



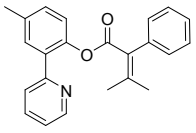
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(3-bromo-4-fluorophenyl)acrylate (7aj), yellow oil, 101.3 mg, yield: 82%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.73 (dd, *J* = 6.5, 2.2 Hz, 1H), 7.69 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.62 (s, 1H), 7.57-7.49 (m, 2H), 7.43 (dq, *J* = 6.8, 2.3 Hz, 1H), 7.29-7.24 (m, 1H), 7.24-7.17 (m, 1H), 7.18-7.08 (m, 2H), 6.46 (d, *J* = 16.0 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.00, 161.09, 159.41, 155.71, 149.59, 145.75, 143.64, 136.24, 133.17, 132.75, 131.93, 131.35, 130.37, 129.00, 123.71, 122.81, 122.15, 118.28, 117.12, 110.00, 20.94; HRMS (ESI) calcd. for $C_{21}H_{16}BrFNO_2$ $[M+H]^+$: 412.0343, found: 412.0341.



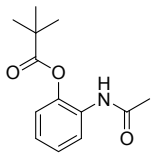
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(naphthalen-2-yl)acrylate (7ak), yellow oil, 85.6 mg, yield: 78%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.68 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.92 (d, *J* = 15.9 Hz, 2H), 7.88-7.82 (m, 3H), 7.73-7.65 (m, 2H), 7.60-7.55 (m, 2H), 7.55-7.49 (m, 2H), 7.29-7.24 (m, 1H), 7.19 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 7.15 (d, *J* = 8.1 Hz, 1H), 6.65 (d, *J* = 16.0 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 165.62, 155.78, 149.67, 146.56, 145.94, 136.15, 134.40, 133.27, 132.89, 131.70, 131.34, 130.33, 128.79, 128.65, 127.81, 127.46, 126.81, 123.76, 123.49, 122.92, 122.07, 117.28, 20.94; HRMS (ESI) calcd. for $C_{25}H_{20}NO_2$ $[M+H]^+$: 366.1489, found: 366.1485.



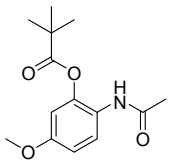
4-Methyl-2-(pyridin-2-yl)phenyl (*E*)-3-(thiophen-2-yl)acrylate (7al), yellow oil, 79.2 mg, yield: 82%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (ddd, *J* = 4.9, 1.9, 1.0 Hz, 1H), 7.88 (d, *J* = 15.7 Hz, 1H), 7.71 (td, *J* = 7.7, 1.9 Hz, 1H), 7.62-7.53 (m, 2H), 7.42 (d, *J* = 5.1 Hz, 1H), 7.33-7.18 (m, 3H), 7.14 (d, *J* = 8.2 Hz, 1H), 7.08 (dd, *J* = 5.1, 3.6 Hz, 1H), 6.36 (d, *J* = 15.7 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.42, 155.60, 149.53, 145.85, 139.28, 138.96, 136.36, 136.04, 132.71, 131.61, 131.36, 130.40, 129.17, 128.25, 123.86, 122.91, 122.21, 115.68, 20.96; HRMS (ESI) calcd. for $C_{19}H_{16}NO_2S$ $[M+H]^+$: 322.0896, found: 322.0888.



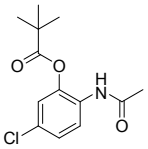
4-Methyl-2-(pyridin-2-yl)phenyl 3-methyl-2-phenylbut-2-enoate (7am), yellow oil, 76.4 mg, yield: 74%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.58 (ddd, *J* = 4.8, 1.9, 1.0 Hz, 1H), 7.54 (d, *J* = 2.3 Hz, 1H), 7.41 (td, *J* = 7.7, 1.8 Hz, 1H), 7.36-7.25 (m, 3H), 7.21 – 7.15 (m, 1H), 7.12 (dddd, *J* = 12.3, 7.5, 3.8, 2.7 Hz, 4H), 7.01 (d, *J* = 8.2 Hz, 1H), 2.35 (s, 3H), 2.12 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 166.13, 155.26, 149.44, 145.97, 137.81, 135.84, 135.68, 132.80, 131.25, 130.04, 129.18, 129.80, 128.15, 127.10, 124.10, 122.79, 121.79, 23.93, 22.61, 20.88; HRMS (ESI) calcd. for C23H22NO2 $[M+H]^+$: 344.1645, found: 344.1639.



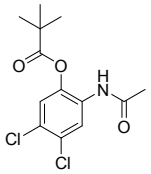
2-Acetamidophenyl pivalate (10a), yellow oil, 46.1 mg, yield: 58%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.27-7.22 (m, 1H), 7.13 (ddd, *J* = 18.9, 7.7, 1.6 Hz, 3H), 2.17 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.24, 167.95, 141.02, 129.79, 126.38, 124.95, 123.15, 121.92, 39.40, 27.16, 24.45; HRMS (ESI) calcd. for $C_{13}H_{18}NO_3$ $[M+H]^+$: 236.1281, found: 236.1276.



2-Acetamido-5-methoxyphenyl pivalate (10b), yellow oil, 49.5 mg, yield: 62%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.9 Hz, 1H), 6.92 (s, 1H), 6.80 (dd, *J* = 8.9, 2.8 Hz, 1H), 6.65 (d, *J* = 2.8 Hz, 1H), 3.80 (s, 3H), 2.13 (s, 3H), 1.40 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 176.36, 168.29, 157.55, 143.62, 125.89, 122.51, 111.80, 107.90, 55.65, 39.35, 27.14, 23.94; HRMS (ESI) calcd. for $C_{14}H_{20}NO_4$ $[M+H]^+$: 266.1387, found: 266.1380.

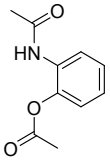


2-Acetamido-5-chlorophenyl pivalate (10c), yellow oil, 53.3 mg, yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.8 Hz, 1H), 7.21 (dd, *J* = 8.8, 2.4 Hz, 1H), 7.17-7.05 (m, 2H), 2.16 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.79, 167.93, 141.23, 129.55, 128.60, 126.46, 123.73, 122.41, 39.45, 27.10, 24.42; HRMS (ESI) calcd. for $C_{13}H_{17}ClNO_3$ $[M+H]^+$: 270.0891, found: 270.0897.

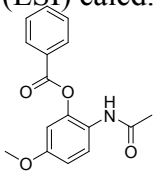


2-Acetamido-4,5-dichlorophenyl pivalate (10d), yellow oil, 51.9 mg, yield: 57%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.24 (s, 1H), 7.16 (s, 1H), 2.17 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.08, 167.95, 139.18，129.98, 129.40, 127.50, 123.64, 123.52, 38.83, 27.06, 24.45; HRMS (ESI) calcd. for $C1_3H_{16}Cl_2NO_3$

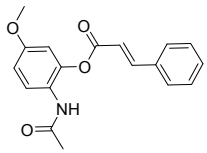
[M+H]$^+$: 304.0502, found: 304.0507.



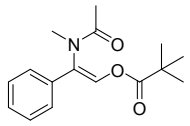
2-Acetamidophenyl acetate[13] **(10e)**, yellow oil, 34.35 mg, yield: 59%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (d, *J* = 8.1 Hz, 1H), 7.25 (dd, *J* = 8.4, 4.3 Hz, 1H), 7.22 (s, 1H), 7.15 (d, *J* = 4.3 Hz, 2H), 2.39 (s, 3H), 2.20 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.73, 168.17, 140.60, 129.65, 126.52, 124.82, 123.05, 122.04, 24.61, 21.11; HRMS (ESI) calcd. for $C_{10}H_{12}NO_3$ [M+H]$^+$: 194.0812, found: 194.0808.



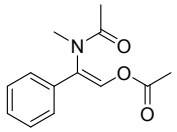
2-Acetamido-5-methoxyphenyl benzoate[13]**(10f)**, yellow oil, 65.5 mg, yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26-8.17 (m, 2H), 7.78 (d, *J* = 8.9 Hz, 1H), 7.68 (t, *J* = 7.4 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.09 (s, 1H), 6.83 (dd, *J* = 6.4, 3.0 Hz, 1H), 6.77 (d, *J* = 2.8 Hz, 1H), 3.79 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.74, 157.60, 143.54, 134.19, 130.34, 128.84, 126.06, 122.72, 121.90, 114.09, 112.16, 108.11, 55.68, 24.02; HRMS (ESI) calcd. for $C_{16}H_{16}NO_4$ [M+H]$^+$: 286.1074, found: 286.1068.



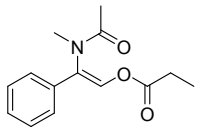
2-Acetamido-5-methoxyphenyl cinnamate (10g), yellow oil, 58.9 mg, yield: 63%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (m, 1H), 7.64-7.60 (m, 3H), 7.47-7.38 (m, 5H), 7.06 (s, 1H), 6.66 (d, *J* = 16.17, 1H), 3.82 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.36, 147.96, 133.79, 131.18, 129.12, 128.49, 125.63, 122.77, 121.89, 116.13, 112.00, 108.02, 55.66, 24.18; HRMS (ESI) calcd. for $C_{18}H_{18}NO_4$ [M+H]$^+$: 312.1230, found: 312.1234.



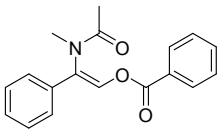
(Z)-2-(*N*-Methylacetamido)-2-phenylvinyl pivalate [14] **(11a)**, yellow oil, 56.3 mg, yield: 68%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (s, 1H), 7.41 (m, 5H), 3.10 (s, 3H), 1.99 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.68, 171.39, 131.65, 129.18, 128.81, 124.87, 34.25, 26.94, 21.08; HRMS (ESI) calcd. for $C_{16}H_{22}NO_3$ [M+H]$^+$: 276.1594, found: 276.1587.



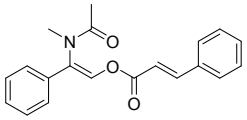
(Z)-2-(*N*-Methylacetamido)-2-phenylvinyl acetate [14] **(11b)**, yellow oil, 48.4 mg, yield: 69%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.43-7.32 (m, 5H), 3.08 (s, 3H), 2.25 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.30, 167.17, 133.30, 131.23, 129.18, 128.87, 128.77, 125.01, 34.33, 21.16, 20.66; HRMS (ESI) calcd. for $C_{13}H_{16}NO_3$ $[M+H]^+$: 234.1125, found: 234.1119.



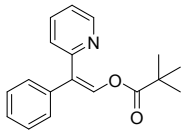
(Z)-2-(*N*-Methylacetamido)-2-phenylvinyl propionate (11c), yellow oil, 49.1 mg, yield: 66%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.45-7.32 (m, 5H), 3.08 (s, 3H), 2.53 (t, J = 7.5 Hz, 2H), 1.96 (s, 3H), 1.23 (t, J = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.31, 170.72, 133.35, 131.28, 129.17, 128.81, 128.78, 124.97, 34.31, 27.41, 21.16, 8.84; HRMS (ESI) calcd. for $C_{14}H_{18}NO_3$ $[M+H]^+$: 248.1281, found: 248.1286.



(Z)-2-(*N*-Methylacetamido)-2-phenylvinyl benzoate [14] **(11d)**, yellow oil, 57.3 mg, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.13 (m, 2H), 8.09 (s, 1H), 7.66 (d, J = 7.1 Hz, 1H), 7.55 (d, J = 7.7 Hz, 2H), 7.47-7.35 (m, 5H), 3.21 (s, 3H), 2.07 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.90, 162.62, 134.36, 133.43, 133.10, 131.41, 130.17, 129.26, 128.98, 128.41, 127.91, 125.01, 34.57, 29.71, 21.24; HRMS (ESI) calcd. for $C_{18}H_{18}NO_3$$[M+H]^+$: 296.1281, found: 296.1273.

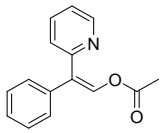


(Z)-2-(*N*-Methylacetamido)-2-phenylvinyl cinnamate (11e), yellow oil, 62.8 mg, yield: 65%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s , 1H) , 7.88 (d , J = 16.0 Hz , 1H) , 7.53-7.63 (m , 4H), 7.39-7.42 (m , 6H) , 6.56 (d , J = 16.0 Hz , 1H) , 3.15 (s , 3H) , 2.03 (s , 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.06, 163.12, 148.29, 133.72, 133.34, 131.42, 131.26, 129.09, 128.86, 128.61, 125.00, 115.47, 114.08, 34.40, 21.27; HRMS (ESI) calcd. for $C_{20}H_{20}NO_3$ [M+H]+: 322.1438, found: 322.1429.

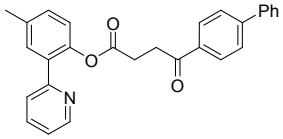


2-Phenyl-2-(pyridin-2-yl)vinyl pivalate (11f), yellow oil, 44.8 mg, yield: 53%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.59 (ddd, J = 4.9, 1.9, 1.0 Hz, 1H), 8.22 (s, 1H), 7.39 (m, 3H), 7.35 (m, 2H), 7.32 (m, 3H), 1.16 (d, J = 0.7 Hz, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.13, 157.00, 149.45, 136.49, 136.31, 130.02, 128.14, 127.61, 122.61, 122.06,

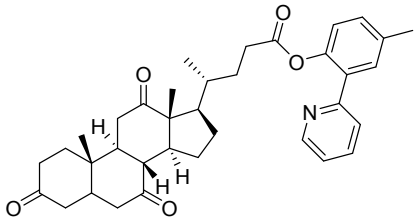
38.86, 26.79; HRMS (ESI) calcd. for $C_{18}H_{20}NO_2$ $[M+H]^+$: 282.1489, found: 282.1477.



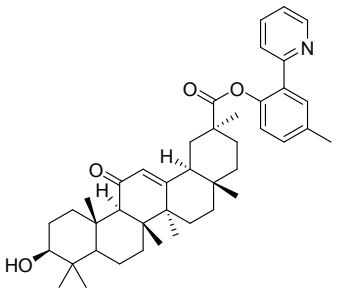
2-Phenyl-2-(pyridin-2-yl)vinyl acetate (11g), yellow oil, 39.6 mg, yield: 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 5.0 Hz, 1H), 7.69 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 2H), 7.43-7.30 (m, 5H), 5.71 (s, 1H), 1.99 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.09, 147.76, 142.65, 137.00, 128.40, 127.65, 126.14, 124.91, 122.64, 121.01, 29.71; HRMS (ESI) calcd. for $C_{15}H_{14}NO_2$ $[M+H]^+$: 240.1019, found: 240.1011.



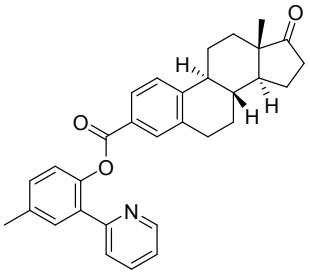
4-Methyl-2-(pyridin-2-yl)phenyl 4-([1,1'-biphenyl]-4-yl)-4-oxobutanoate (12), yellow oil, 82.3 mg, yield: 65%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 5.9 Hz, 1H), 8.19-8.13 (m, 1H), 8.11 (s, 1H), 8.06 (s, 2H), 7.70 (s, 2H), 7.62 (s, 3H), 7.55 (t, *J* = 6.7 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.40 (s, 1H), 7.32-7.29 (m, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 3.36 (d, *J* = 6.5 Hz, 2H), 2.85 (d, *J* = 6.5 Hz, 2H), 2.37 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.47, 175.76, 145.03, 141.01, 140.21, 138.82, 134.87, 134.12, 127.93, 127.63, 127.25, 126.27, 126.25, 124.05, 121.63, 119.59, 119.34, 32.27, 26.86, 19.72; HRMS (ESI) calcd. for $C_{28}H_{24}NO_3$ $[M+H]^+$: 422.1751, found: 422.1746.



4-Methyl-2-(pyridin-2-yl)phenyl(4R)-4-((8R,9S,10S,13R,14S,17R)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate (13)，white solid, mp: 180.5-181.5 °C, 136.8 mg, yield: 80%; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.2 Hz, 1H), 7.72 (tt, *J* = 7.8, 1.9 Hz, 1H), 7.55-7.44 (m, 2H), 7.27-7.17 (m, 2H), 7.08-6.93 (m, 1H), 2.90 (q, *J* = 4.3, 3.5 Hz, 3H), 2.57-2.48 (m, 1H), 2.39 (d, *J* = 3.0 Hz, 3H), 2.35-2.18 (m, 9H), 2.02 (s, 4H), 1.86-1.81 (m, 2H), 1.61-1.58 (m, 1H), 1.39 (d, *J* = 3.3 Hz, 3H), 1.38-1.28 (m, 4H), 1.03 (d, *J* = 2.9 Hz, 3H), 0.82 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 211.93, 209.04, 208.67, 172.42, 155.77, 149.39, 145.89, 136.22, 135.84, 132.62, 131.21, 130.25, 123.84, 122.82, 122.13, 62.15, 56.85, 51.75, 48.92, 46.75, 45.63, 45.50, 44.93, 42.74, 38.60, 36.42, 35.97, 35.30, 31.37, 30.17, 27.52, 25.07, 21.83, 20.85, 18.59, 11.82; HRMS (ESI) calcd. for $C_{36}H_{44}NO_5$ $[M+H]^+$: 570.3214, found: 570.3215.



4-Methyl-2-(pyridin-2-yl)phenyl(2S,4aS,6aS,6bR,10S,12aS,12bR,14bS)-10-hydroxy-2,4a,6a,6b,9,9,12a-heptamethyl-13-oxo-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,12b,13,14b-icosahydropicene-2-carboxylate (14), yellow oil, 135.9 mg, yield: 71%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.66 (ddd, *J* = 4.9, 1.8, 0.9 Hz, 1H), 7.69 (td, *J* = 7.7, 1.8 Hz, 1H), 7.46 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.42 (d, *J* = 2.1 Hz, 1H), 7.26-7.17 (m, 2H), 6.95 (d, *J* = 8.2 Hz, 1H), 5.56 (s, 1H), 3.18 (dd, *J* = 11.2, 5.0 Hz, 1H), 2.82-2.69 (m, 1H), 2.39 (s, 3H), 2.30 (s, 1H), 2.21-2.13 (m, 1H), 2.03-1.92 (m, 3H), 1.80 (d, *J* = 4.6 Hz, 1H), 1.69-1.55 (m, 5H), 1.46-1.28 (m, 8H), 1.21-1.08 (m, 11H), 0.98 (m, 5H), 0.78 (d, *J* = 5.3 Hz, 6H), 0.72-0.63 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 200.01, 174.90, 168.77, 155.86, 149.47, 145.88, 136.11, 135.76, 133.43, 131.33, 130.21, 128.53, 124.26, 122.49, 122.20, 78.41, 62.16, 61.75, 54.88, 47.92, 45.32, 44.05, 43.12, 40.96, 39.09, 37.57, 37.02, 32.70, 31.77, 31.02, 28.51, 28.11, 27.87, 27.20, 26.37, 26.30, 23.41, 20.87, 18.64, 17.46, 16.34, 15.65; HRMS (ESI) calcd. for $C_{42}H_{56}NO_4$ $[M+H]^+$: 638.4204, found: 638.4193.



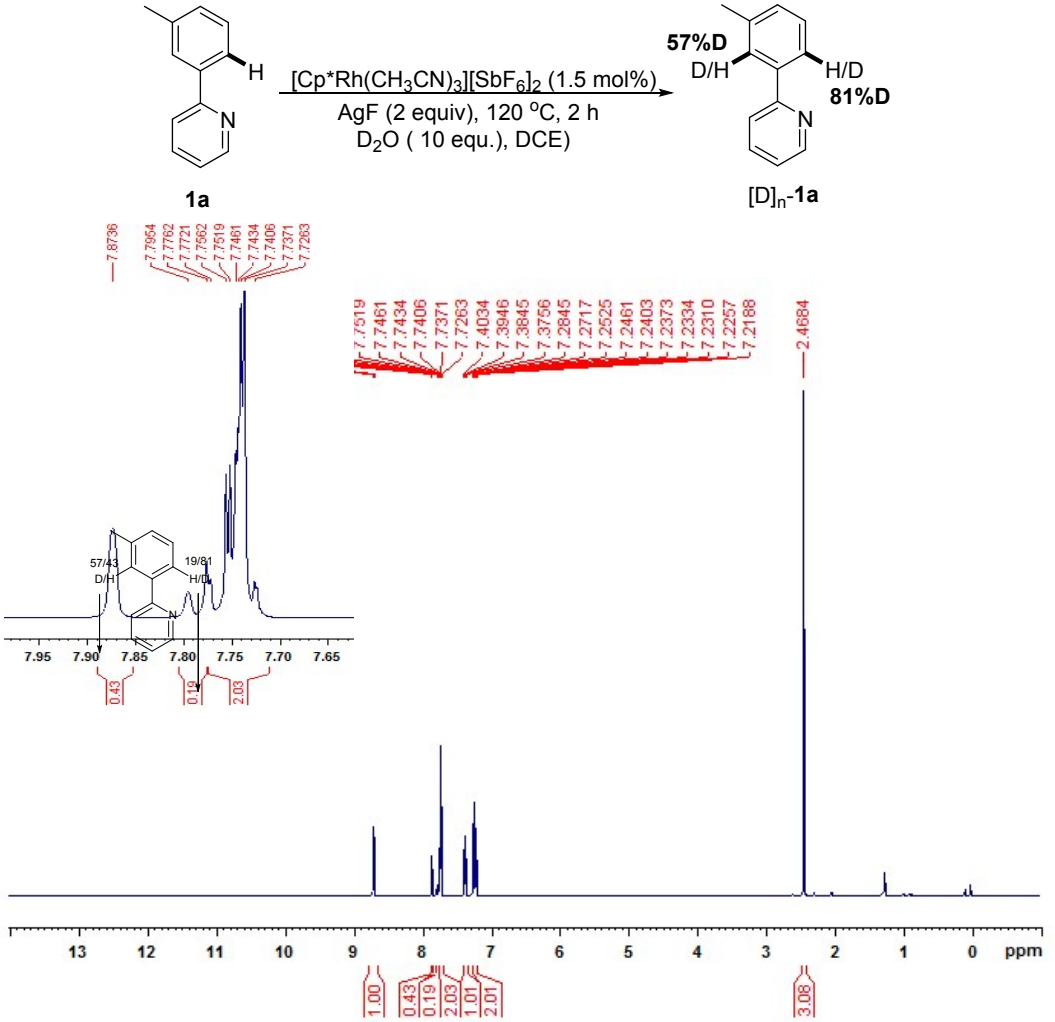
4-Methyl-2-(pyridin-2-yl)phenyl(8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthrene-3-carboxylate (15), yellow oil, 109.0 mg, yield: 78%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.7 Hz, 1H), 7.90-7.79 (m, 2H), 7.63-7.52 (m, 3H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.32 – 7.24 (m, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 3.05-2.88 (m, 2H), 2.59-2.51 (m, 1H), 2.44 (s, 3H), 2.36 (d, *J* = 4.1 Hz, 1H), 2.18 (d, *J* = 9.3 Hz, 1H), 2.10-1.97 (m, 4H), 1.66-1.57 (m, 2H), 1.57-1.45 (m, 4H), 0.93 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 220.52, 165.39, 155.56, 149.57, 146.06, 145.80, 136.92, 136.14, 136.00, 132.81, 131.33, 130.82, 130.35, 127.42, 126.91, 125.57, 123.81, 123.00, 122.07, 50.50, 47.87, 44.72, 37.76, 35.82, 31.54, 29.20, 26.24, 25.56, 21.59, 20.96, 13.82; HRMS (ESI) calcd. for $C_{31}H_{32}NO_3$ $[M+H]^+$: 466.2377, found: 466.2365.

5. The mechanistic studies

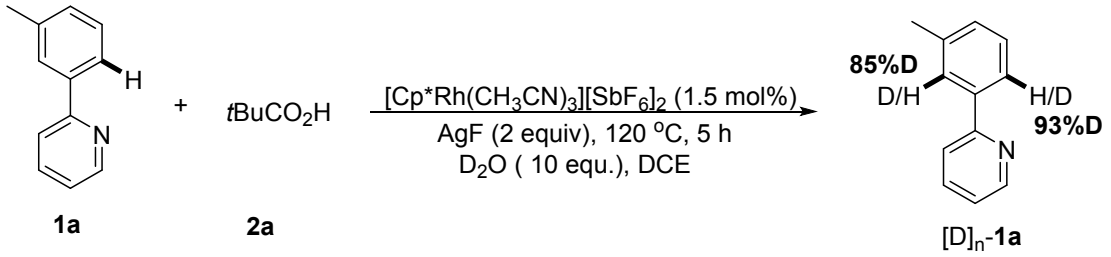
a) H/D exchange experiment

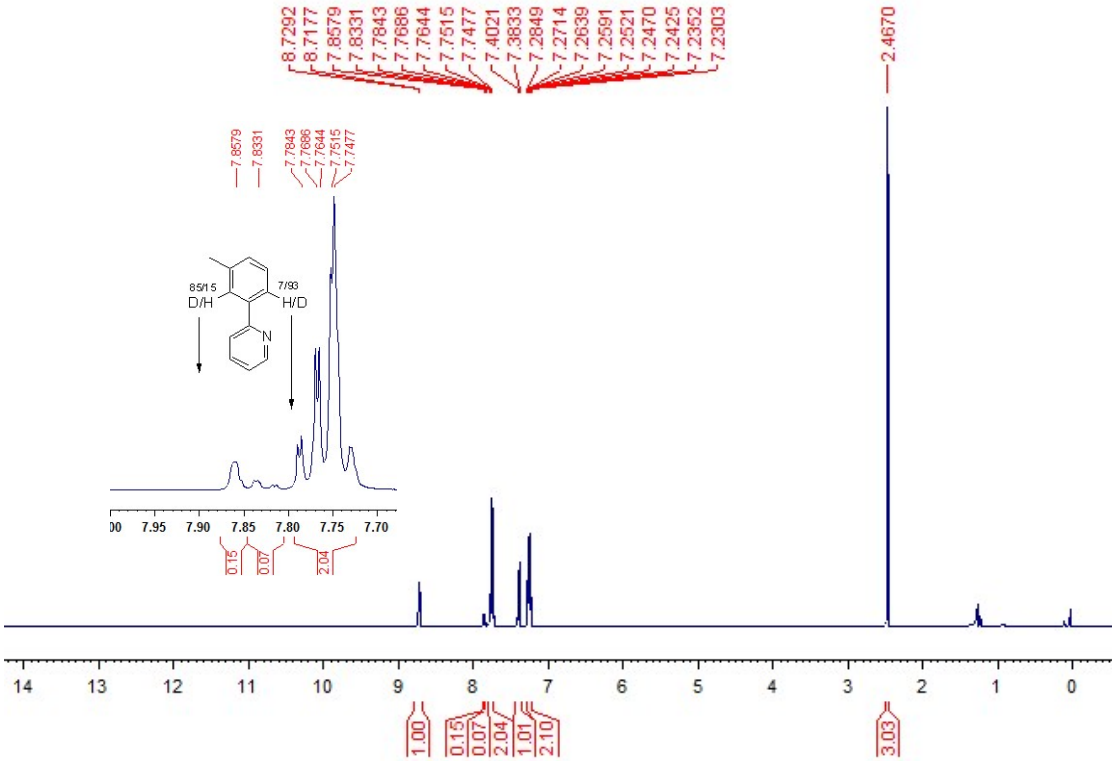
To an oven-dried pressure tube were sequentially added 2-(*m*-tolyl)pyridine (**1a**) (50.77 mg, 0.30 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.74 mg, 0.0045 mmol), AgF (76.12 mg, 0.60 mmol), D_2O (60.06 mg, 3.0 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously

at 120 °C for 20 h in an oil bath under nitrogen atmosphere. The ratio of H/D was determined on the basis of ^{1}H NMR analysis.



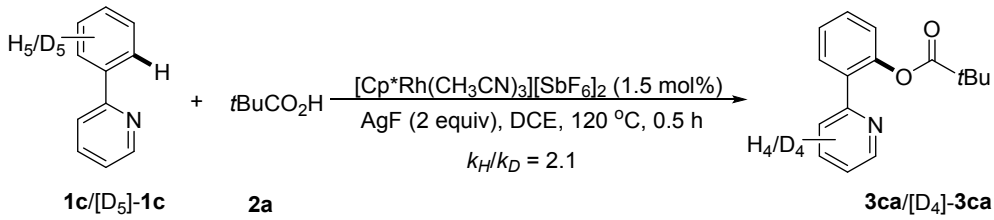
To an oven-dried pressure tube were sequentially added 2-(*m*-tolyl)pyridine (**1a**) (50.77 mg, 0.30 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.74 mg, 0.0045 mmol), pivalic acid (**2a**) (61.28 mg, 0.60 mmol), AgF (76.12 mg, 0.60 mmol), D_2O (60.06 mg, 3.0 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 5 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3ca** as an inseparable mixture (37.8 mg, 47%) and [Dn]-**1a**(25.9 mg, 51%). The ratio of H/D was determined on the basis of ^{1}H NMR analysis.



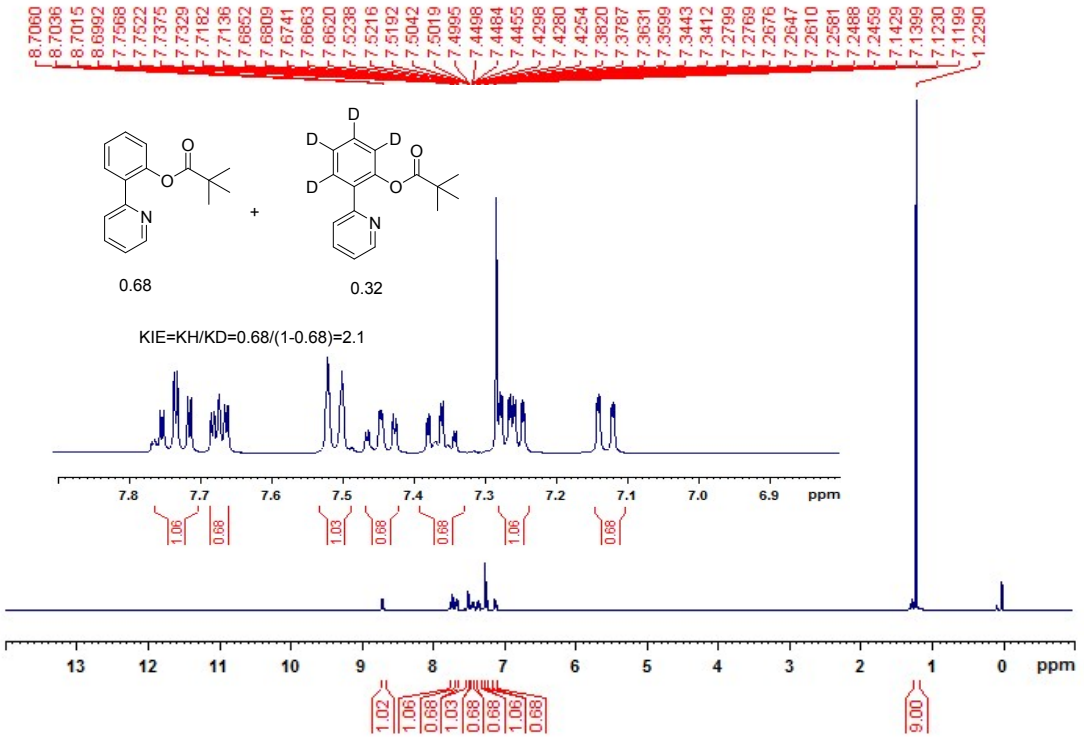


b) Kinetic isotope effect

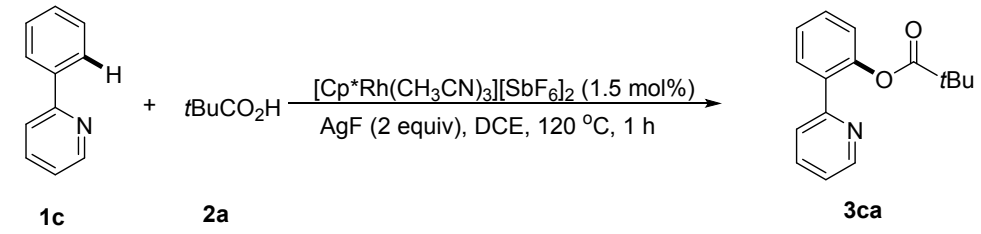
To an oven-dried pressure tube were sequentially added d^5-2-Phenylpyridine ([D5]-**1c**) (48.10 mg, 0.30 mmol), 2-phenylpyridine (**1c**) (46.56 mg, 0.30 mmol), pivalic acid (**2a**) (61.28 mg, 0.60 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (7.49 mg, 0.009 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.5 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 0.5 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3ca** and [D4]-**3ca** as an inseparable mixture (18.5 mg, 23%). KIE value (k_H/k_D = 2.1) was determined on the basis of ^{1}H NMR analysis.



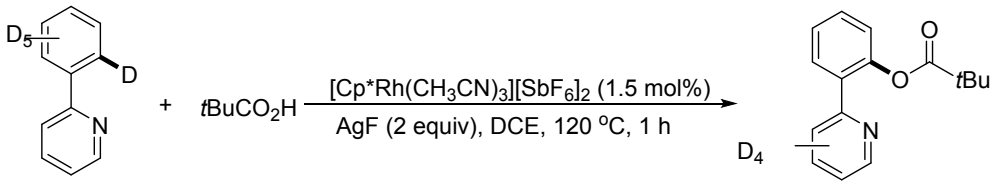
1c/[D_5]-**1c** **2a** **3ca**/[D_4]-**3ca**



To an oven-dried pressure tube were sequentially added d^5-2-Phenylpyridine ([D5]-**1c**) (48.10 mg, 0.30 mmol) or 2-phenylpyridine (**1c**) (46.56 mg, 0.30 mmol), pivalic acid (**2a**) (61.28 mg, 0.60 mmol), [Cp*Rh(CH_3CN)$_3$][SbF_6]$_2$ (7.49 mg, 0.009 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.5 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for designated time (10, 20, 30, 40, 50 min) in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3ca** or [D4]-**3ca**. KIE value (k_H/k_D = 1.44) was determined on the basis of ^{1}H NMR analysis.

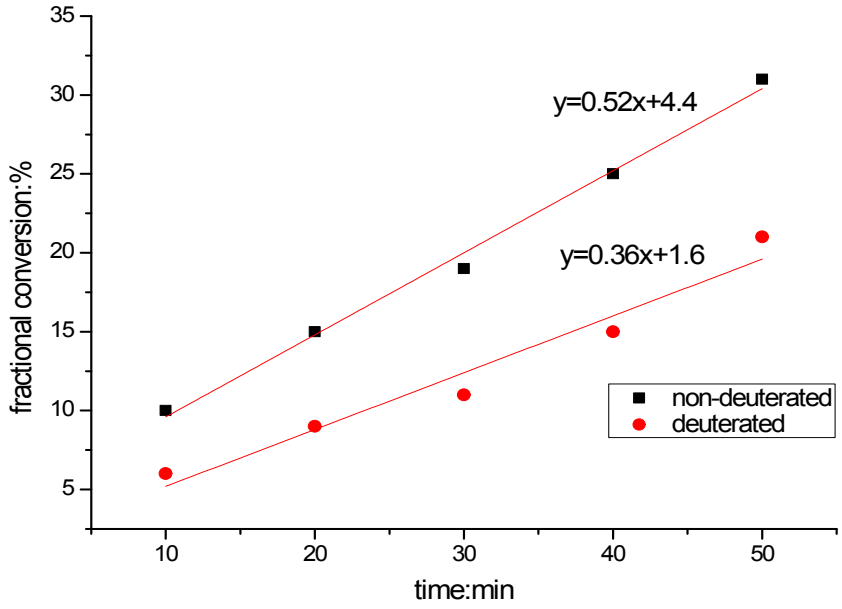


1c **2a** **3ca**



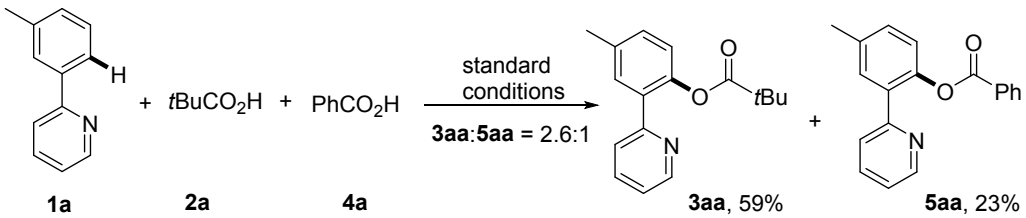
[D_5]-**1c** **2a** [D_4]-**3ca**

Time(min)	10	20	30	40	50
3ca(%)	10	15	19	25	31
[D4]-**3ca**(%)	6	9	11	15	21



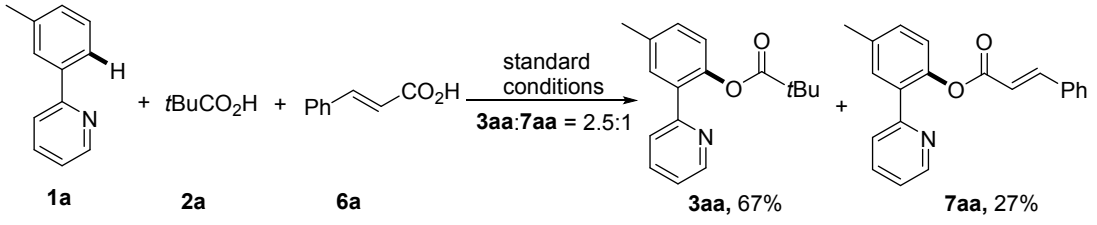
KIE=0.52/0.36=1.44

c) Competition experiments

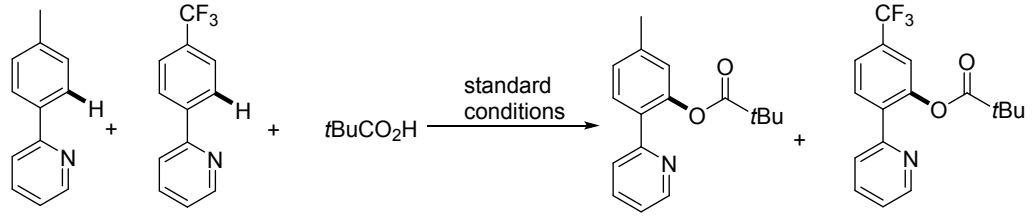


1a **2a** **4a** **3aa**, 59% **5aa**, 23%

To an oven-dried pressure tube were sequentially added 2-(*m*-tolyl)pyridine (**1a**) (50.77 mg, 0.30 mmol), pivalic acid (**2a**) (61.28 mg, 0.6 mmol), benzoic acid (**4a**) (73.27 mg, 0.6 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.74 mg, 0.0045 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 20 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3aa**(47.67 mg, 59%) and **5aa**(19.96 mg, 23%), respectively.

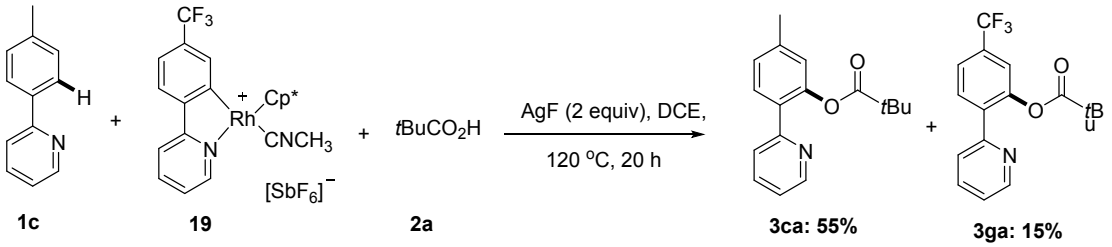


To an oven-dried pressure tube were sequentially added 2-(*m*-tolyl)pyridine (**1a**) (50.77 mg, 0.30 mmol), pivalic acid (**2a**) (61.28 mg, 0.6 mmol), cinnamic acid (**6a**) (88.90 mg, 0.6 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.74 mg, 0.0045 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 20 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3aa**(54.14 mg, 67%) and **7aa**(25.54 mg, 27%), respectively.

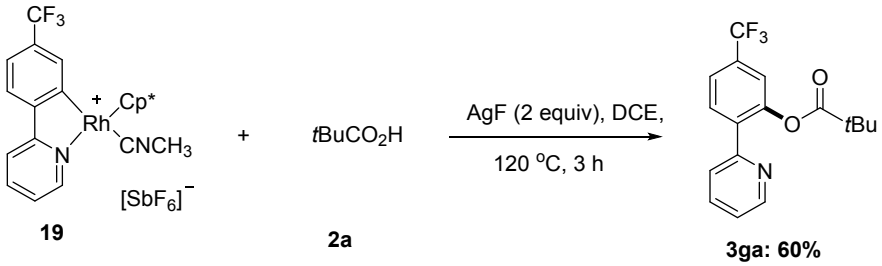


To an oven-dried pressure tube were sequentially added 2-(*p*-tolyl)pyridine (**1c**) (50.77 mg, 0.30 mmol), 2-(4-(trifluoromethyl)phenyl)pyridine (**1g**) (66.96 mg, 0.30 mmol), pivalic acid (**2a**) (61.28 mg, 0.6 mmol), $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (3.74 mg, 0.0045 mmol), AgF (76.12 mg, 0.60 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 20 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature,

the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3ca** (63.83 mg, 79%).



To an oven-dried pressure tube were sequentially added 2-(*p*-tolyl)pyridine (**1c**) (25.35 mg, 0.15 mmol), **19** (110.50 mg, 0.15 mmol), pivalic acid (**2a**) (30.63 mg, 0.3 mmol), AgF (38.05 mg, 0.30 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 20 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products **3ca** (22.20 mg, 55%) and 3**ga** (7.26 mg, 15%).

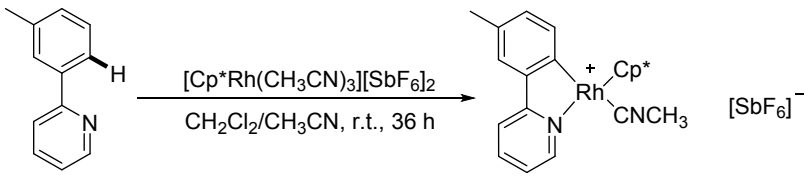


To an oven-dried pressure tube were sequentially added **19** (110.50 mg, 0.15 mmol), pivalic acid (**2a**) (30.63 mg, 0.3 mmol), AgF (38.05 mg, 0.30 mmol) and 1,2-dichloroethane (1.50 mL). After being degassed three times, the reaction mixture was heated and stirred vigorously at 120 °C for 3 h in an oil bath under nitrogen atmosphere. After cooling to ambient temperature, the reaction mixture was diluted with saturated aqueous $NaHCO_3$ (10.0 mL) and extracted with CH_2Cl_2 (5.0 mL × 3). The combined organic layer was dried with anhydrous Na_2SO_4 and filtered. The filtrate was concentrated by vacuum evaporation and the residue was purified by column chromatography on silica gel using a mixture of ethyl acetate and hexane to give the pure products 3**ga** (29.05 mg, 60%).

d) Preparation of rhodacycle complexes

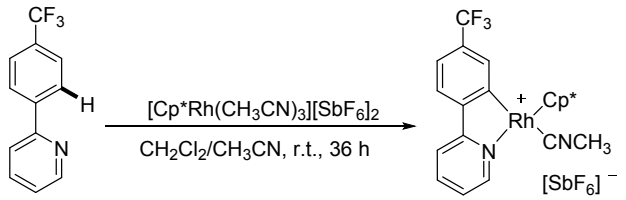
Preparation of 16[15]: A mixture of $[Cp^*RhCl_2]_2$ (62.0 mg, 0.1 mmol), NaOAc (20.0 mg, 0.23 mmol), 2-(*m*-tolyl)pyridine (**1a**) (33.85 mg, 0.2 mmol) were stirred at room temperature in dichloromethane (10.0 mL) for 24 h. Then the mixture was filtered through a pad of celite and evaporated to dryness and purified by column chromatography on silica gel using a mixture of dichloromethane and hexane to afford the desire product as a red-orange solid (86.43 mg, 98%).

Preparation of 17: A mixture of $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (83.40 mg, 0.1mmol), 2-(*m*-tolyl)pyridine (**1a**) (25.40 mg, 0.15 mmol) were stirred at room temperature in dichloromethane (5.0 mL) and acetonitrile (0.50 mL) for 36 h. Then the mixture was filtered through a pad of celite and evaporated to dryness and purified by column chromatography on silica gel using a mixture of dichloromethane and methanol to afford the desire product as an orange solid (56.70 mg, 83%); ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 8.96 (d, *J* = 5.6 Hz, 1H), 8.17 (t, *J* = 7.9 Hz, 1H), 8.09-8.04 (m, 1H), 7.77-7.72 (m, 2H), 7.50 (ddd, *J* = 7.2, 5.6, 1.4 Hz, 1H), 7.20 (dd, *J* = 7.7, 1.9 Hz, 1H), 2.38 (s, 3H), 2.35 (s, 3H), 1.72 (s, 15H); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 165.39, 152.20, 139.25, 136.26, 133.53, 131.95, 129.57, 124.91, 123.55, 119.85, 101.37, 98.18, 20.03, 8.47, 2.47; HRMS (ESI) calcd. for $C_{22}H_{25}NRh$ $[Cp^*RhAr]^+$: 406.1042, found: 406.1027.



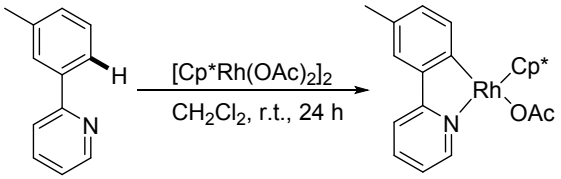
1a **17**, 83%

Preparation of 18: A mixture of $[Cp^*Rh(CH_3CN)_3][SbF_6]_2$ (125.12 mg, 0.15 mmol), 2-(4-(trifluoromethyl)phenyl)pyridine (**1g**) (33.45 mg, 0.15 mmol) were stirred at room temperature in dichloromethane (5.0 mL) and acetonitrile (0.50 mL) for 36 h. Then the mixture was filtered through a pad of celite and evaporated to dryness and purified by column chromatography on silica gel using a mixture of dichloromethane and methanol to afford the desire product as an brown solid (88.44 mg, 80%); ^{1}H NMR (400 MHz, $(CD_3)_2CO$) δ 9.04 (d, *J* = 5.5 Hz, 1H), 8.31 (d, *J* = 8.0 Hz, 1H), 8.21 (m, 1H), 8.10 (m, 2H), 7.95 (m, 1H), 7.55 (m, 1H), 2.33 (s, 3H), 1.73 (s, 15H); ^{13}C NMR (101 MHz, $(CD_3)_2CO$) δ 174.08, 163.65, 152.73, 148.64, 139.83, 132.76, 128.90, 128.54, 125.13, 124.24, 120.98, 118.49, 98.72, 98.66, 8.25, 2.30; HRMS (ESI) calcd. for $C_{22}H_{22}F_3NRh$ $[Cp^*RhAr]^+$: 460.3174, found: 406.2744.



1g **18**, 80%

Preparation of 19: A mixture of $[Cp^*Rh(OAc)_2]_2$ (71.24 mg, 0.10 mmol), 2-(*m*-tolyl)pyridine (**1a**) (33.85 mg, 0.20 mmol) were stirred at room temperature in dichloromethane (5.0 mL) for 24 h. Then the mixture was filtered through a pad of celite and evaporated to dryness and purified by column chromatography on silica gel using a mixture of dichloromethane and hexane to afford the desire product as a red-orange solid (81.86 mg, 88%); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 5.7 Hz, 1H), 7.86 (d, J = 7.0 Hz, 1H), 7.78 (d, J = 8.1 Hz, 2H), 7.45 (s, 1H), 7.12 (d, J = 9.5 Hz, 2H), 2.36 (s, 3H), 1.67 (s, 3H), 1.65 (s, 15H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 164.50, 150.29, 142.51, 135.90, 135.55, 130.78, 128.89, 123.17, 120.75, 117.94, 94.82, 94.78, 30.88, 19.99, 8.36; HRMS (ESI) calcd. for $C_{22}H_{25}NRh$ $[Cp^*RhAr]^+$: 406.1042, found: 406.1031.



1a **19**, 88%

6. References:

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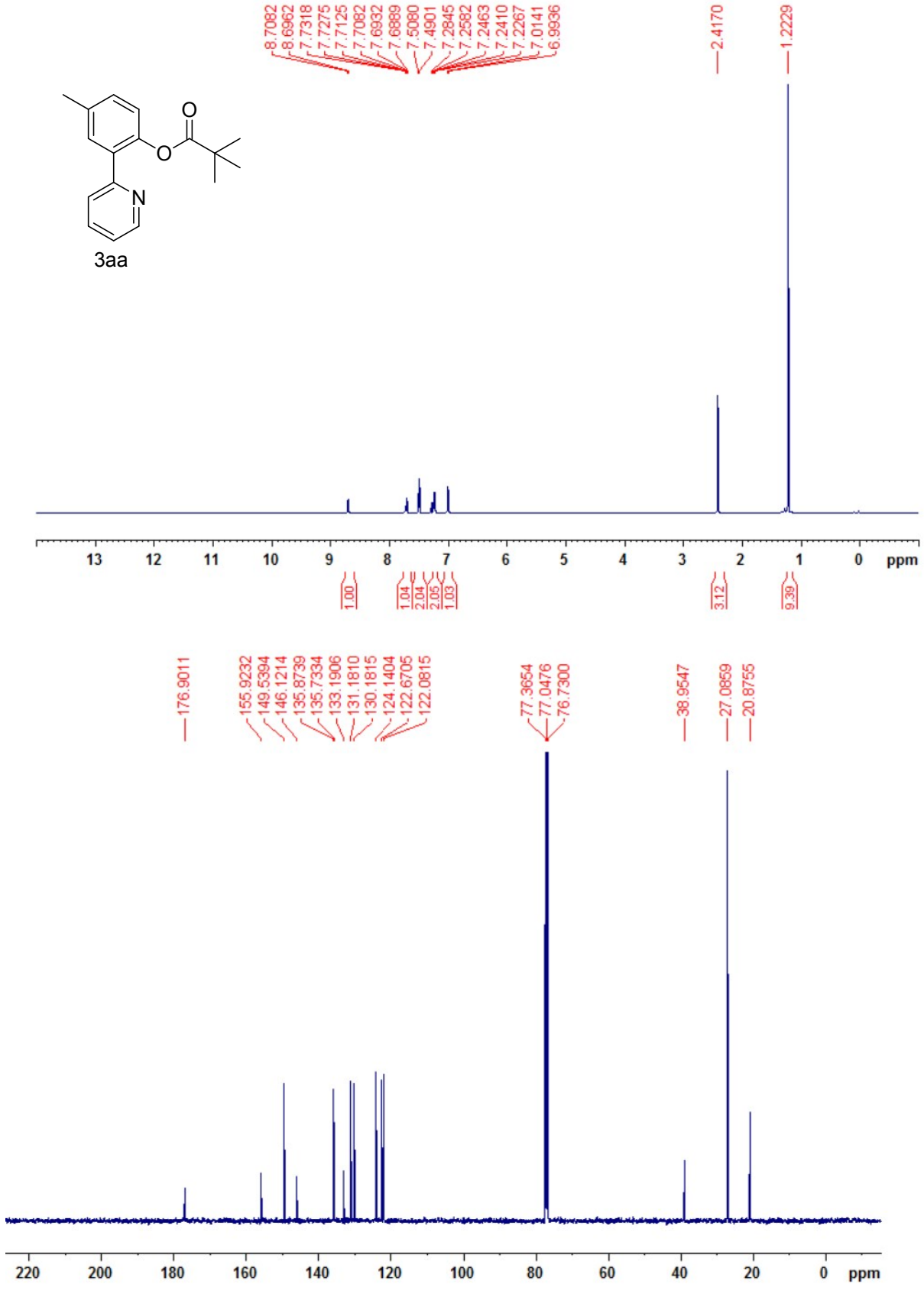
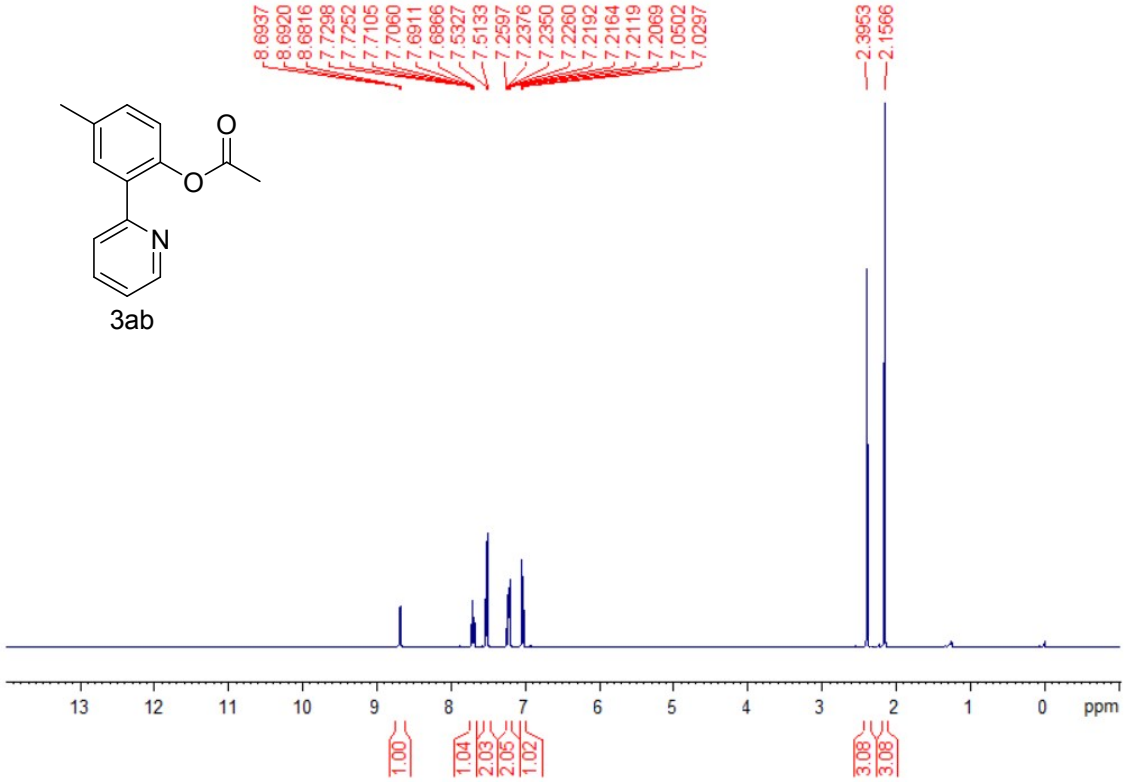
7. ^{1}H and ^{13}C NMR spectra of products

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O
O
N
13
12
11
10
9
8
7
6
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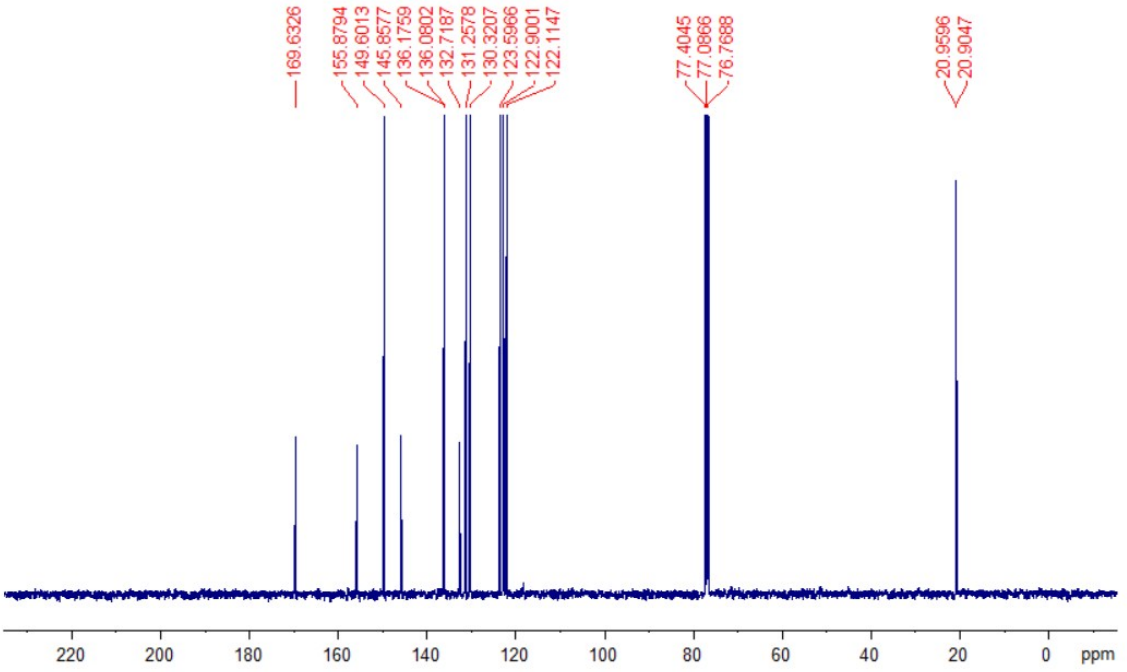
3.08

3ab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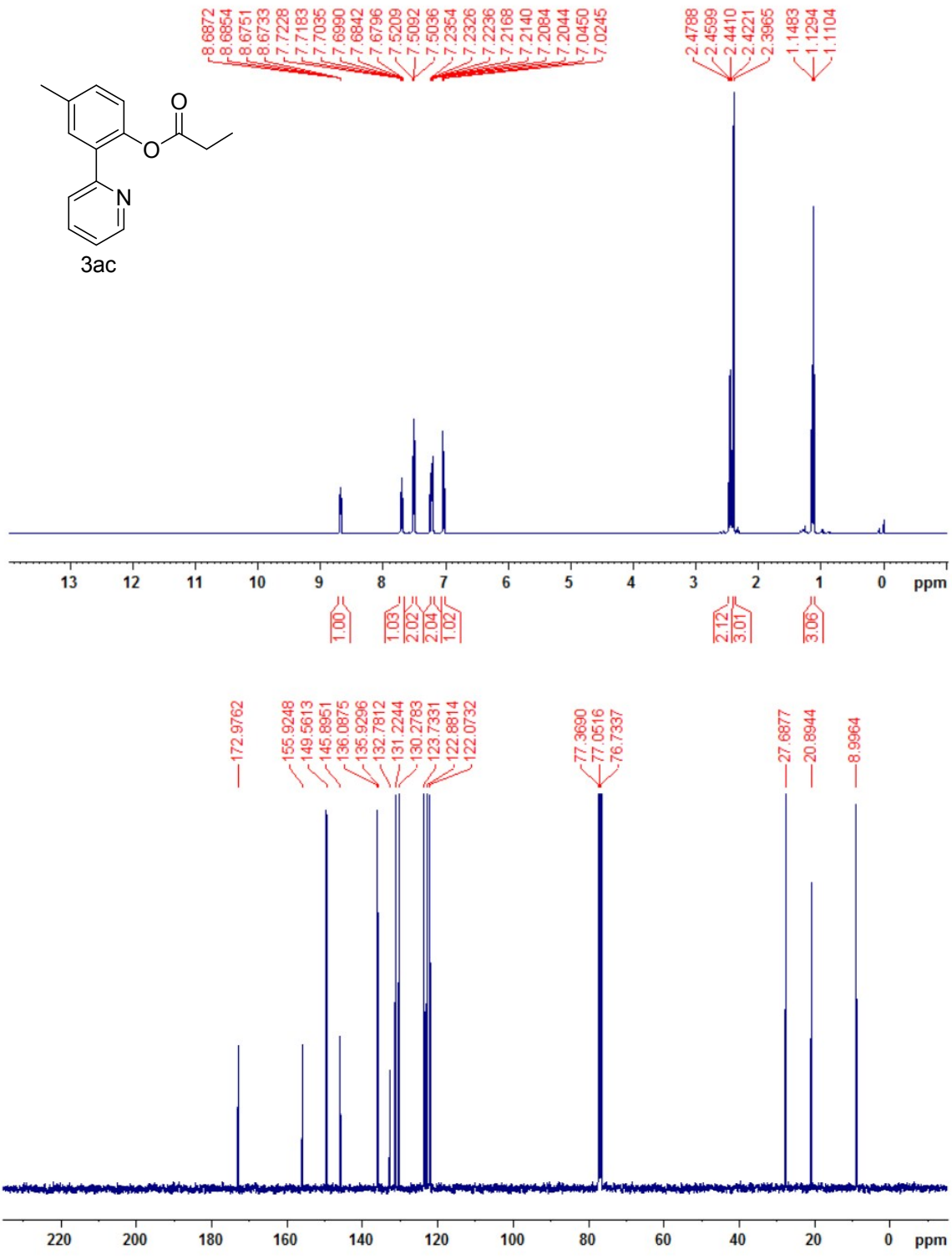
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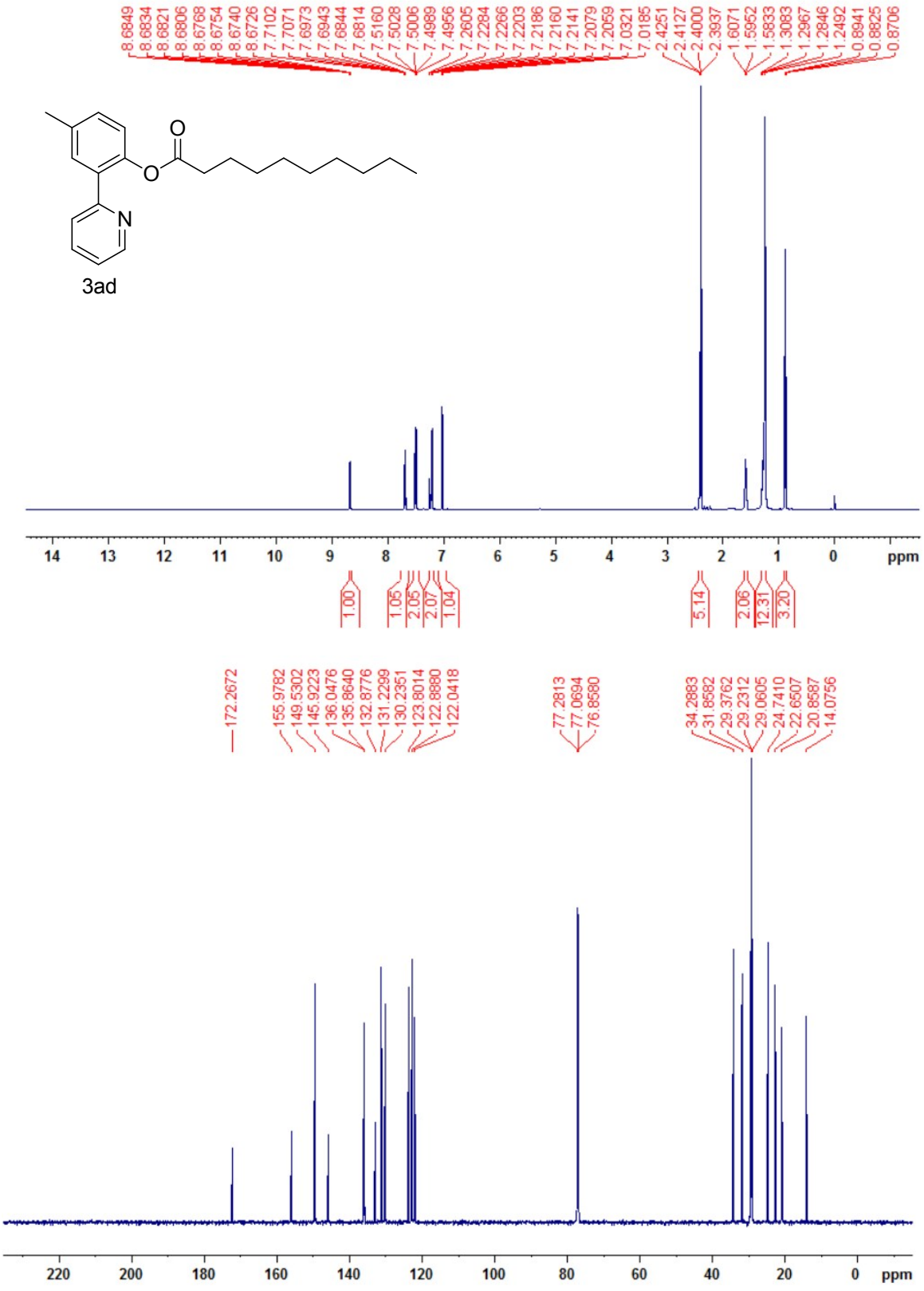
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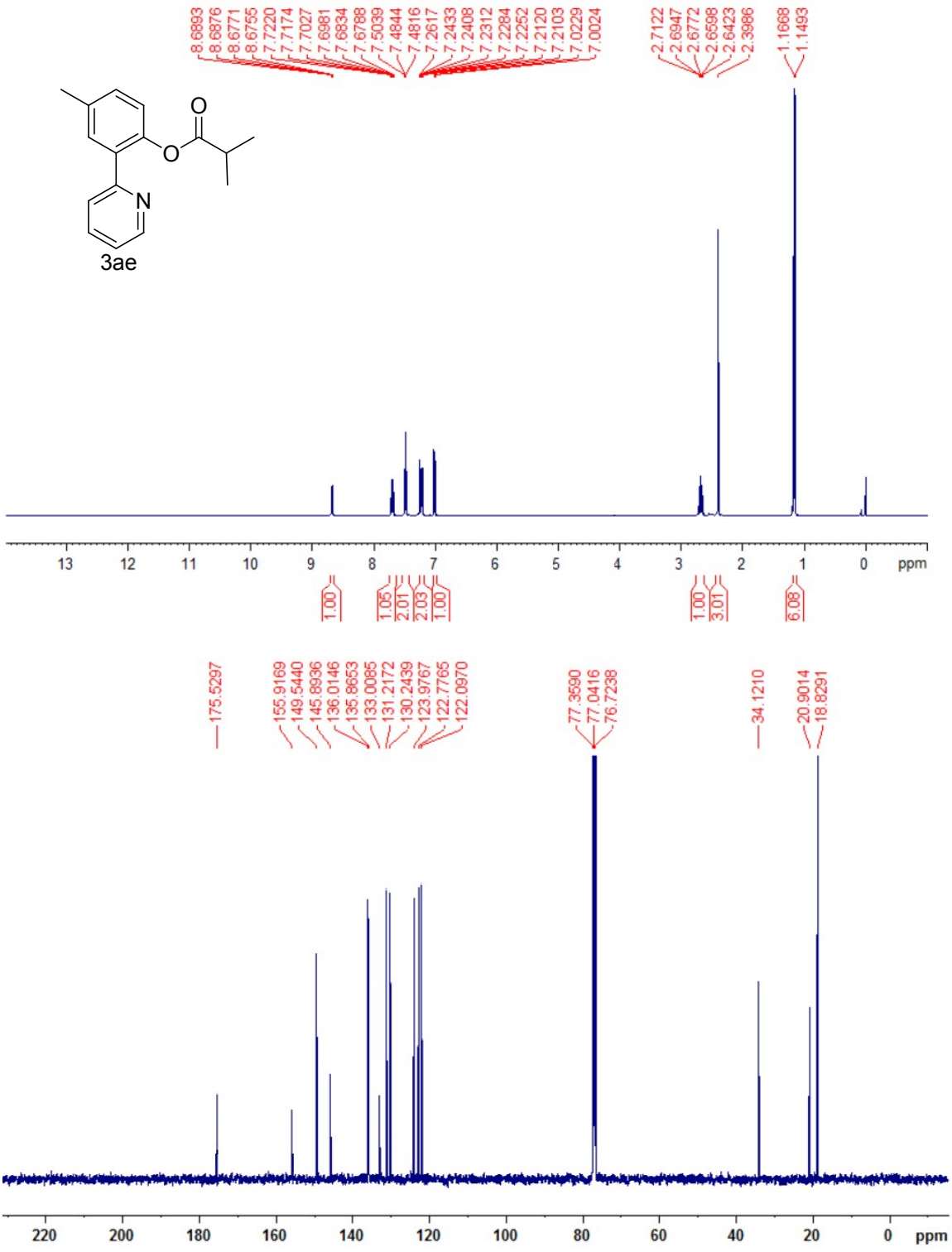
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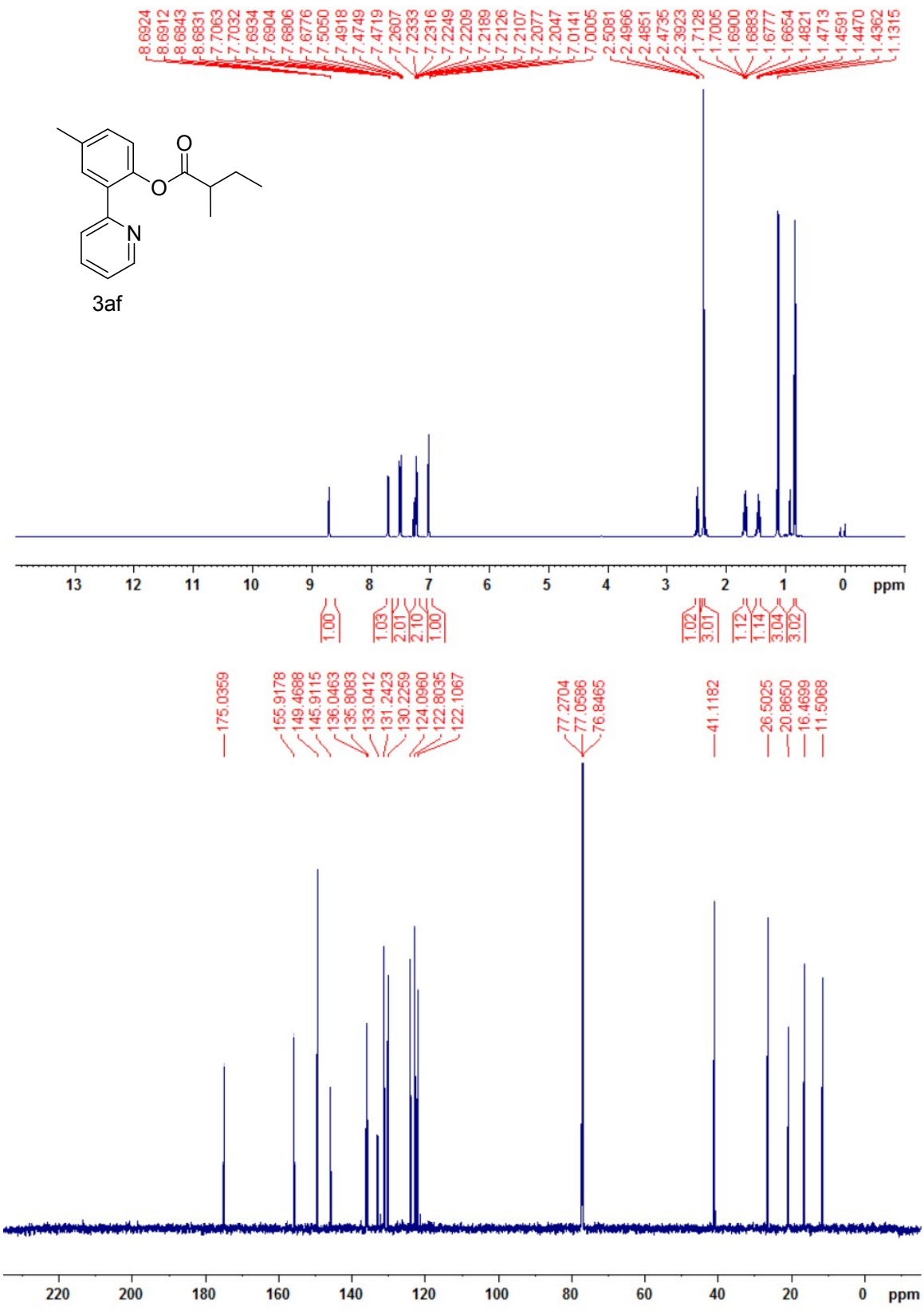
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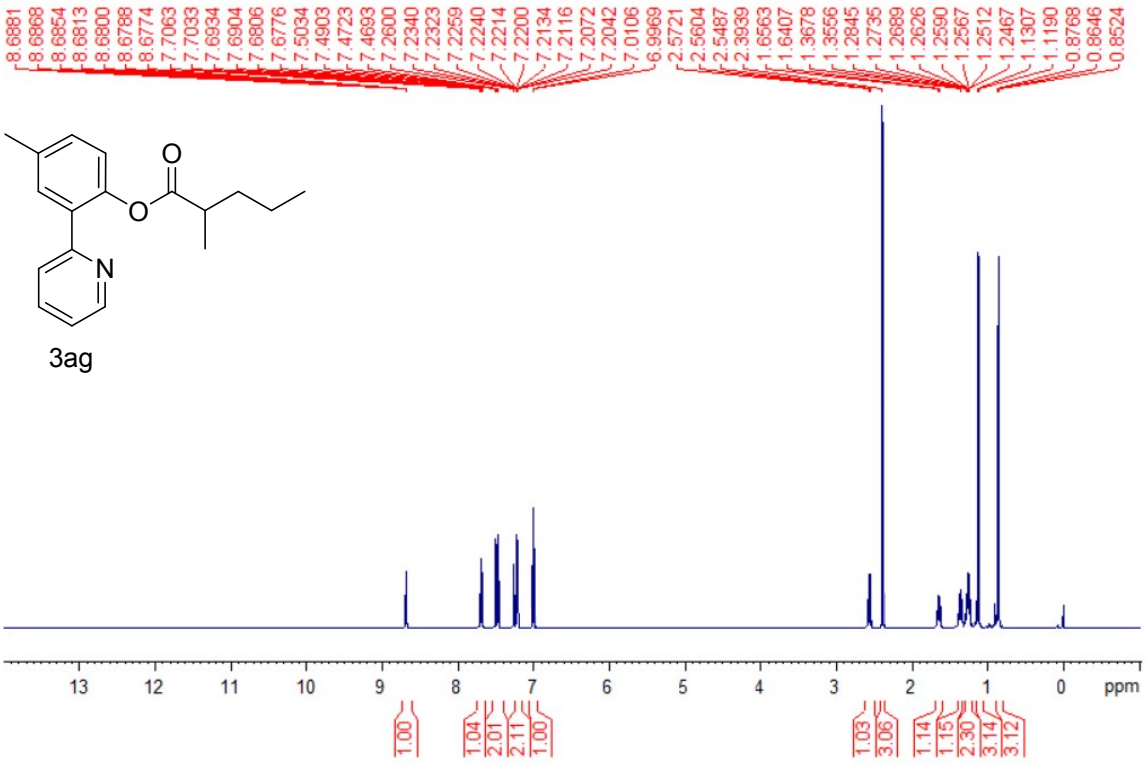
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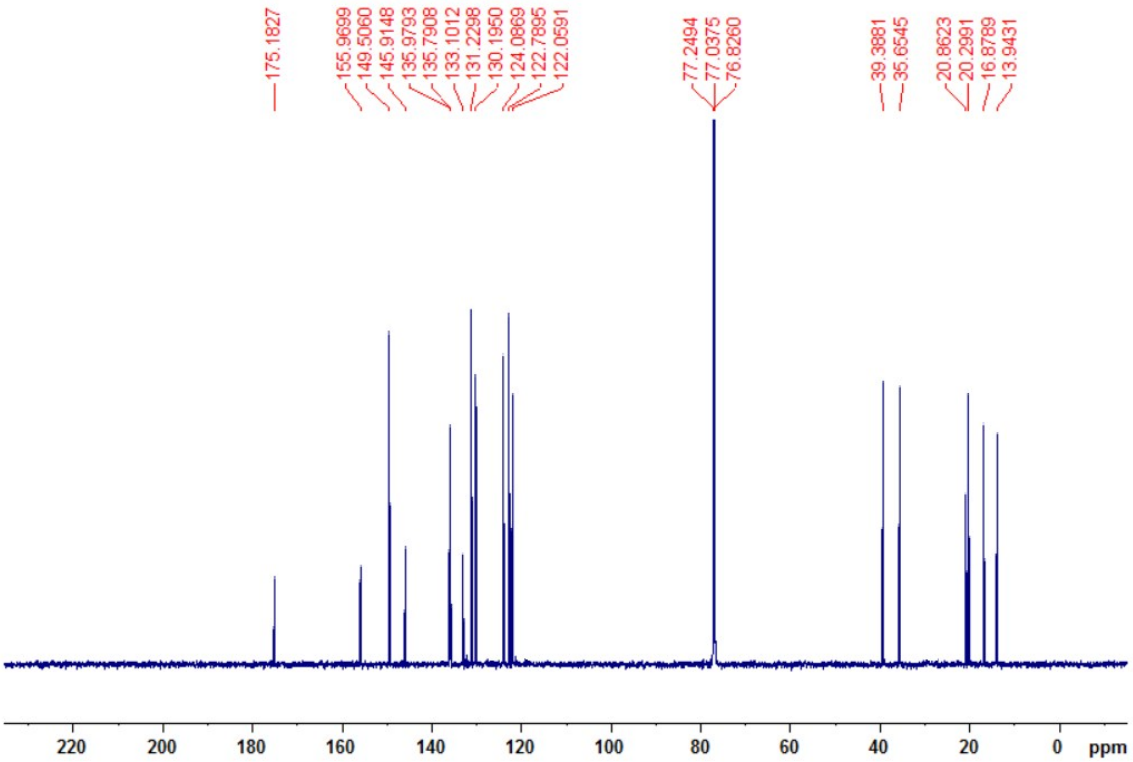
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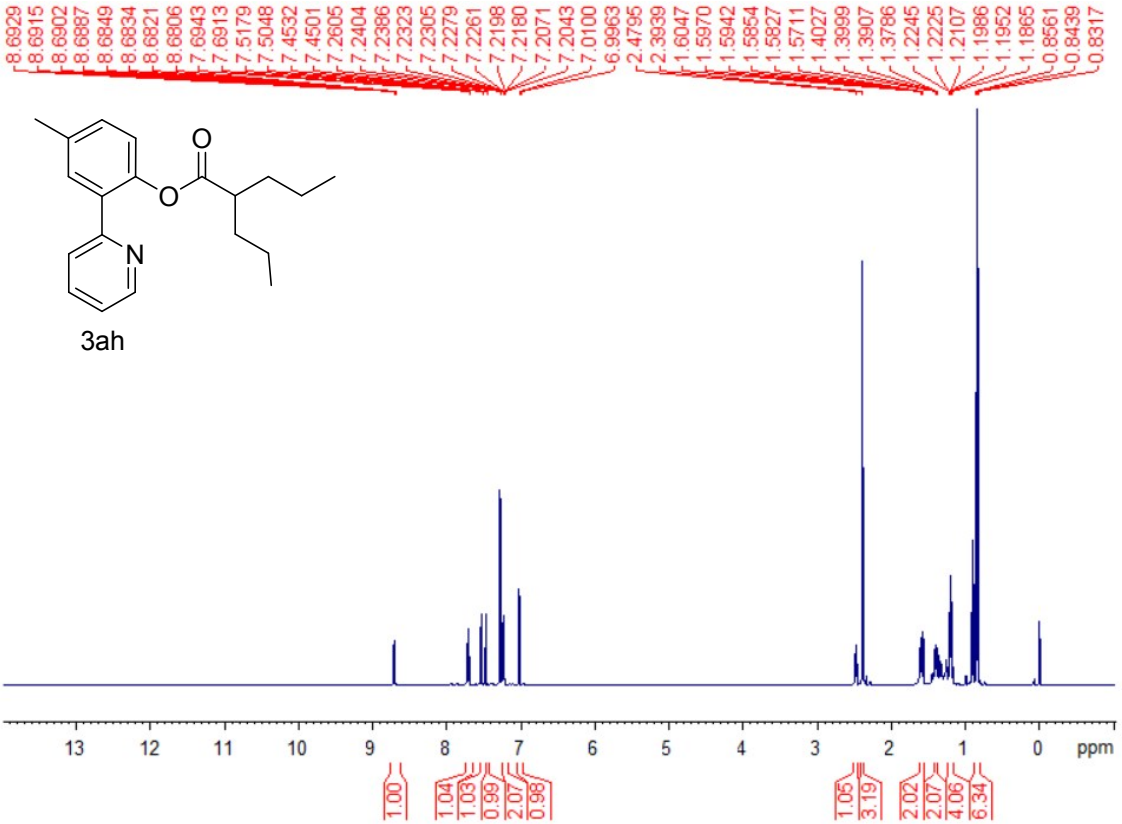
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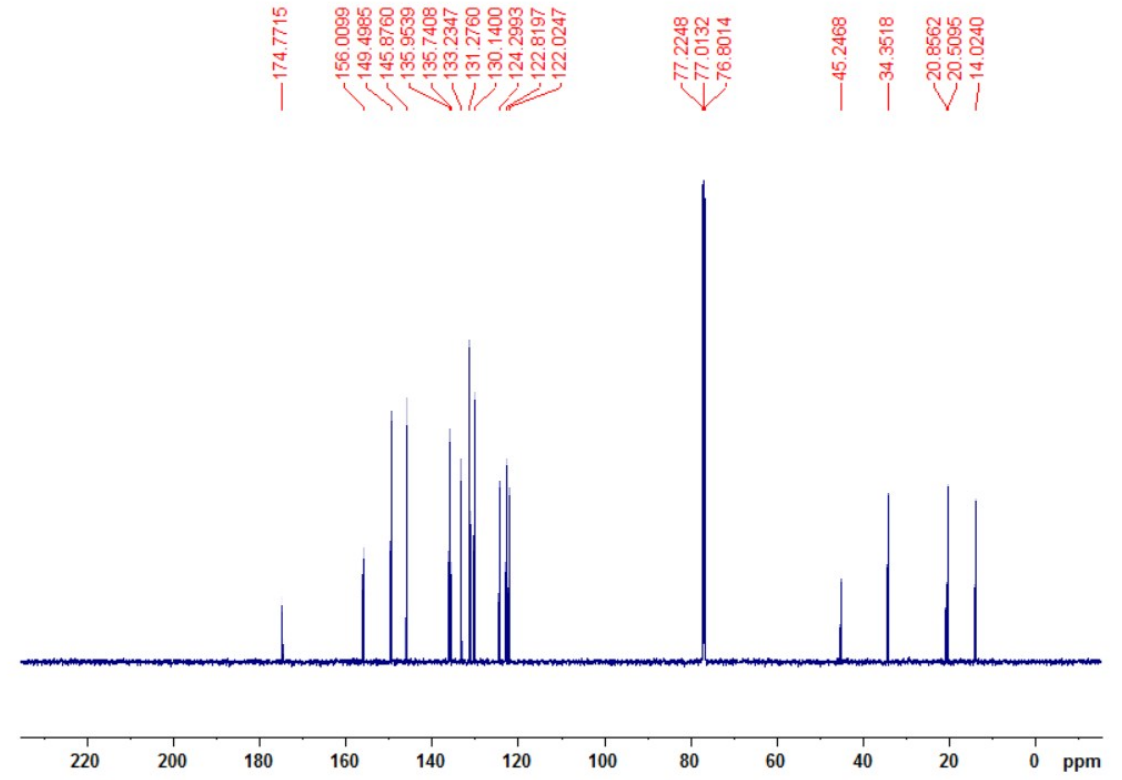
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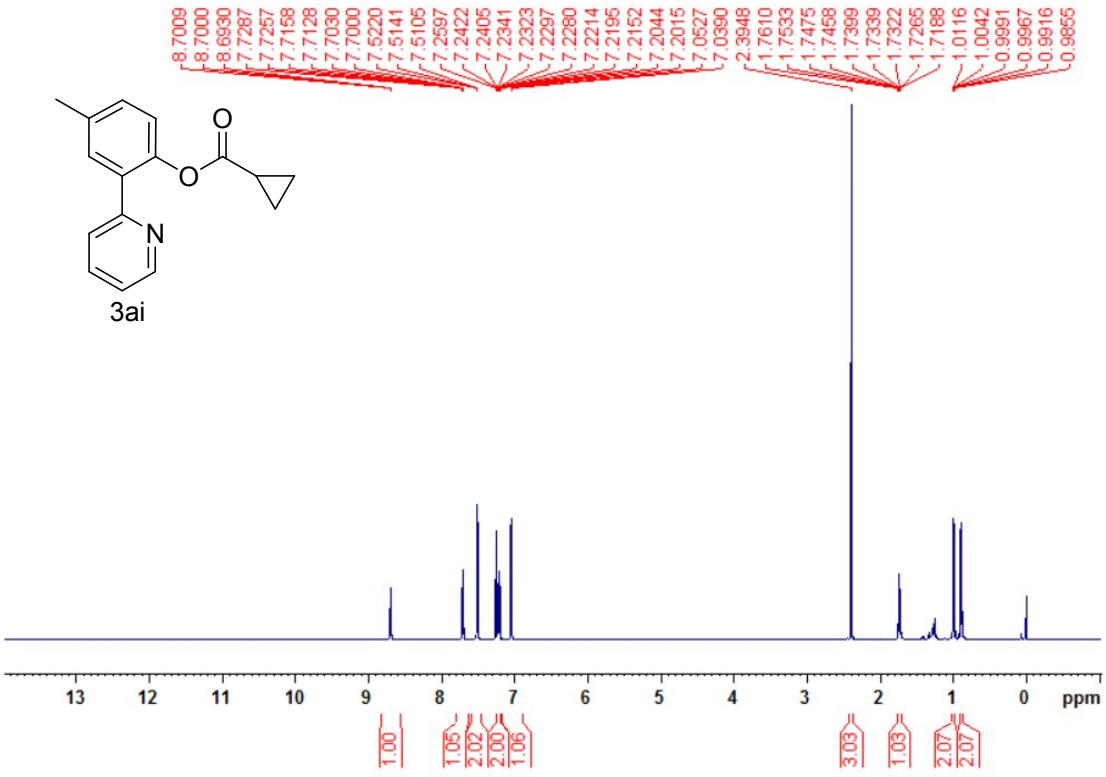
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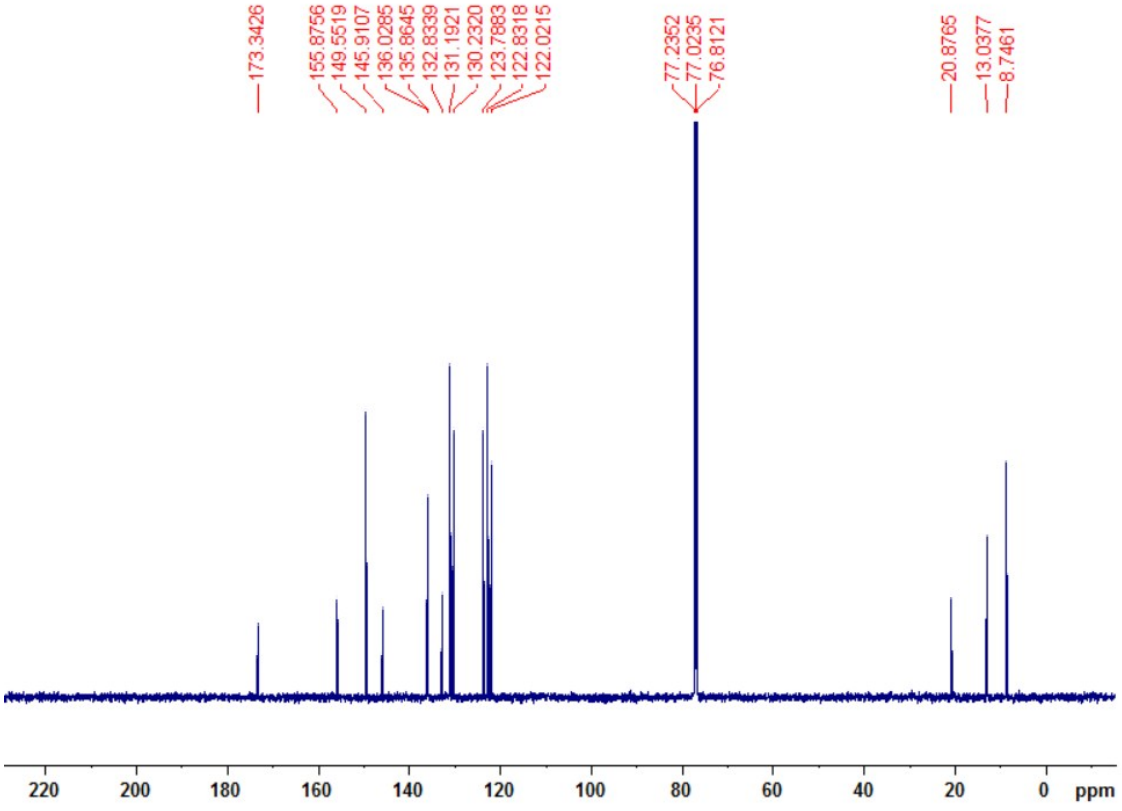
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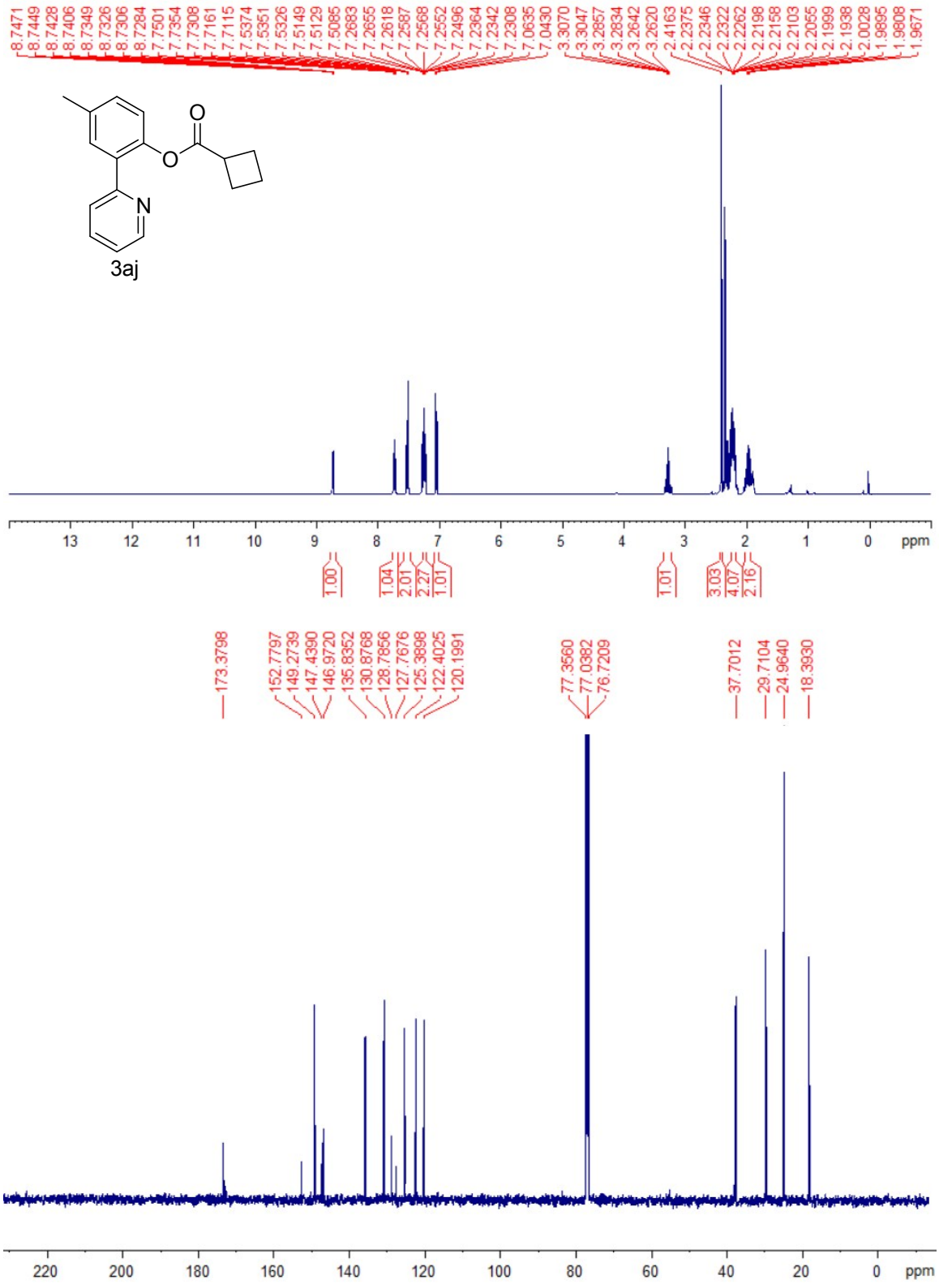
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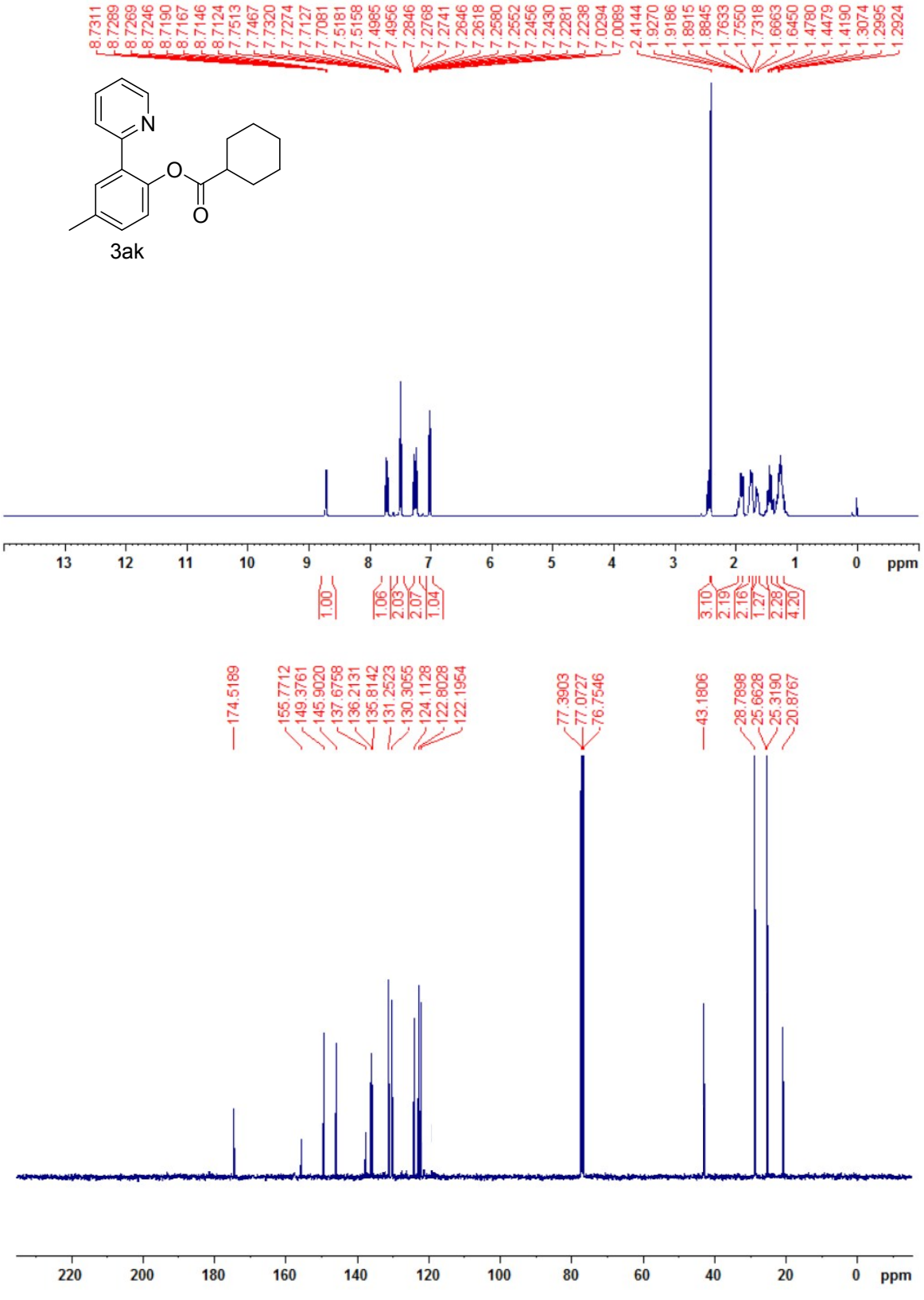
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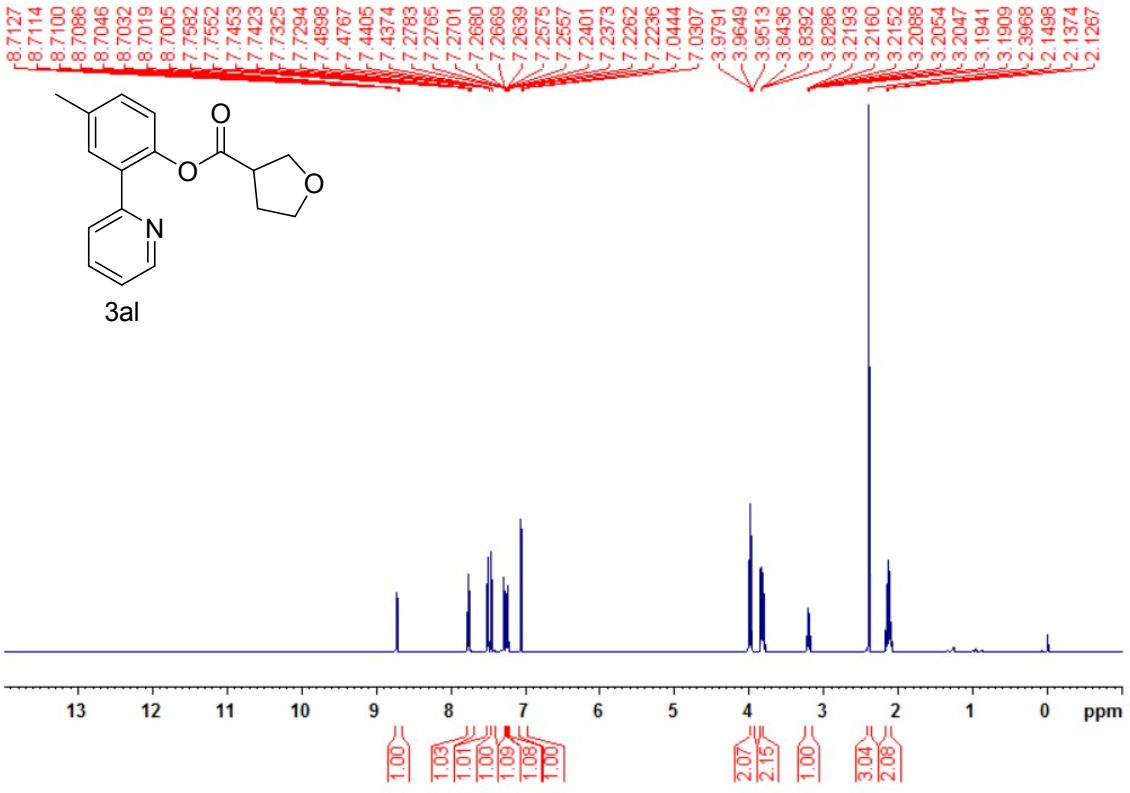
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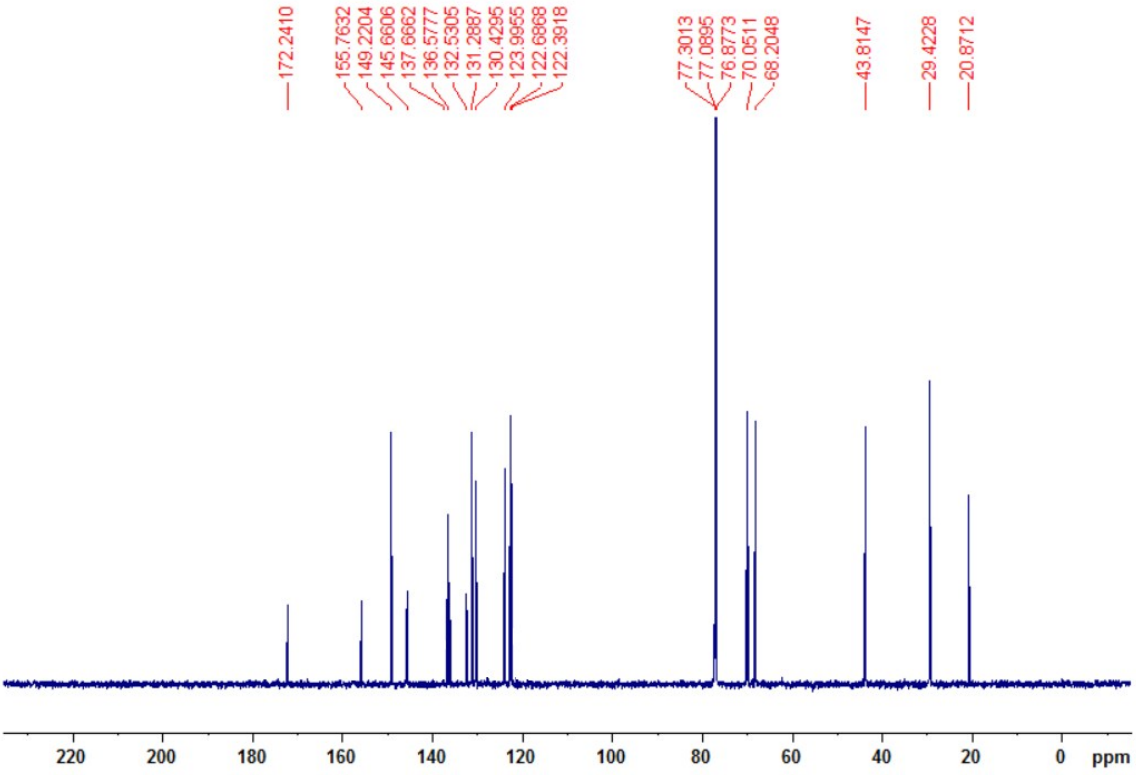
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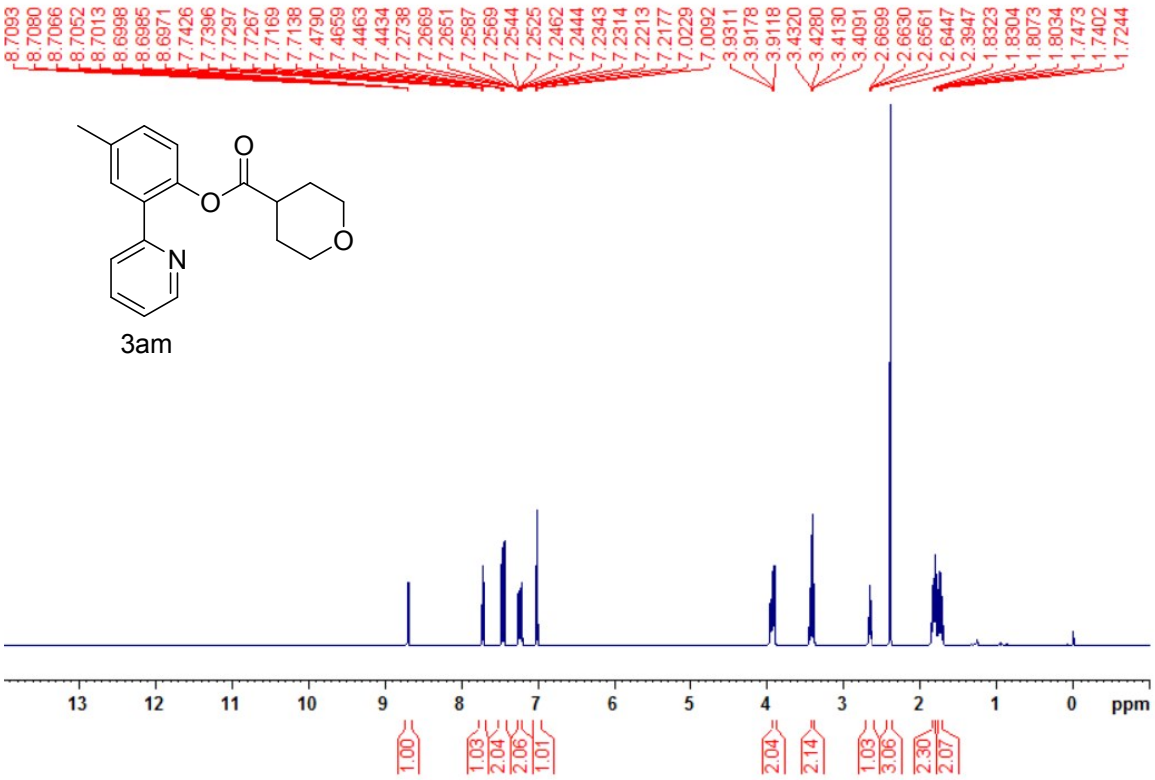
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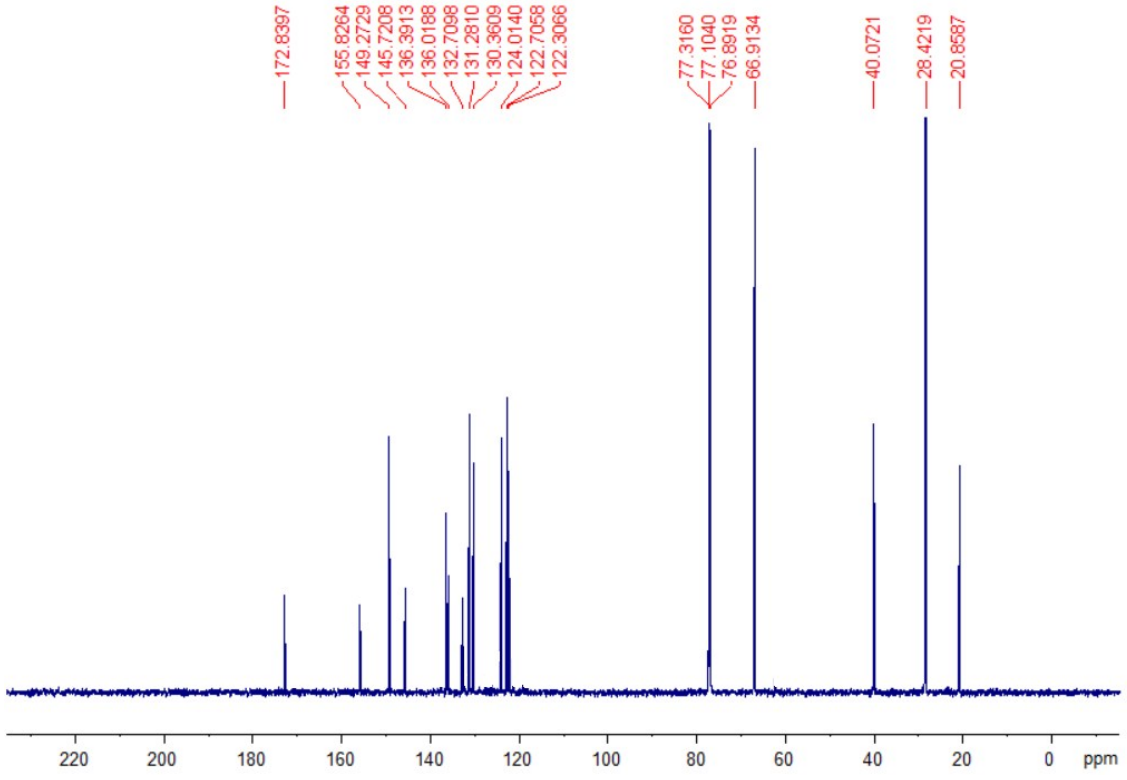
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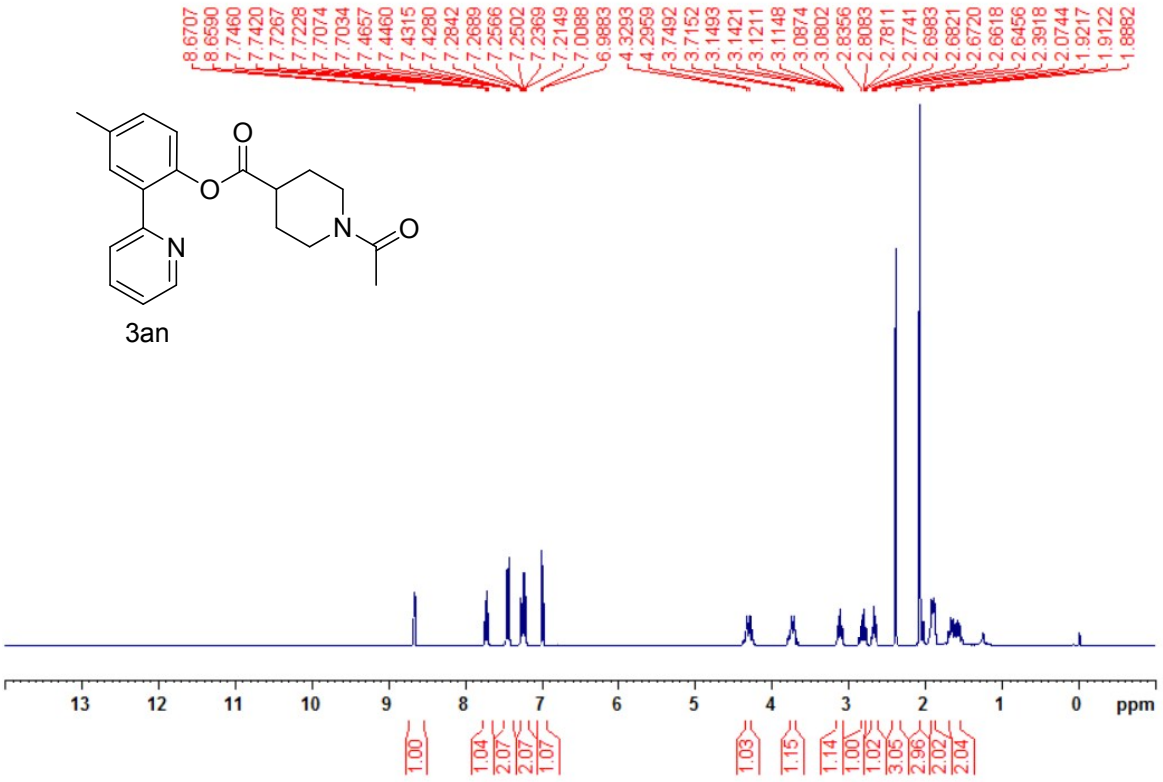
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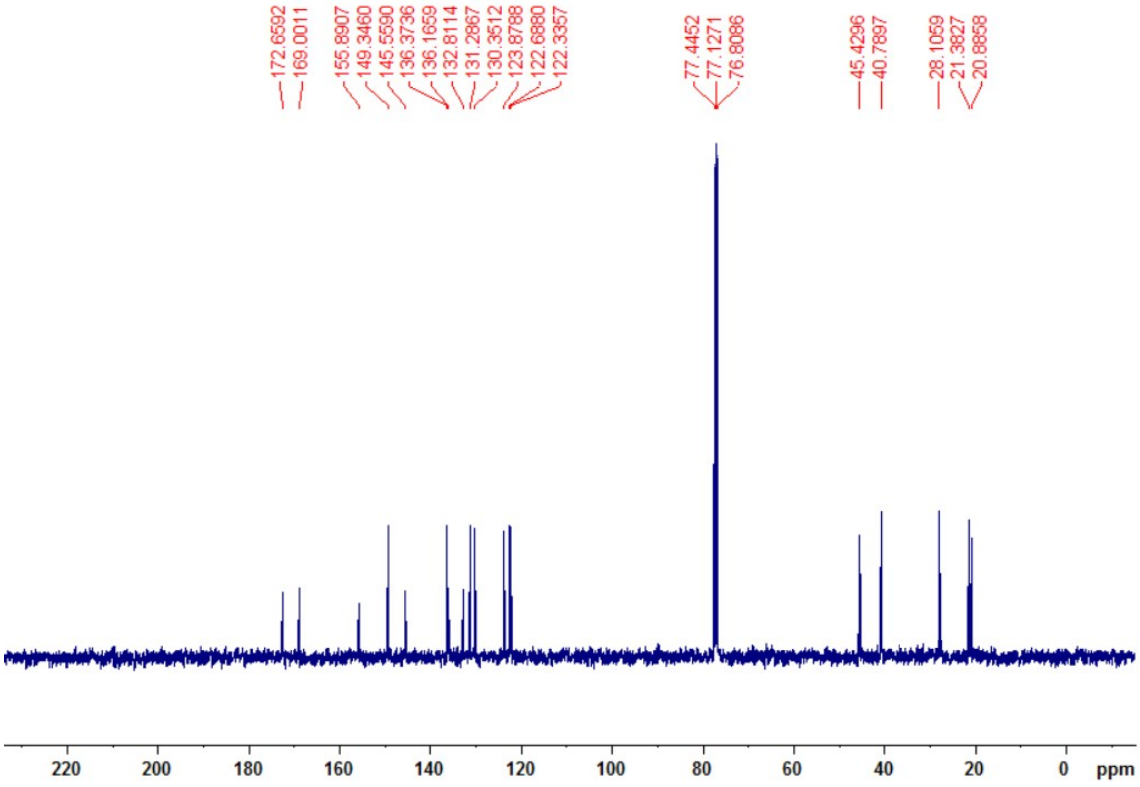
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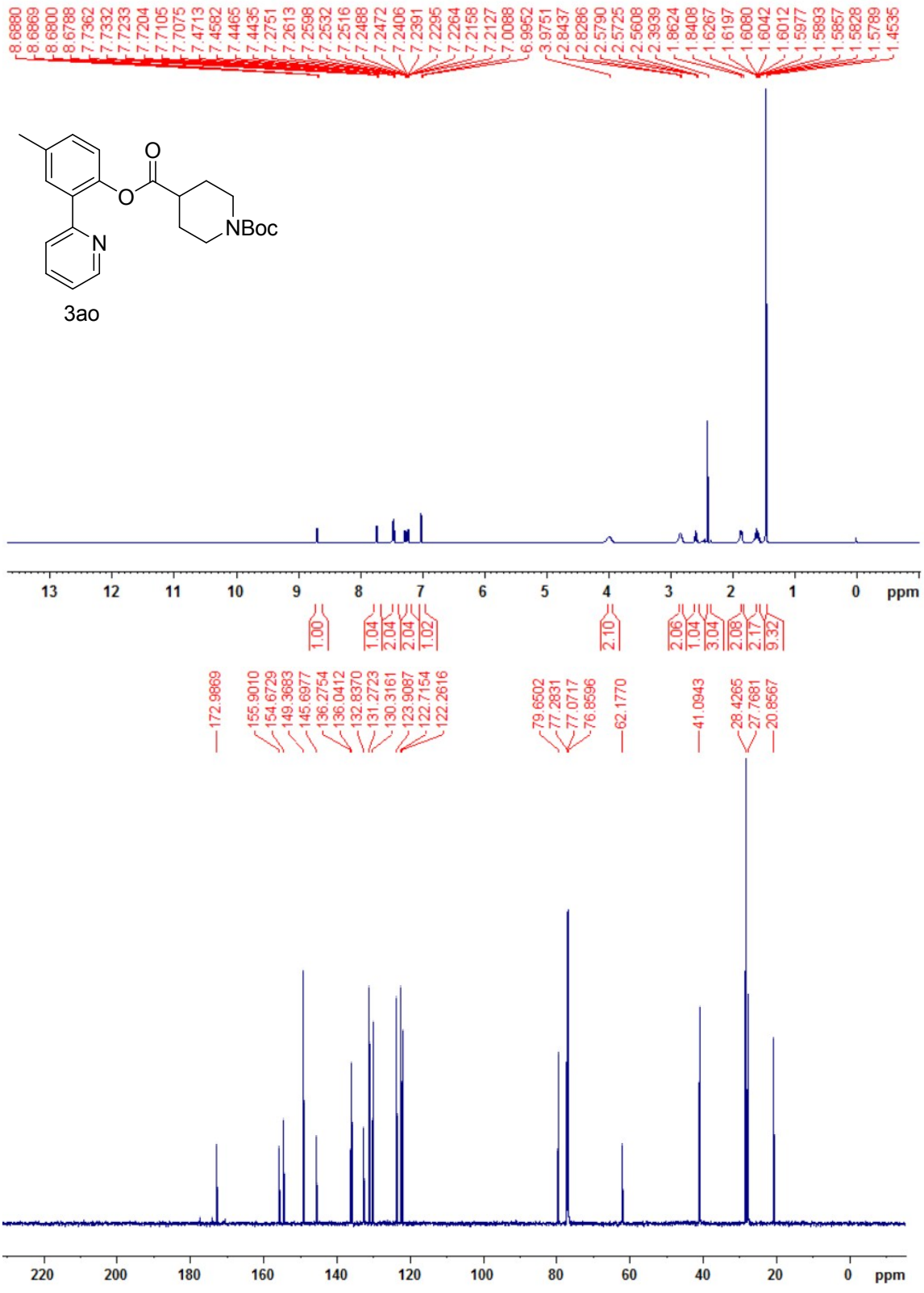
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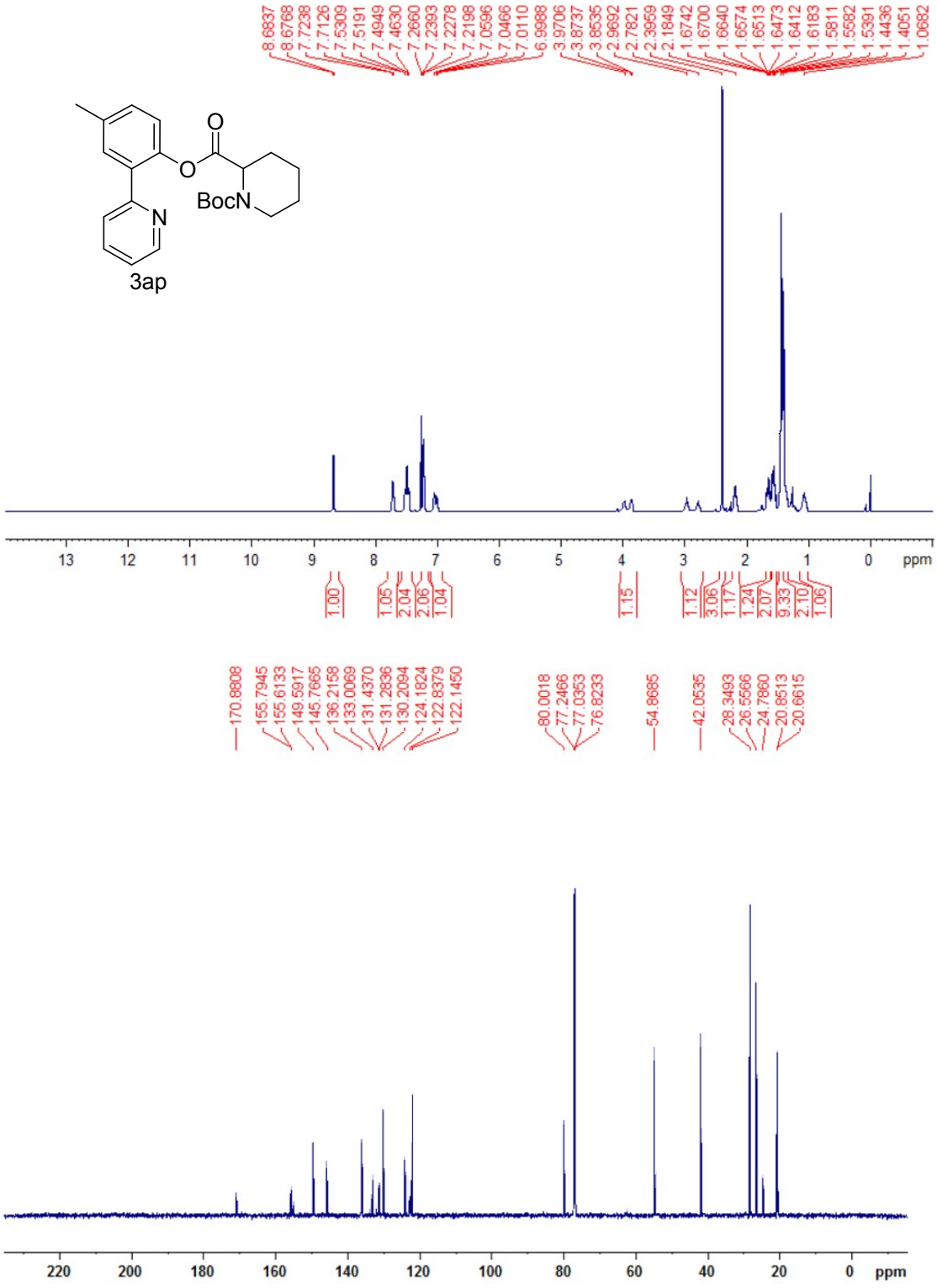
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O
BocN
N
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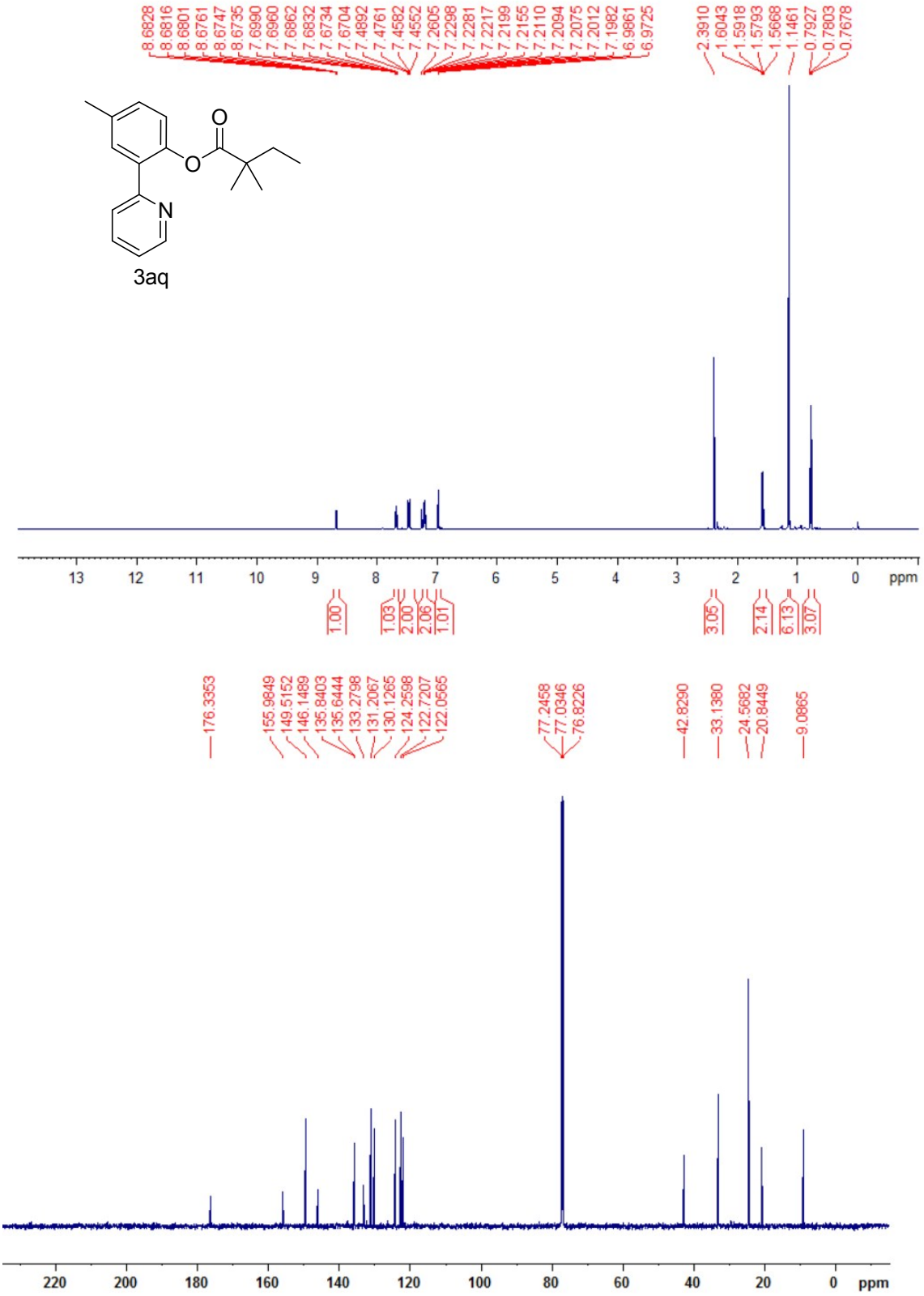
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O
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3.07
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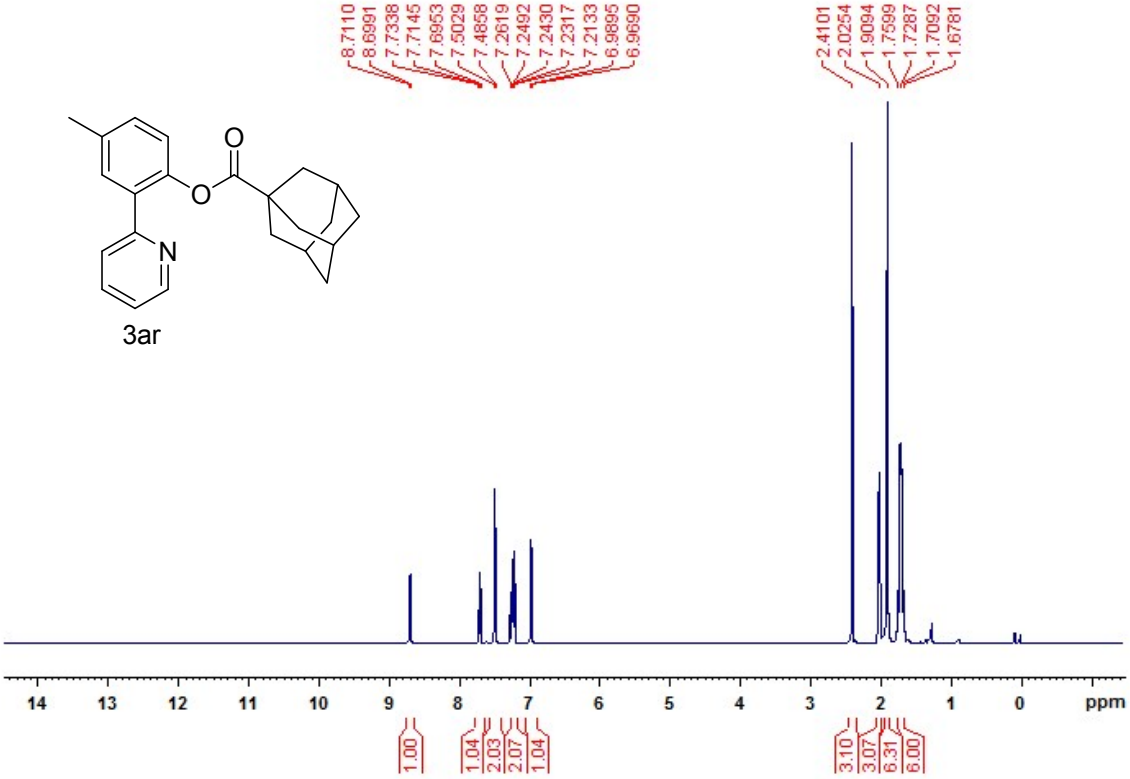
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O
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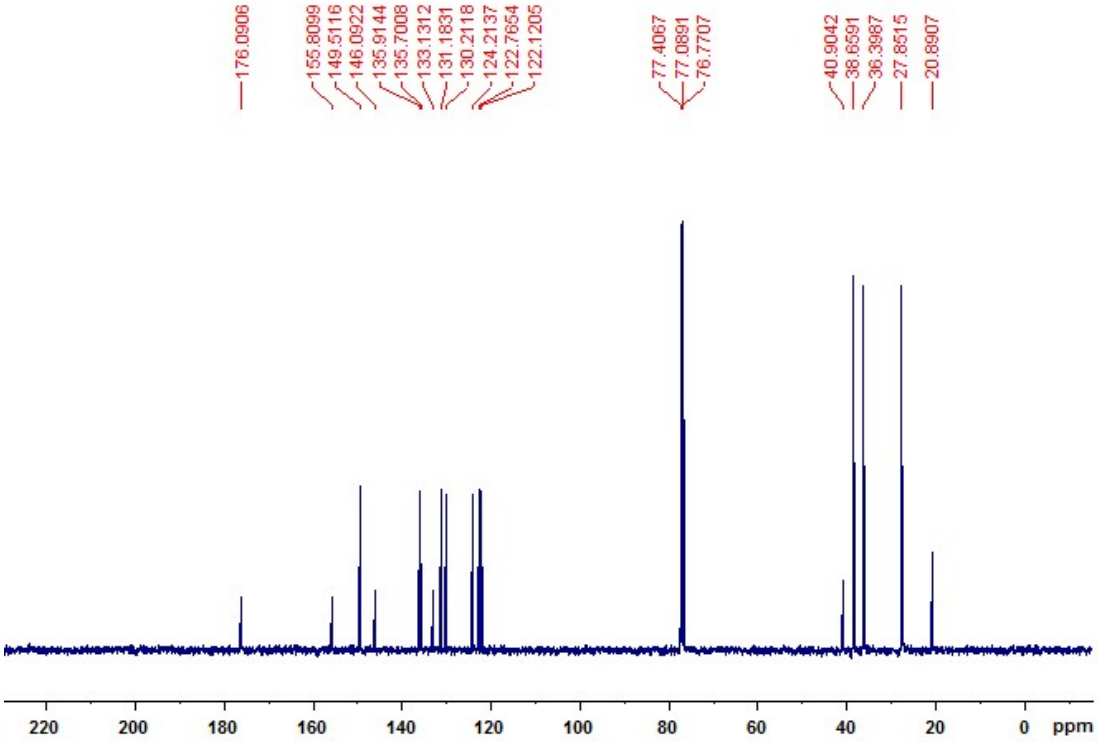
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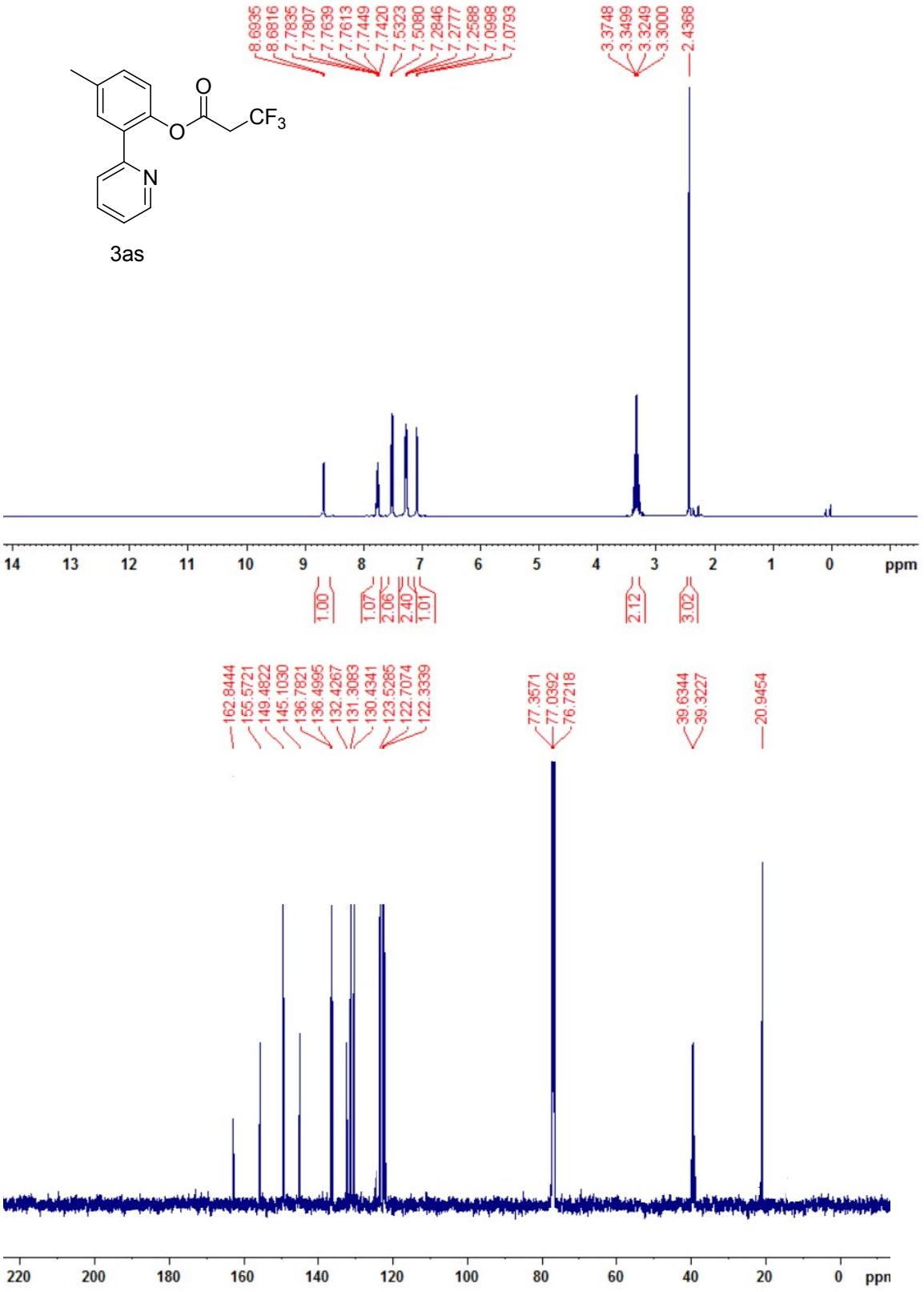
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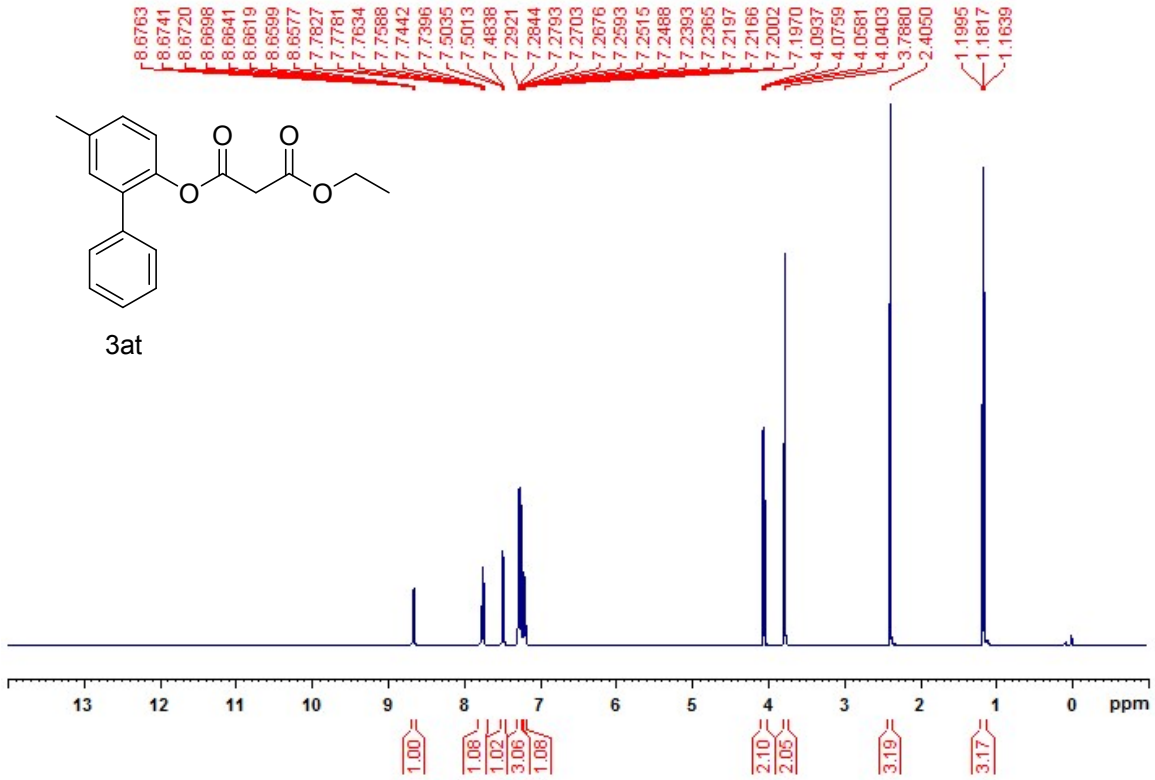
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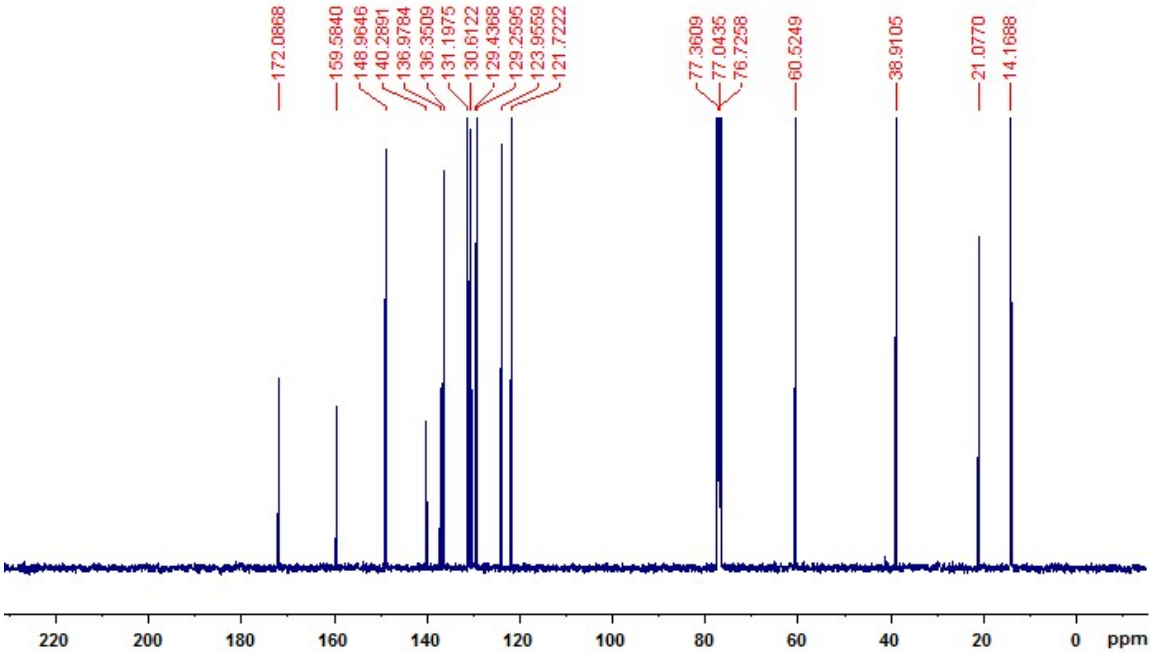
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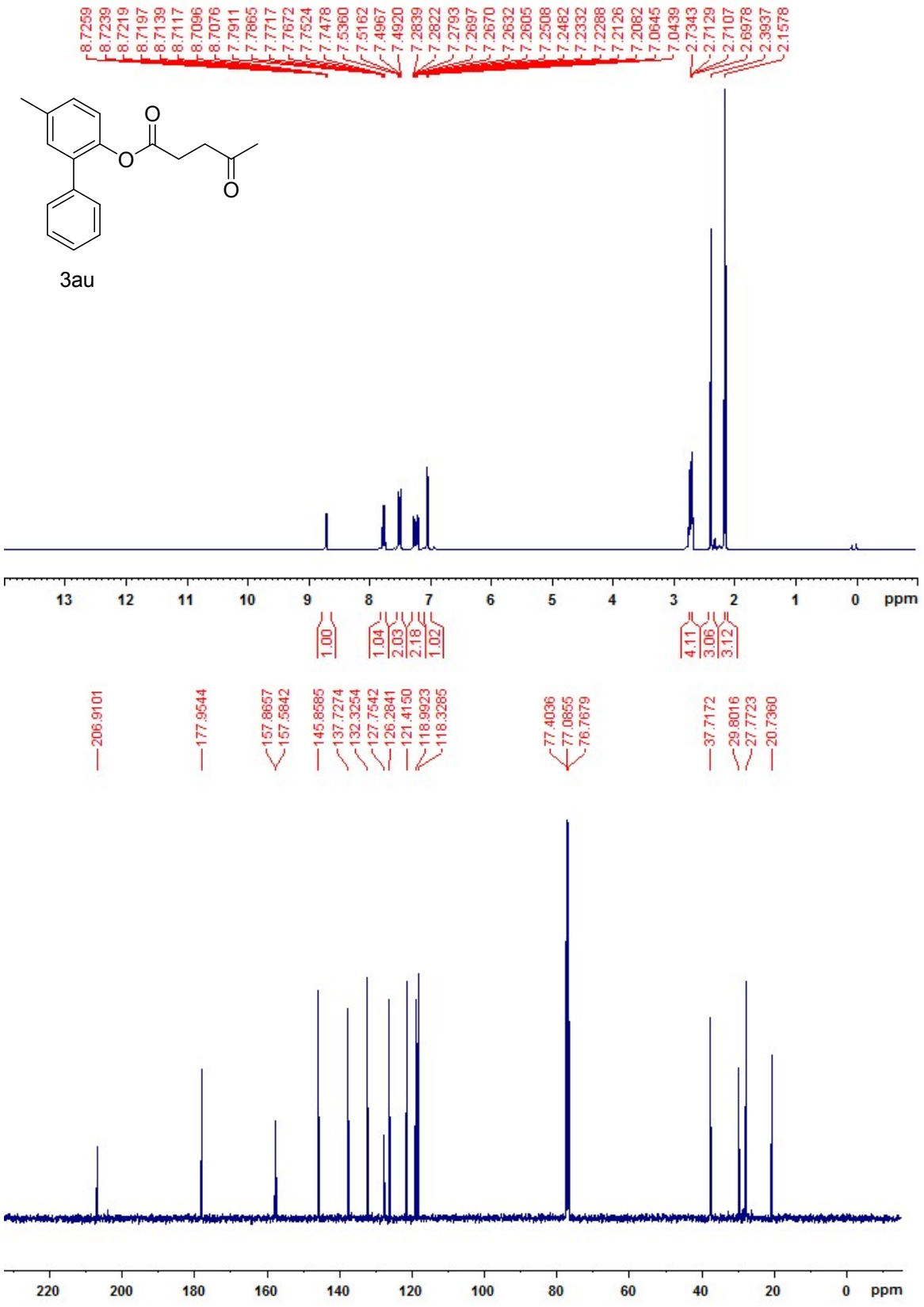
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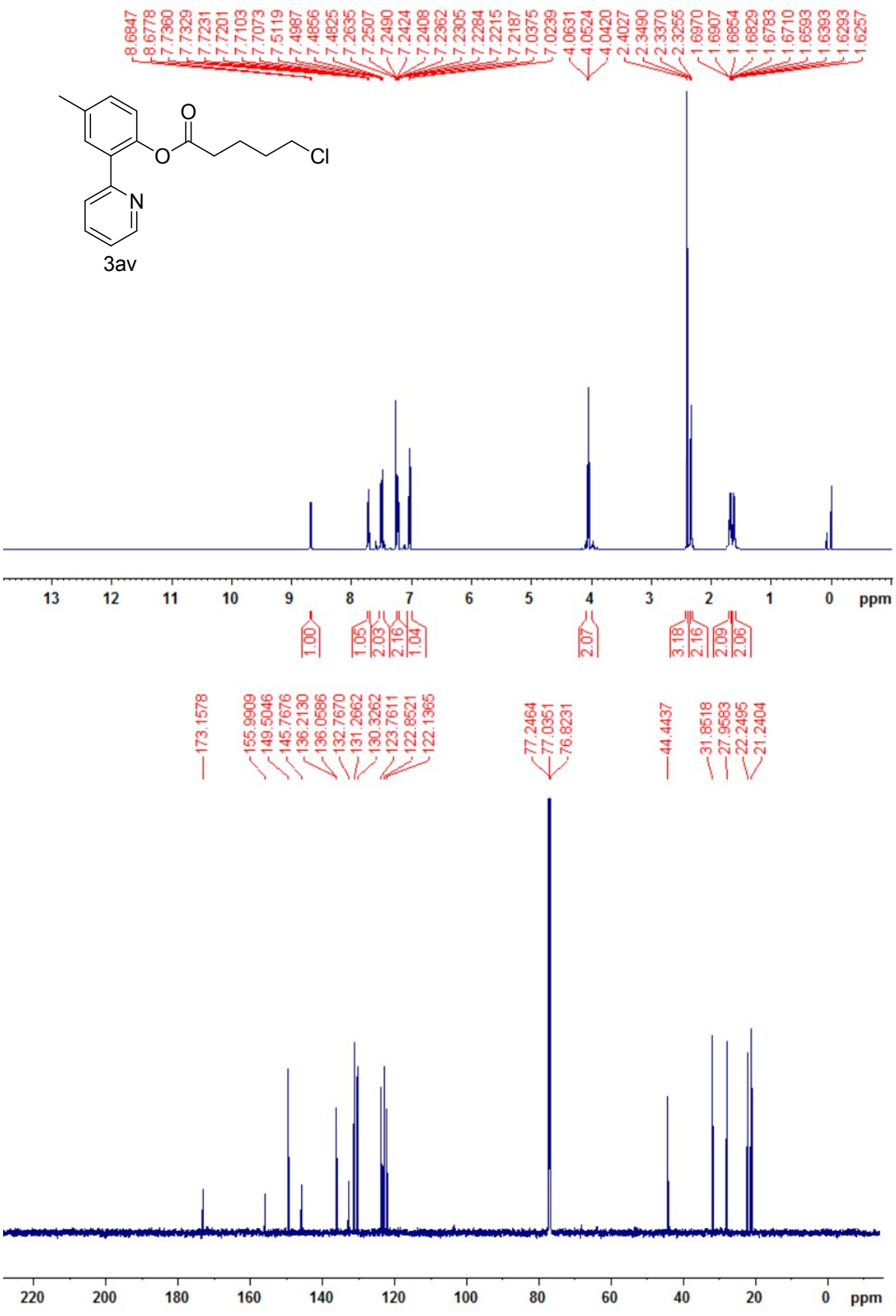
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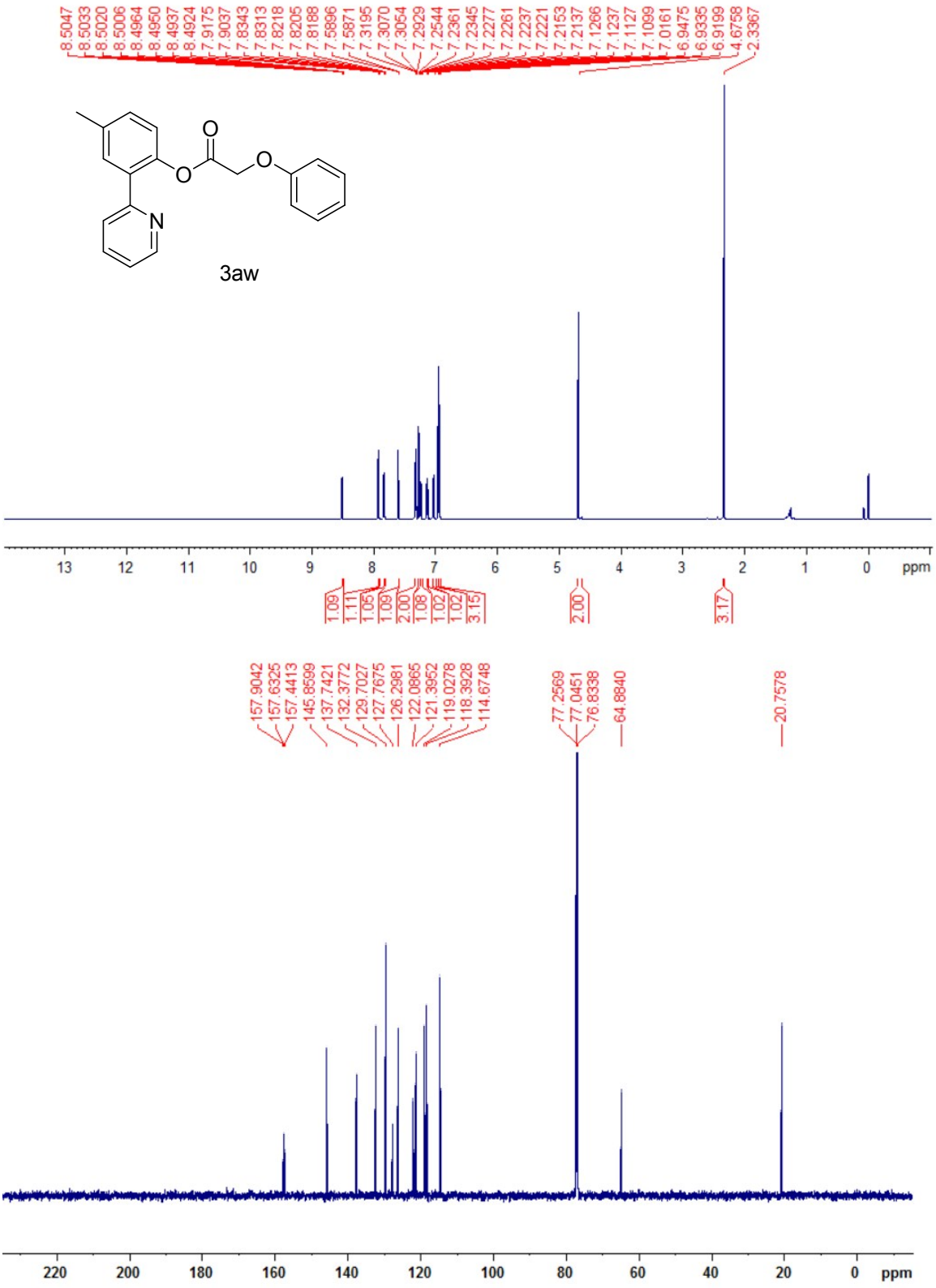
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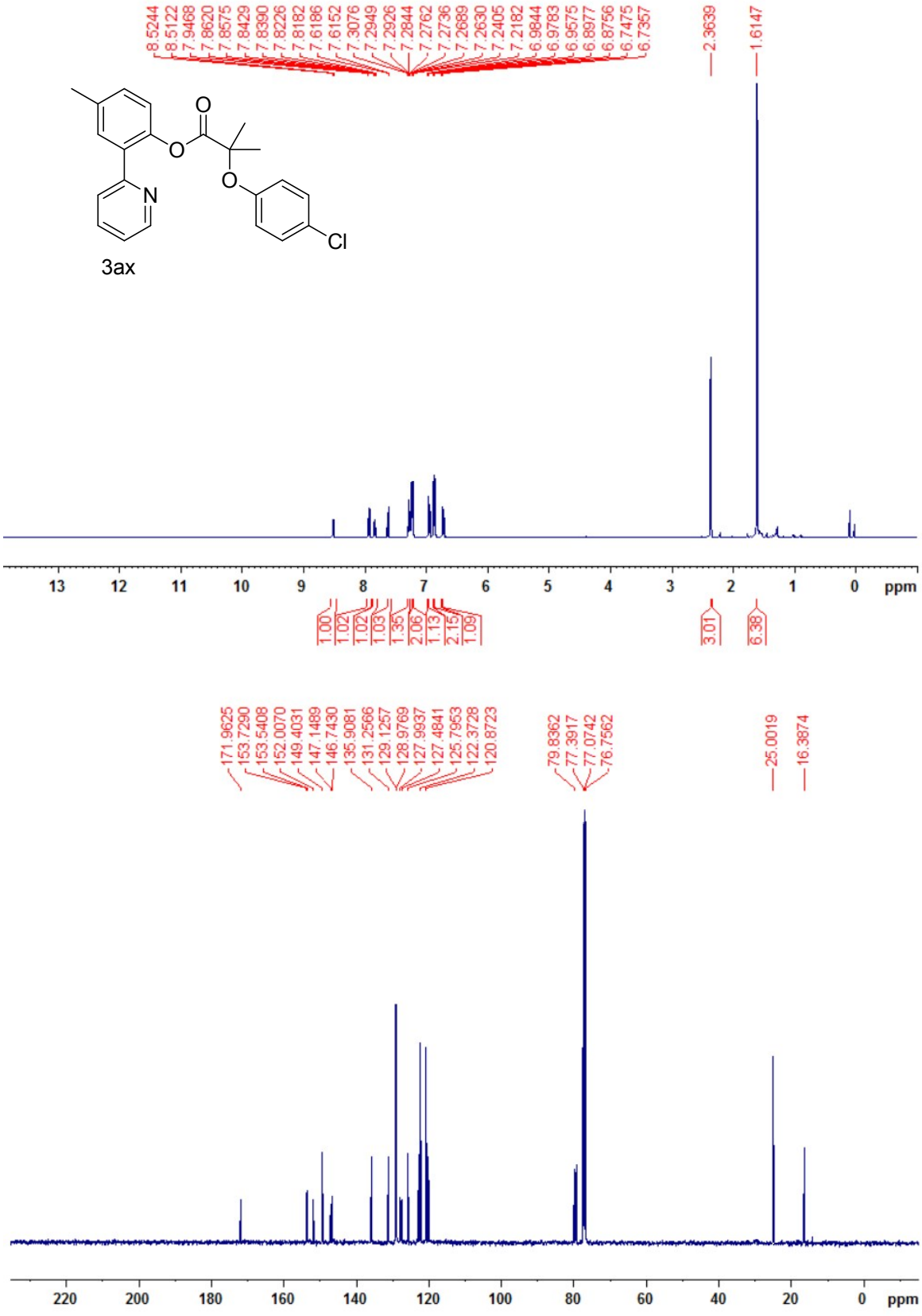
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O
O
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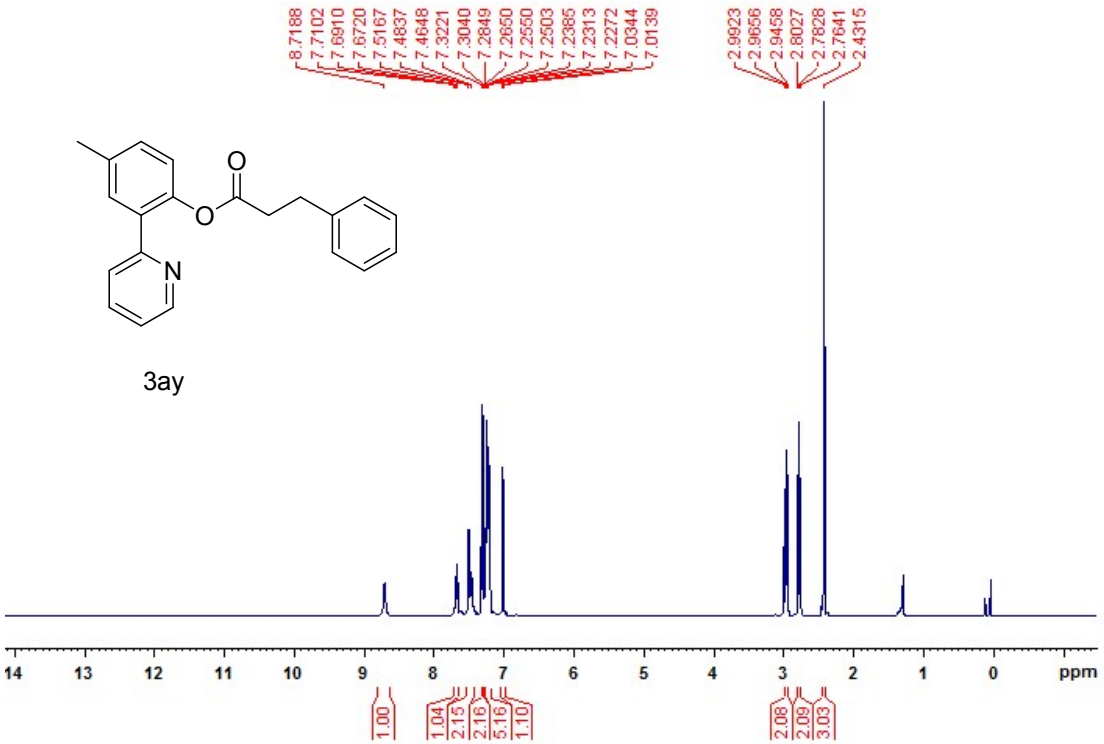
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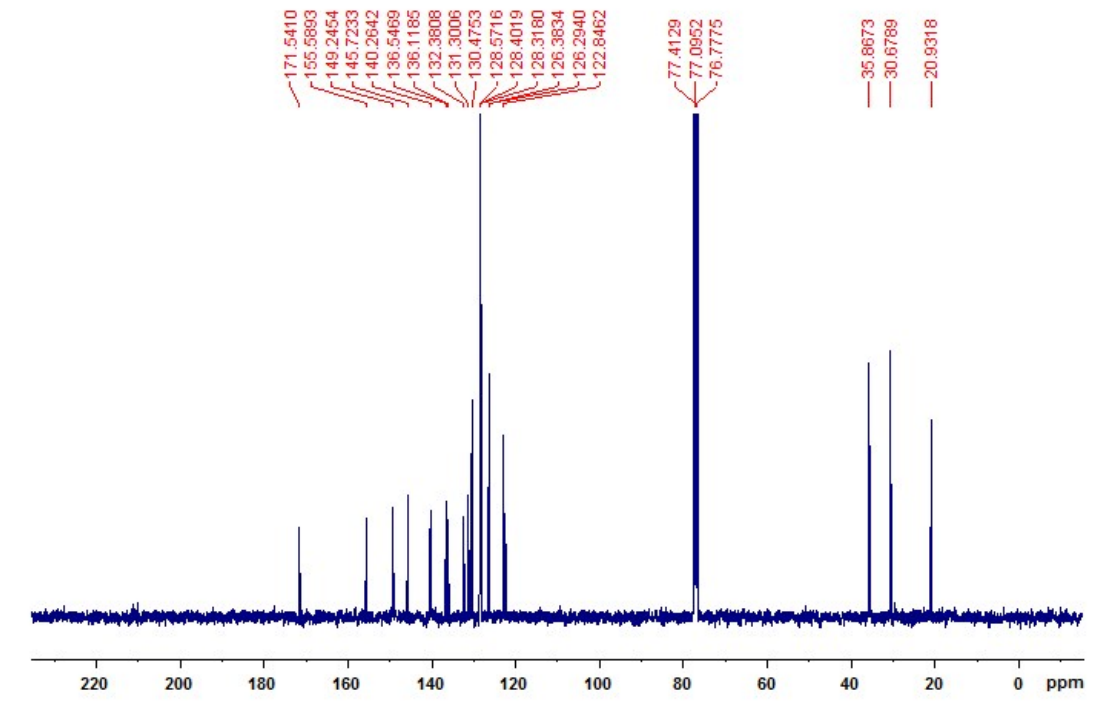
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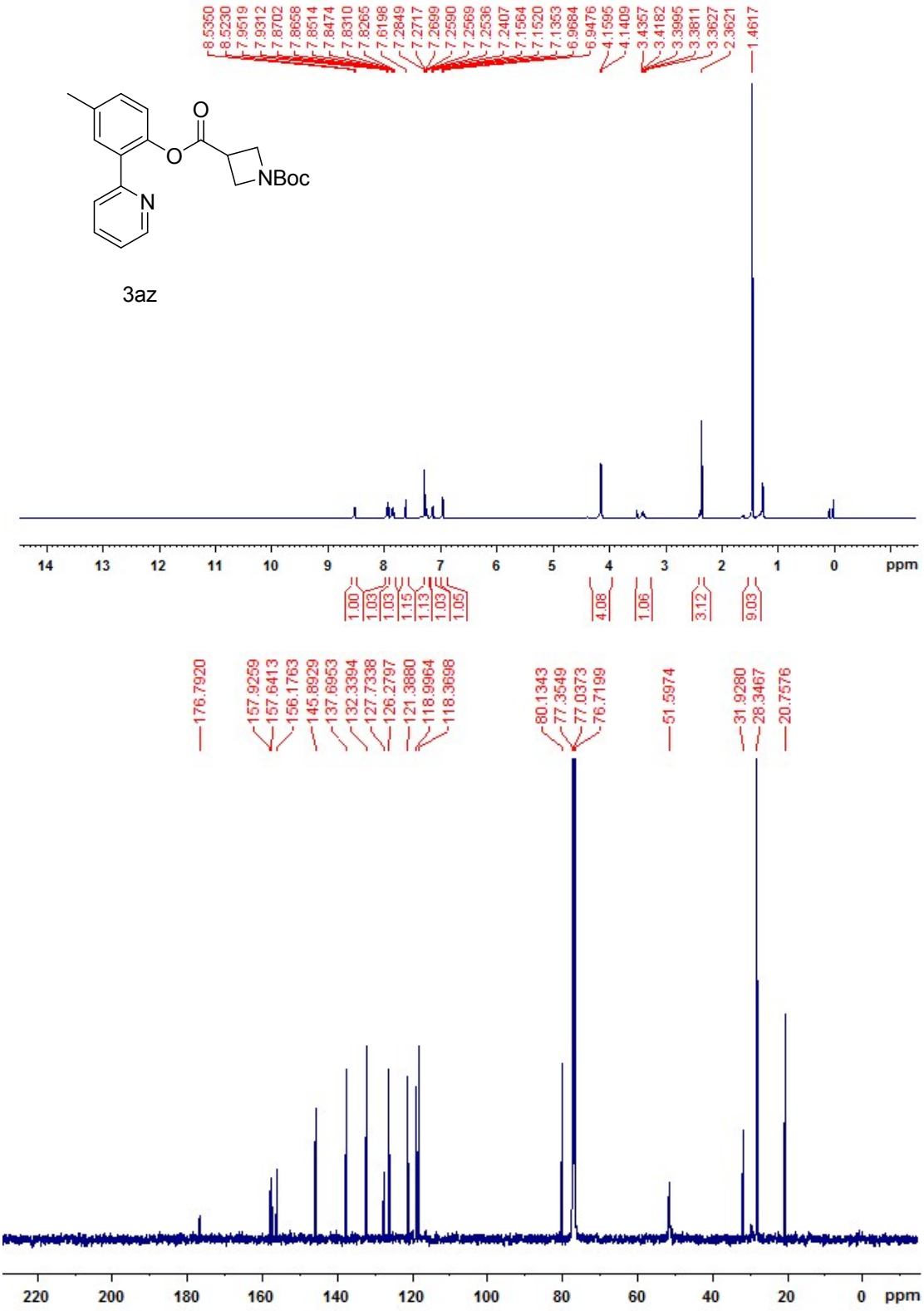
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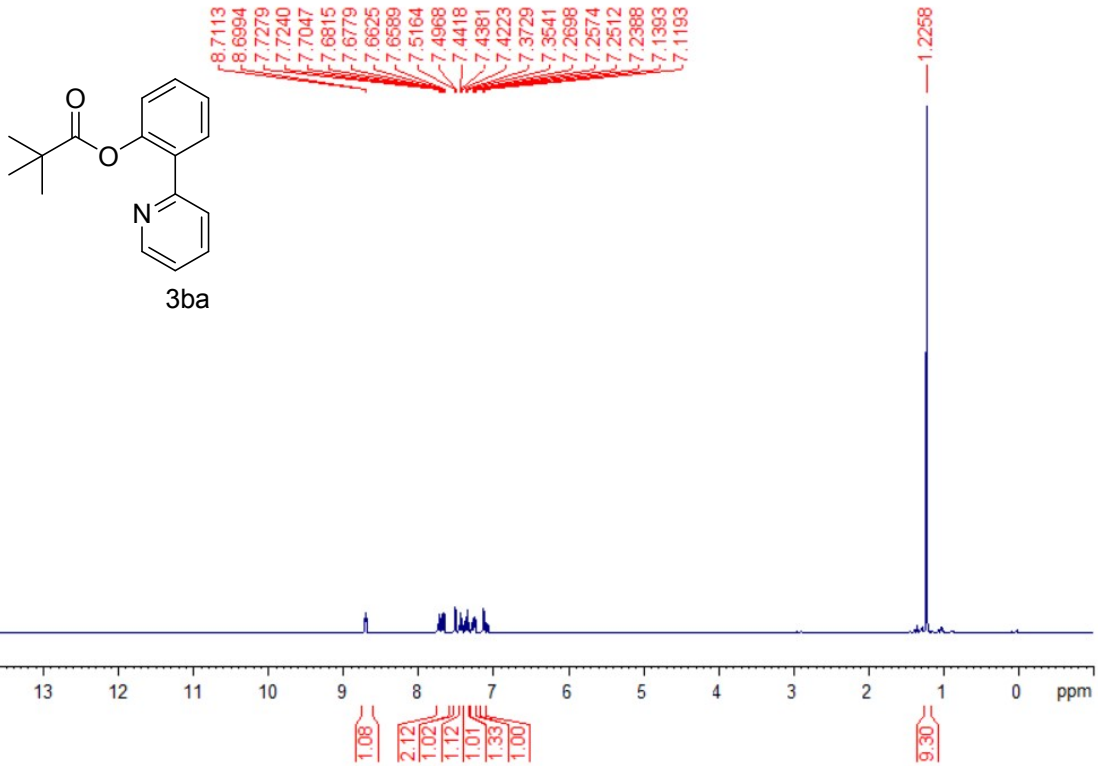
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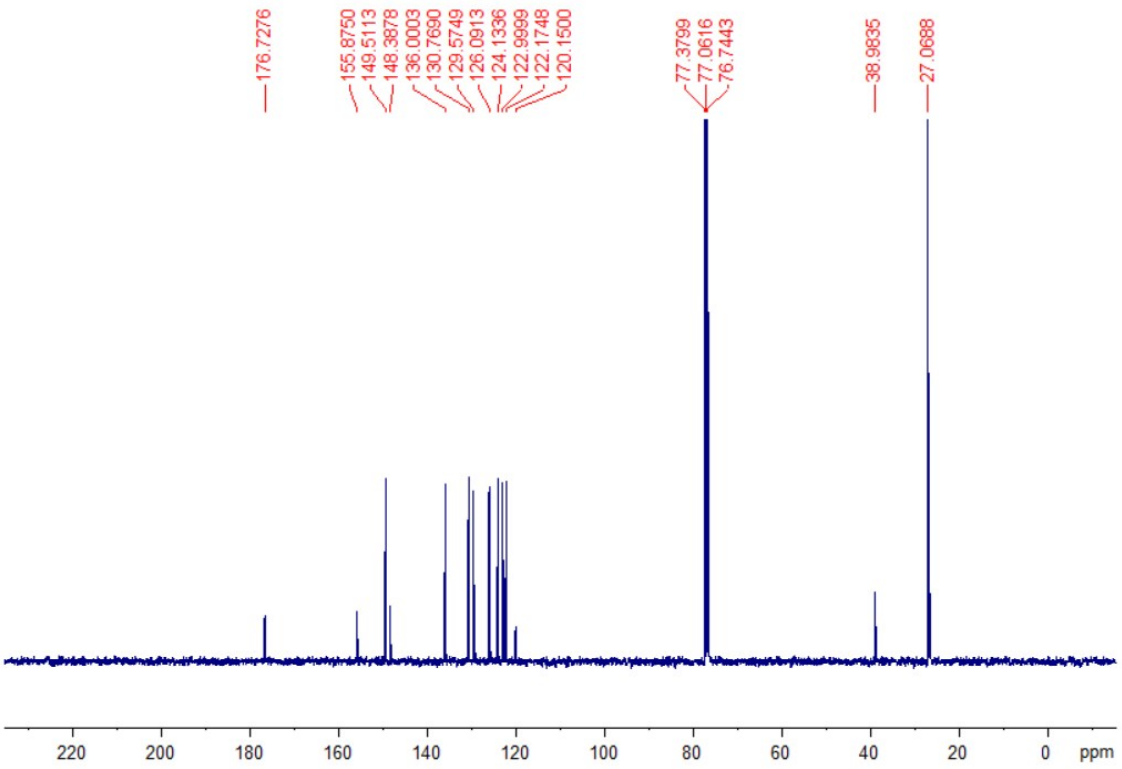
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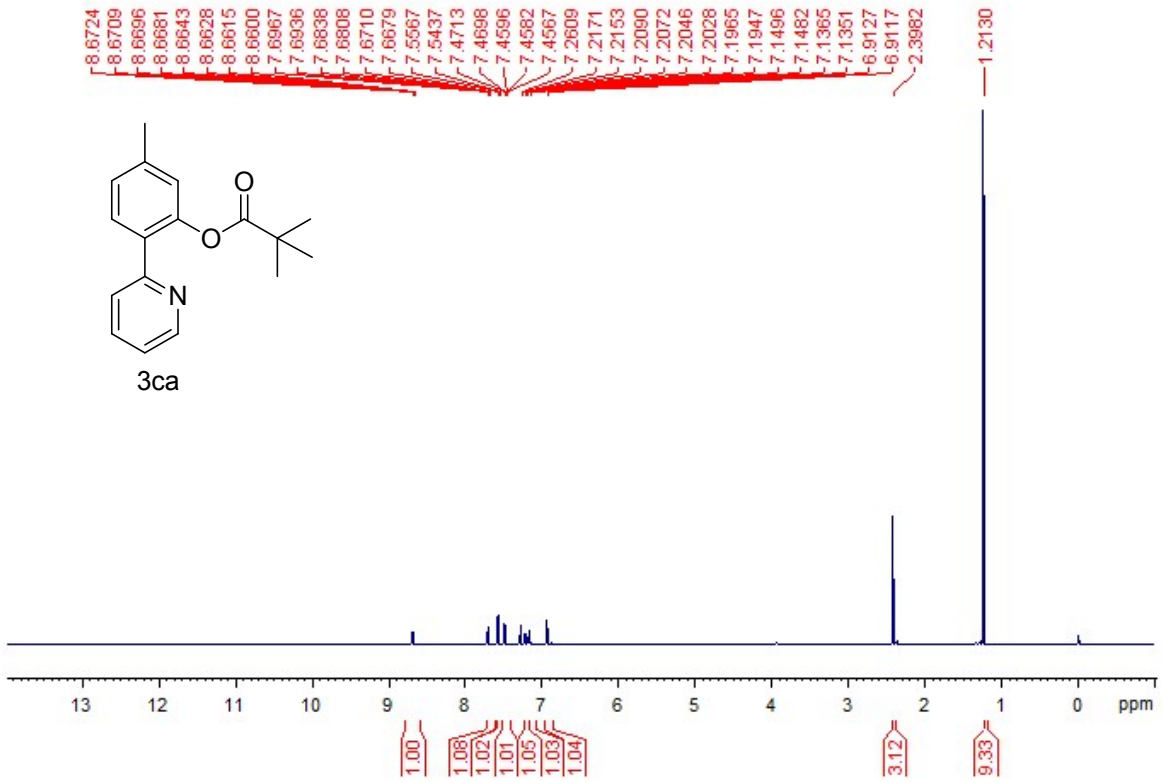
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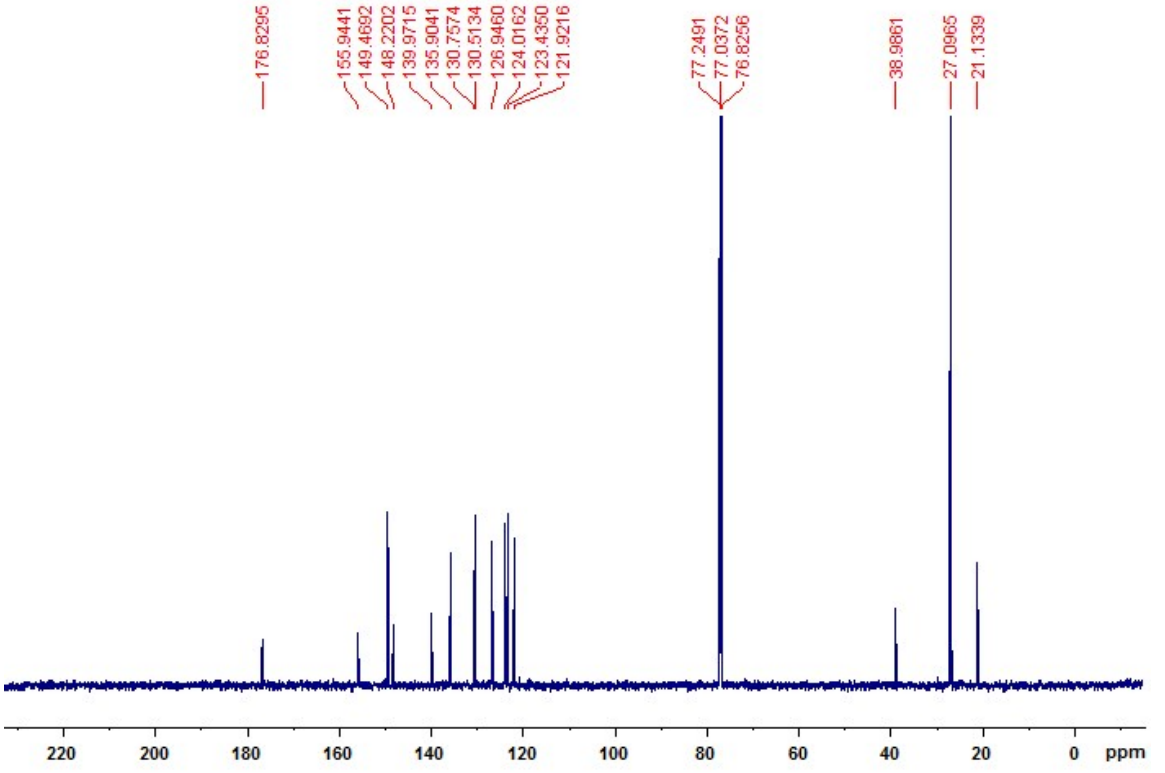
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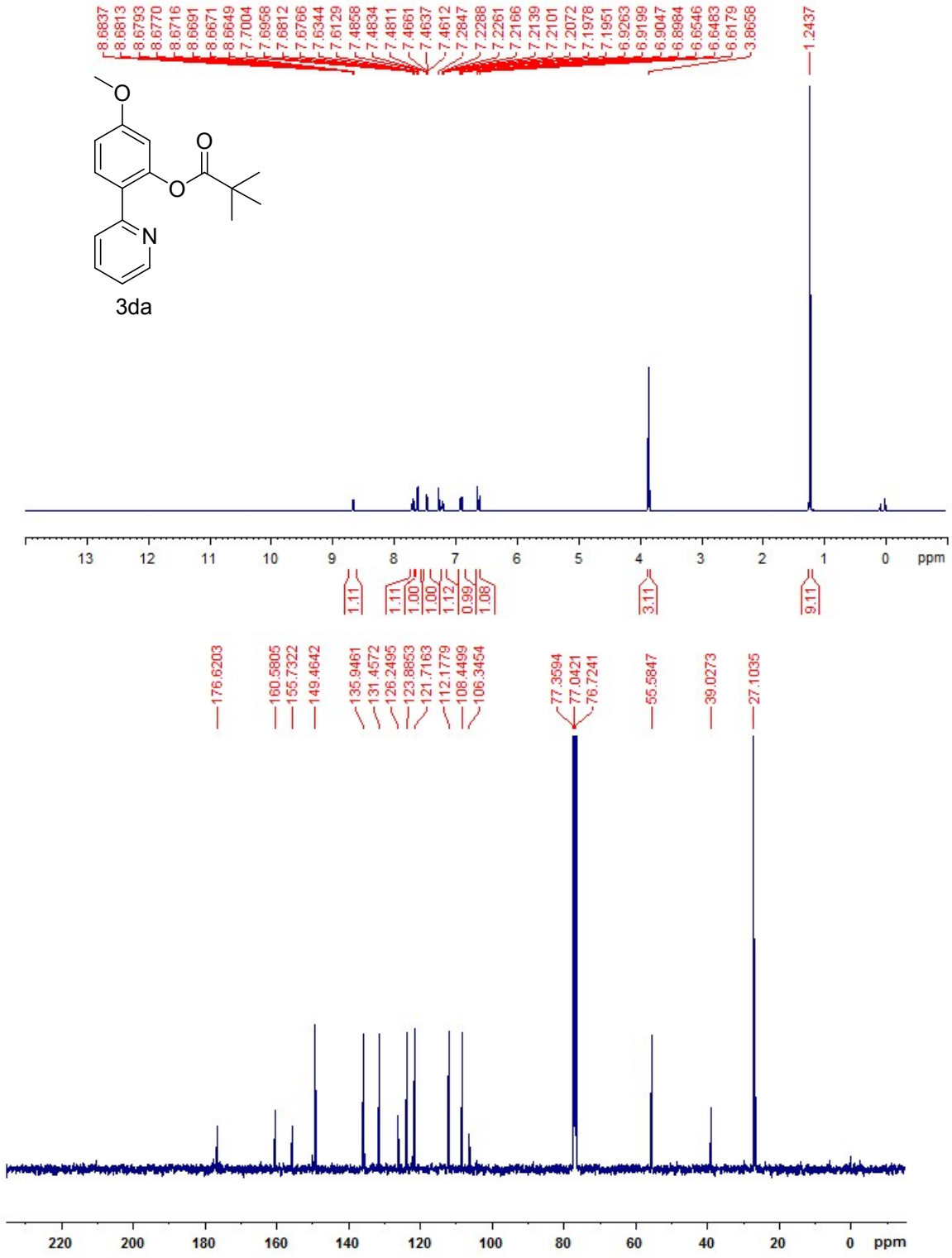
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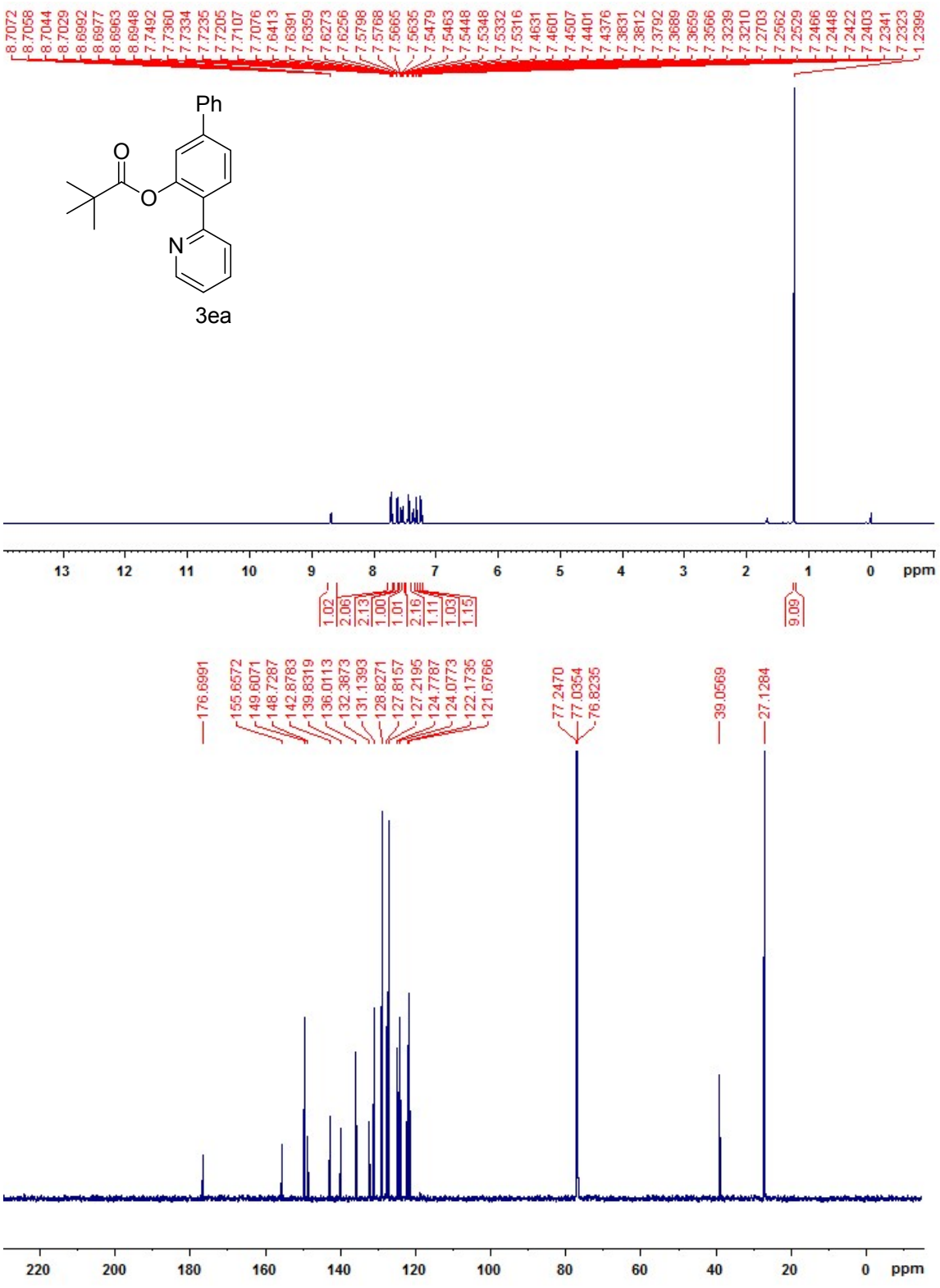
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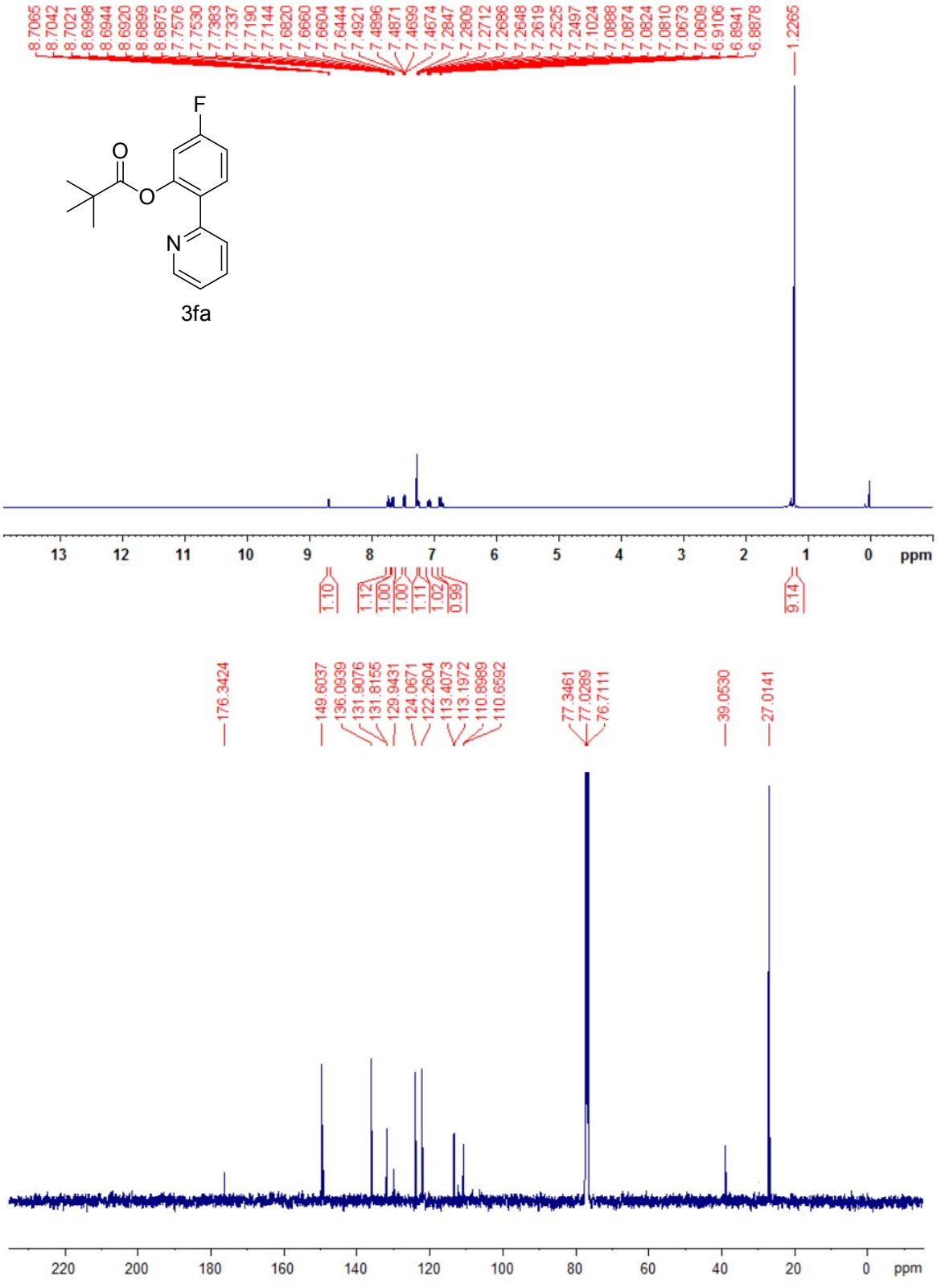
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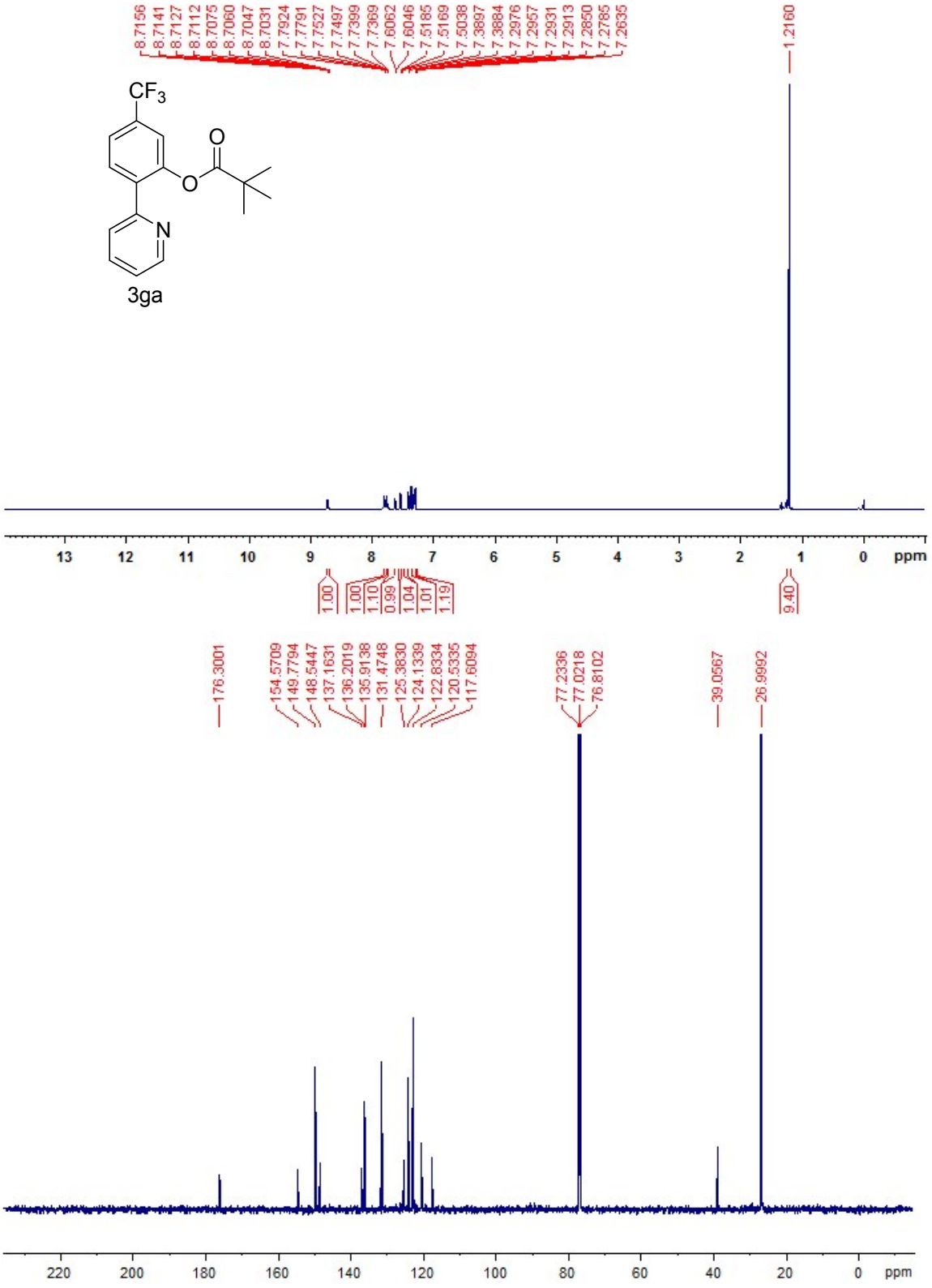
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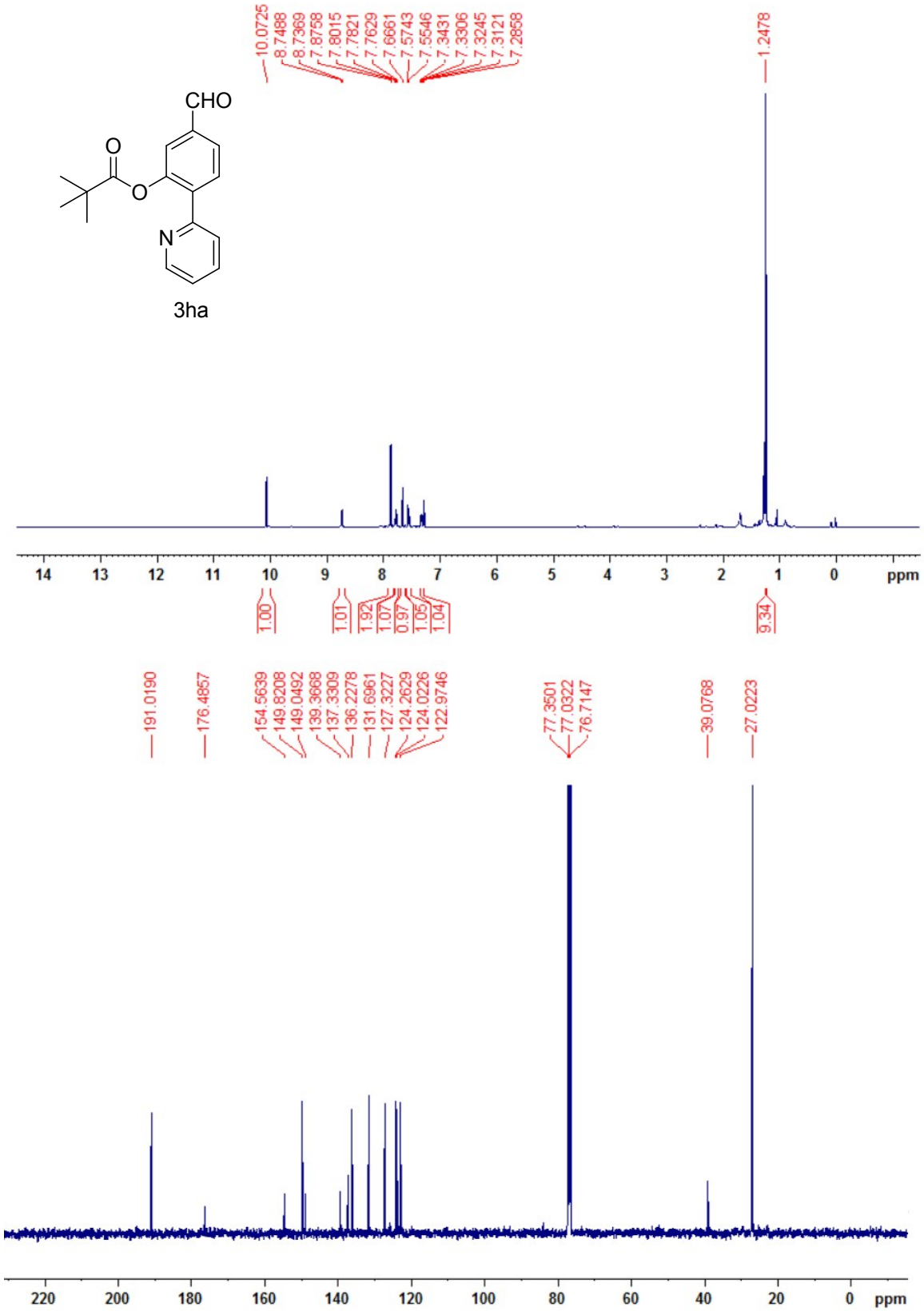
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O
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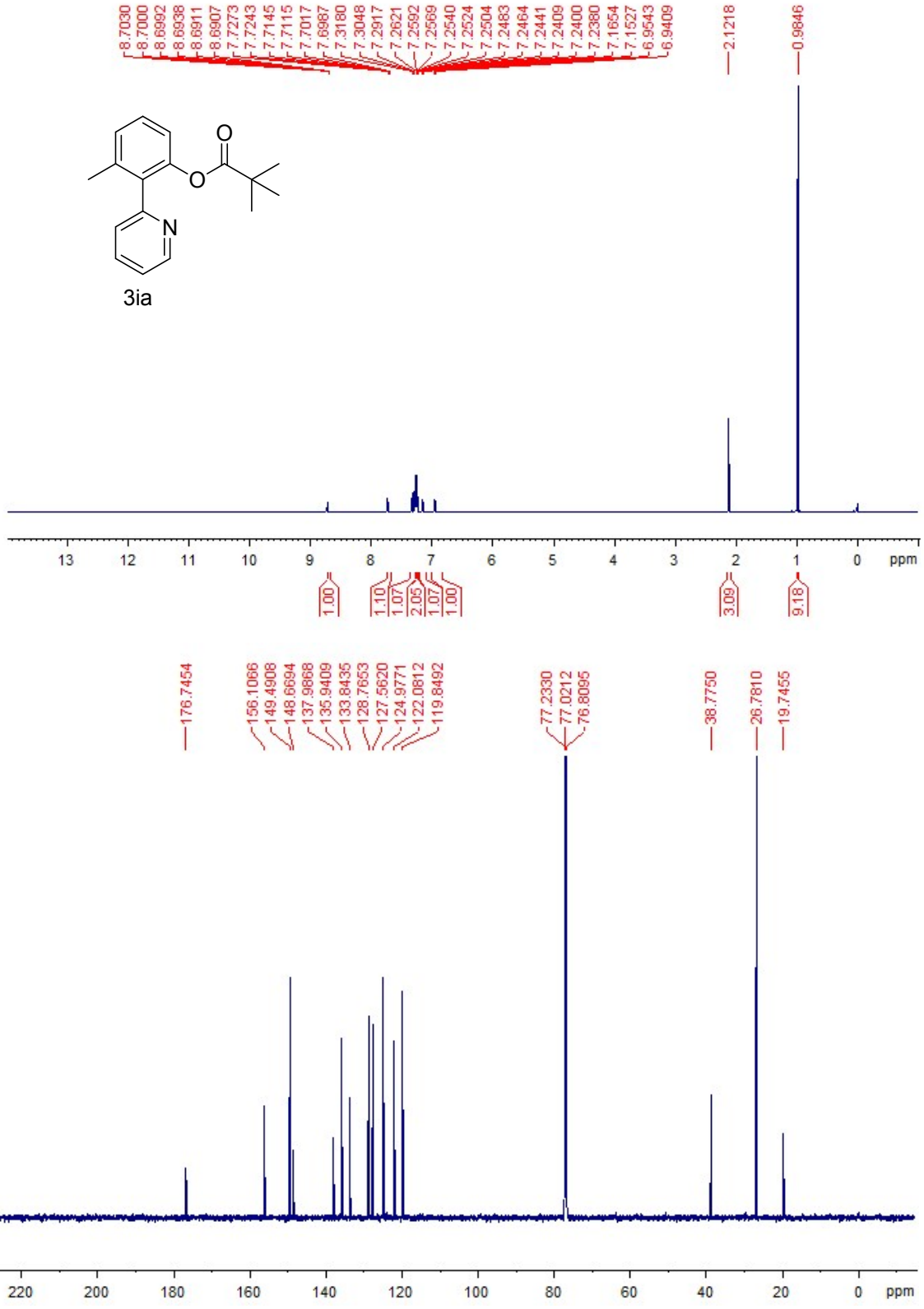
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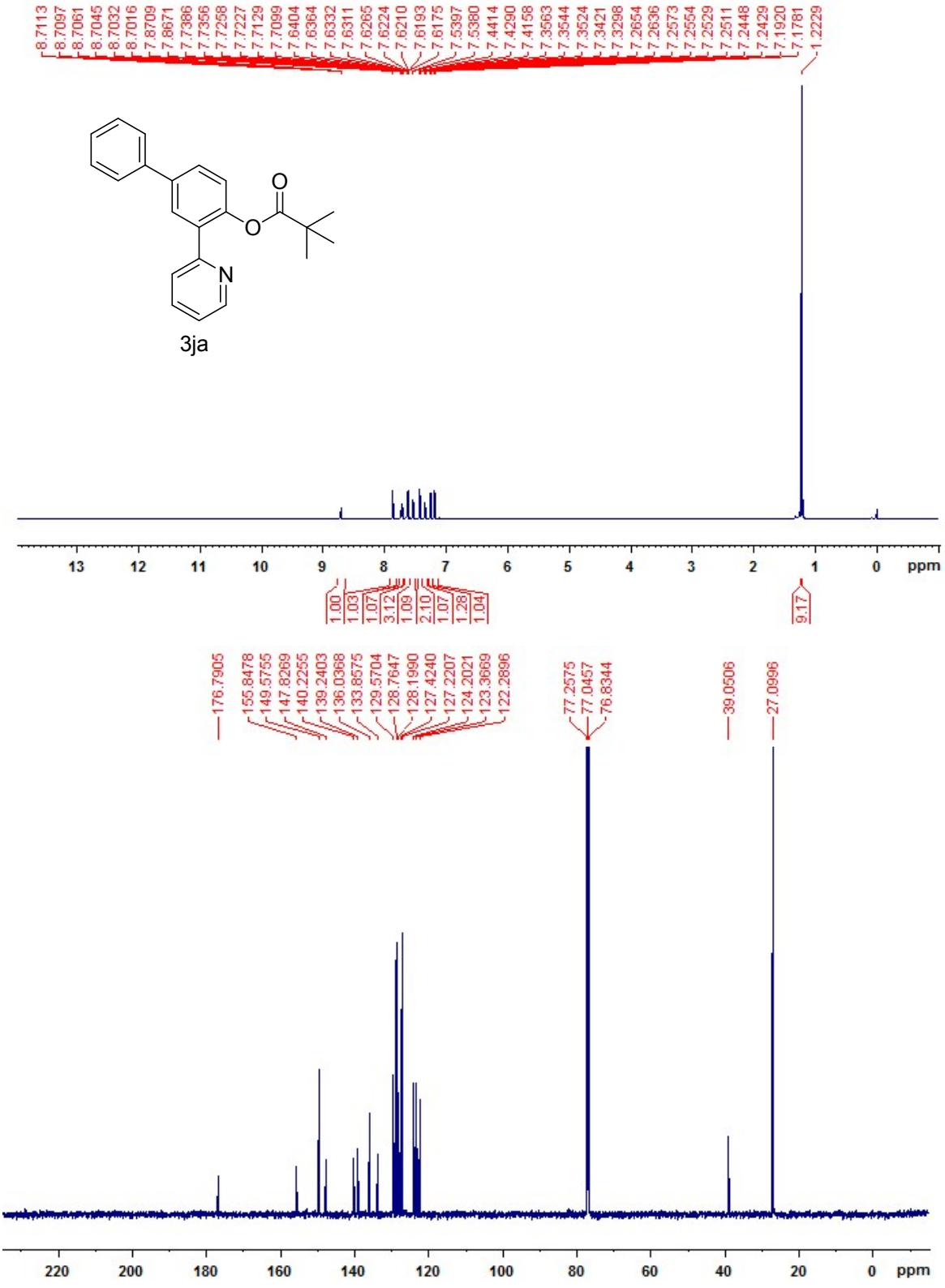
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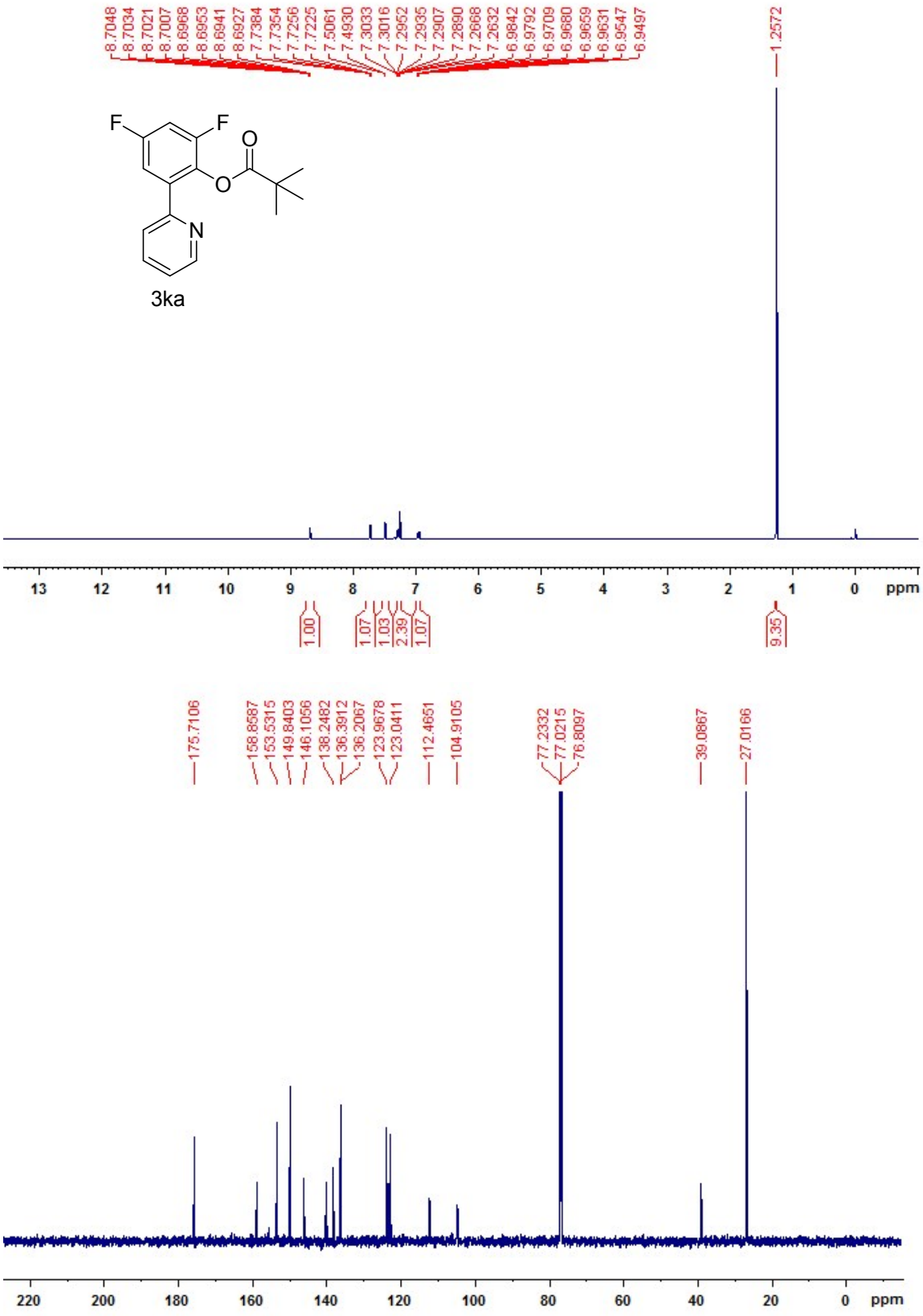
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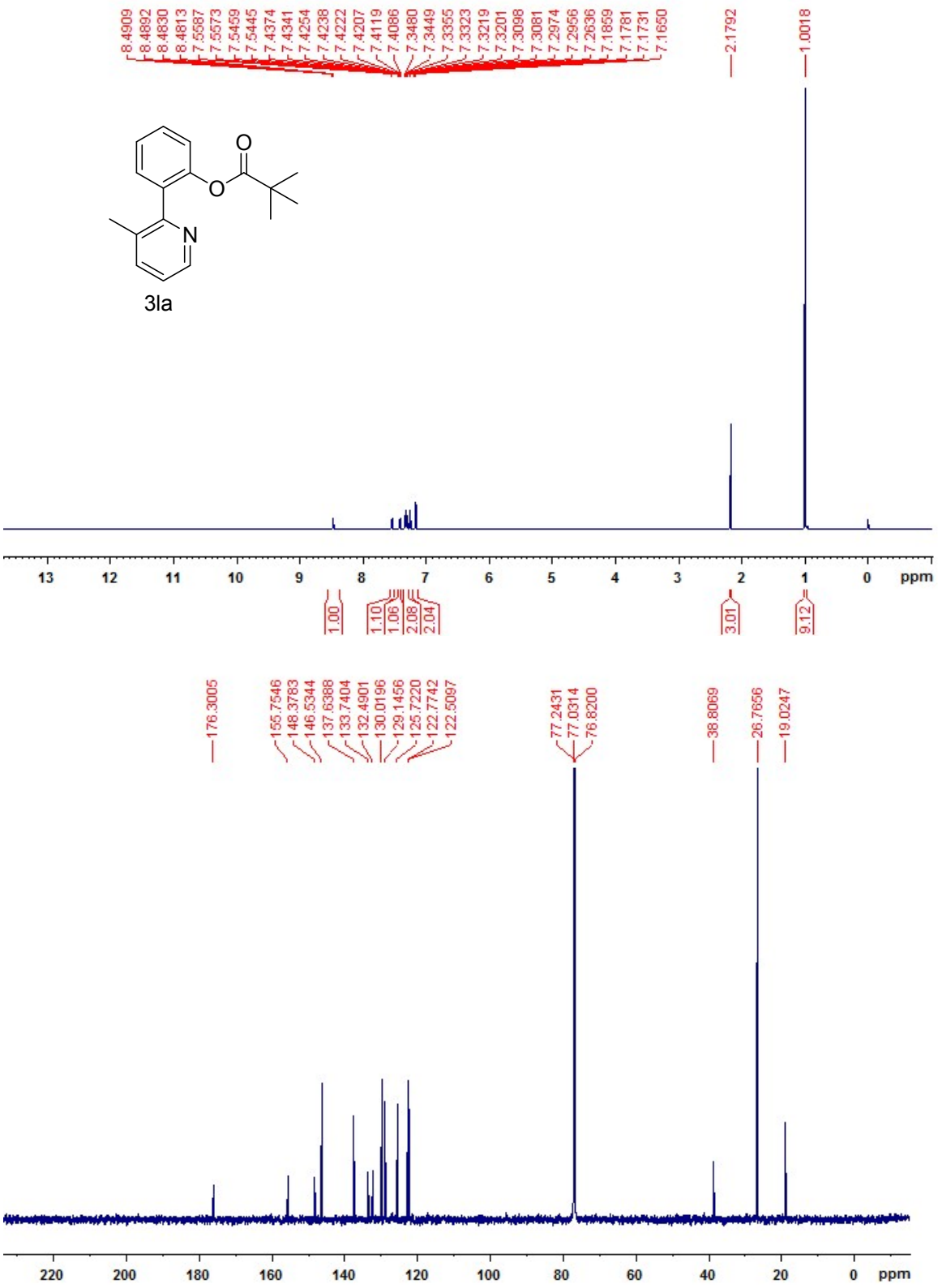
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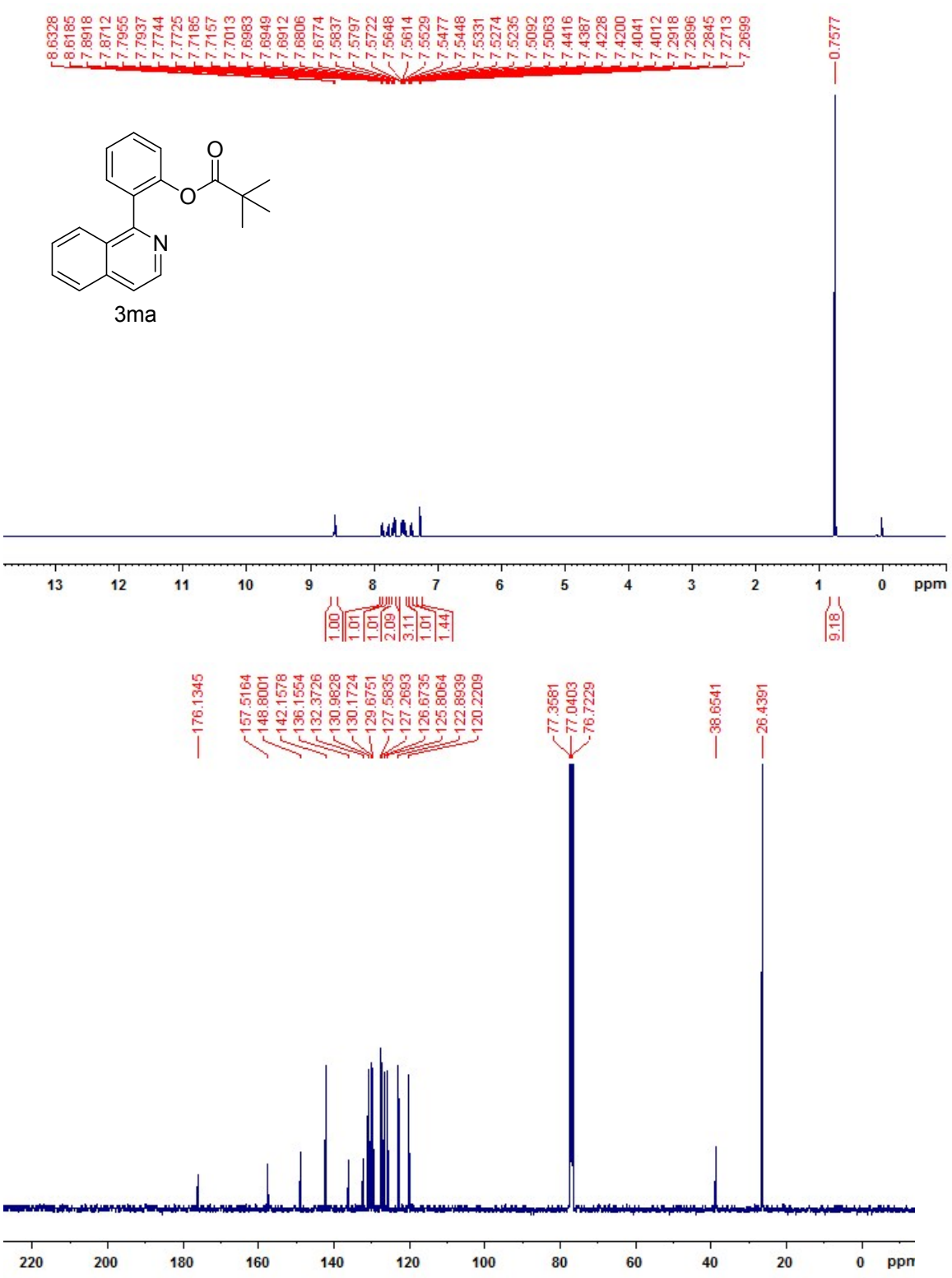
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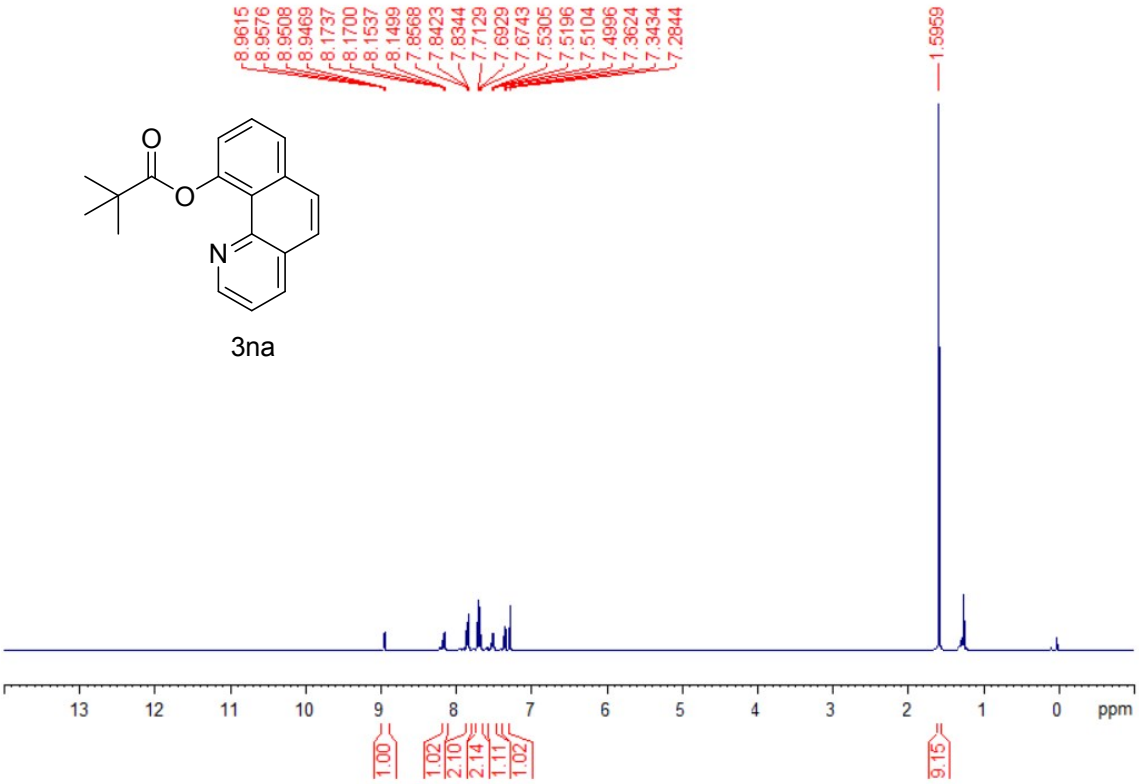
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O
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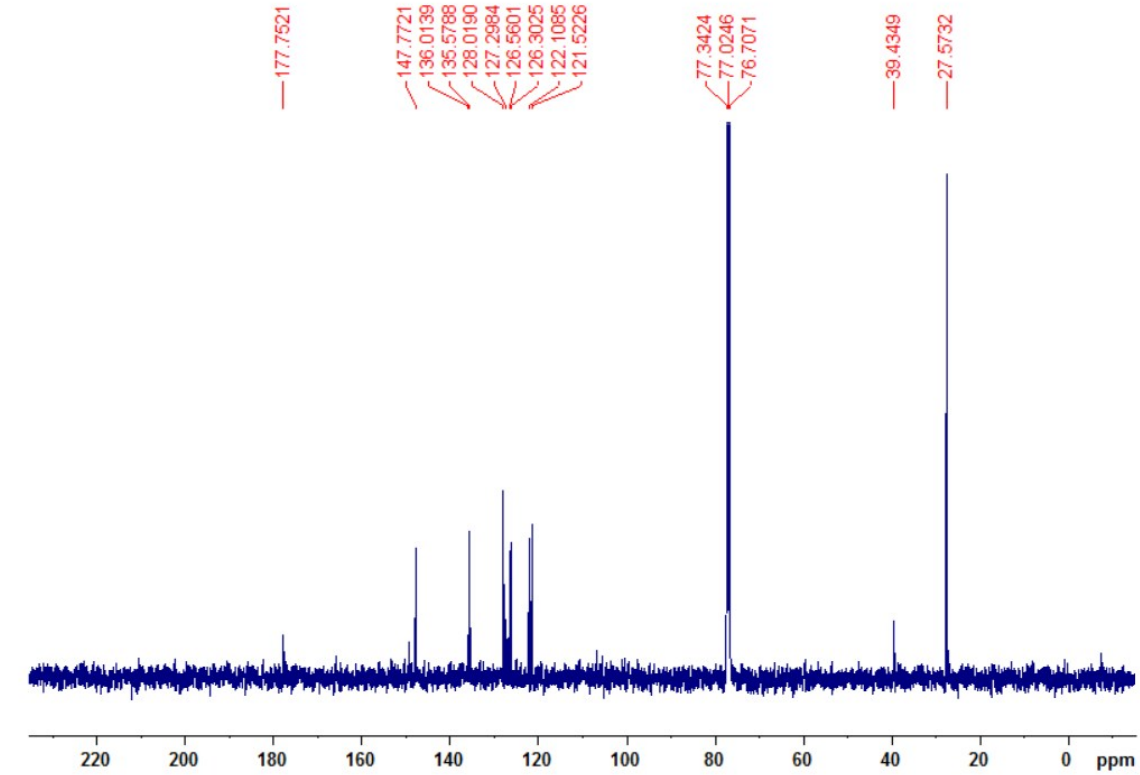
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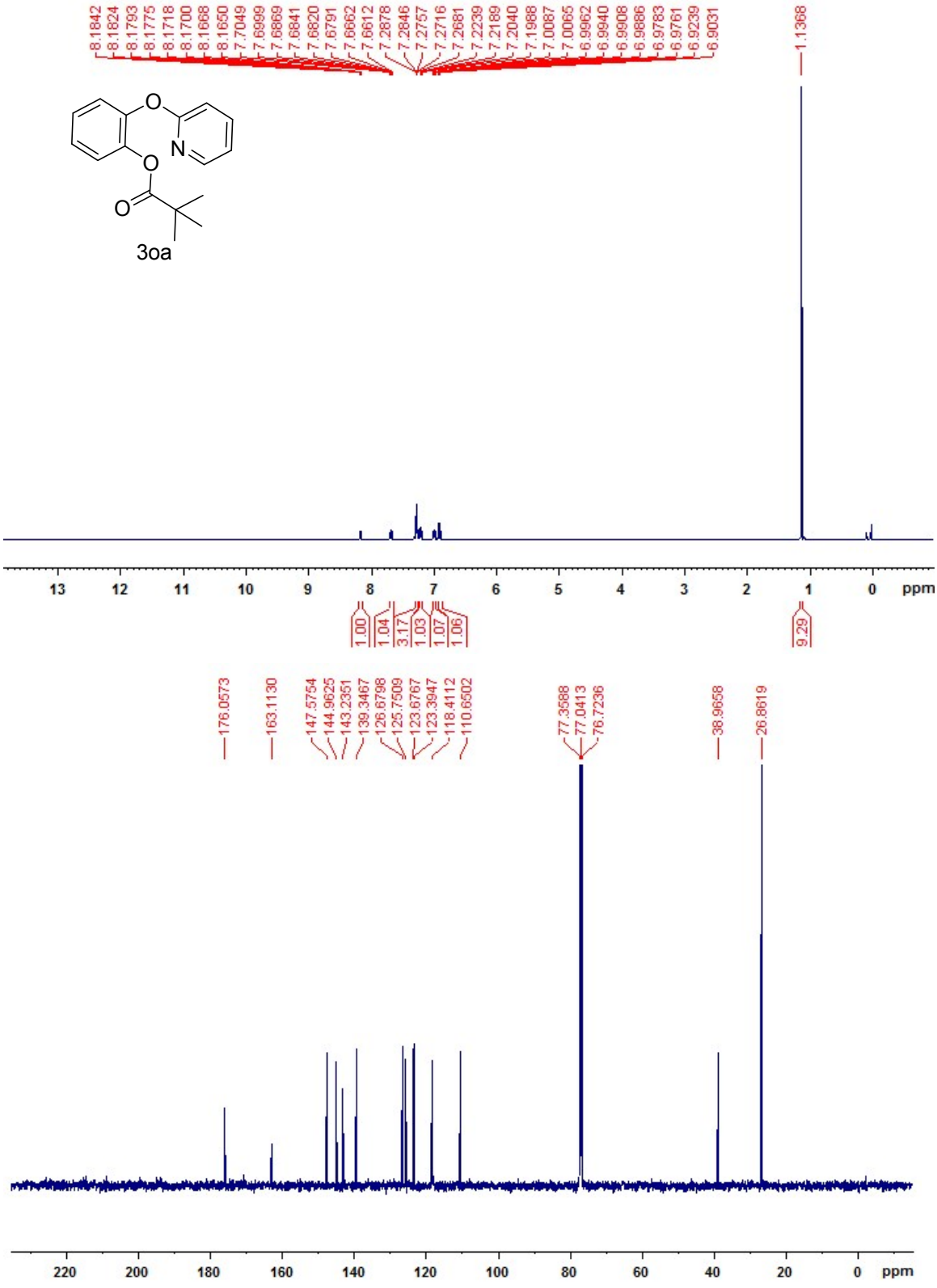
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O
O
3oa
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3.17
1.03
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1.06
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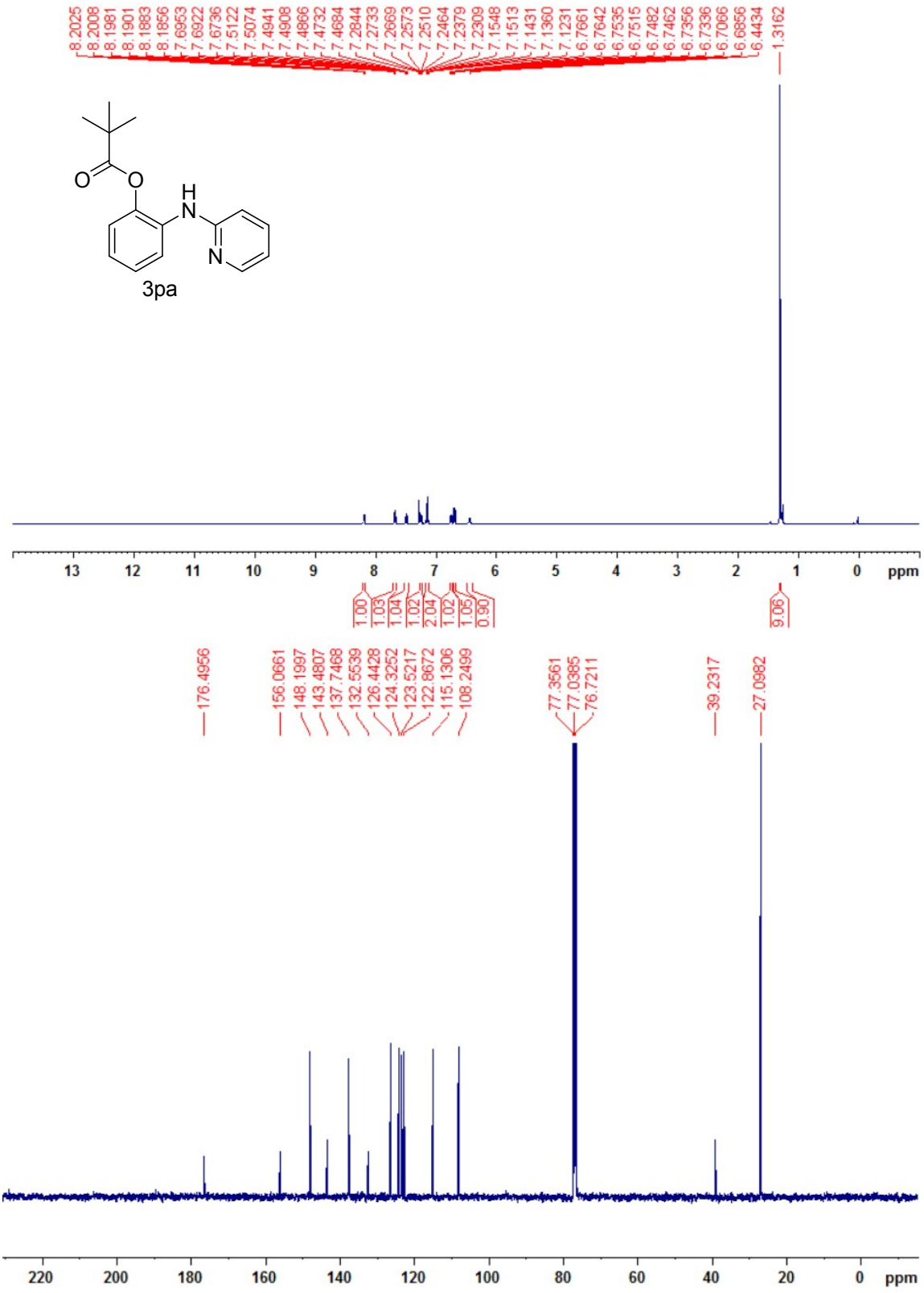
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O
H
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N
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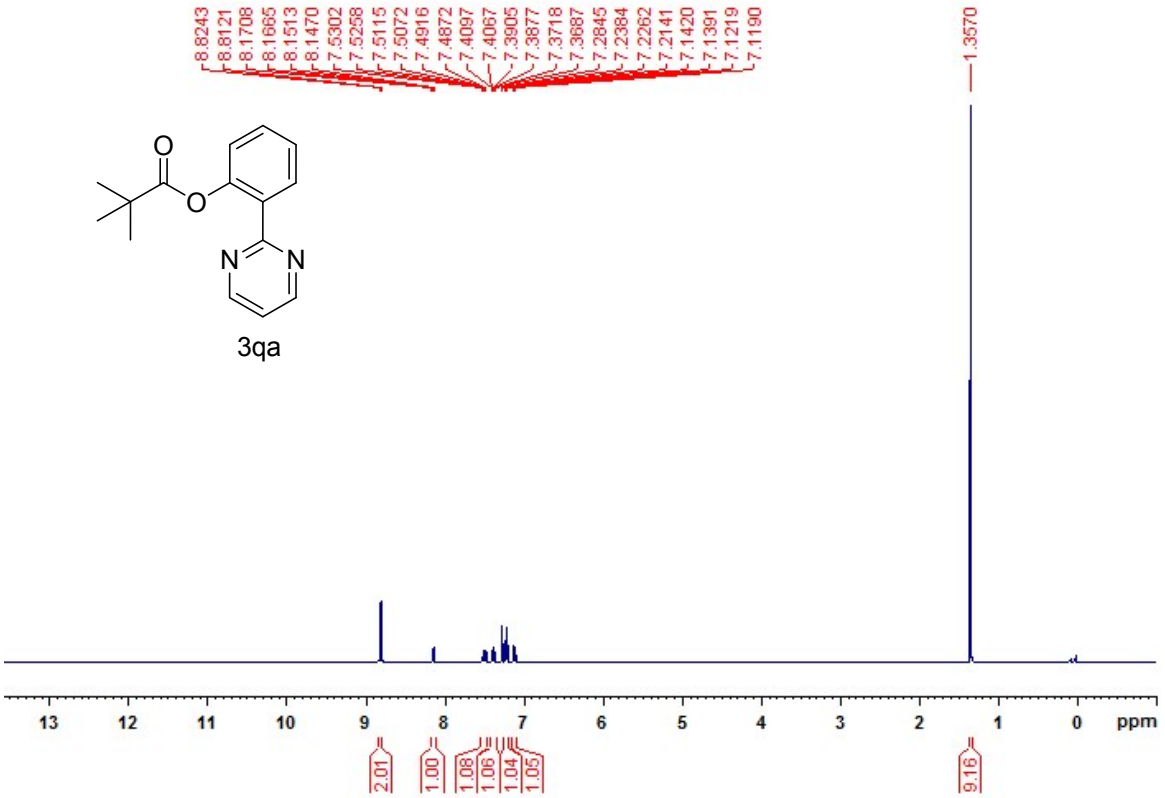
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O
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N
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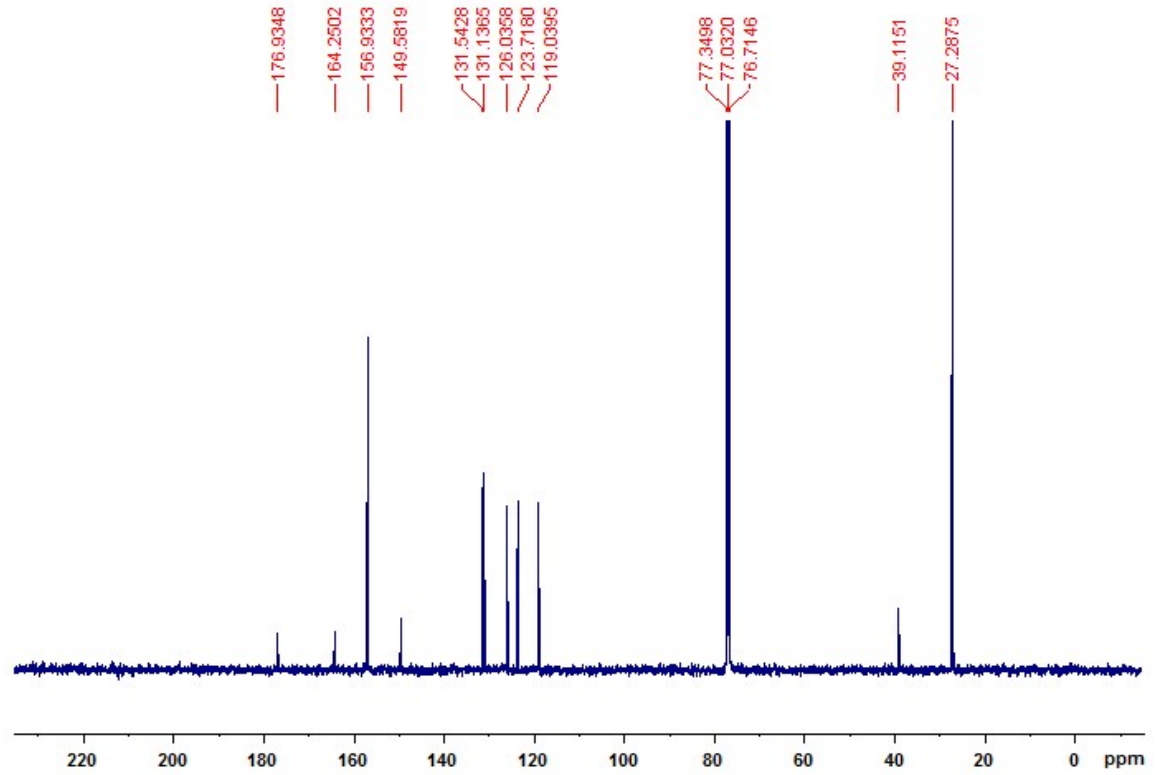
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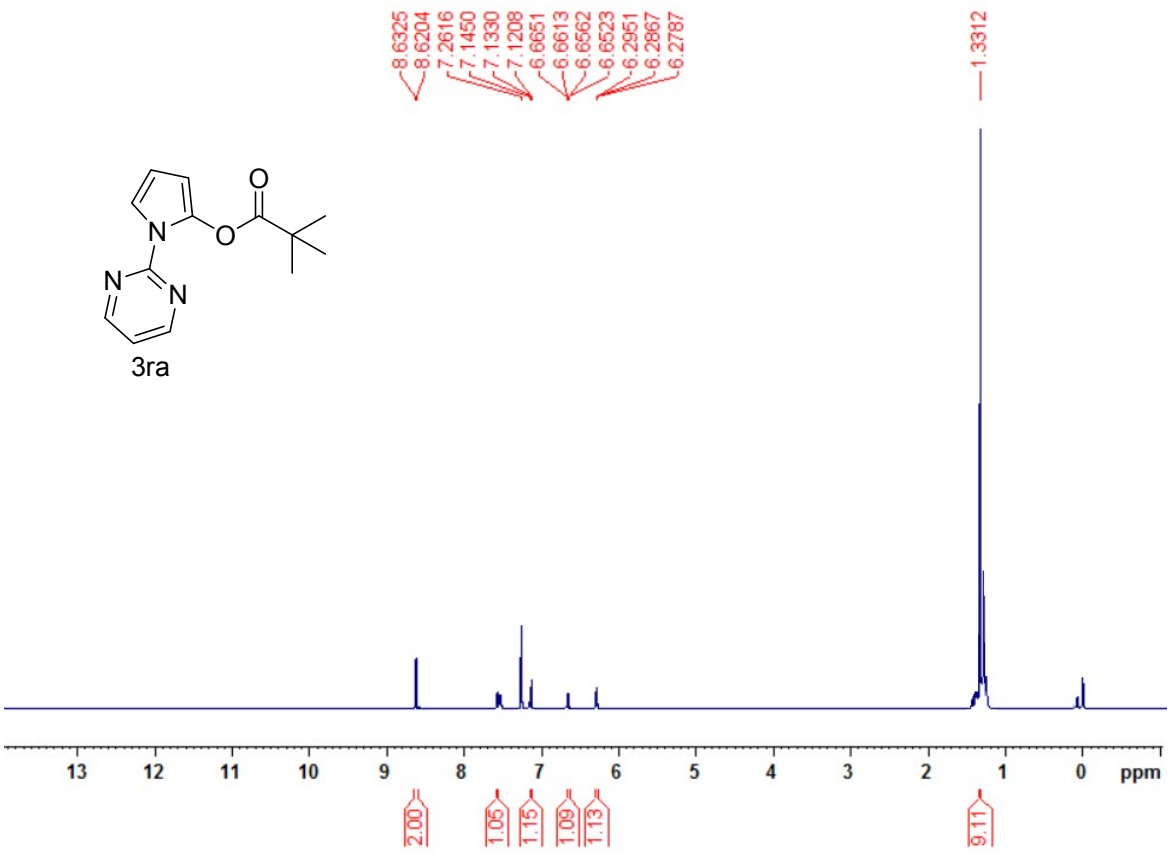
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6.2787
1.3312
O
N
O
N
N
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12
11
10
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8
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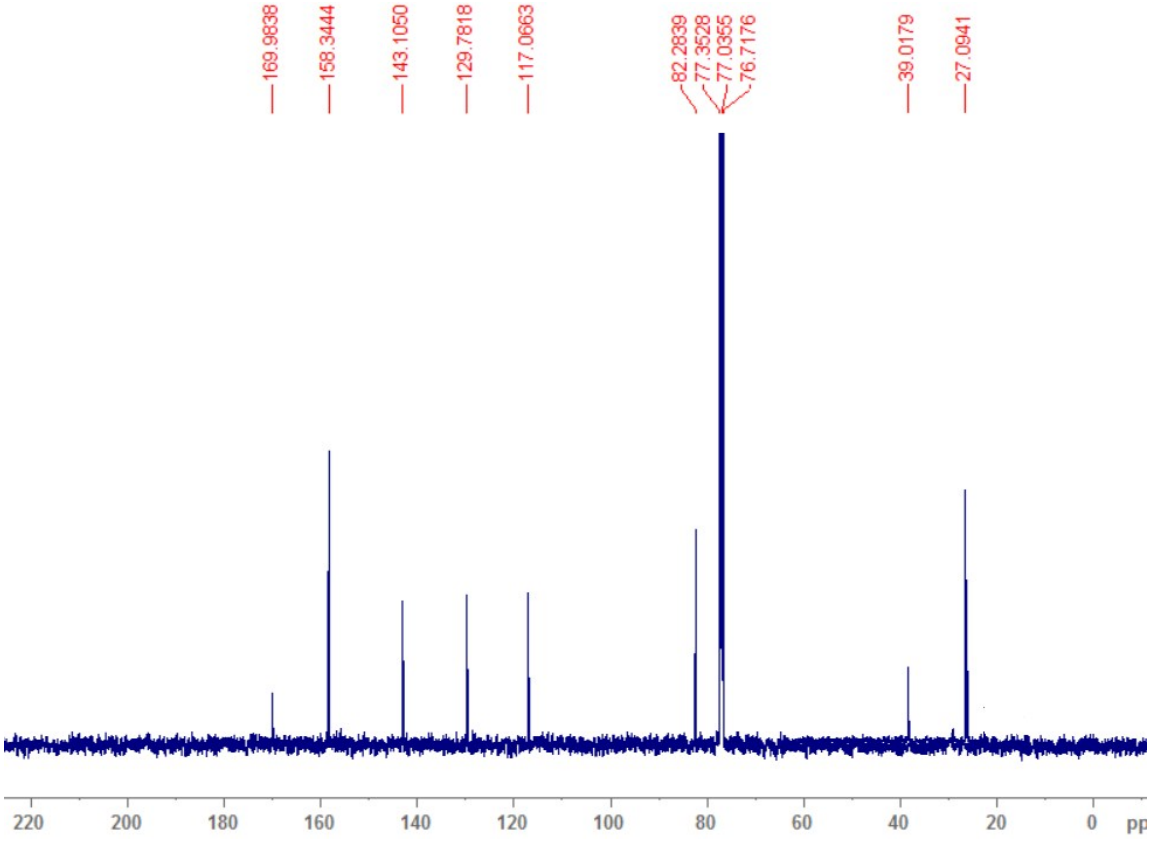
3ra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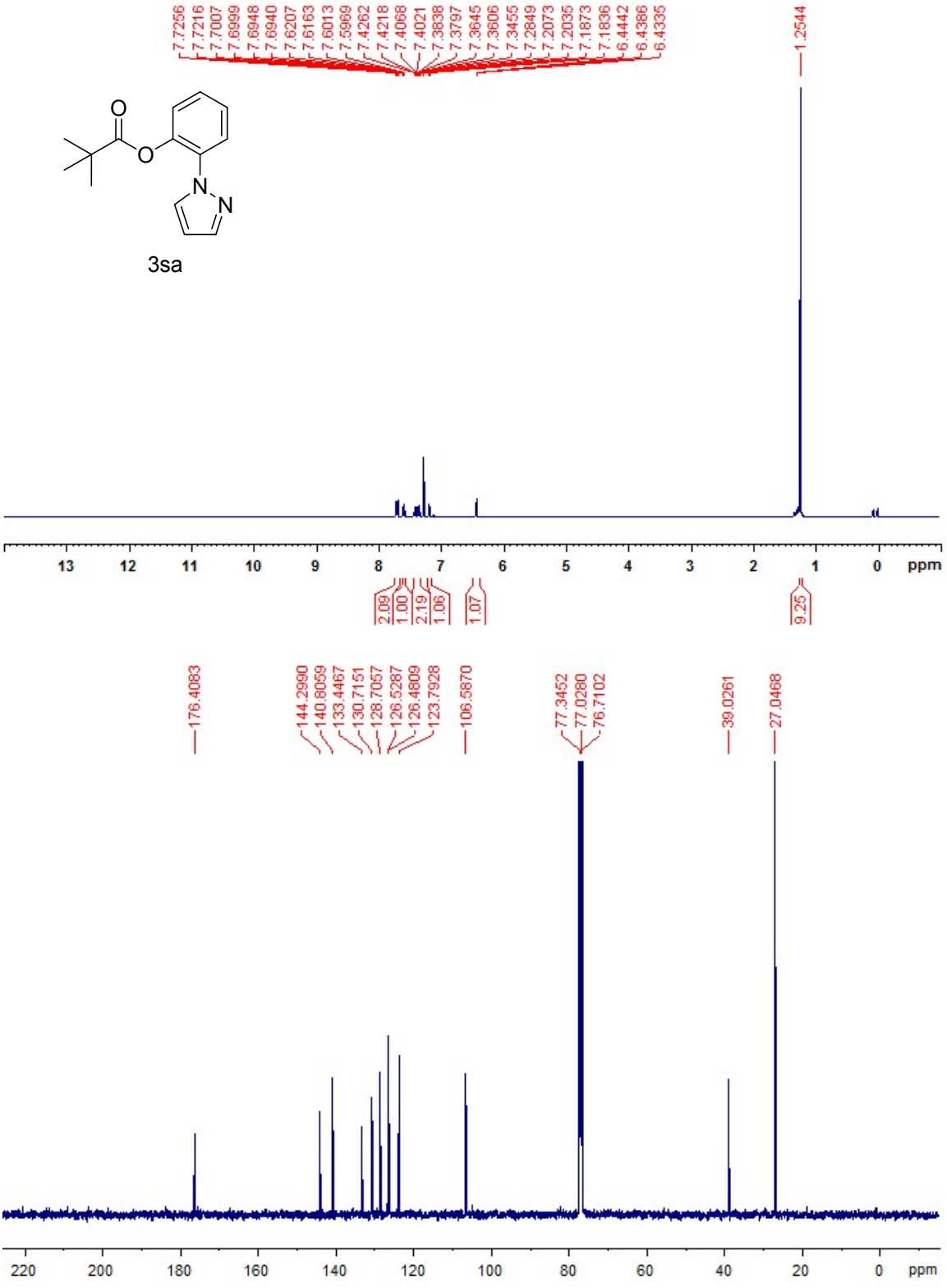
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O
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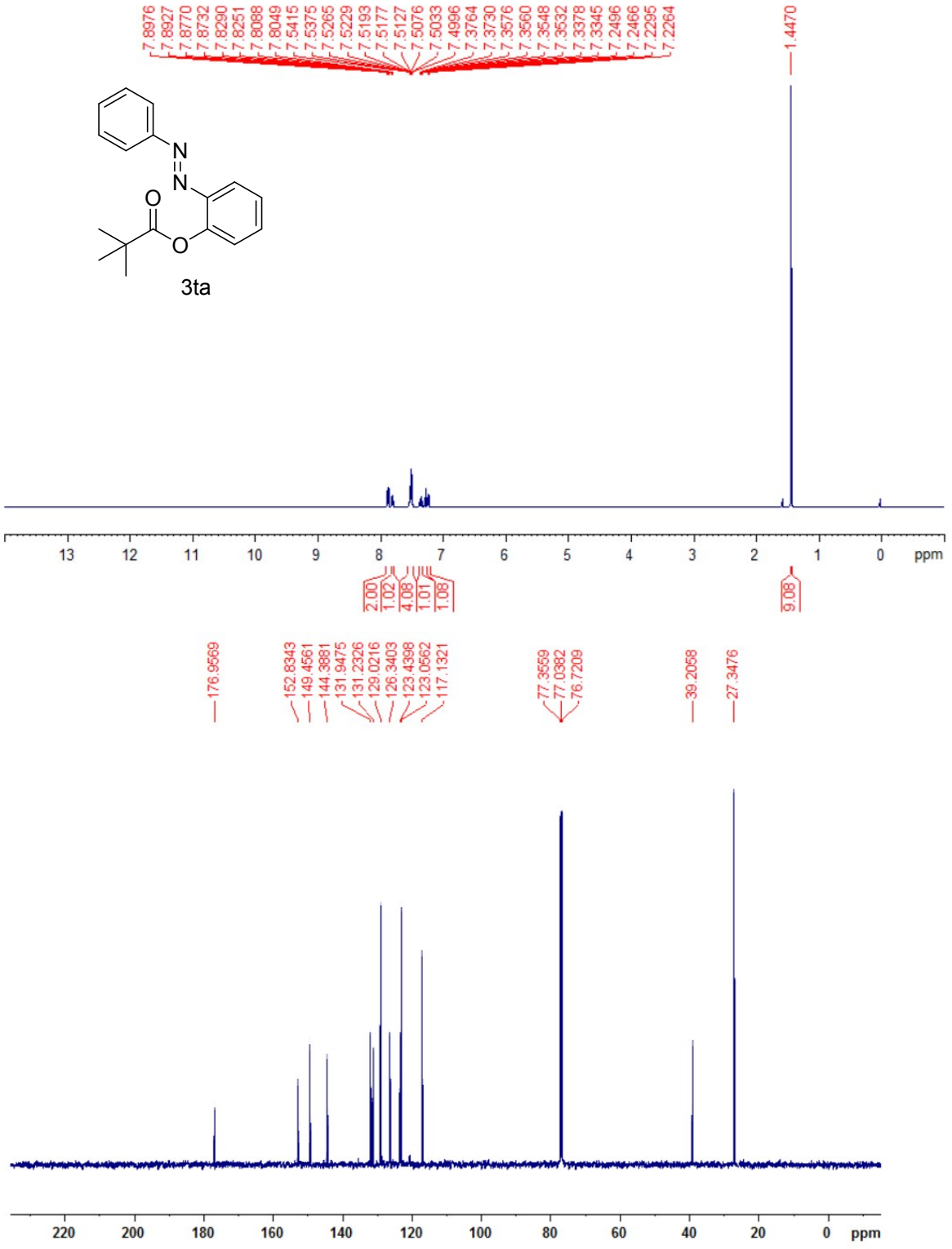
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7.3560
7.3548
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7.3378
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7.2496
7.2466
7.2295
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O
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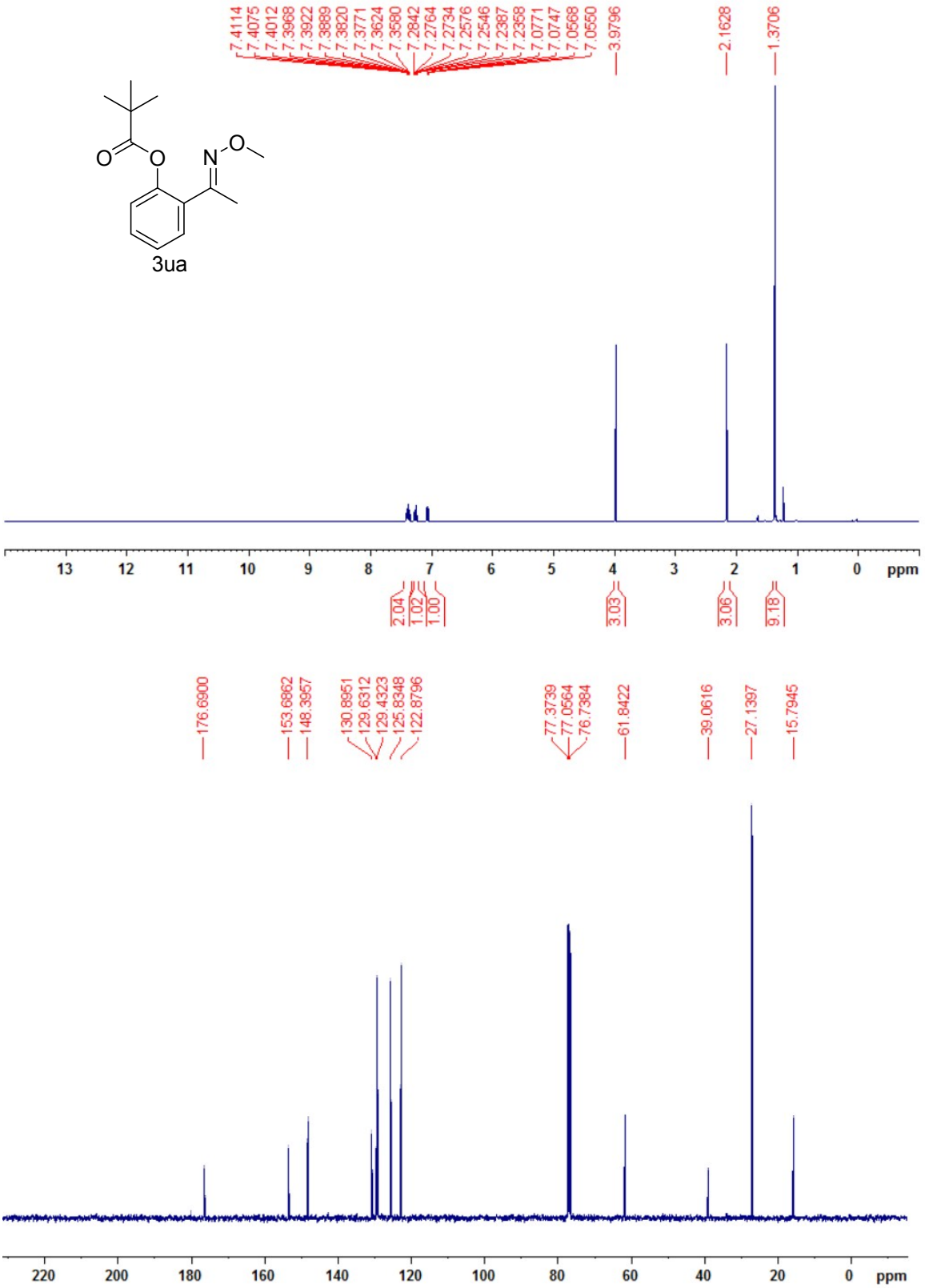
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7.0550
3.9796
2.1628
1.3706
O
O
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O
3ua
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7
6
5
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3
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ppm
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1.00
3.03
3.06
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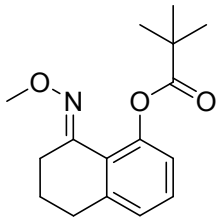

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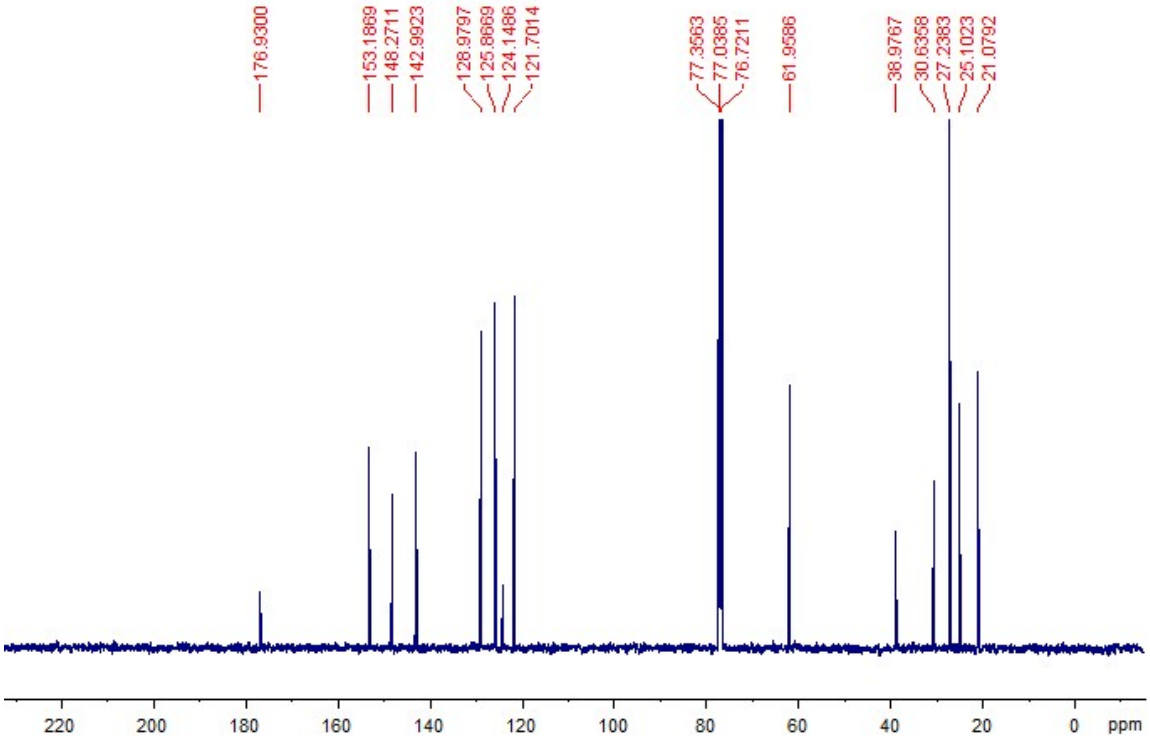
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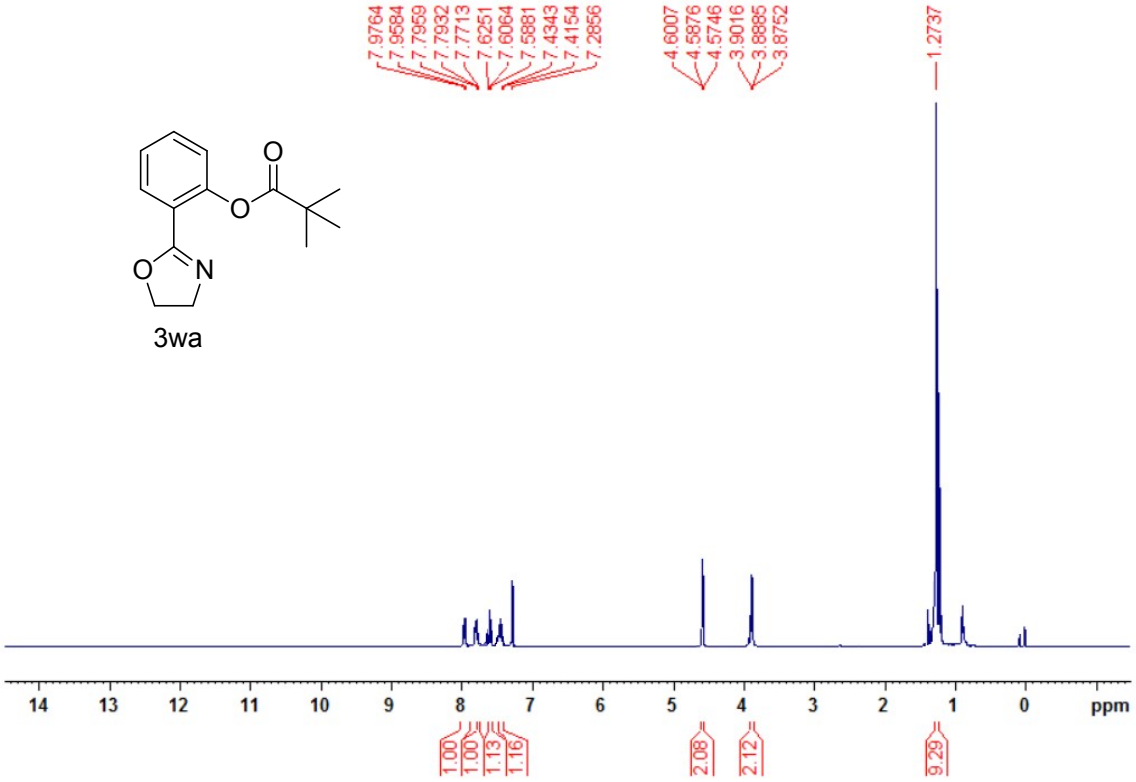
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O
O
N
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12
11
10
9
8
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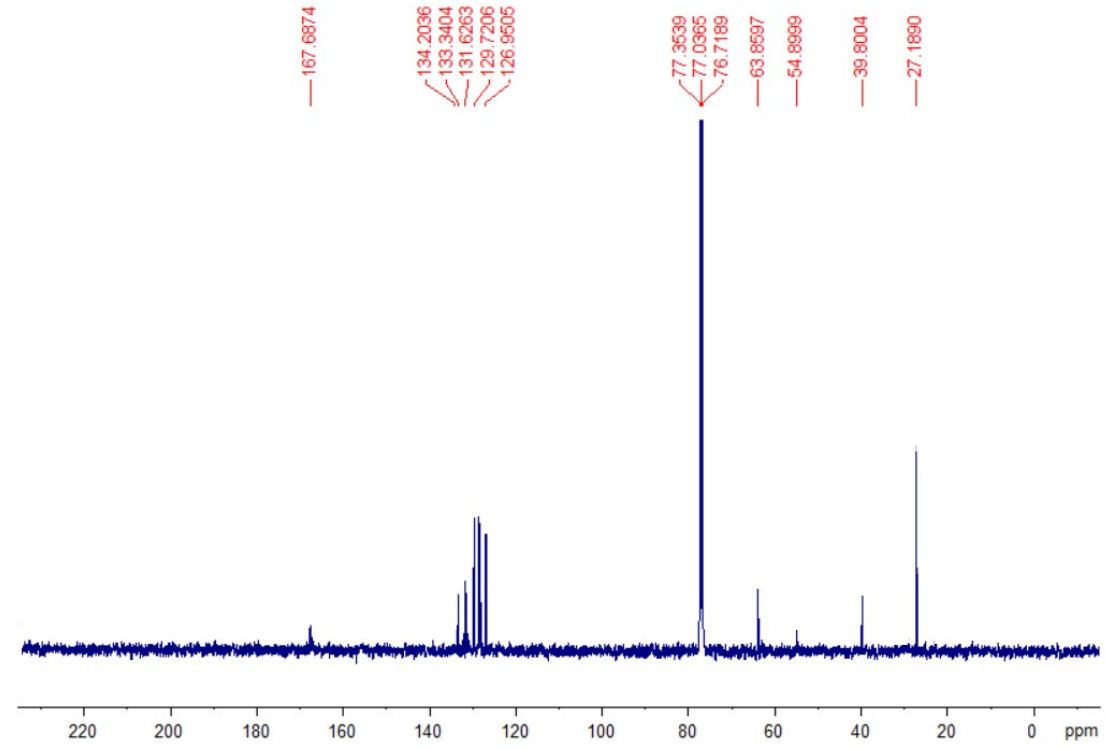
2.12
9.29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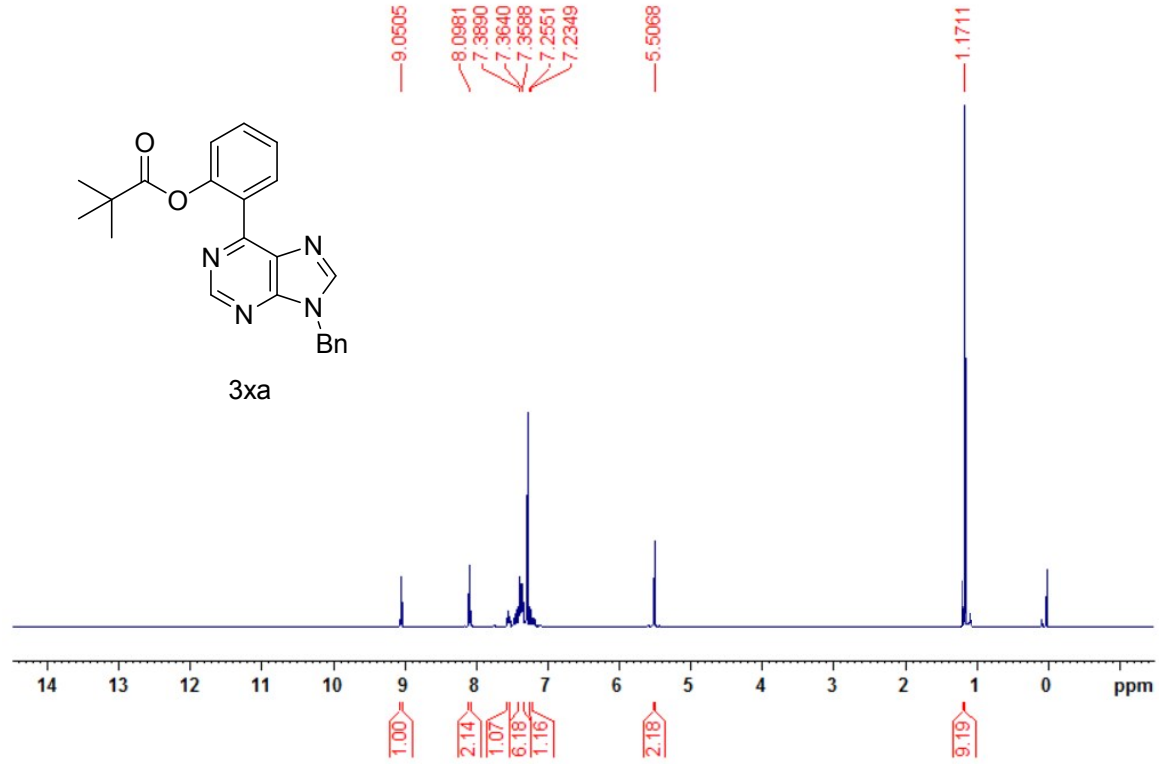
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N
N
N
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6.18
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2.18
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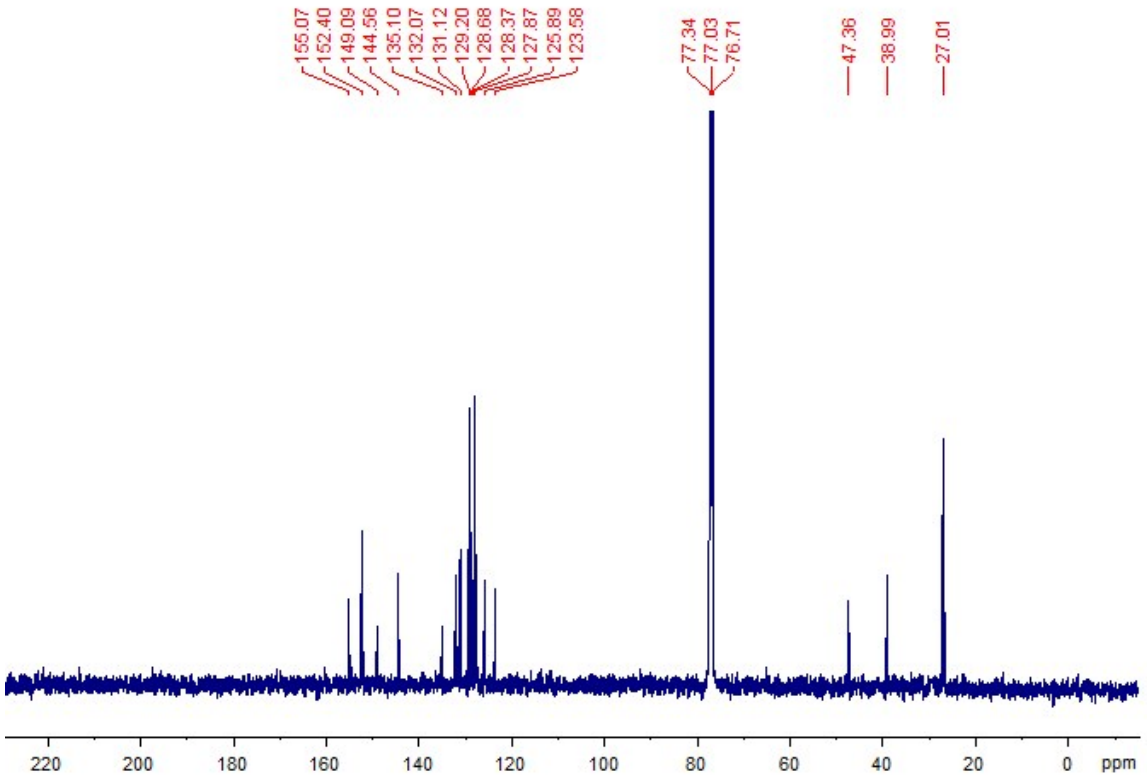
3xa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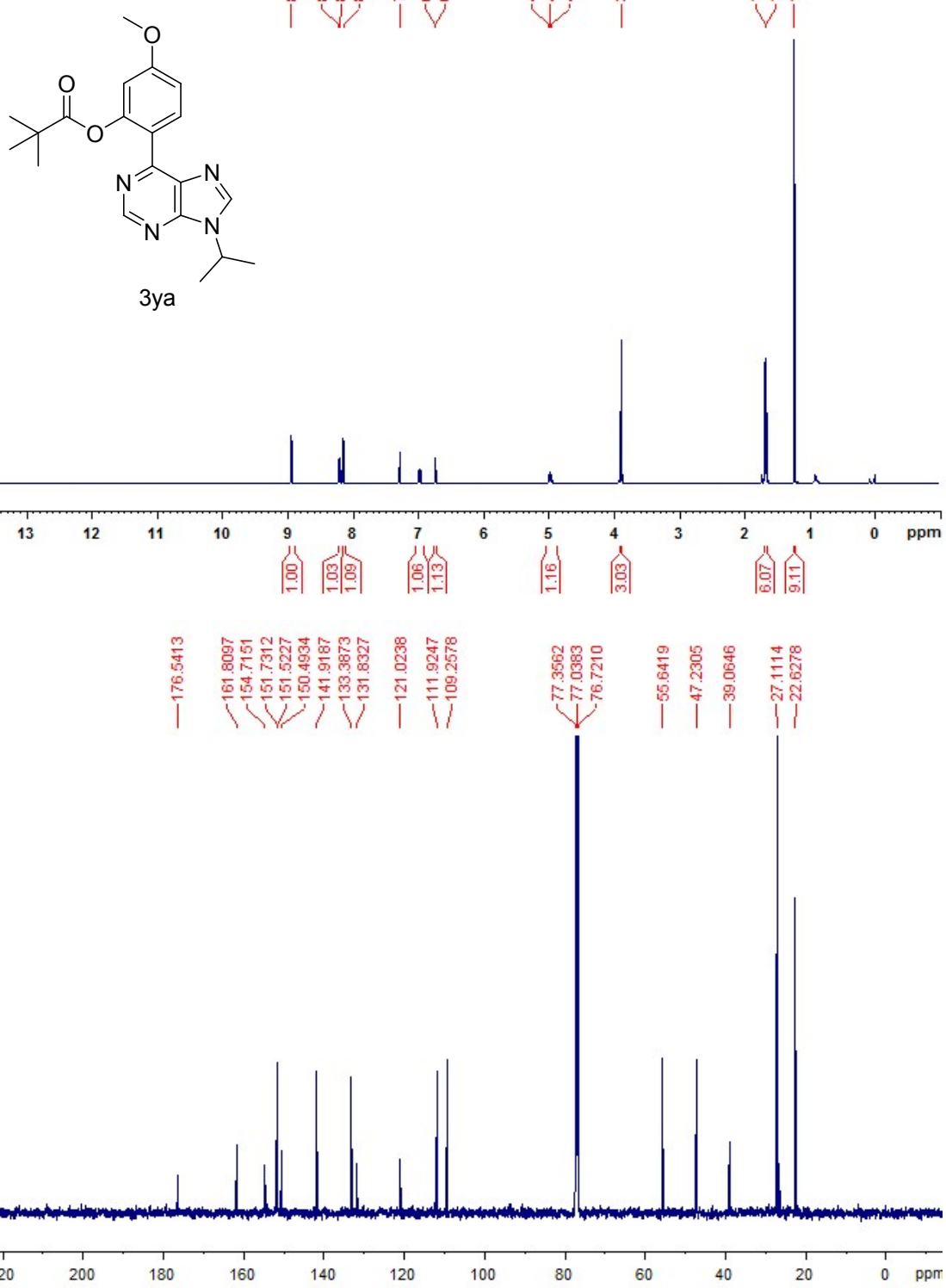
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1.06
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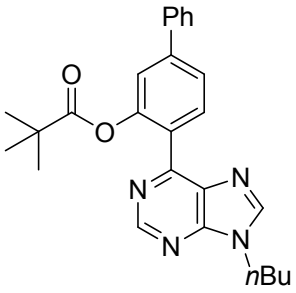
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3za

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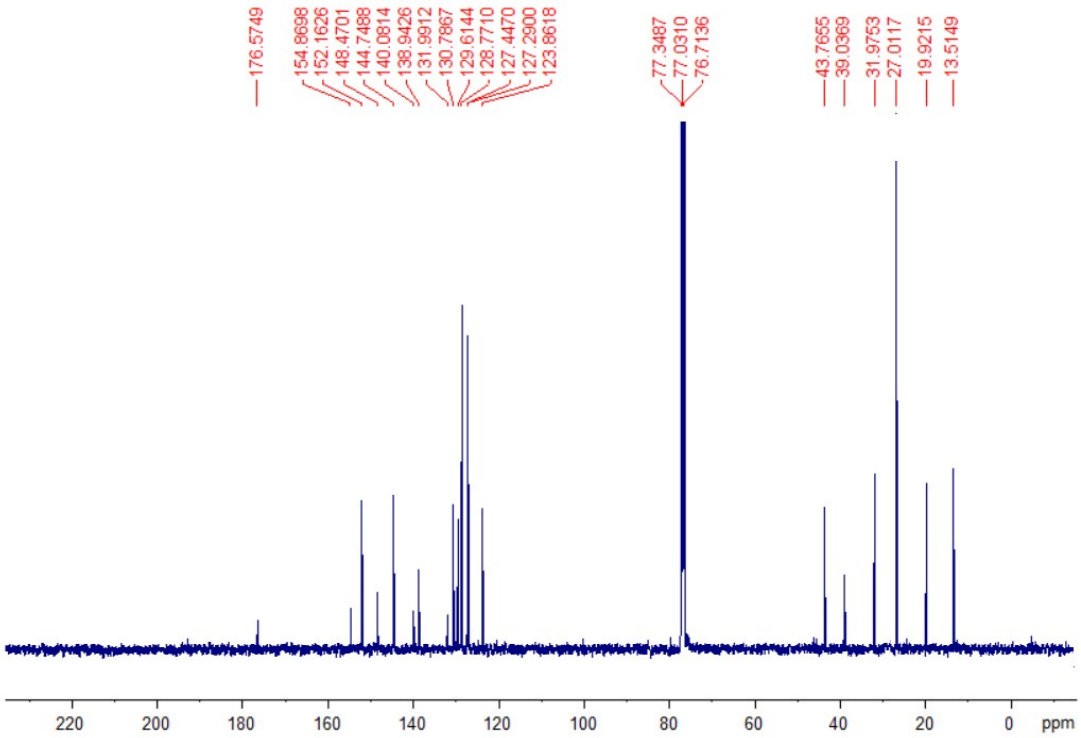
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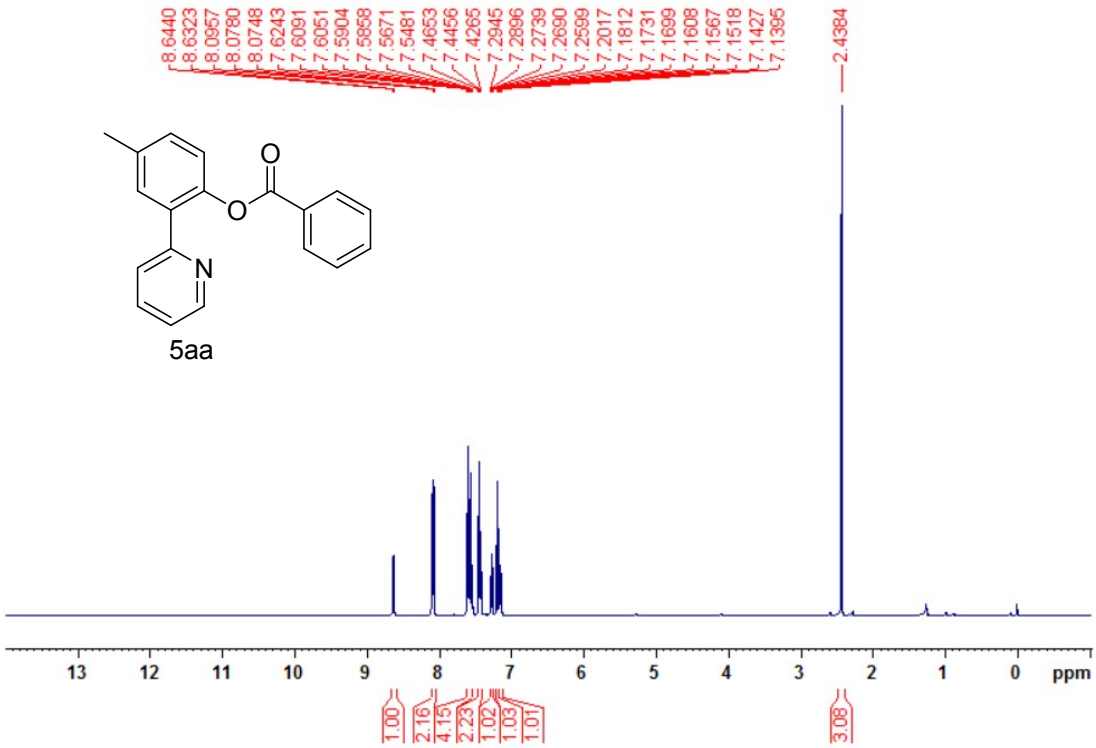
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4.15
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1.03
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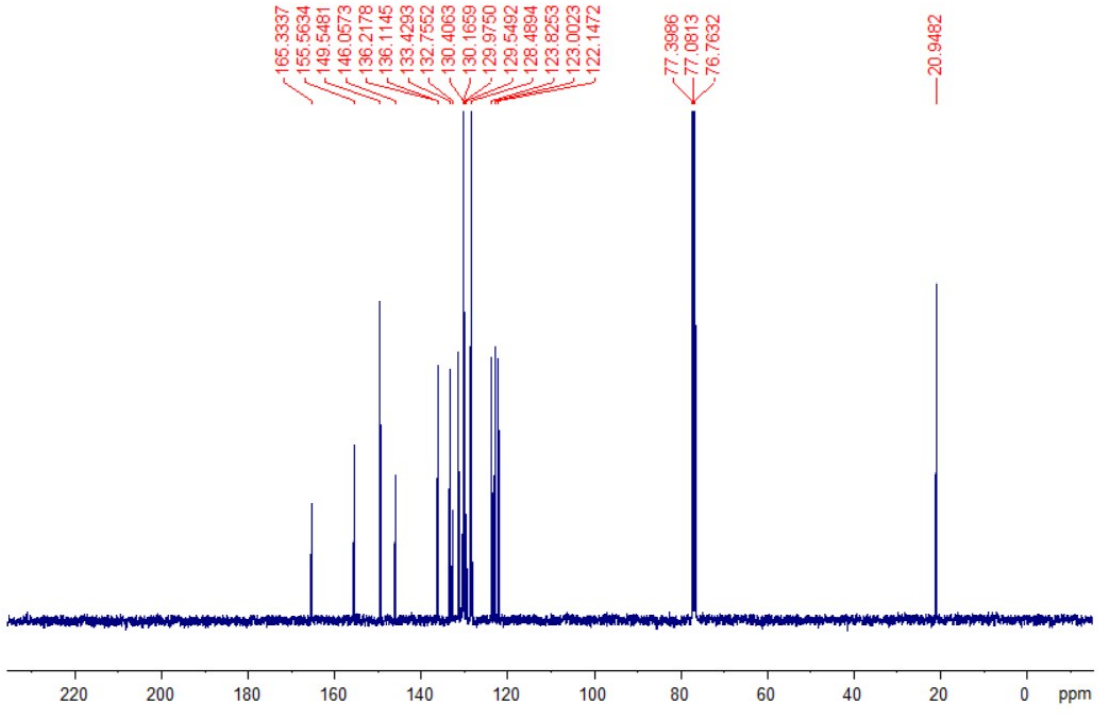
3.08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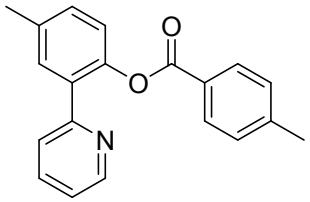
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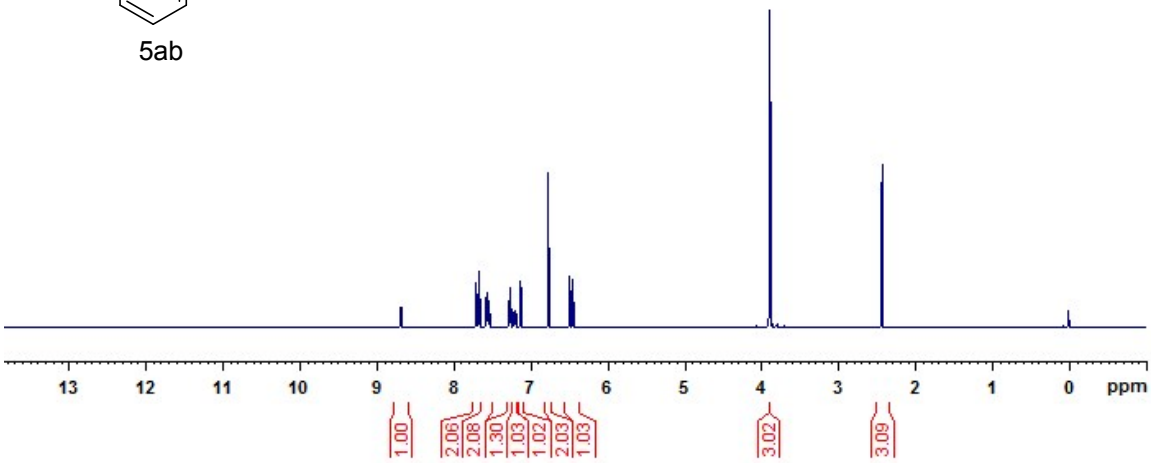
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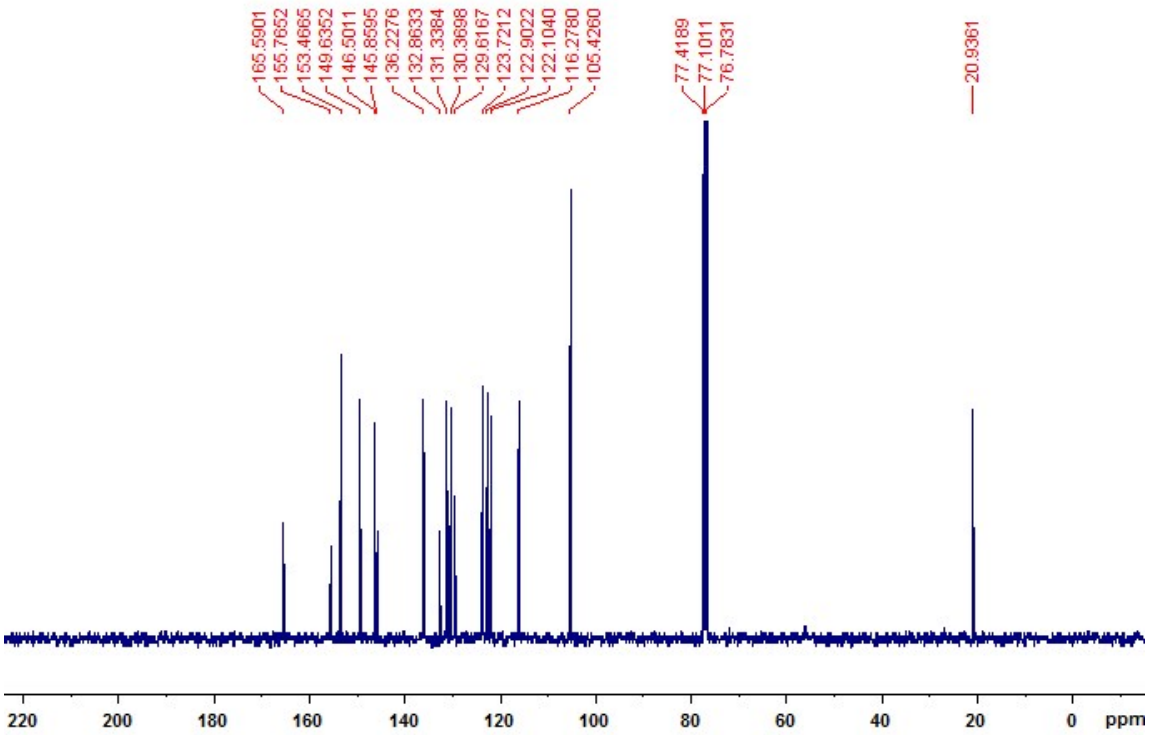
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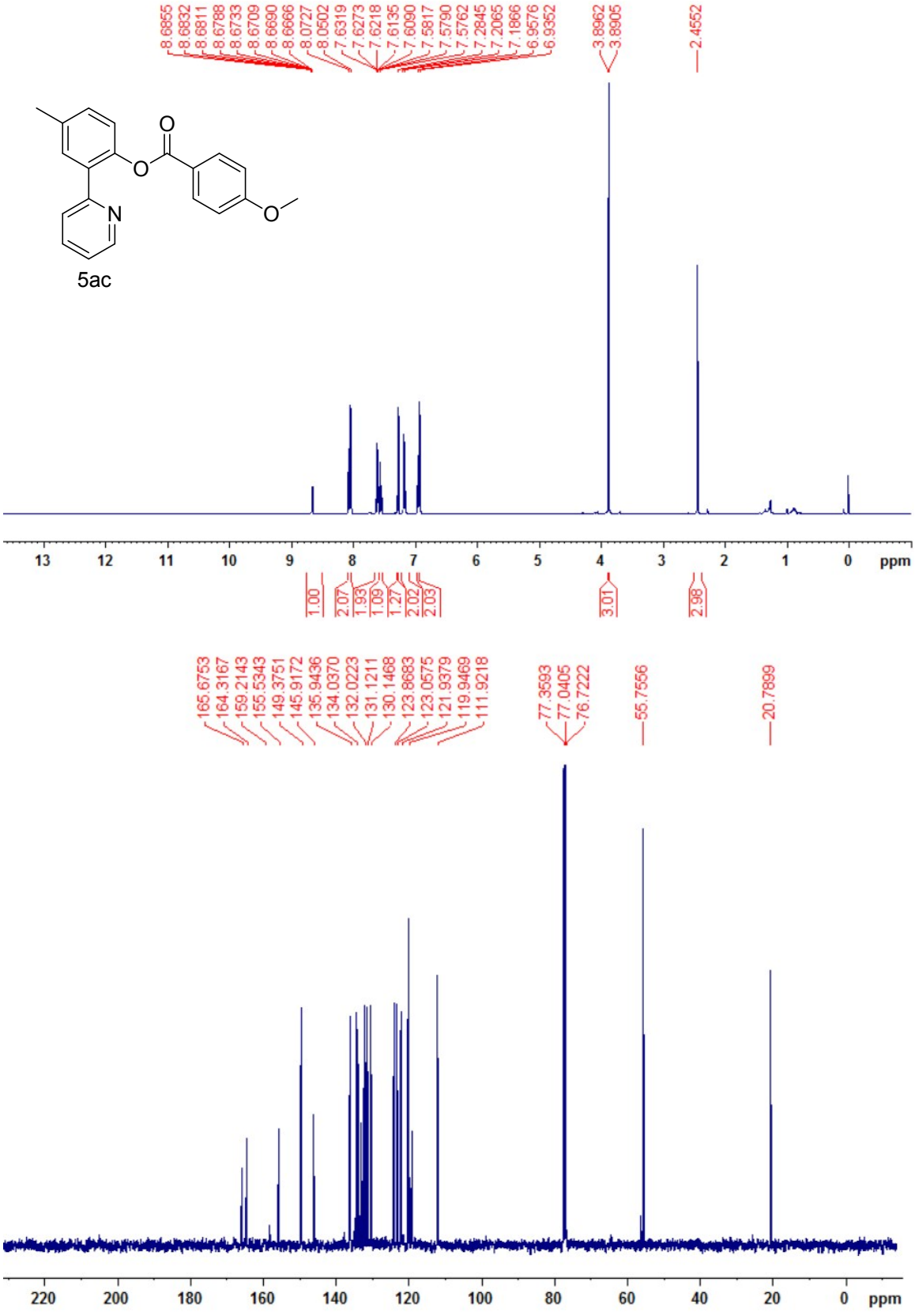
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7.1866
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2.4552
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O
N
O
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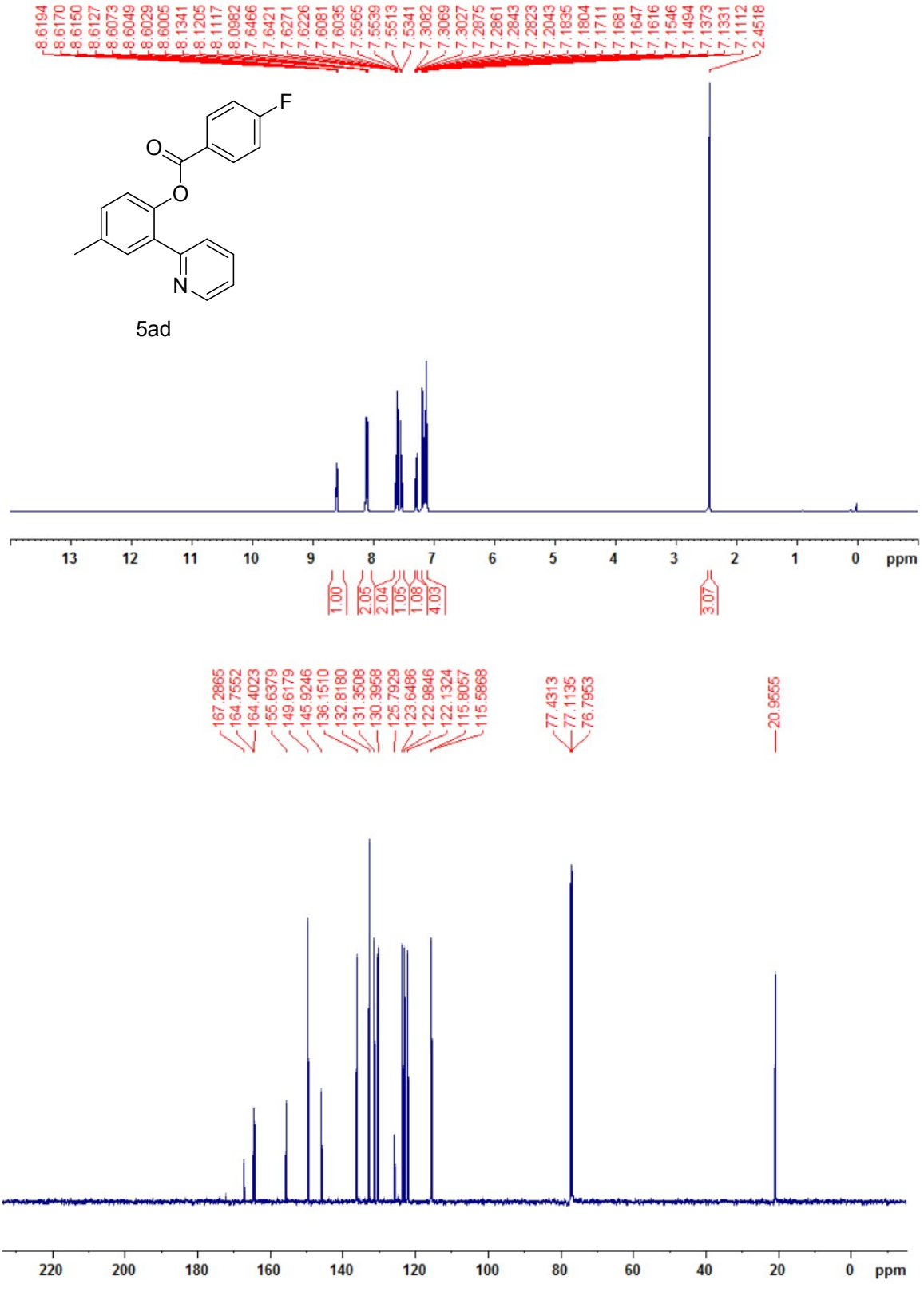
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7.3027
7.2875
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7.2823
7.2043
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7.1804
7.1711
7.1681
7.1647
7.1616
7.1546
7.1494
7.1373
7.1331
7.1112
2.4518
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O
O
N
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2.04
1.05
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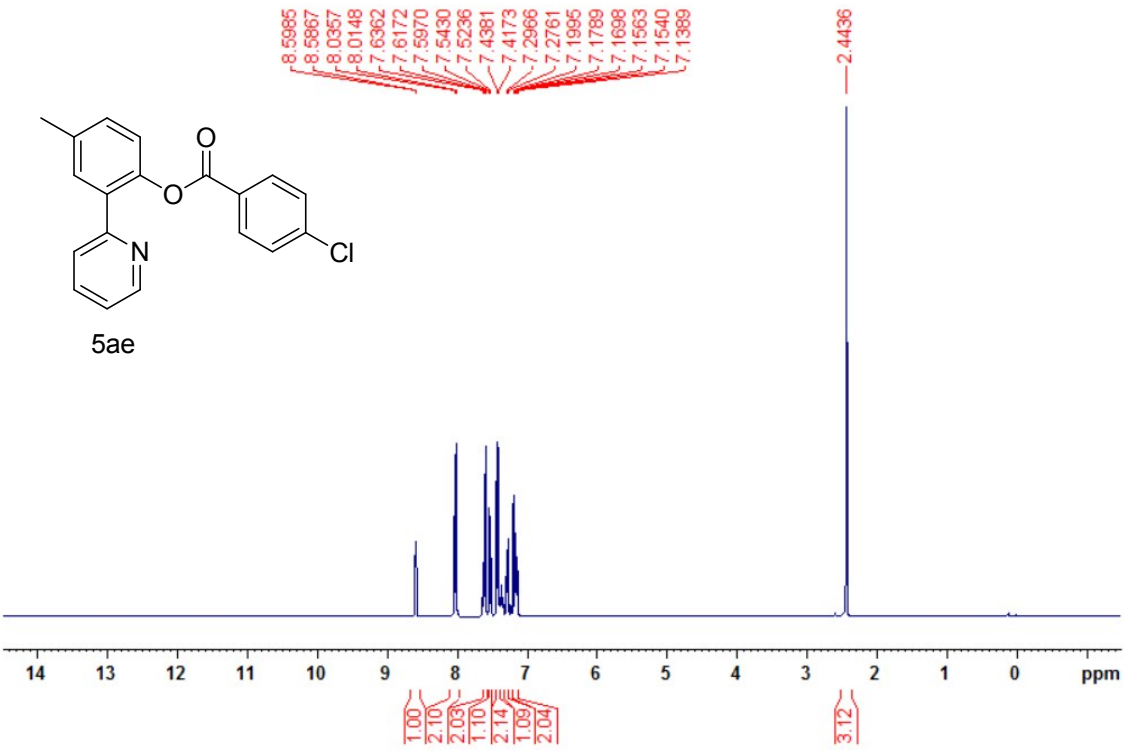
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O
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Cl
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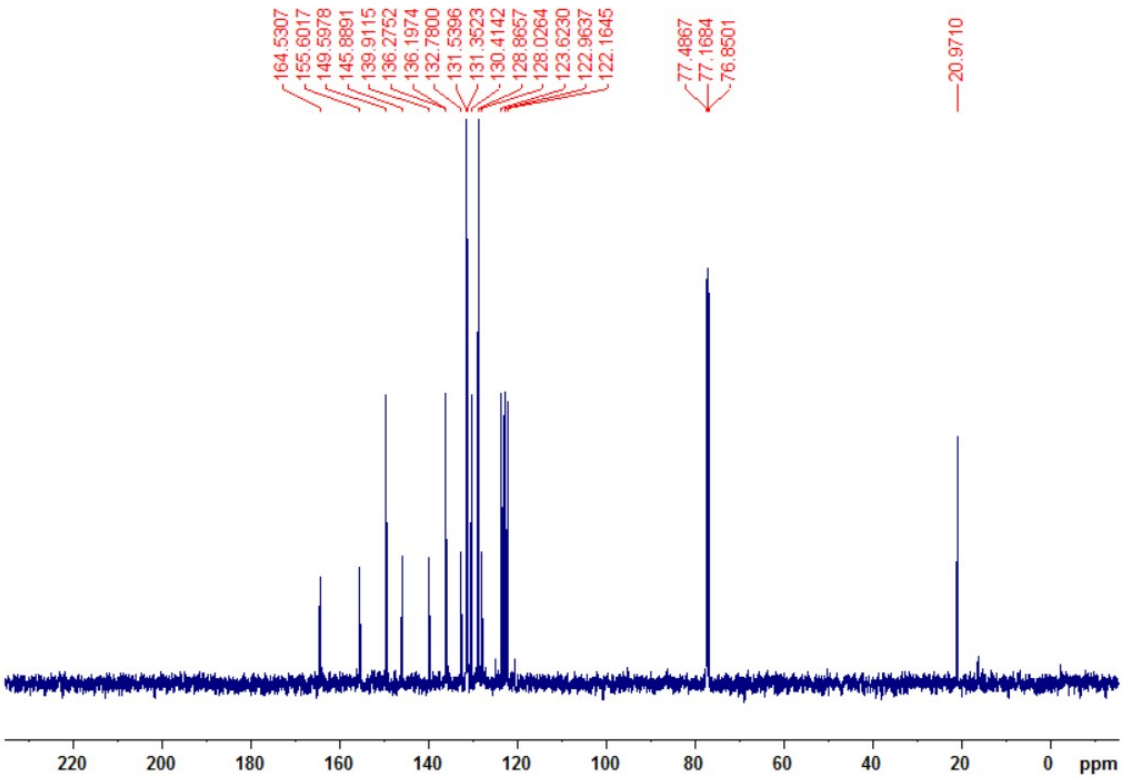
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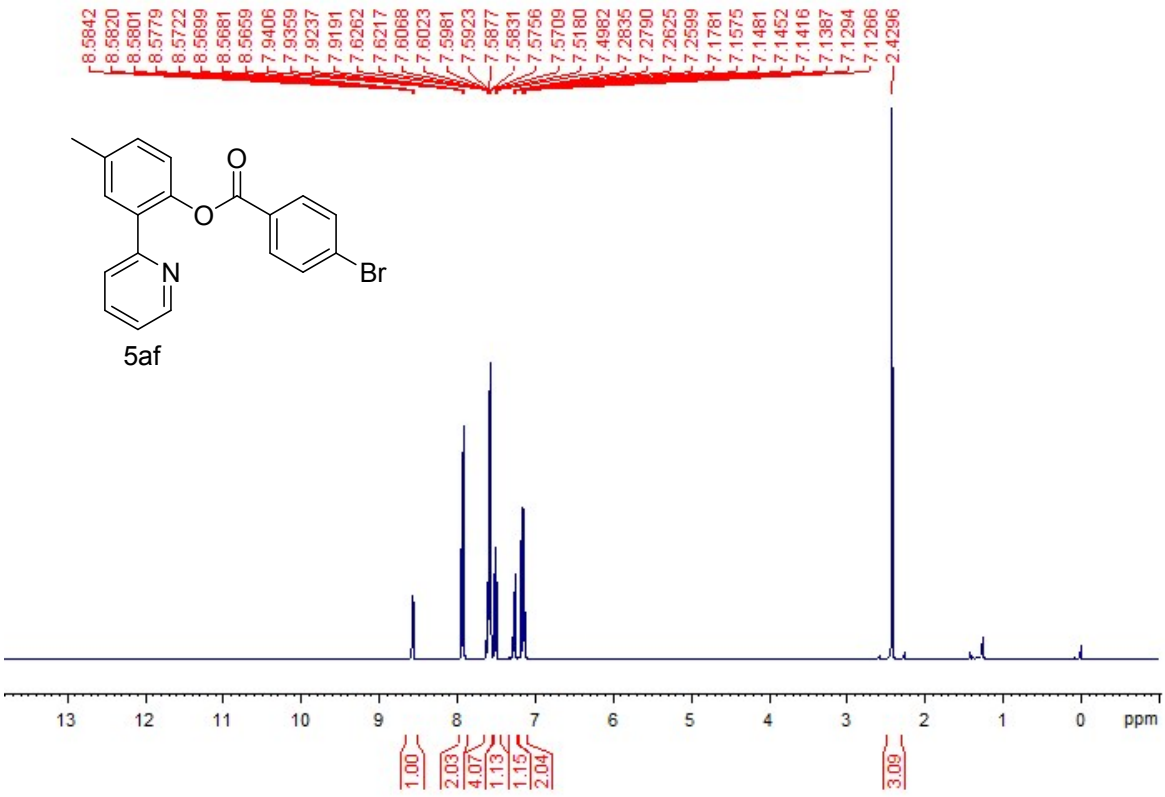
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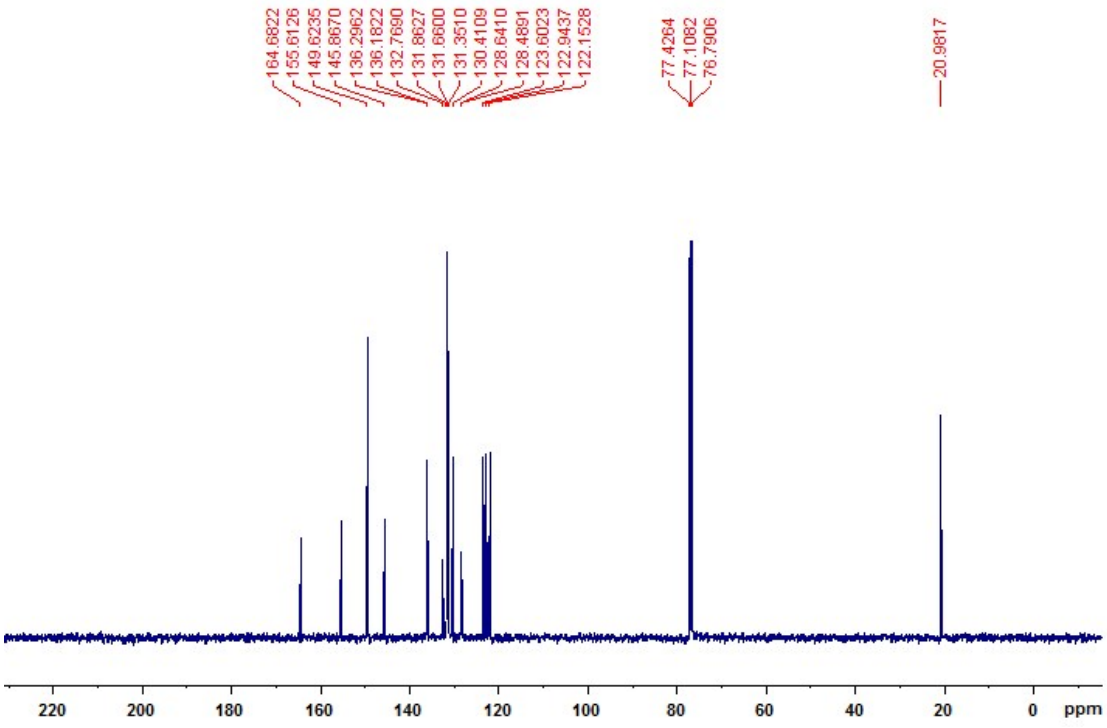
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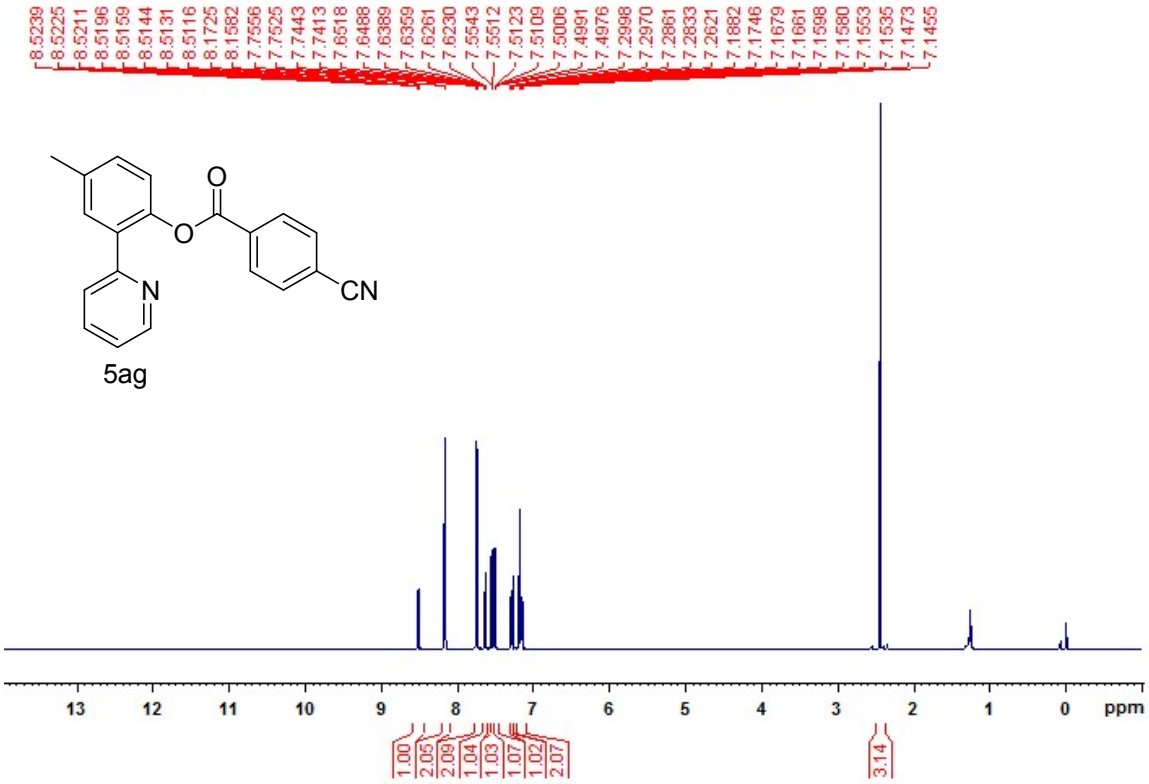
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O
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CN
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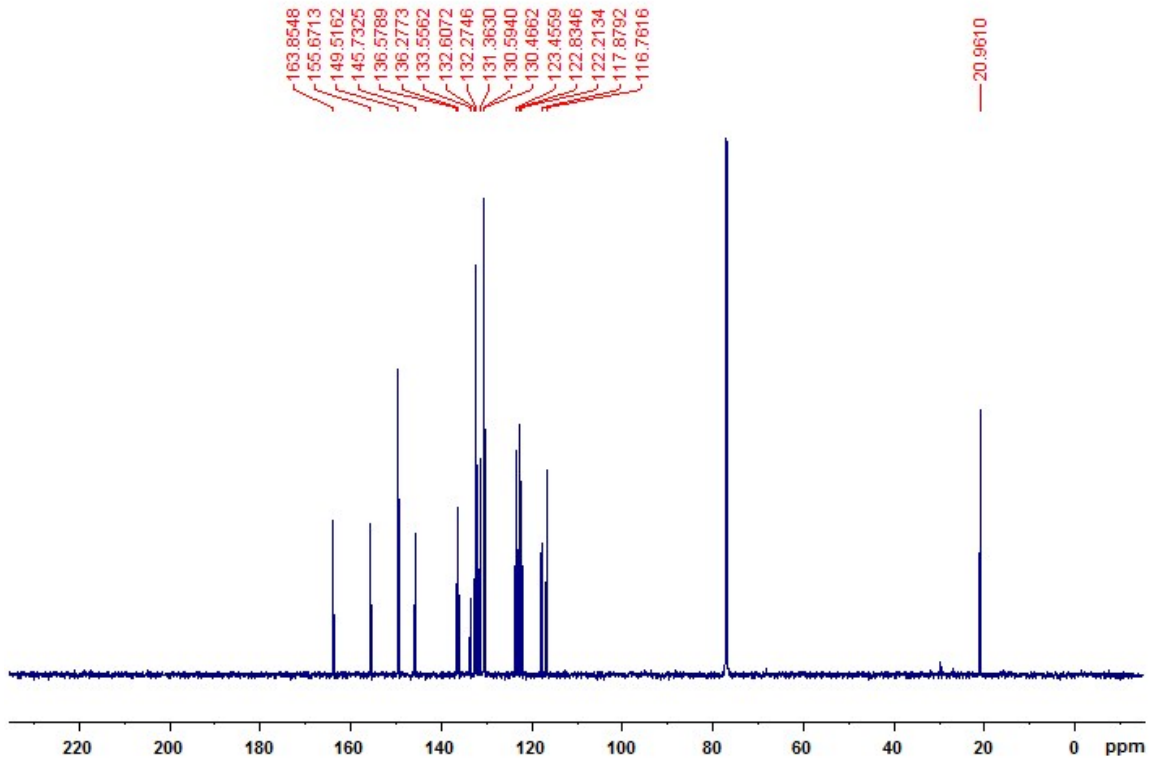
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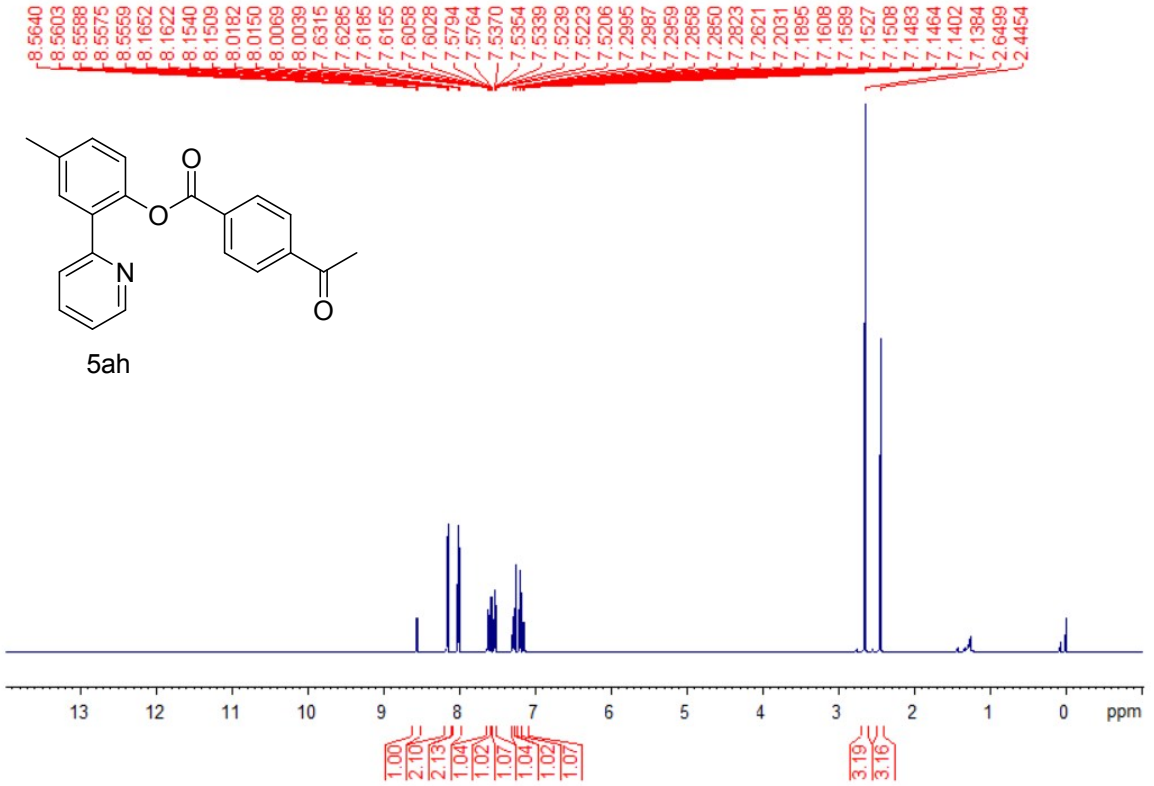
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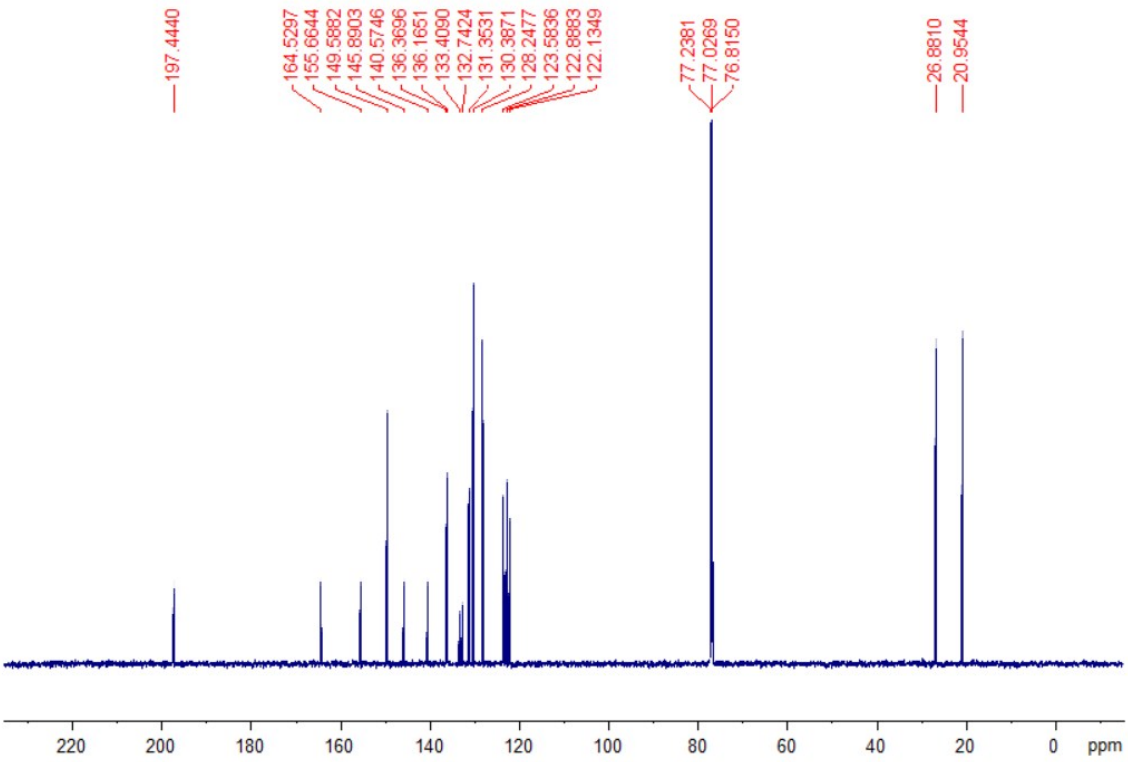
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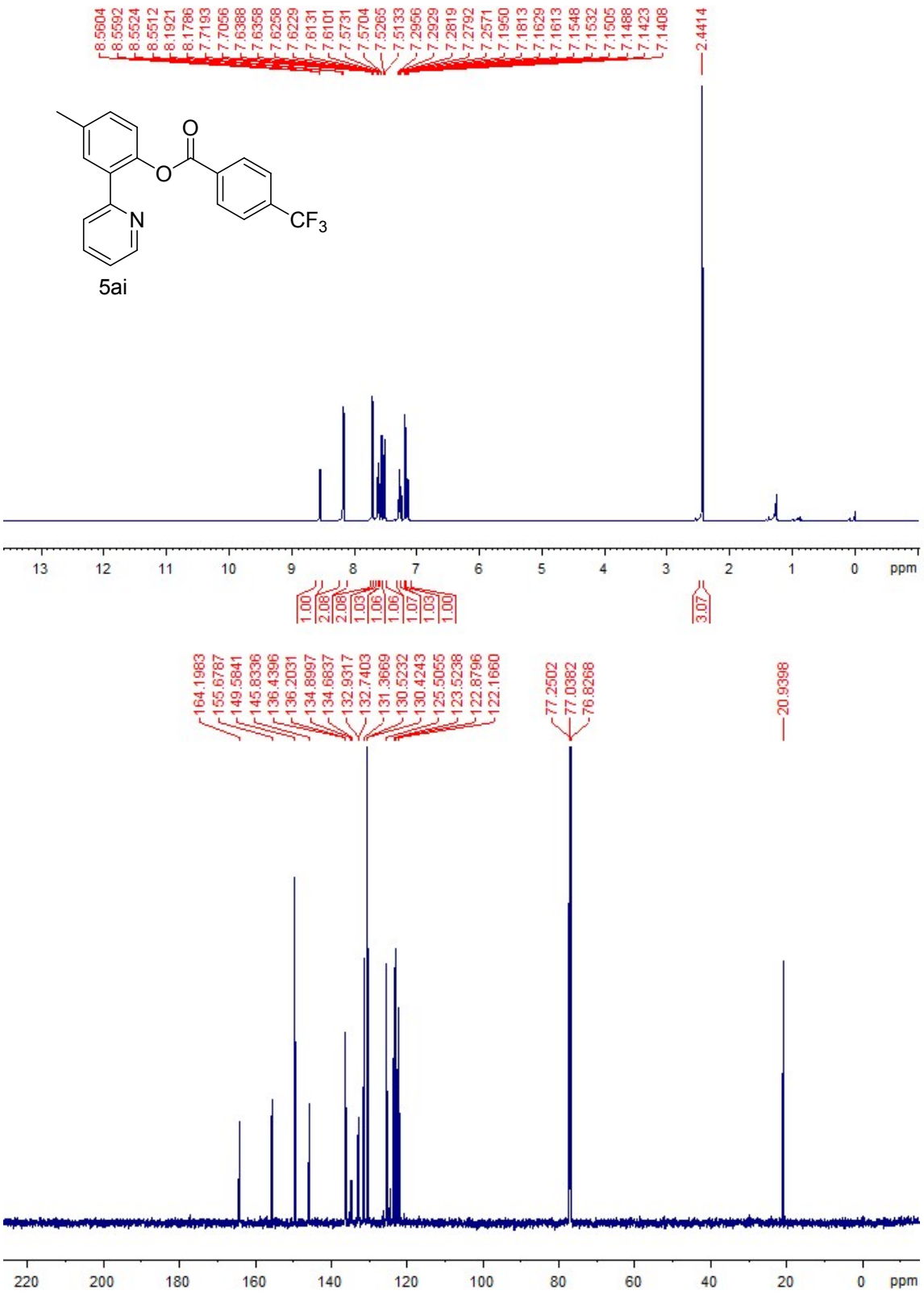
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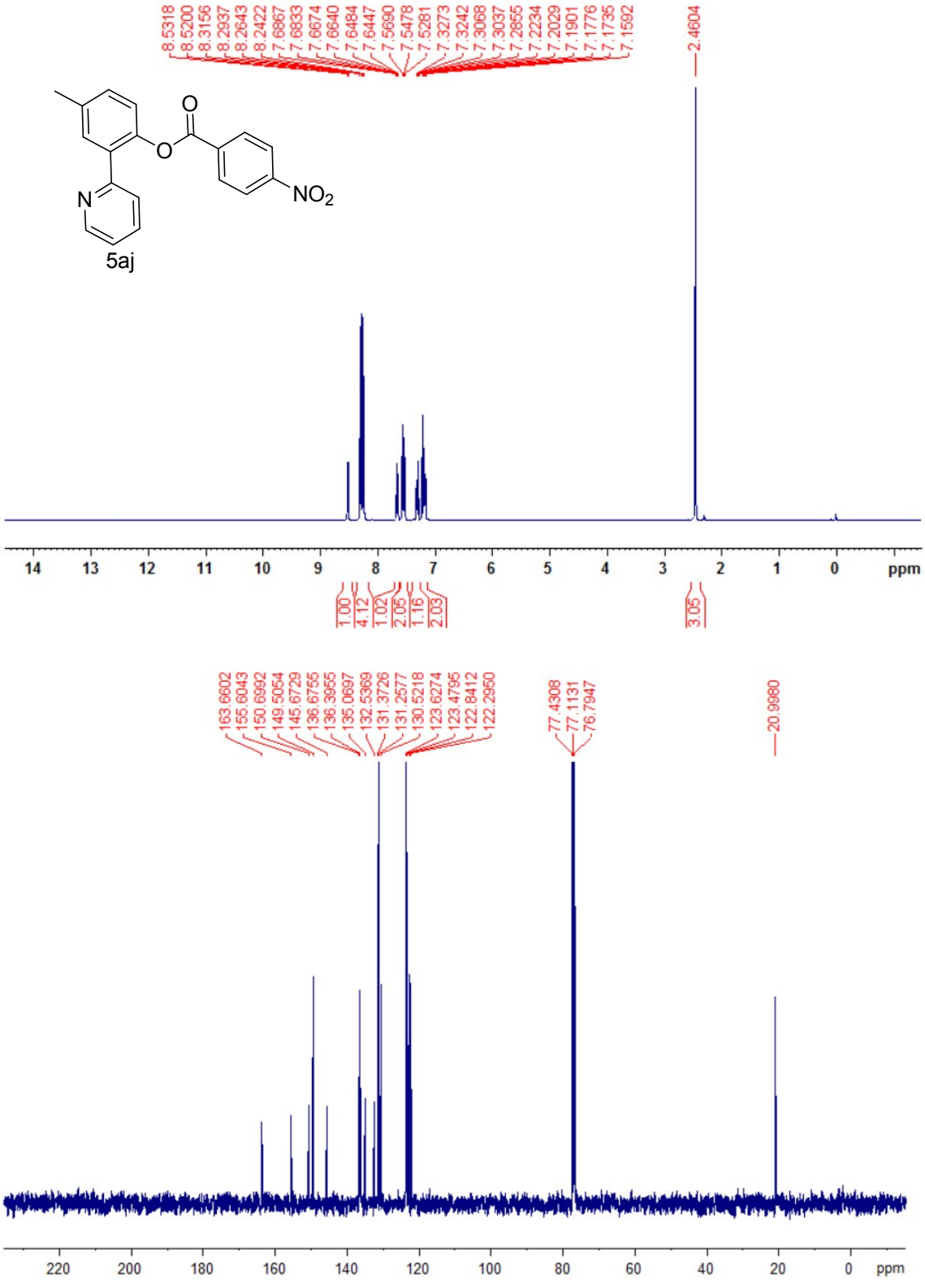
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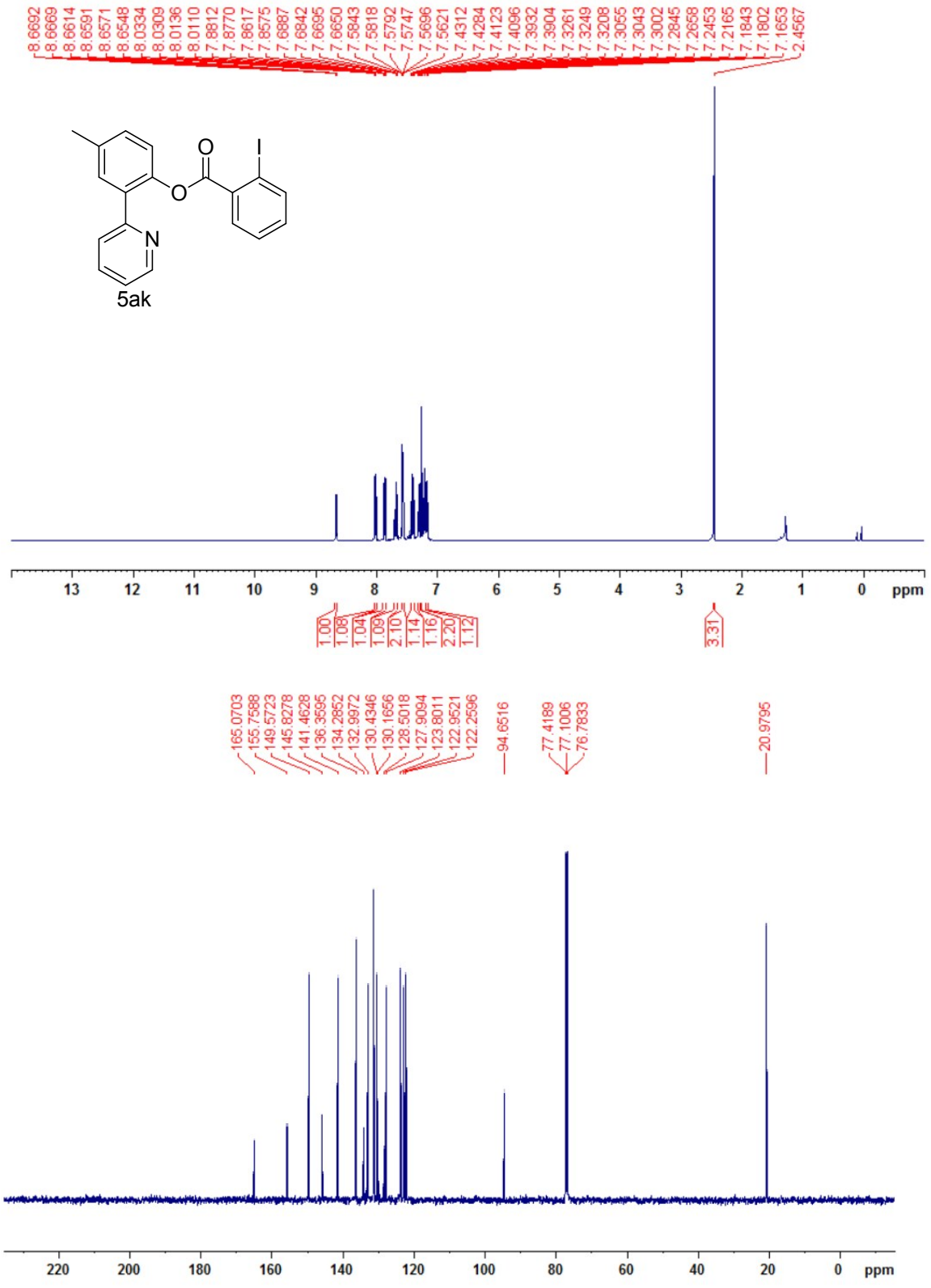
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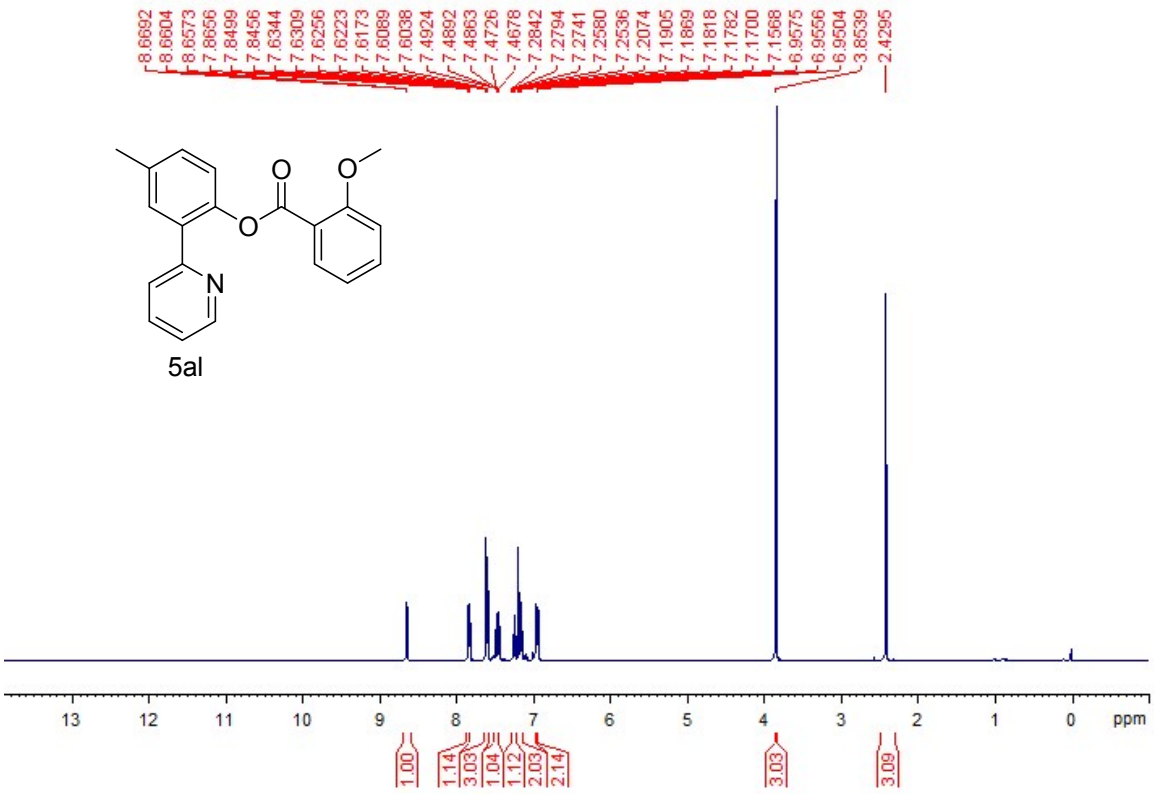
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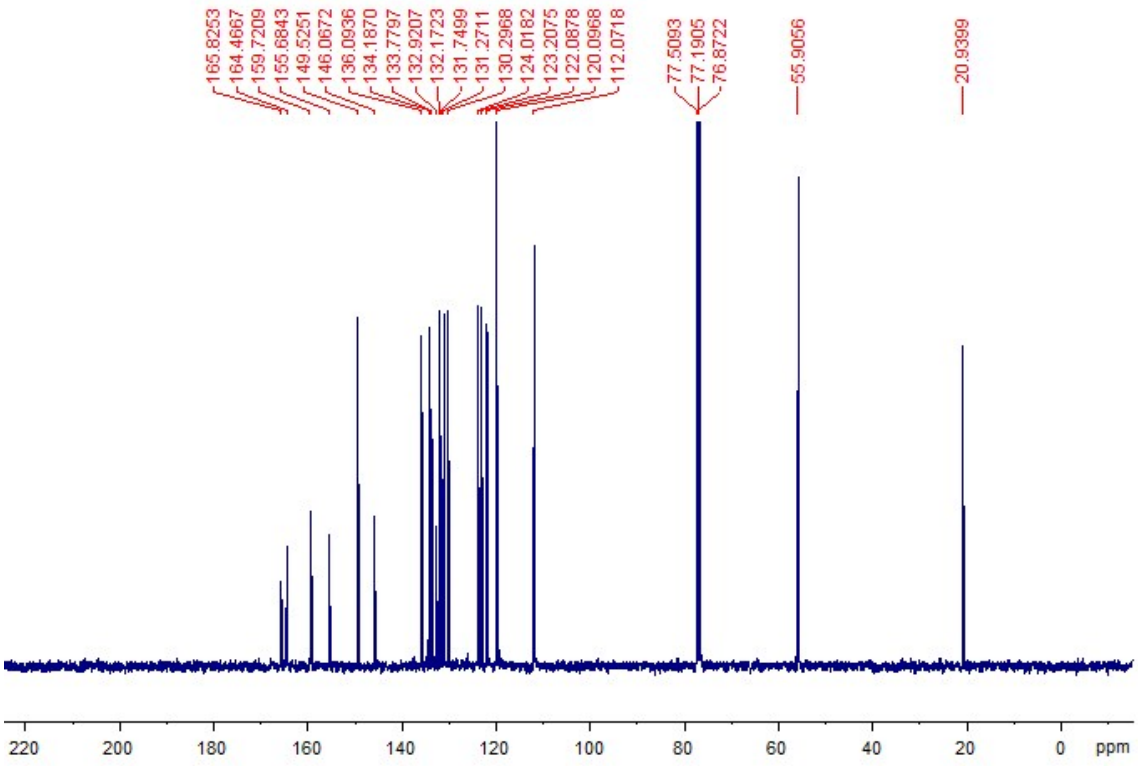
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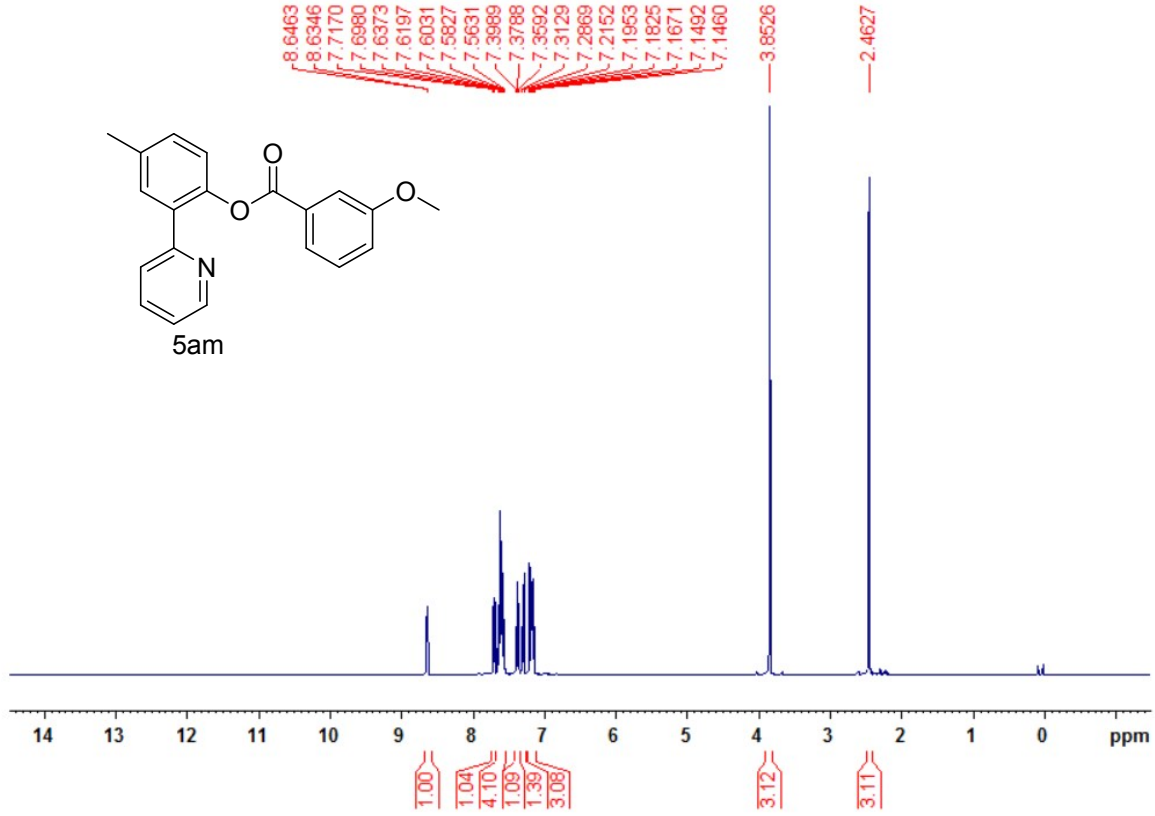
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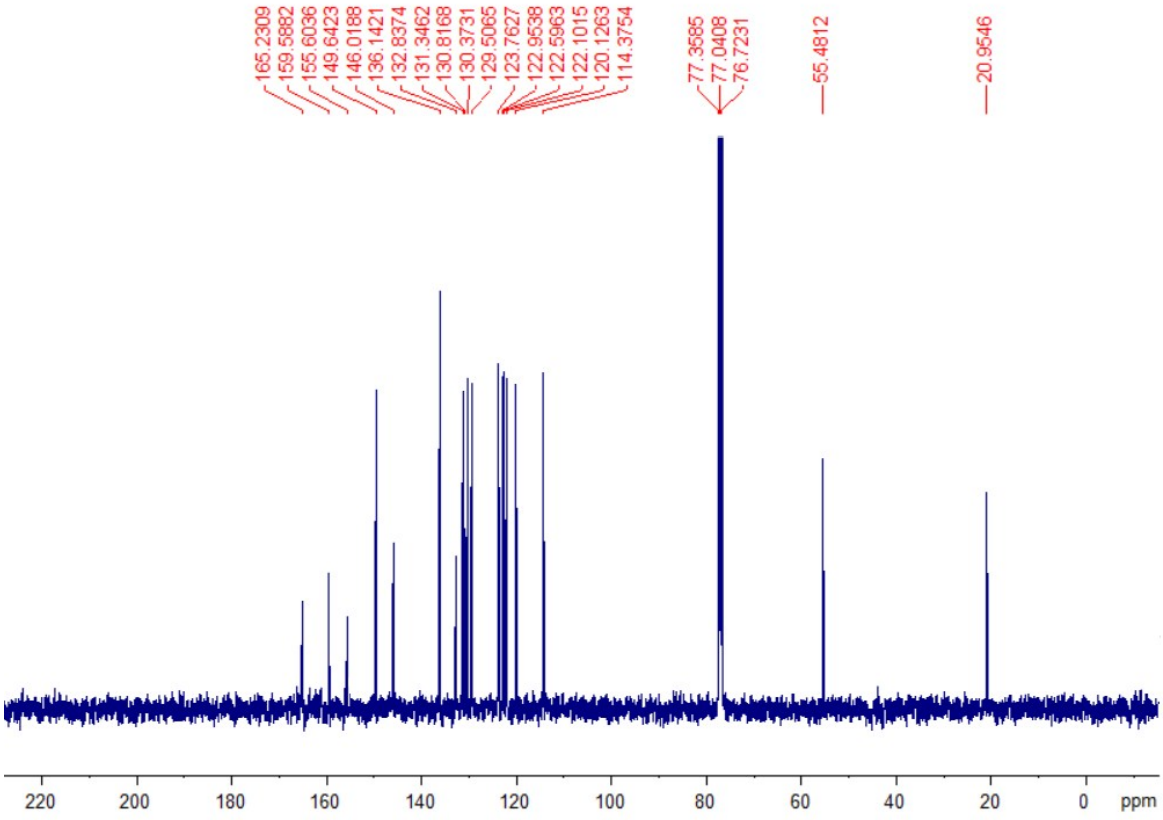
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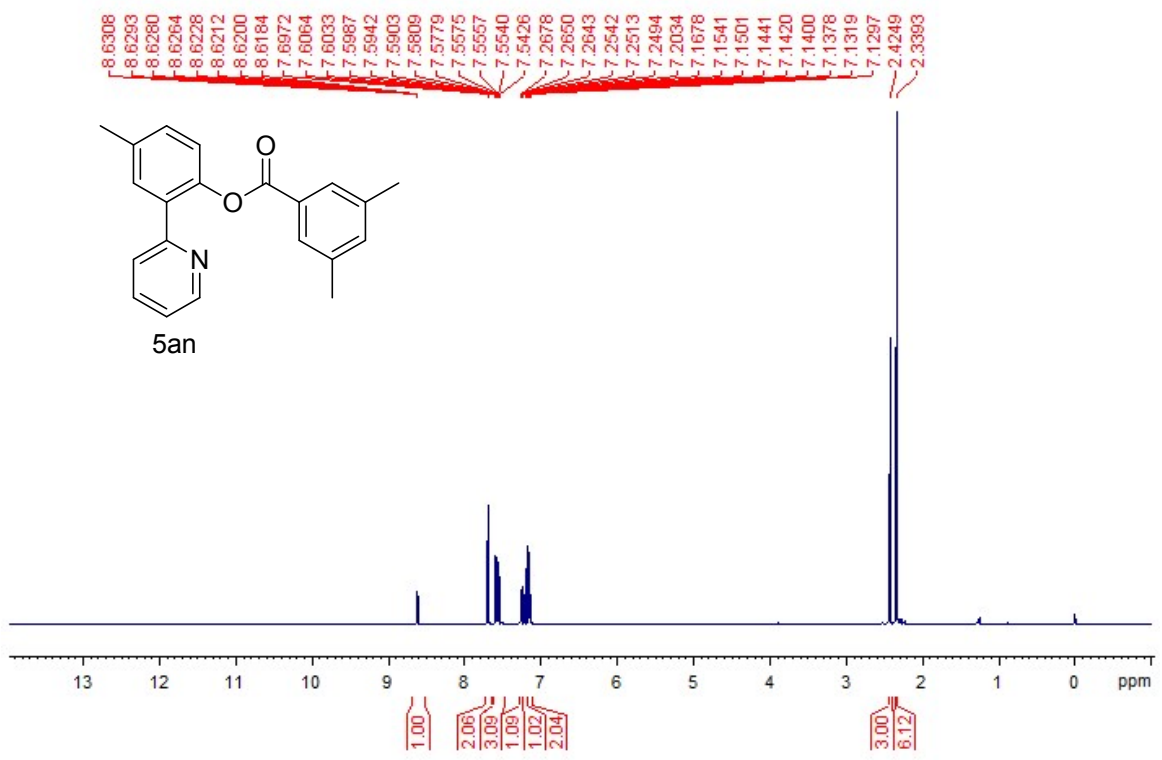
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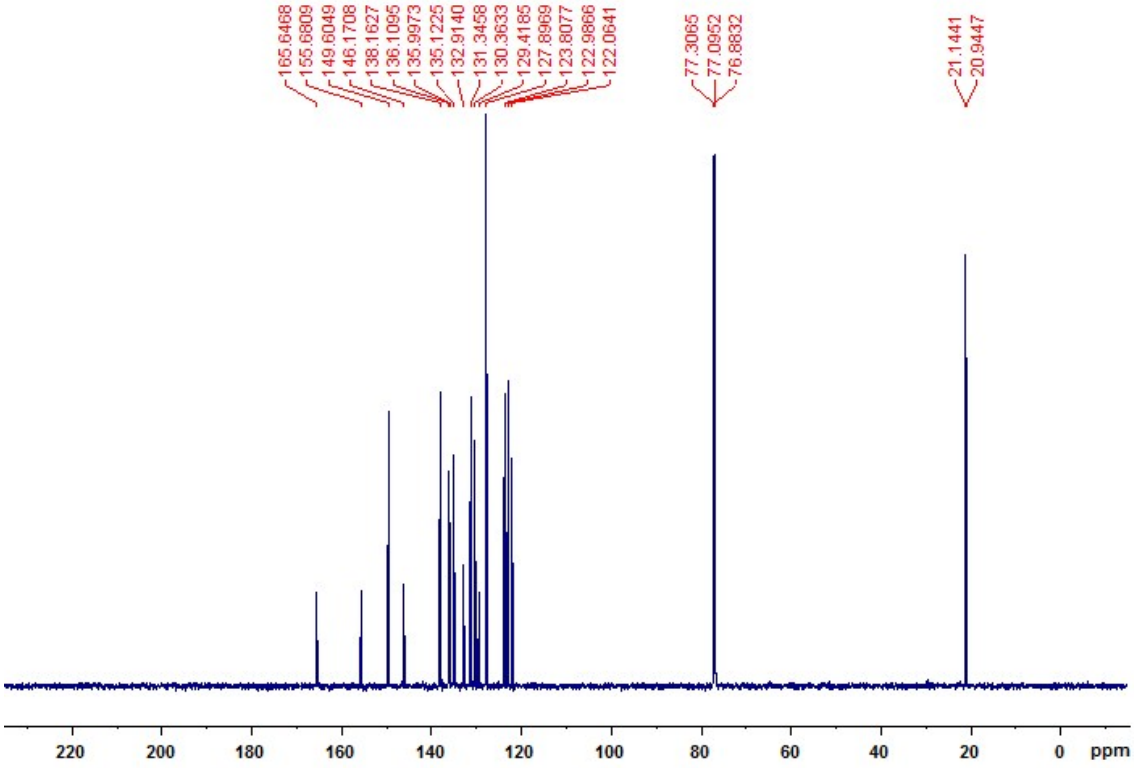
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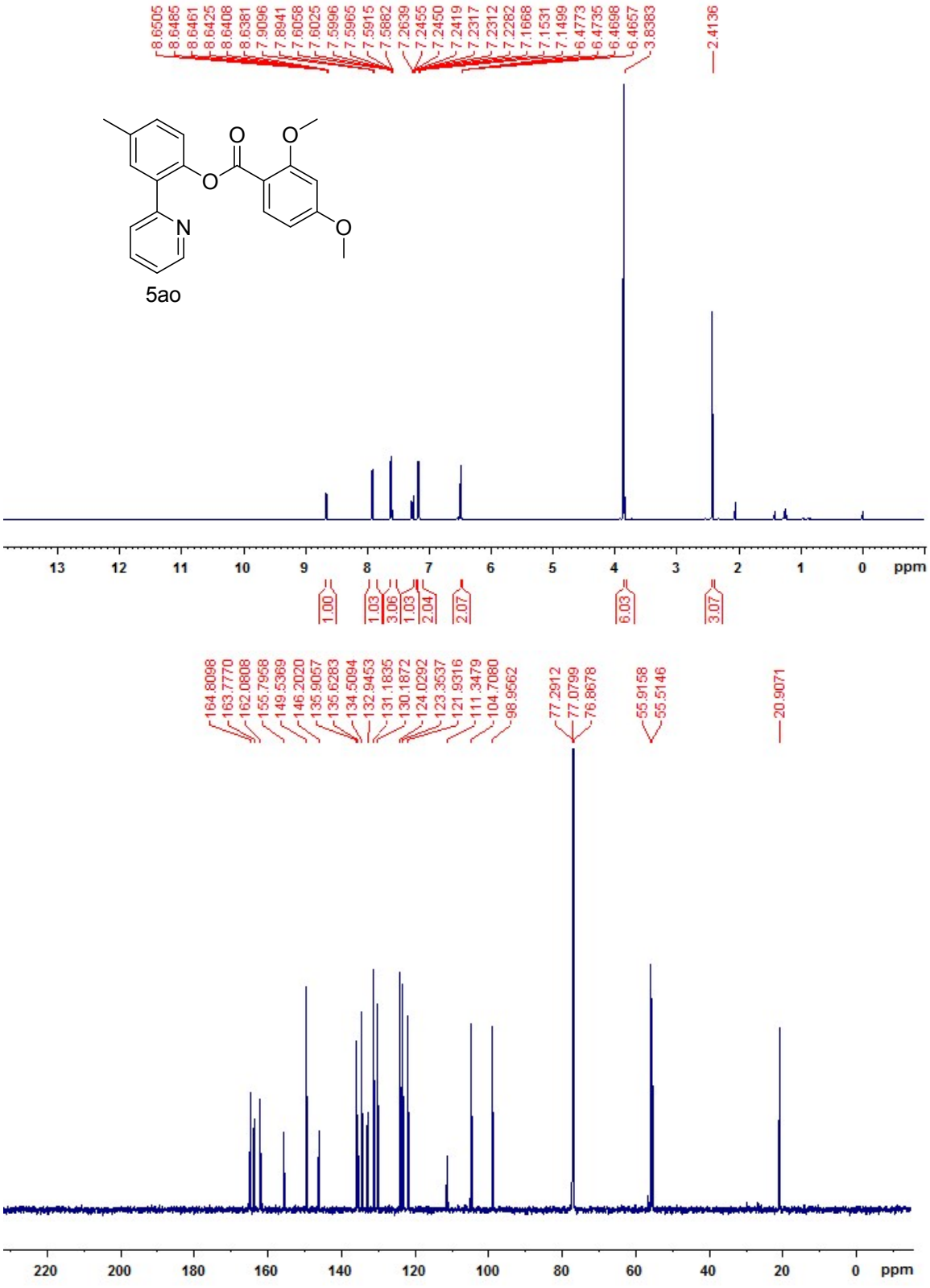
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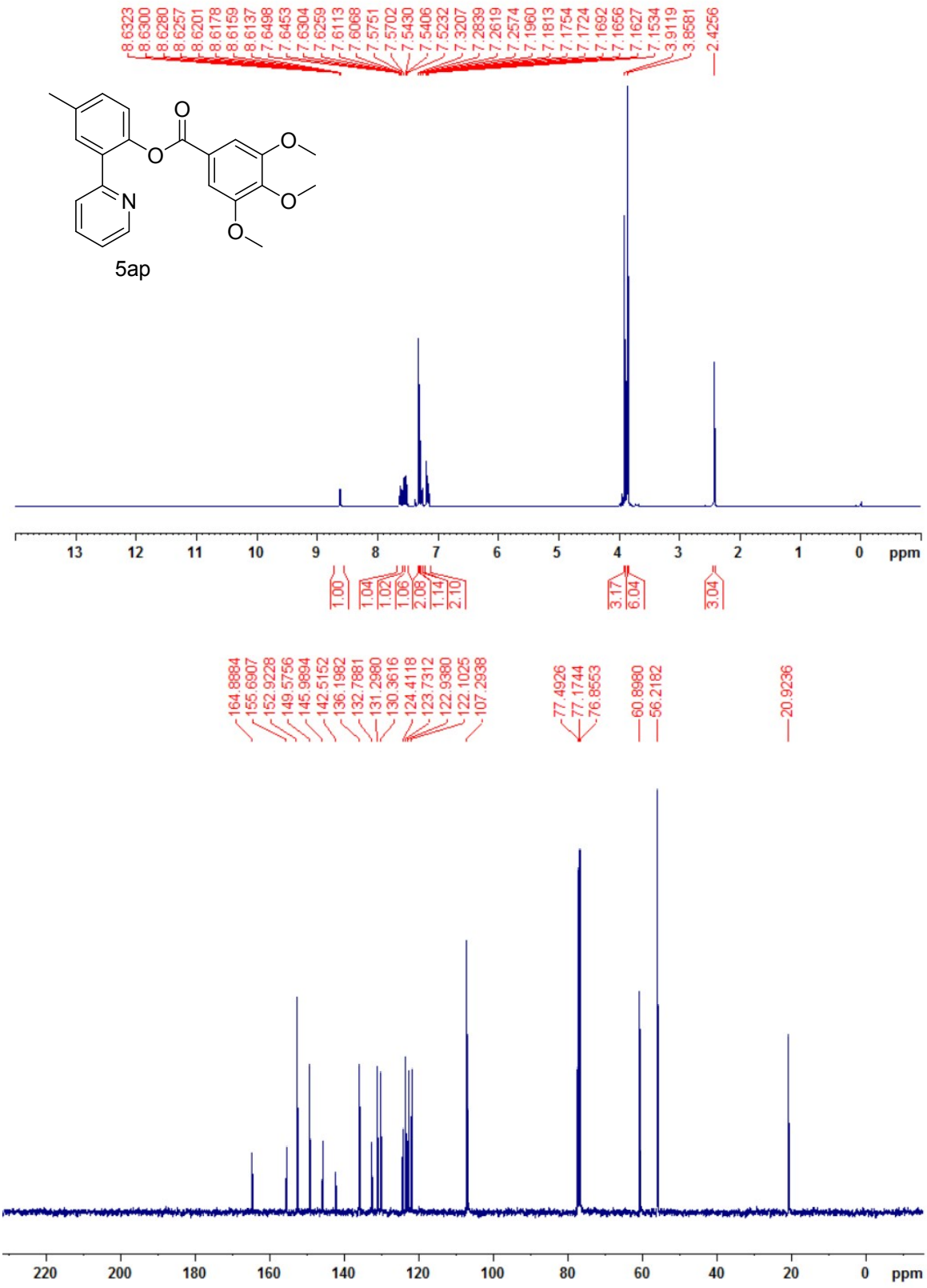
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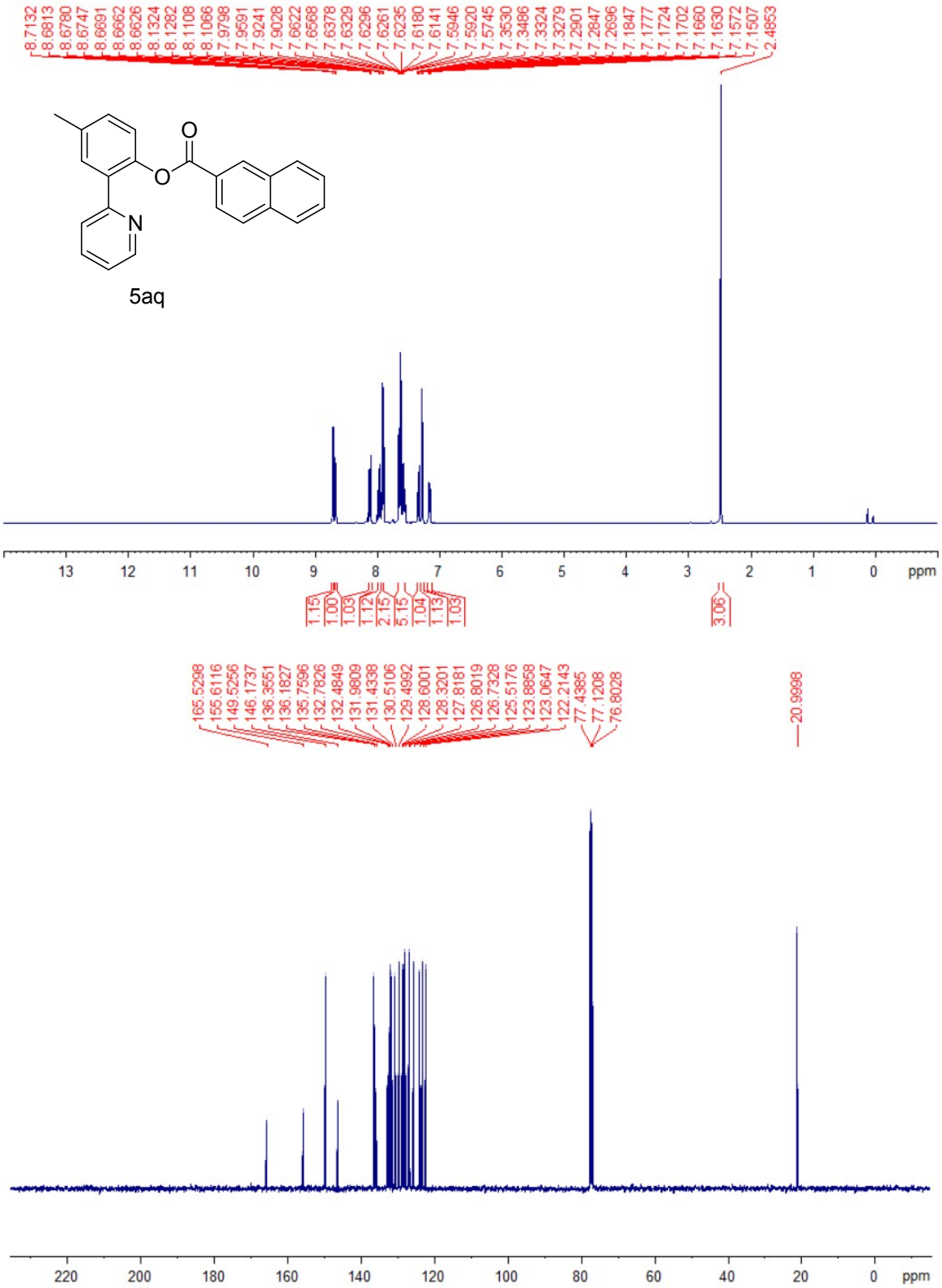
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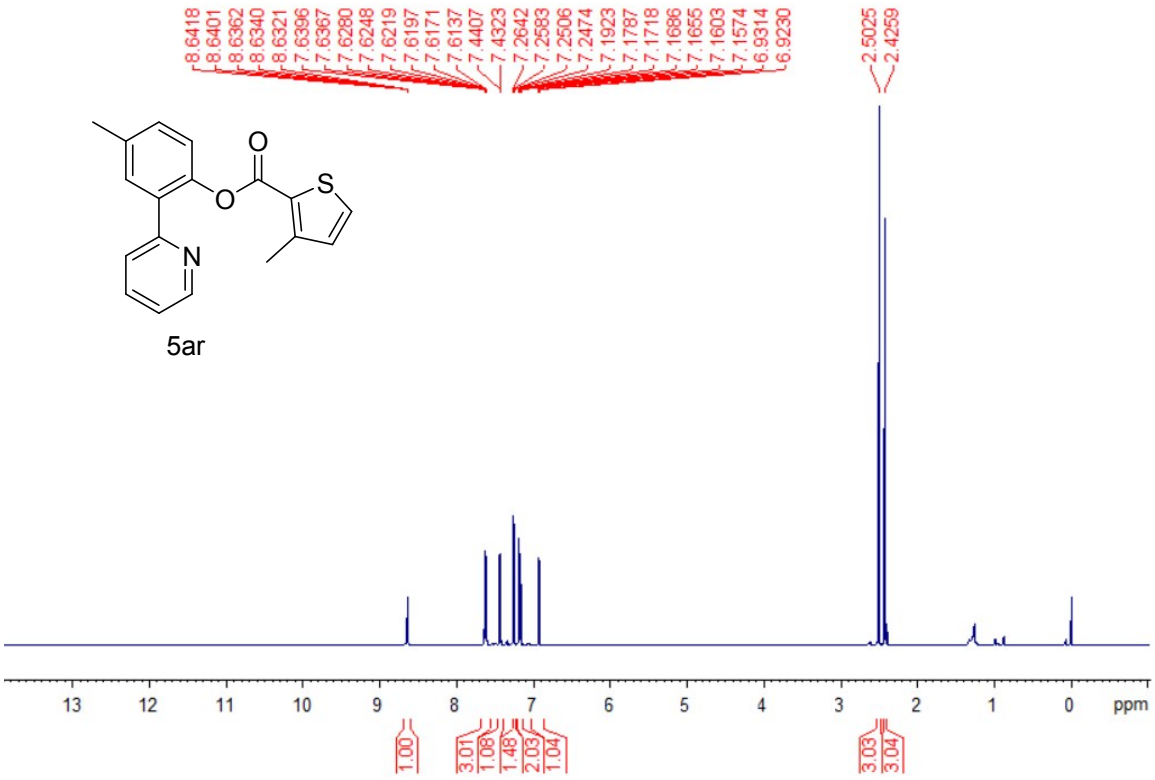
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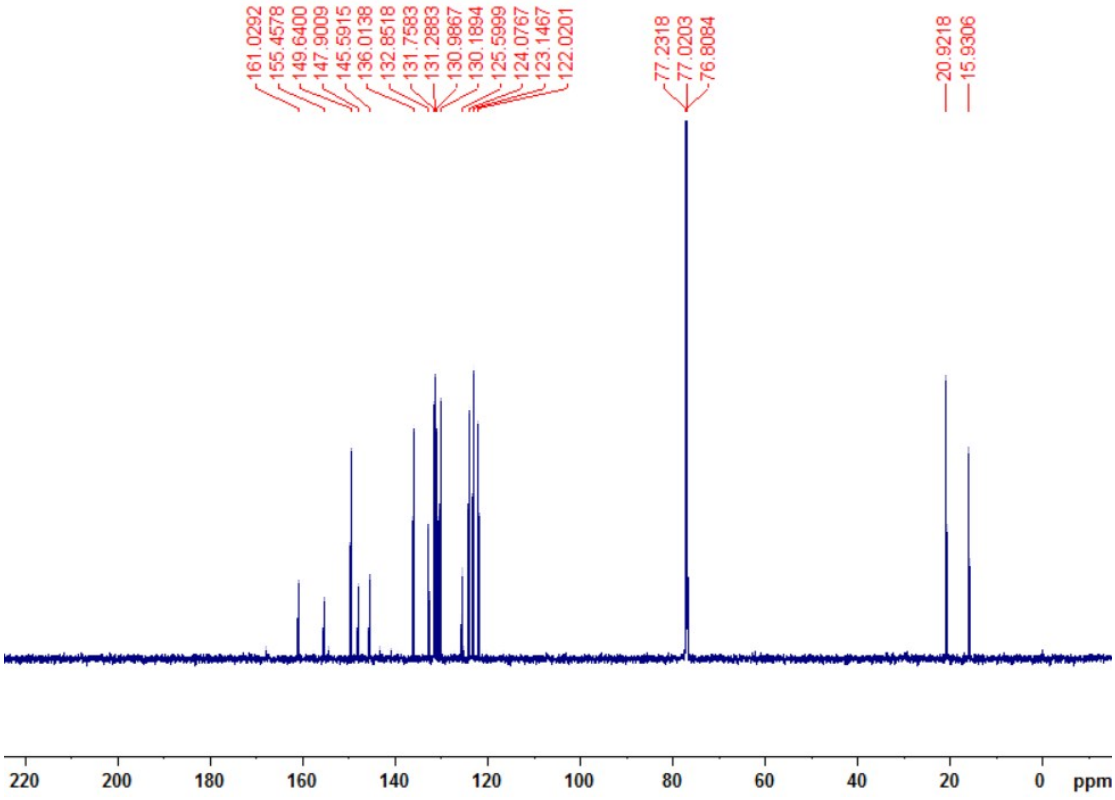
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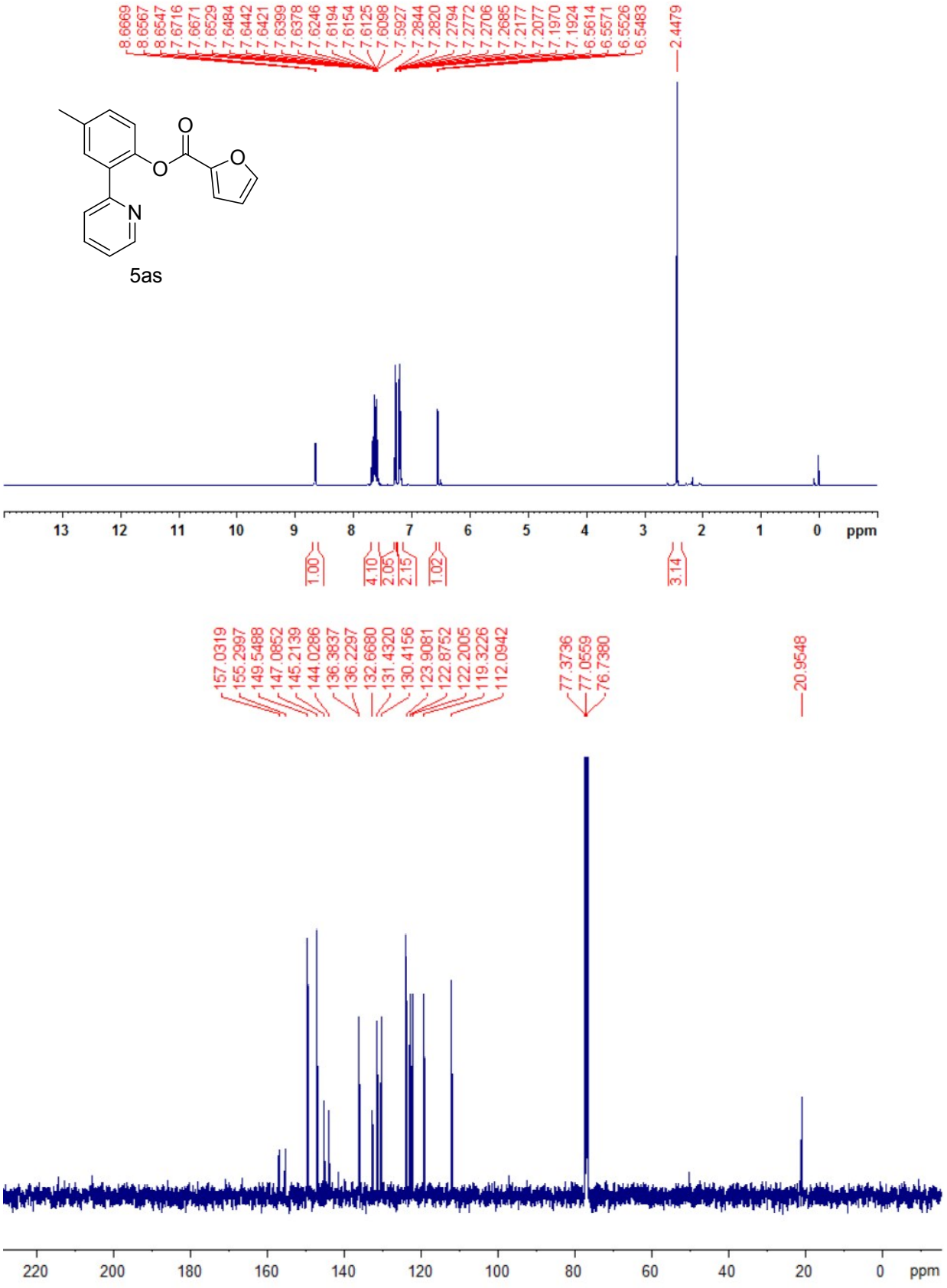
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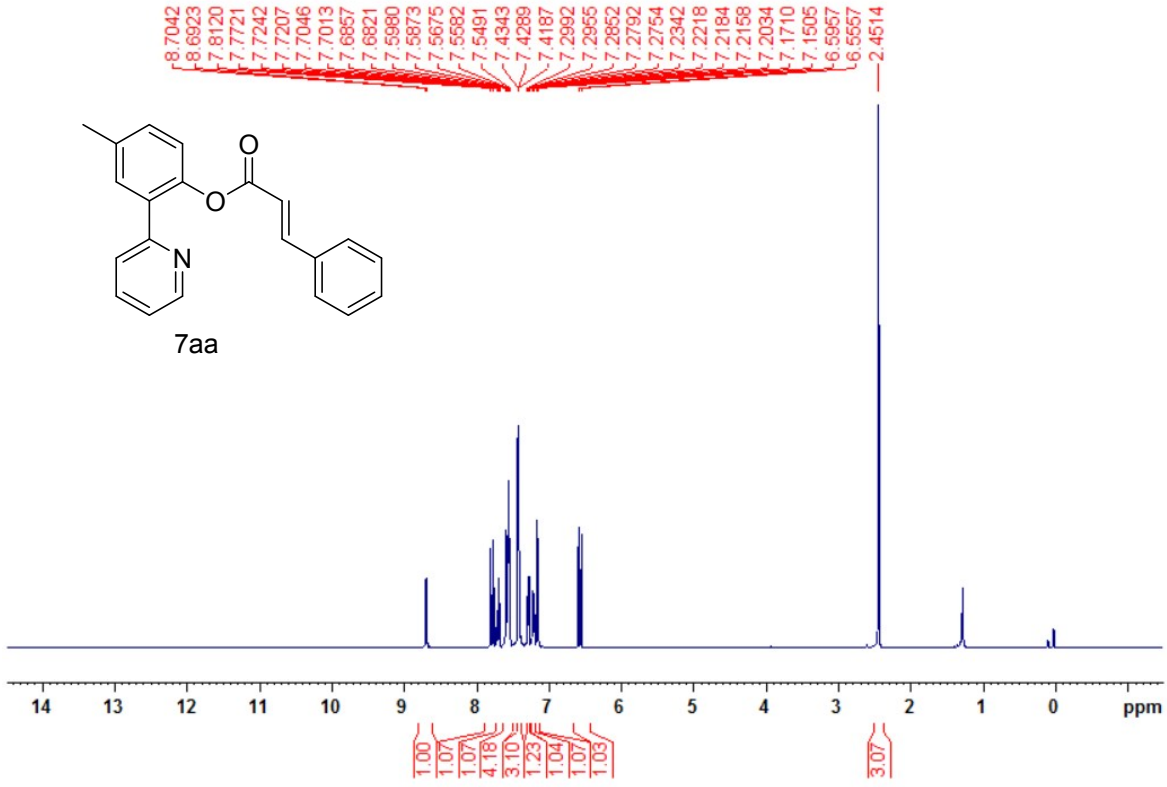
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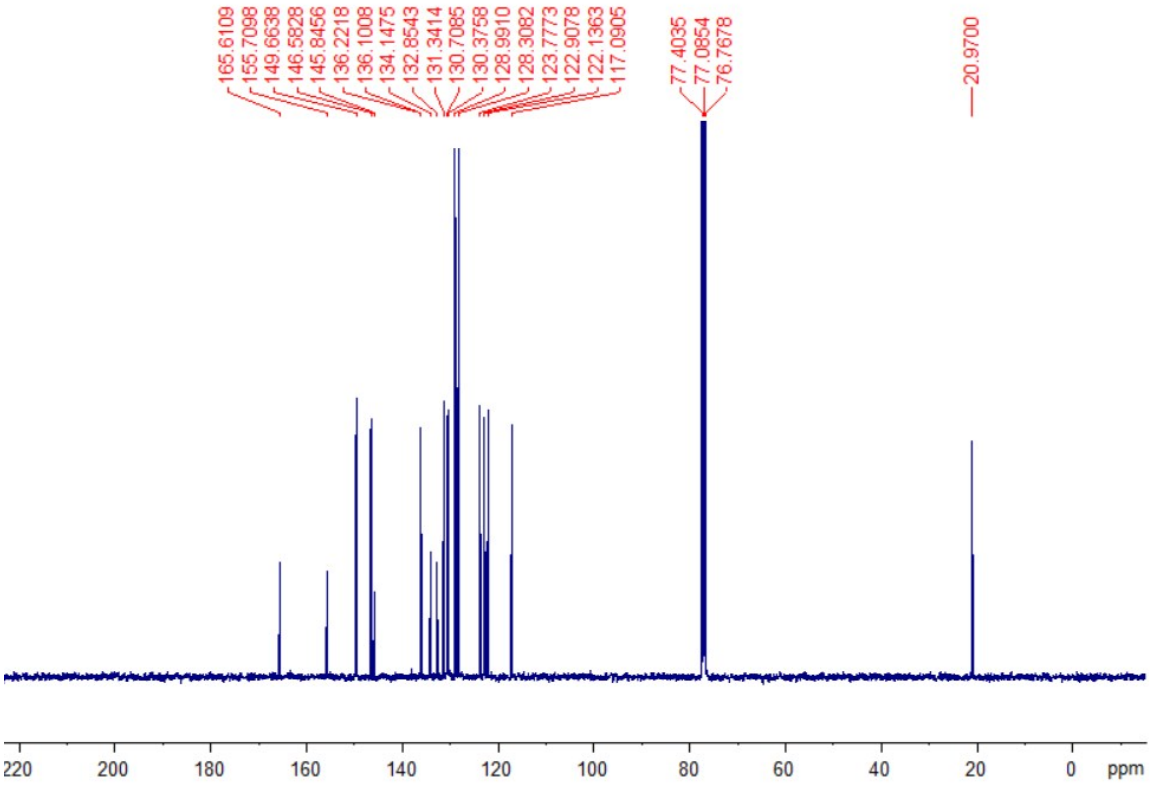
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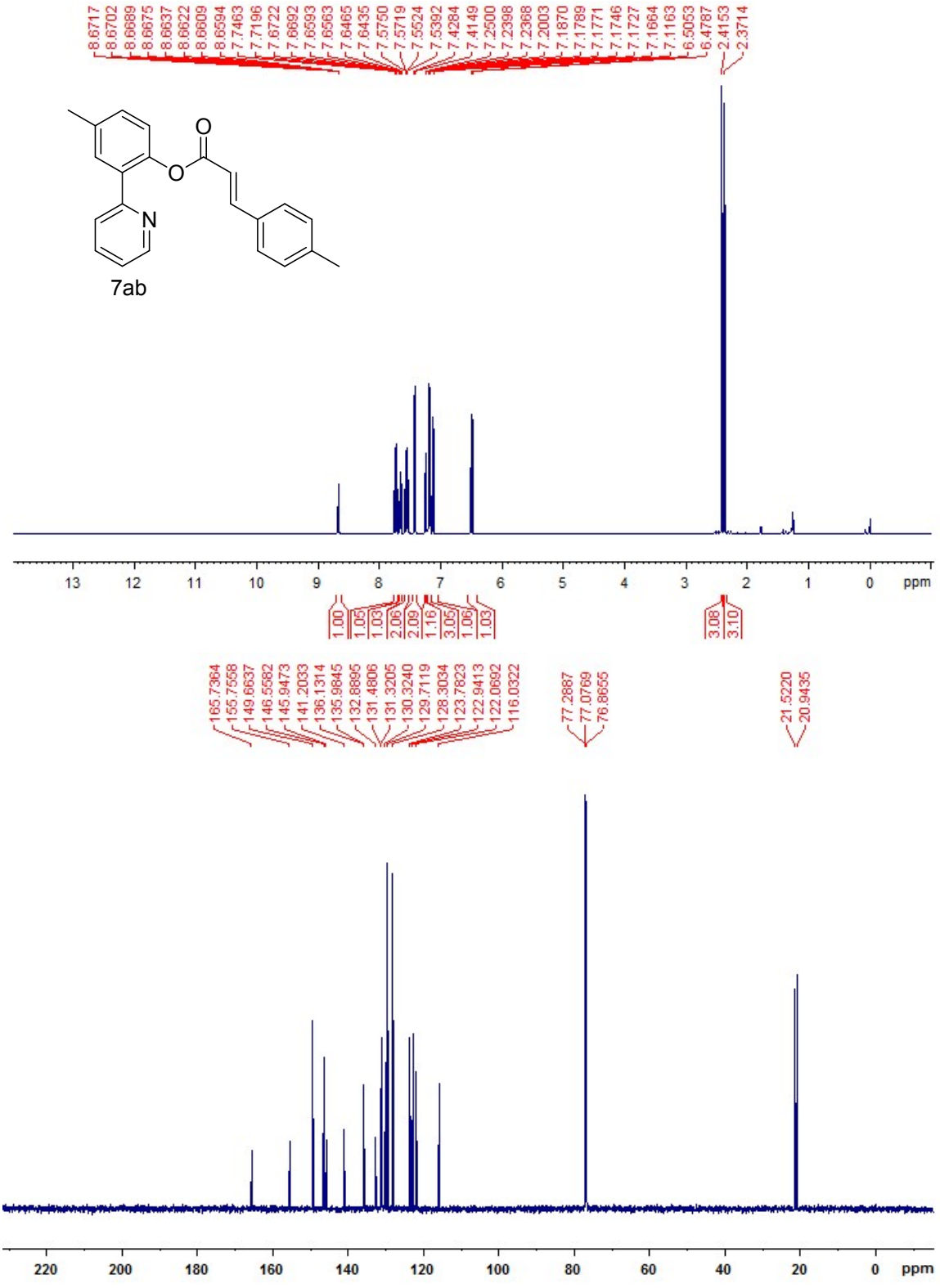
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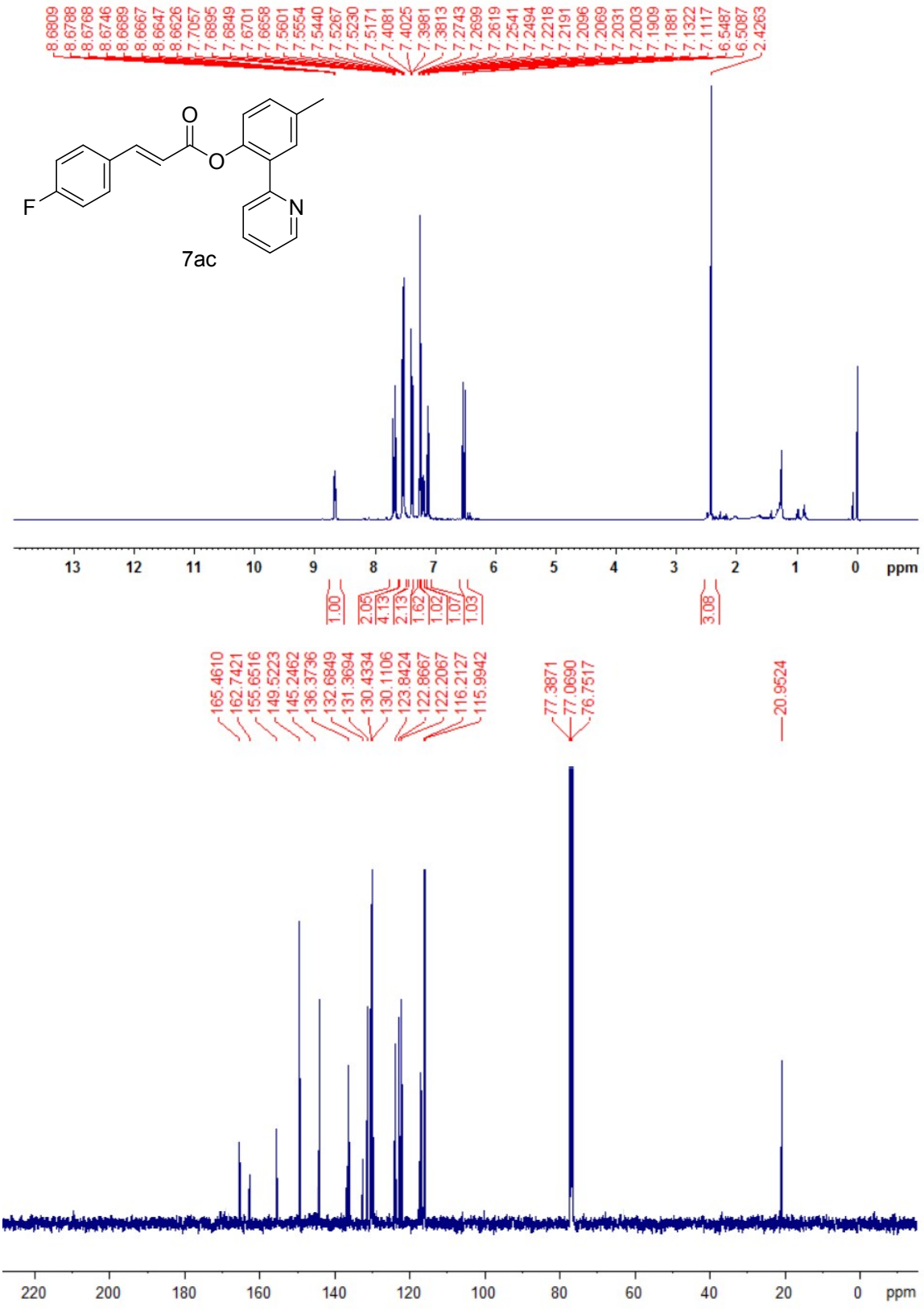
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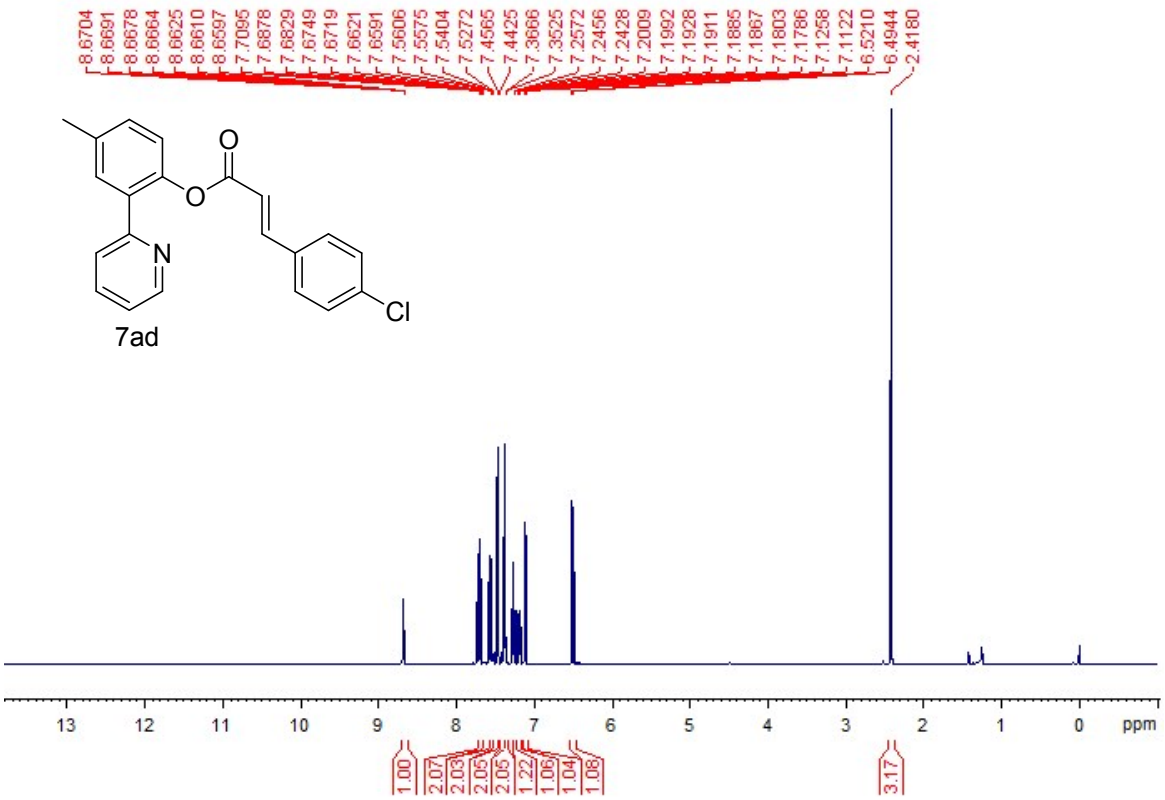
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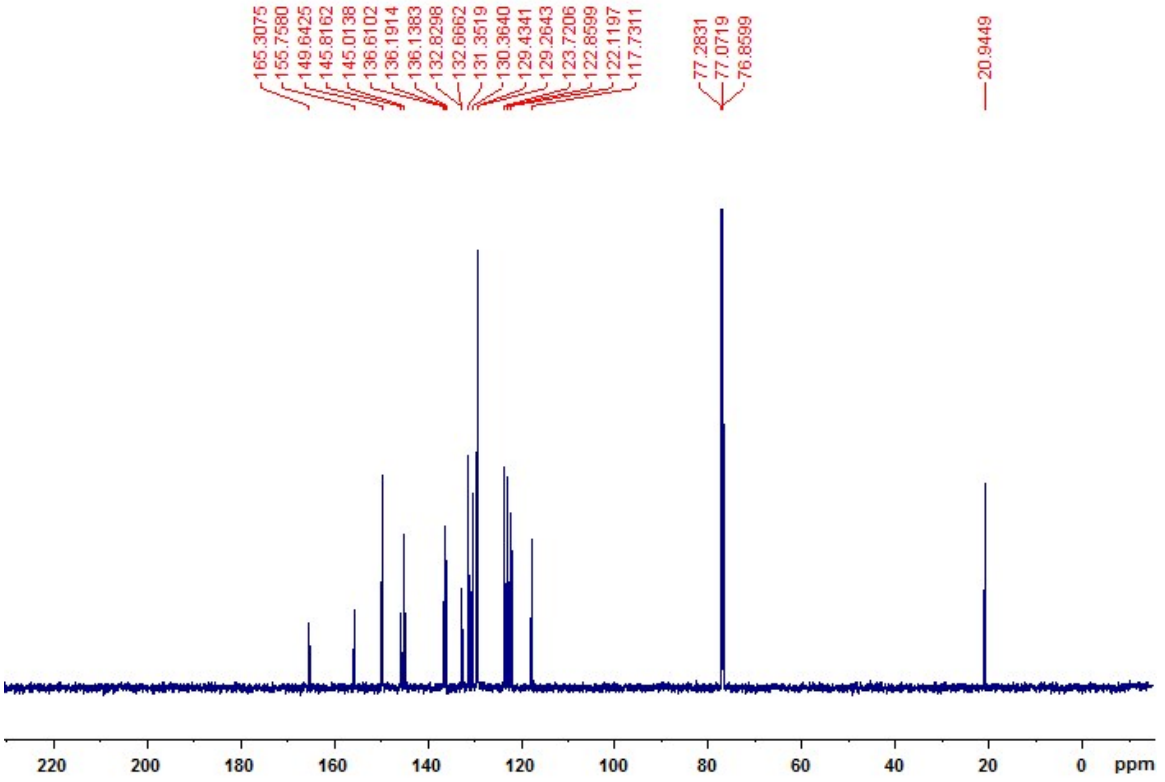
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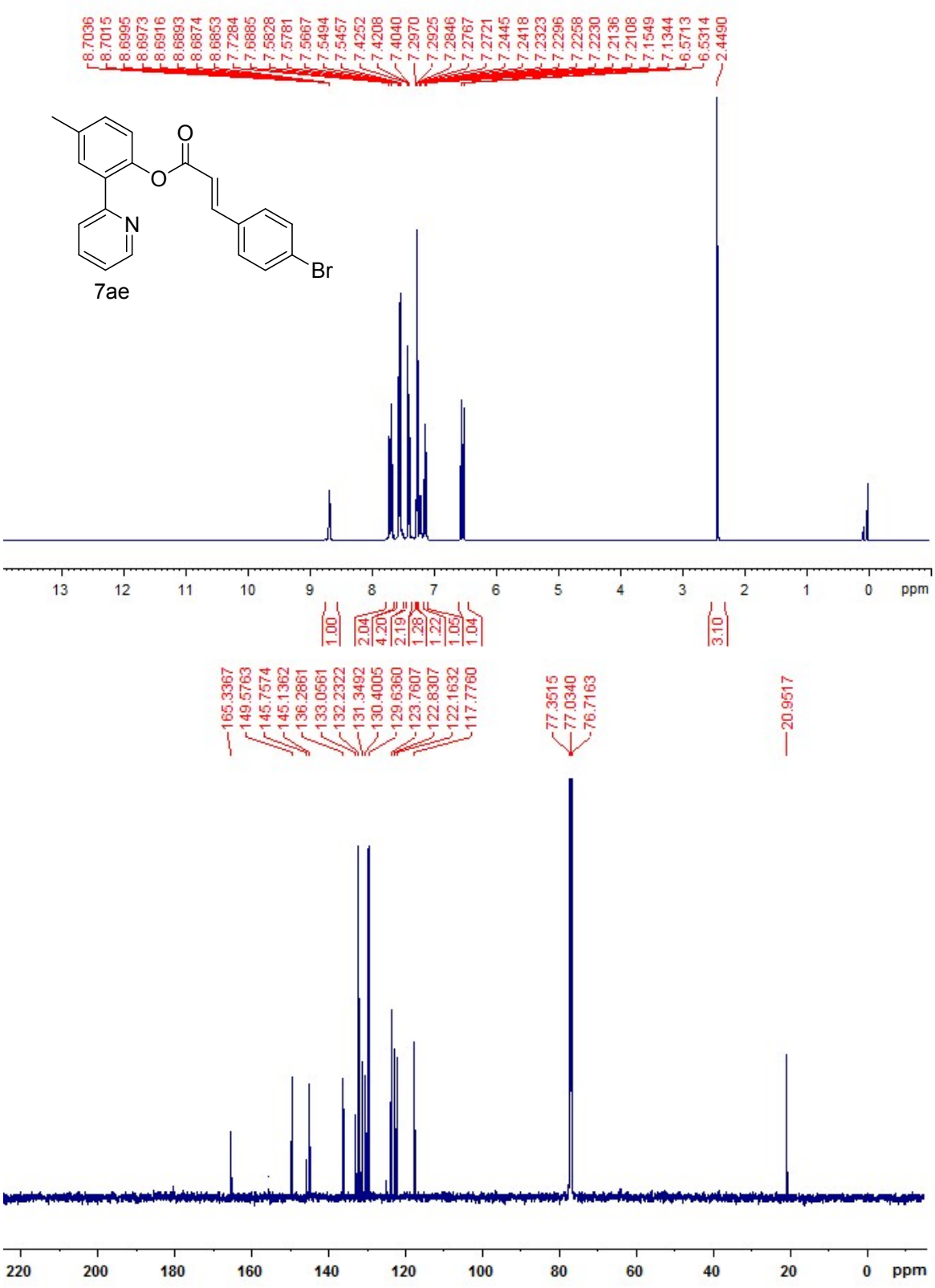
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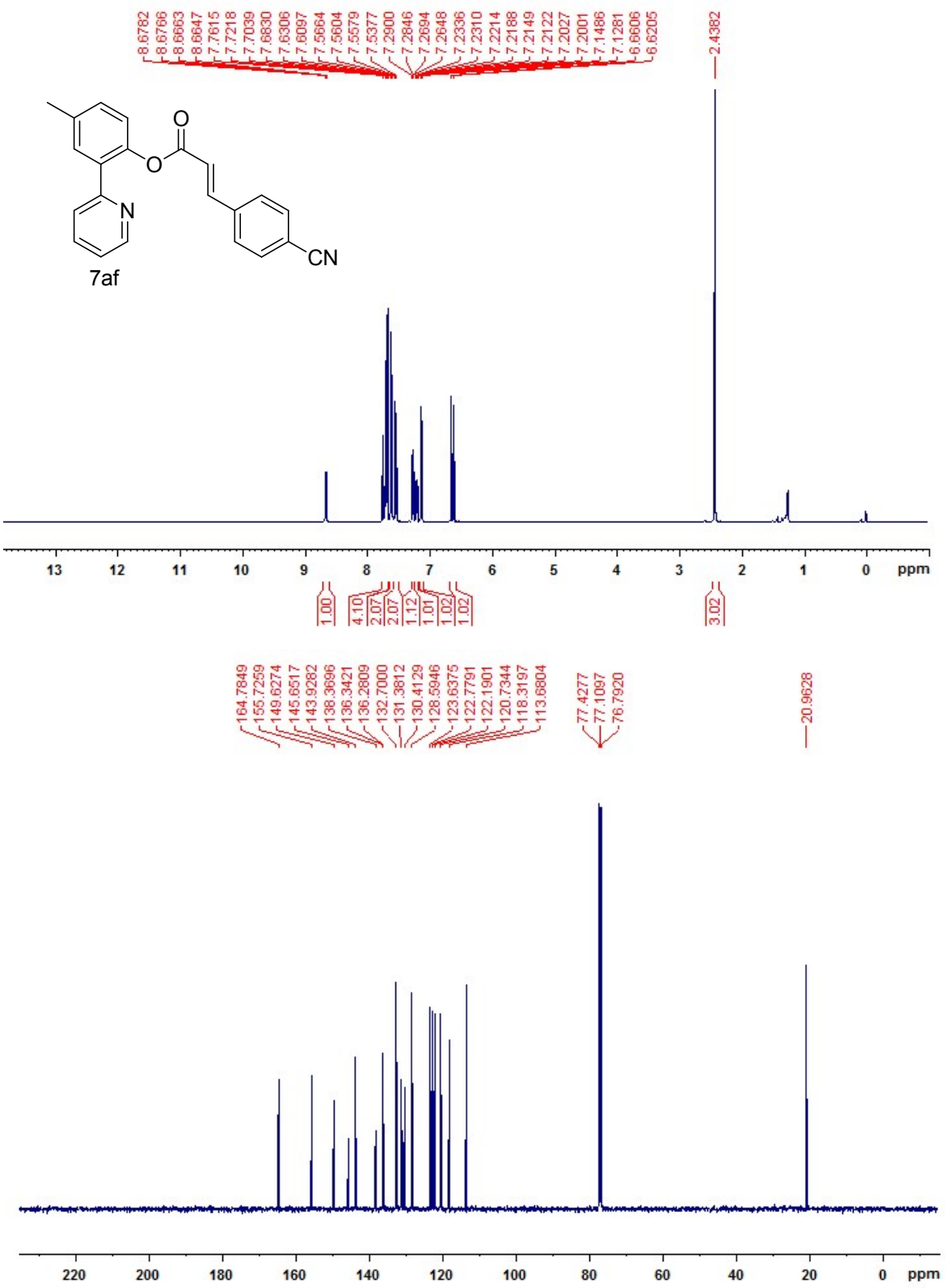
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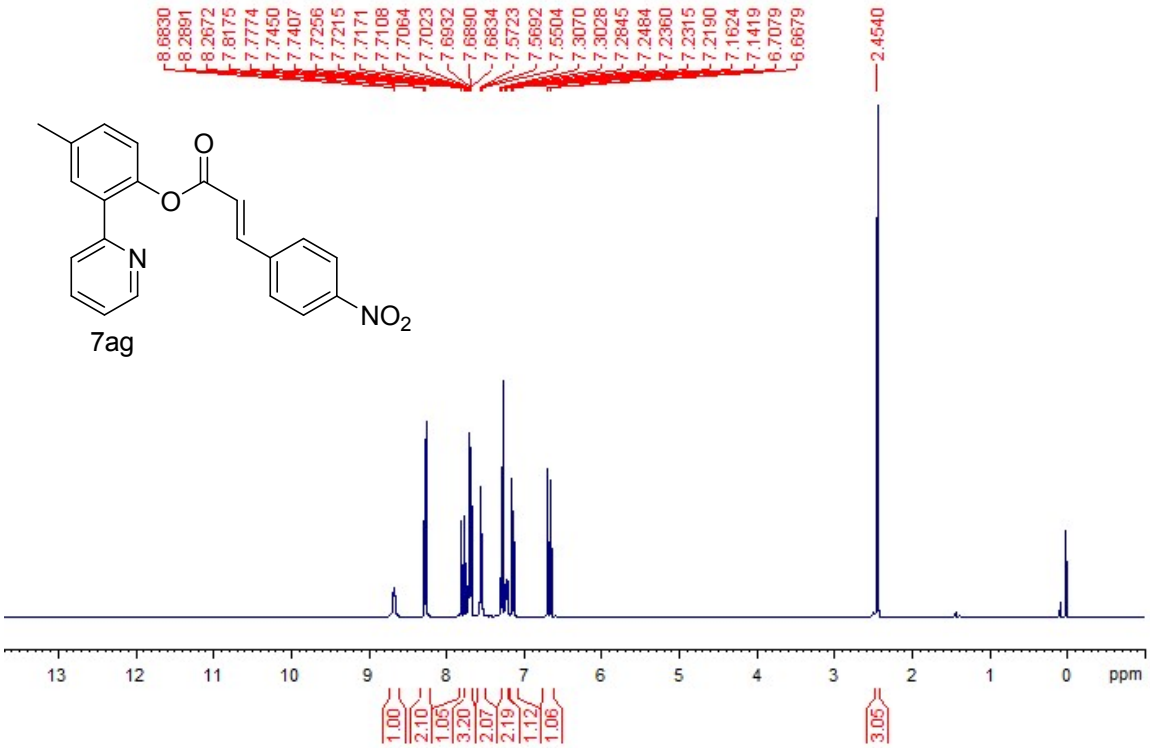
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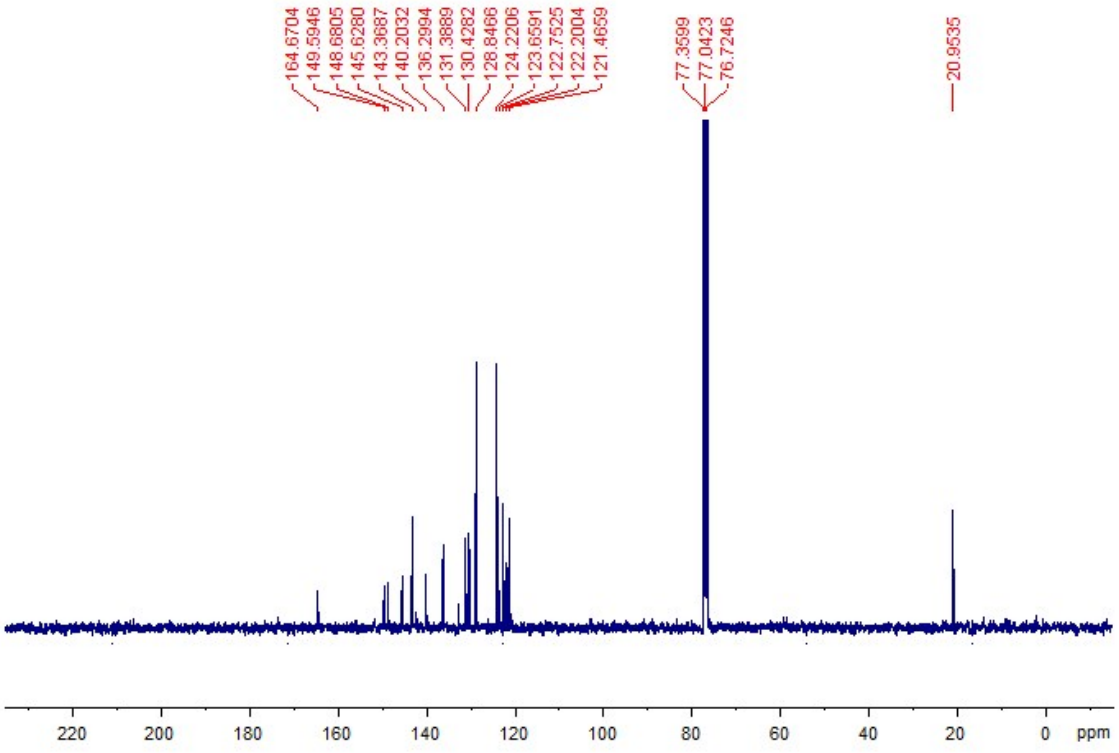
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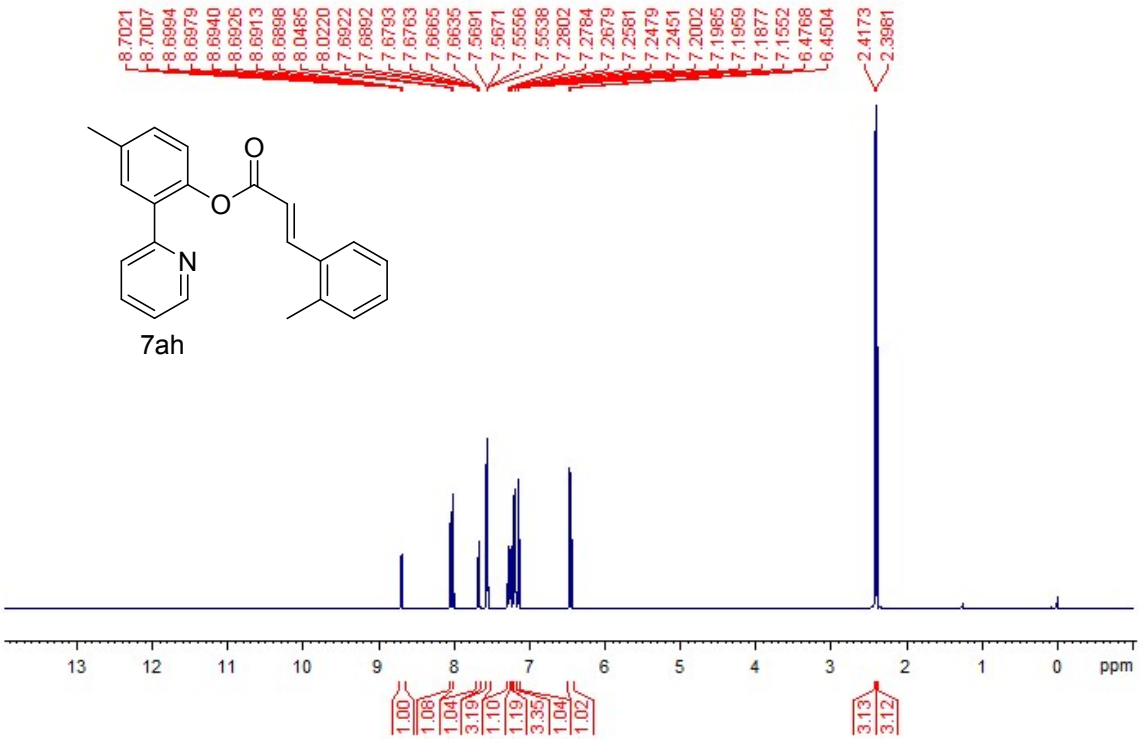
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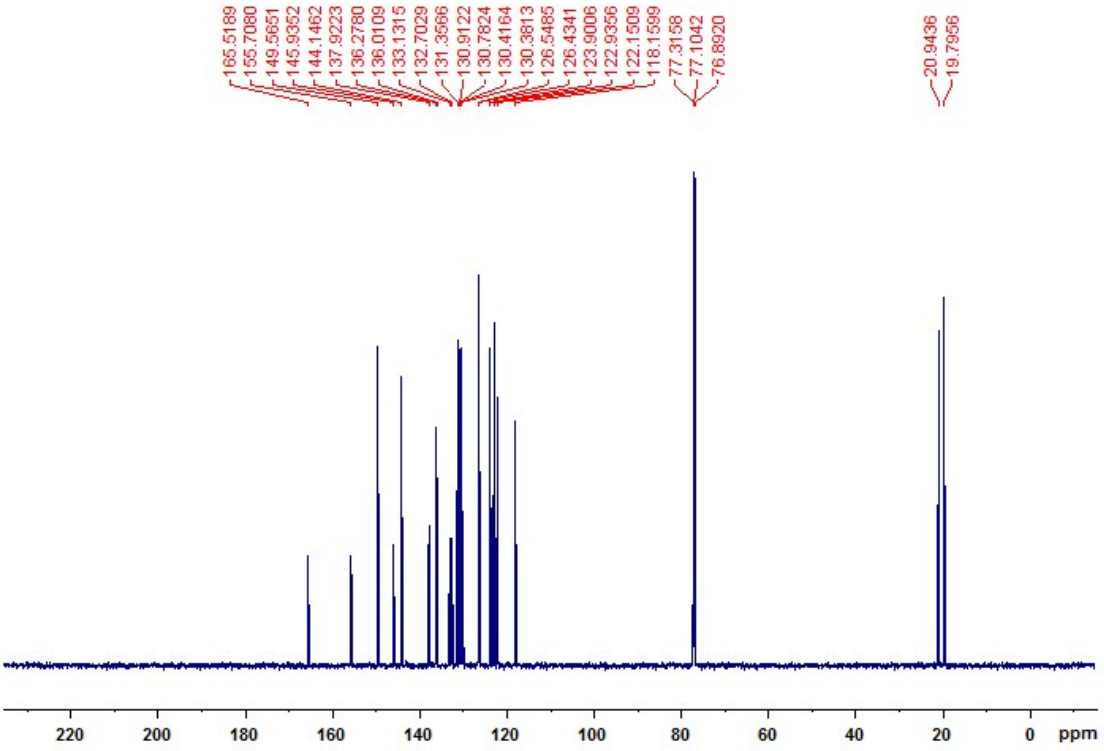
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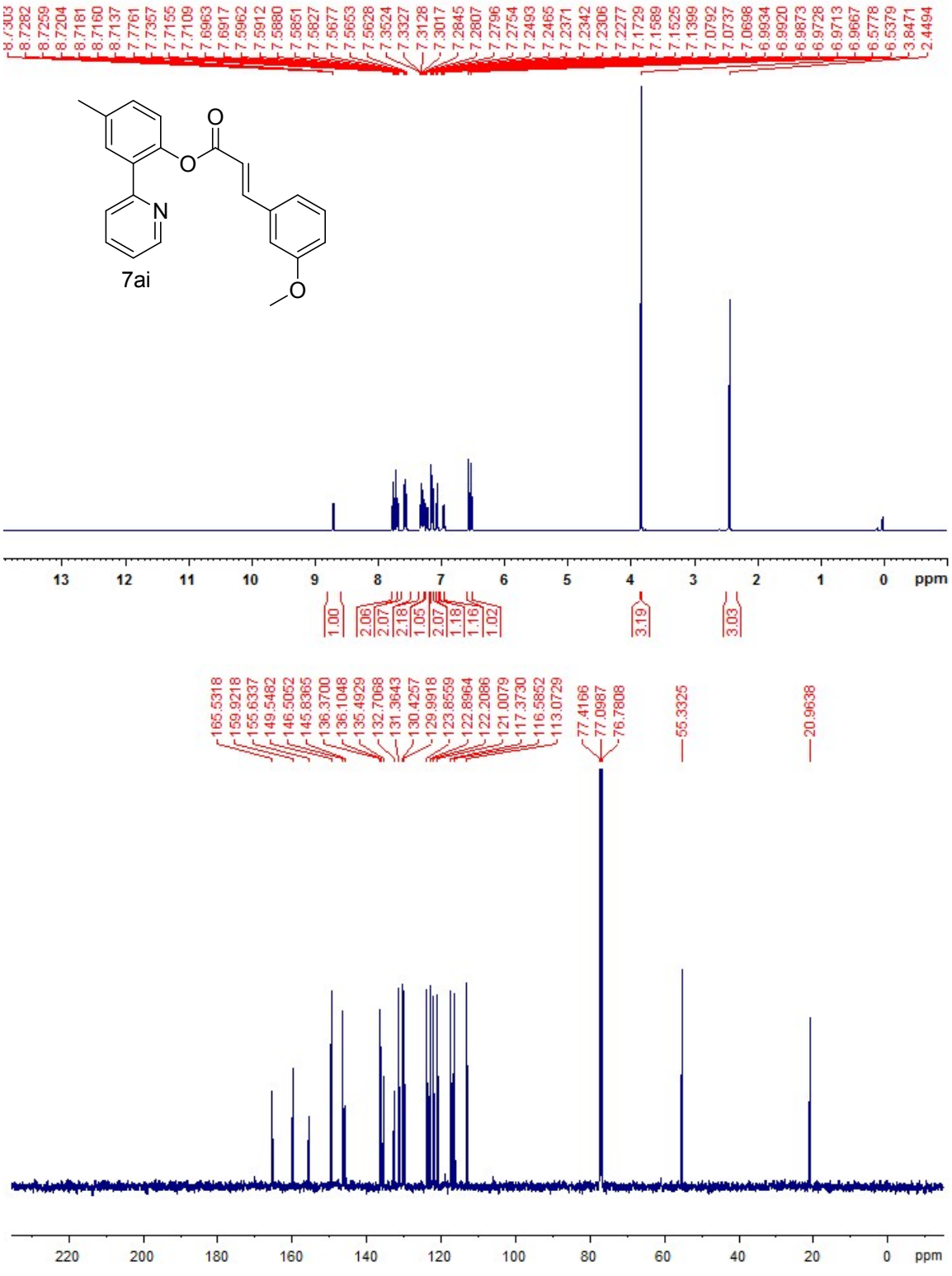
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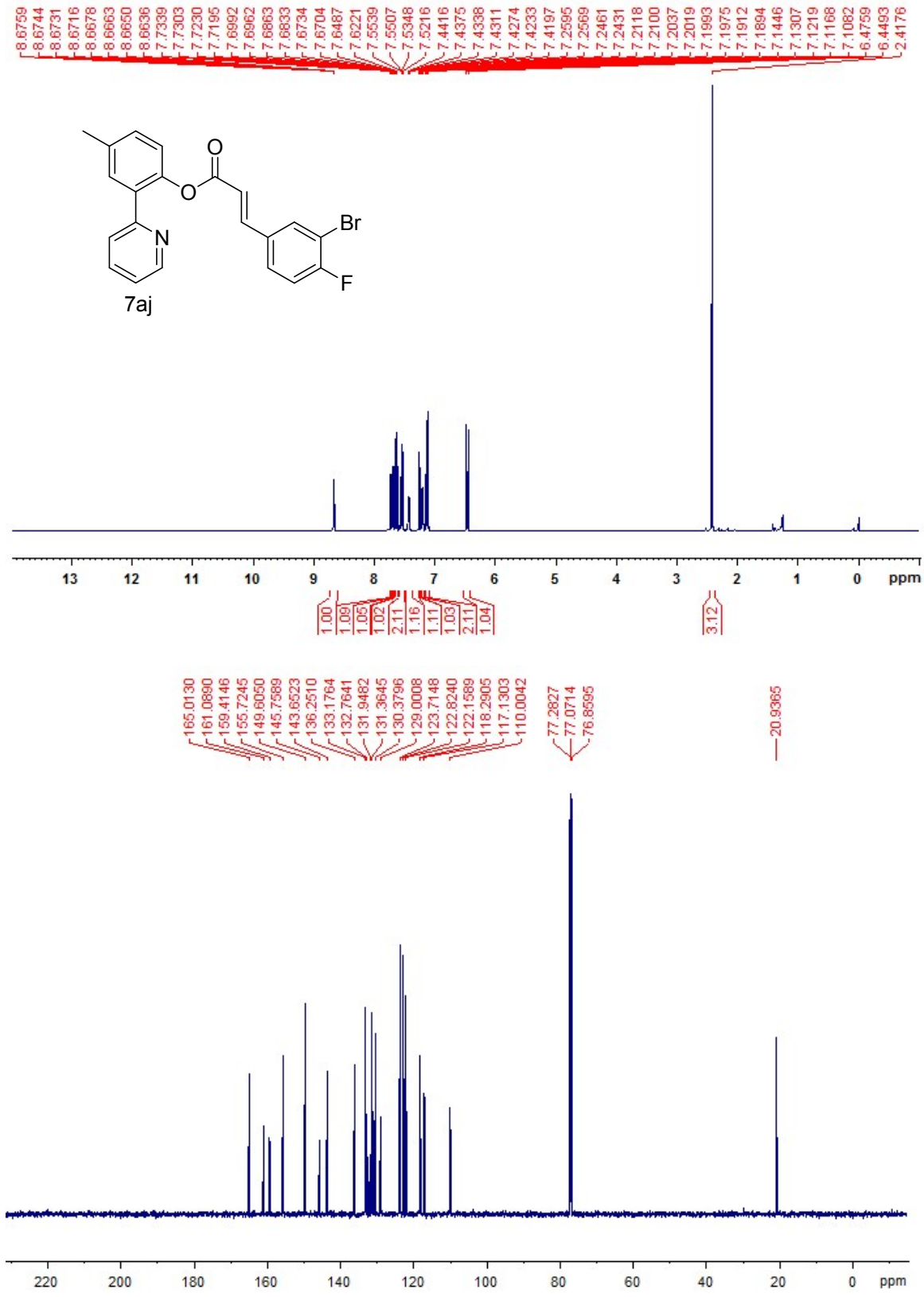
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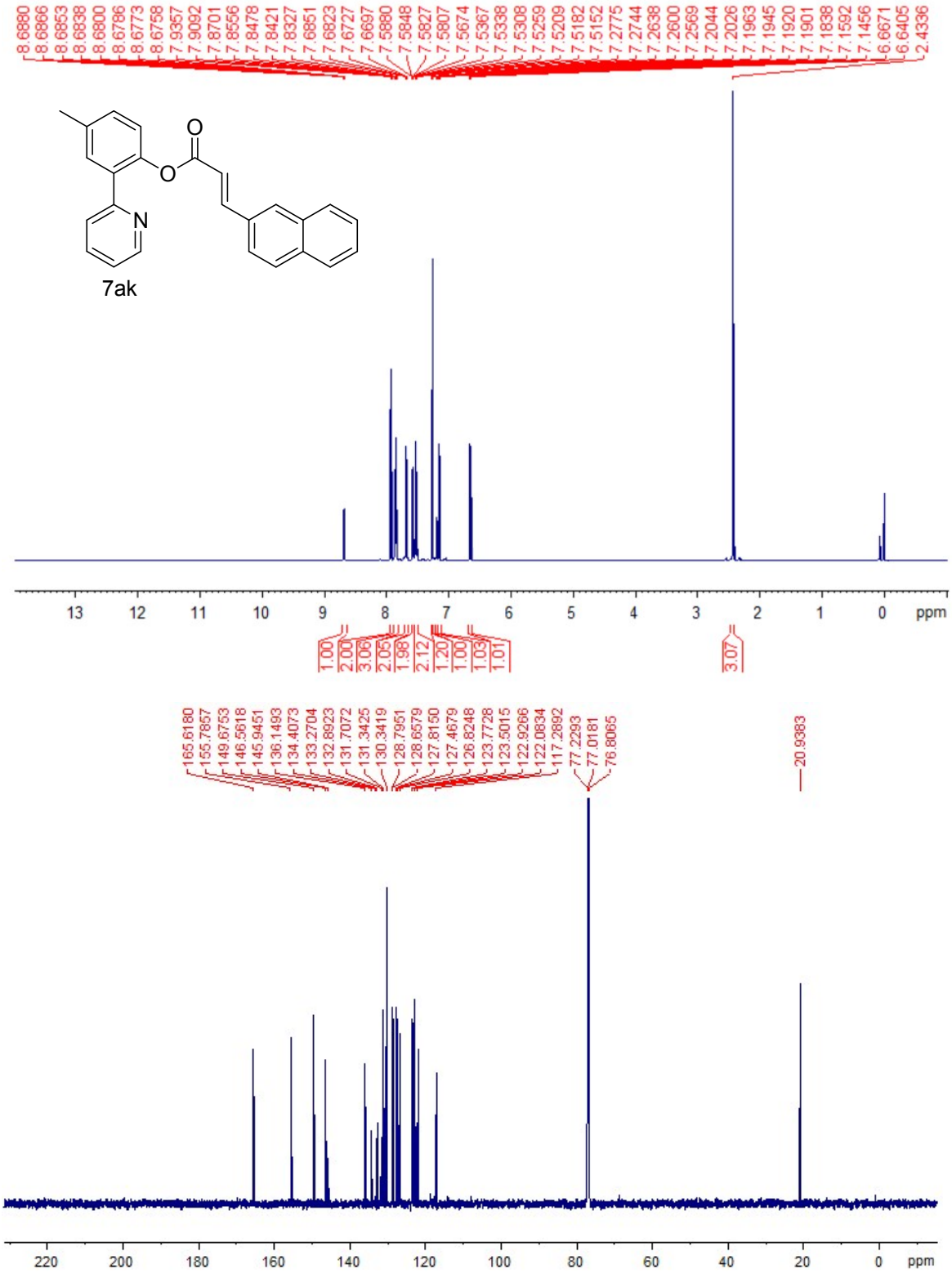
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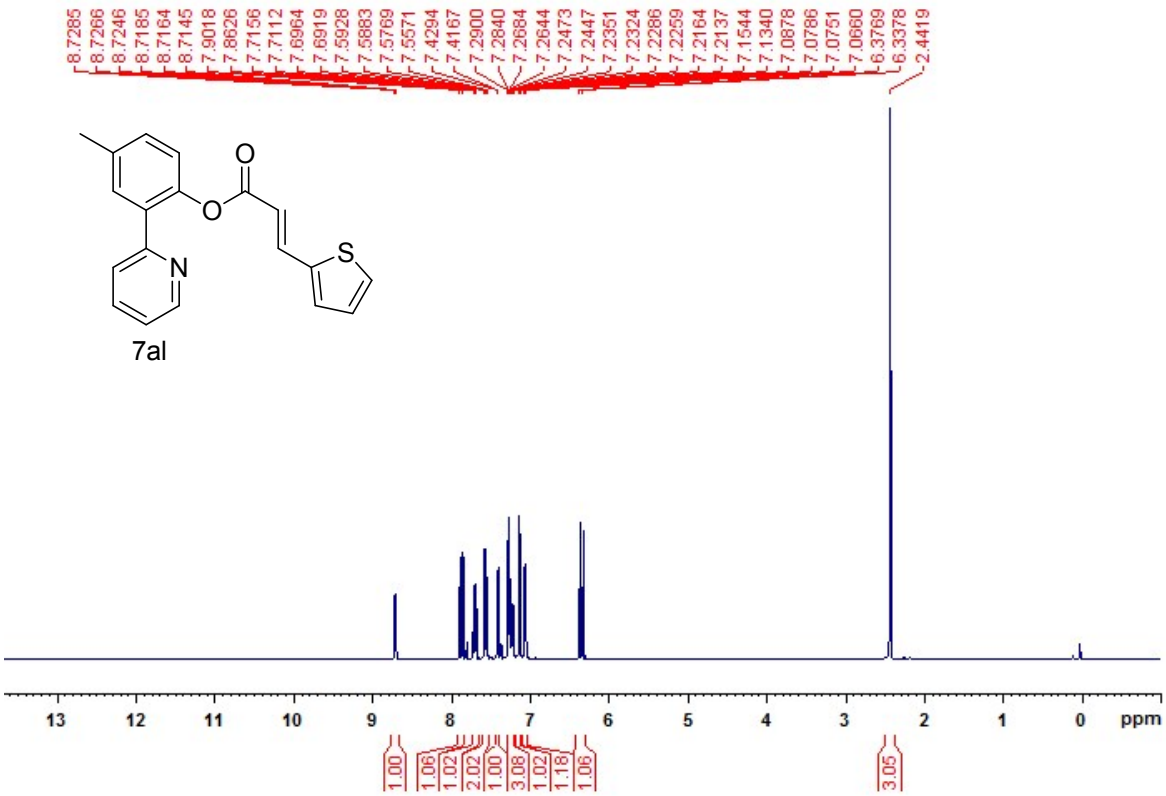
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O
O
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S
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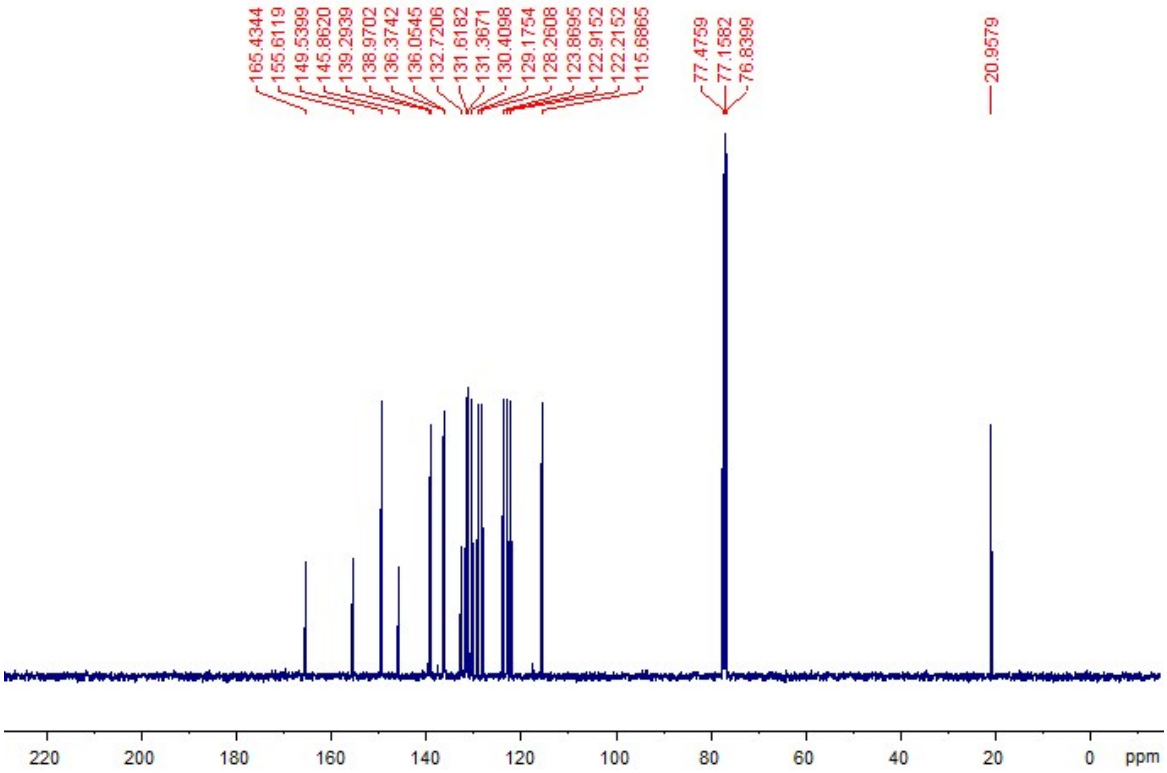
3.05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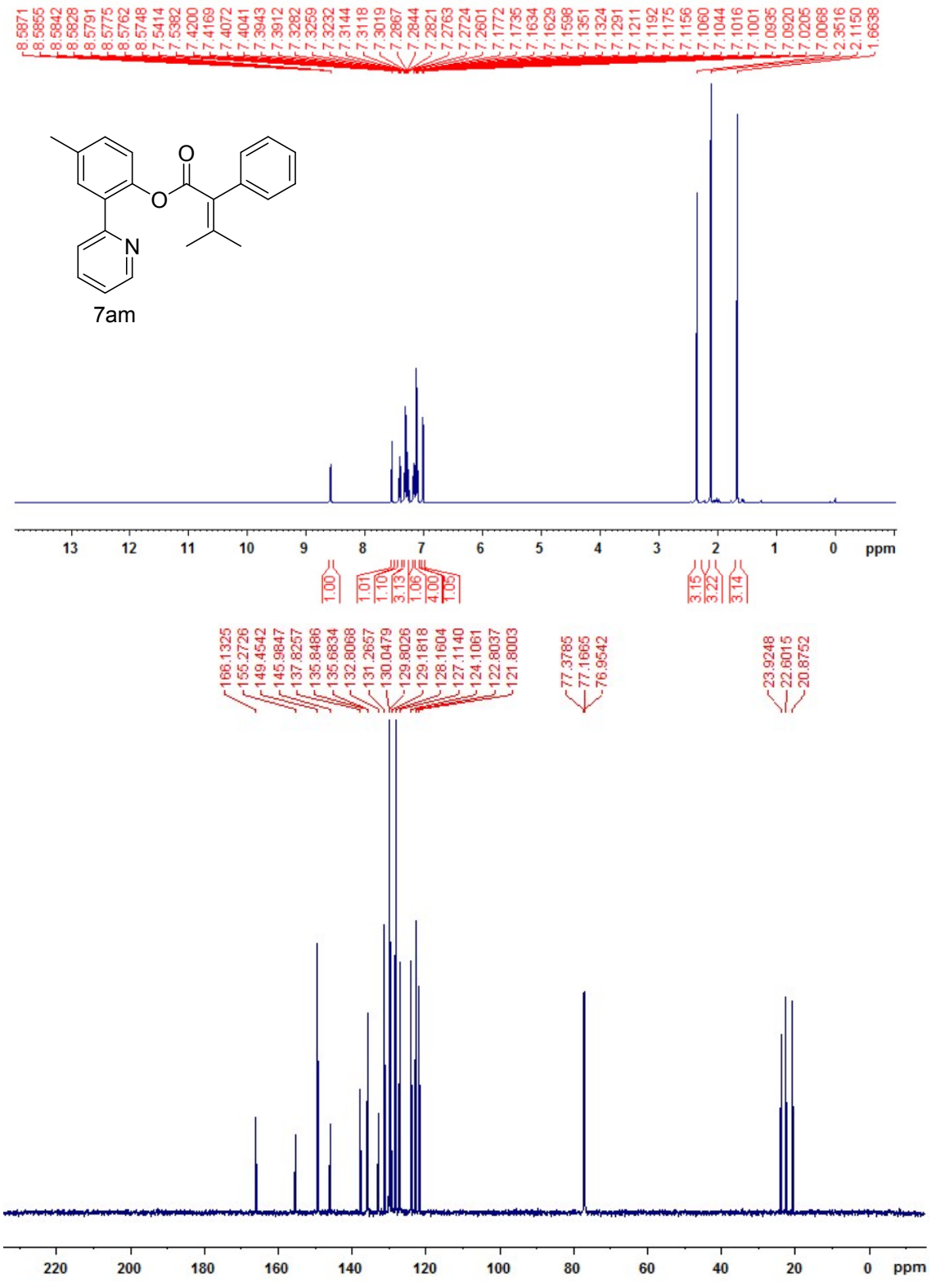
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O
O
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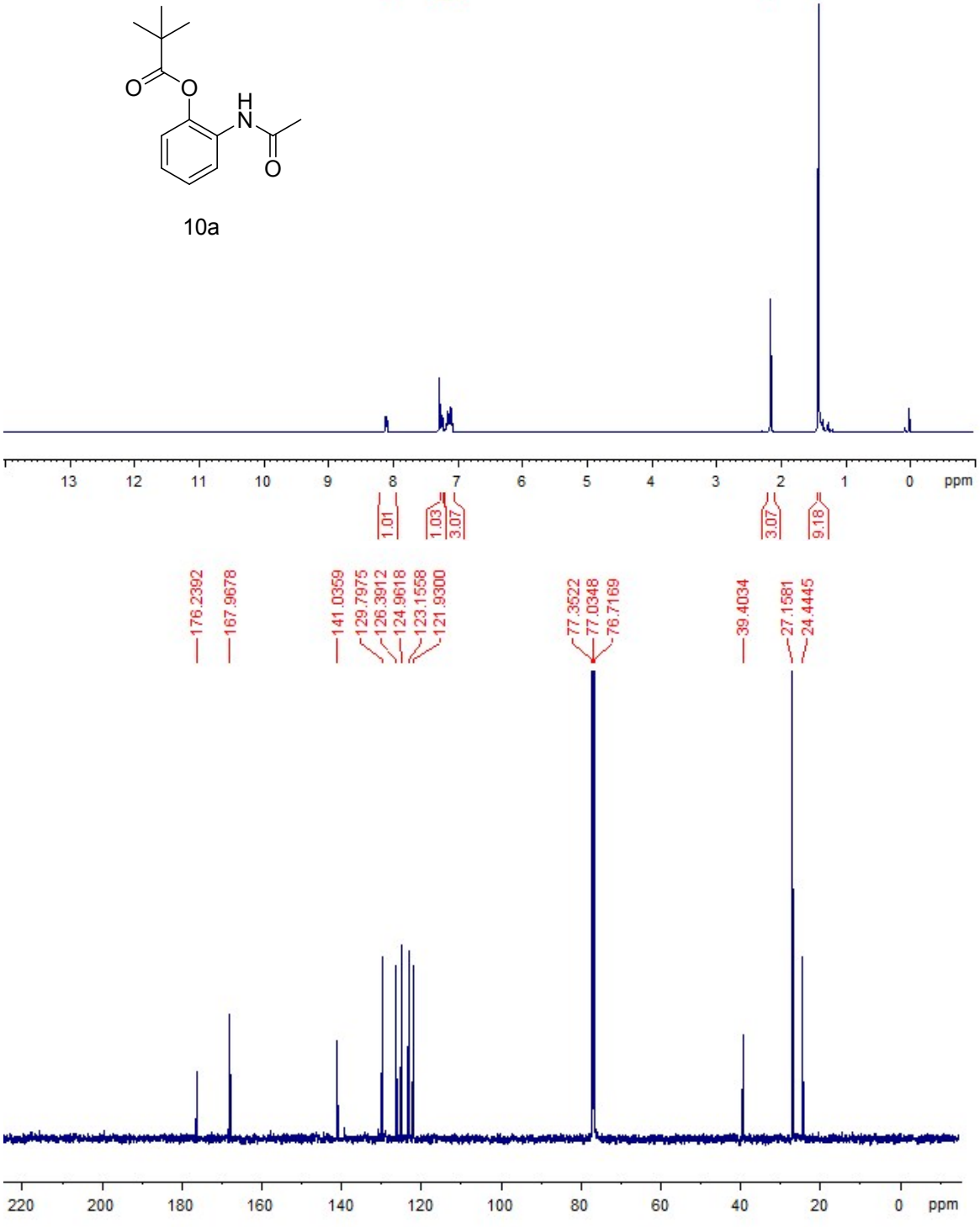
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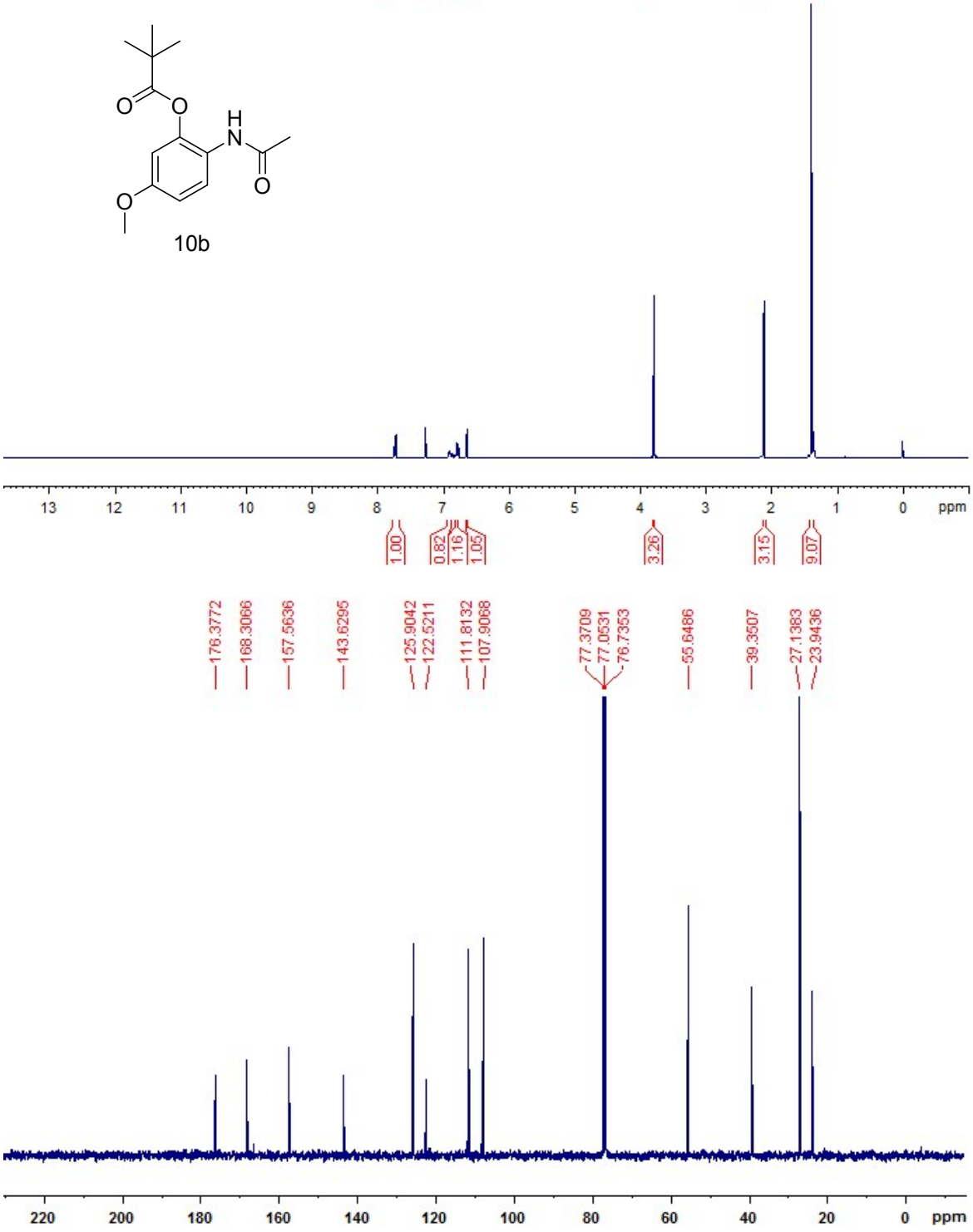
10a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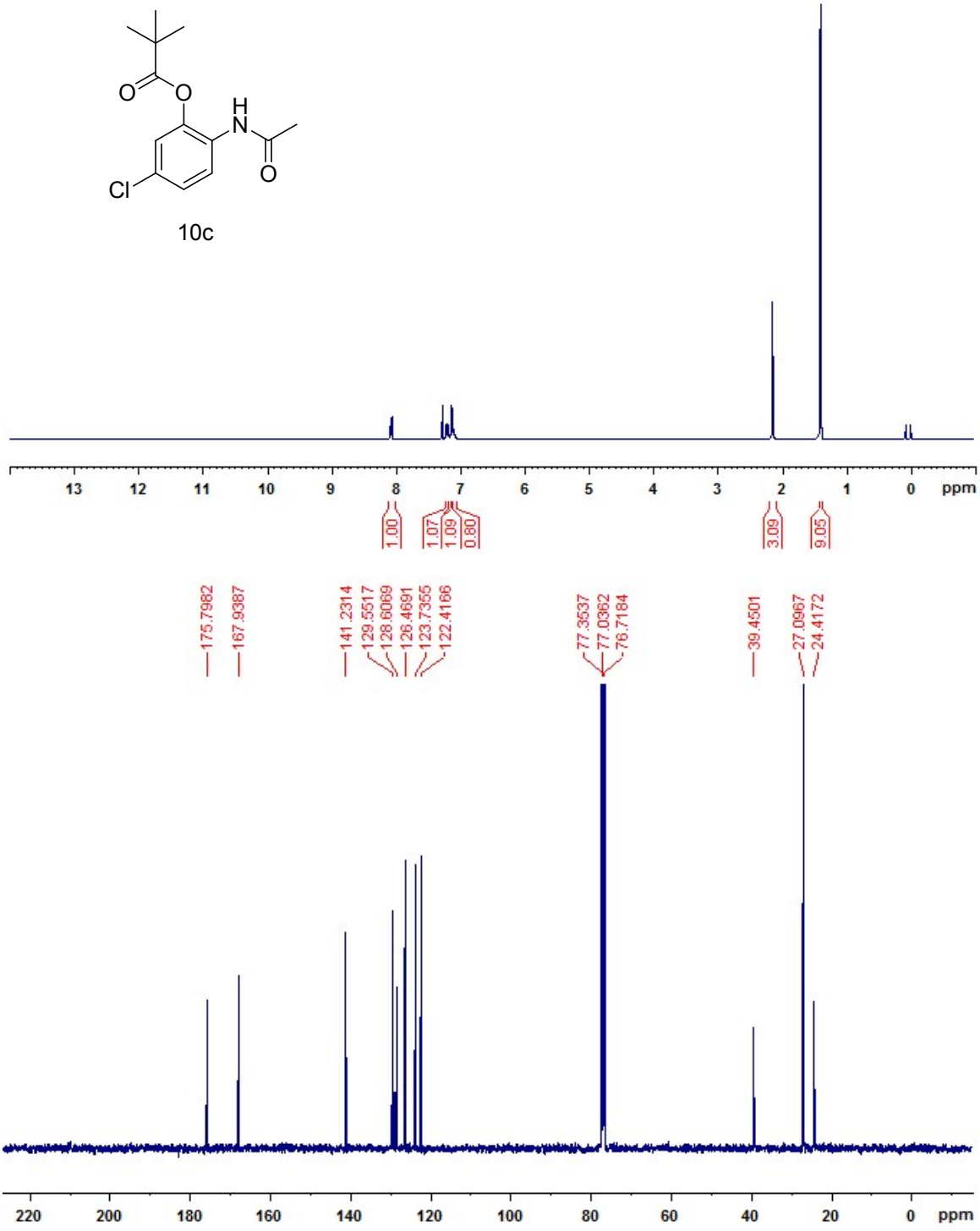
10b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O
O
H
N
O
Cl
10c
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8
7
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120
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60
40
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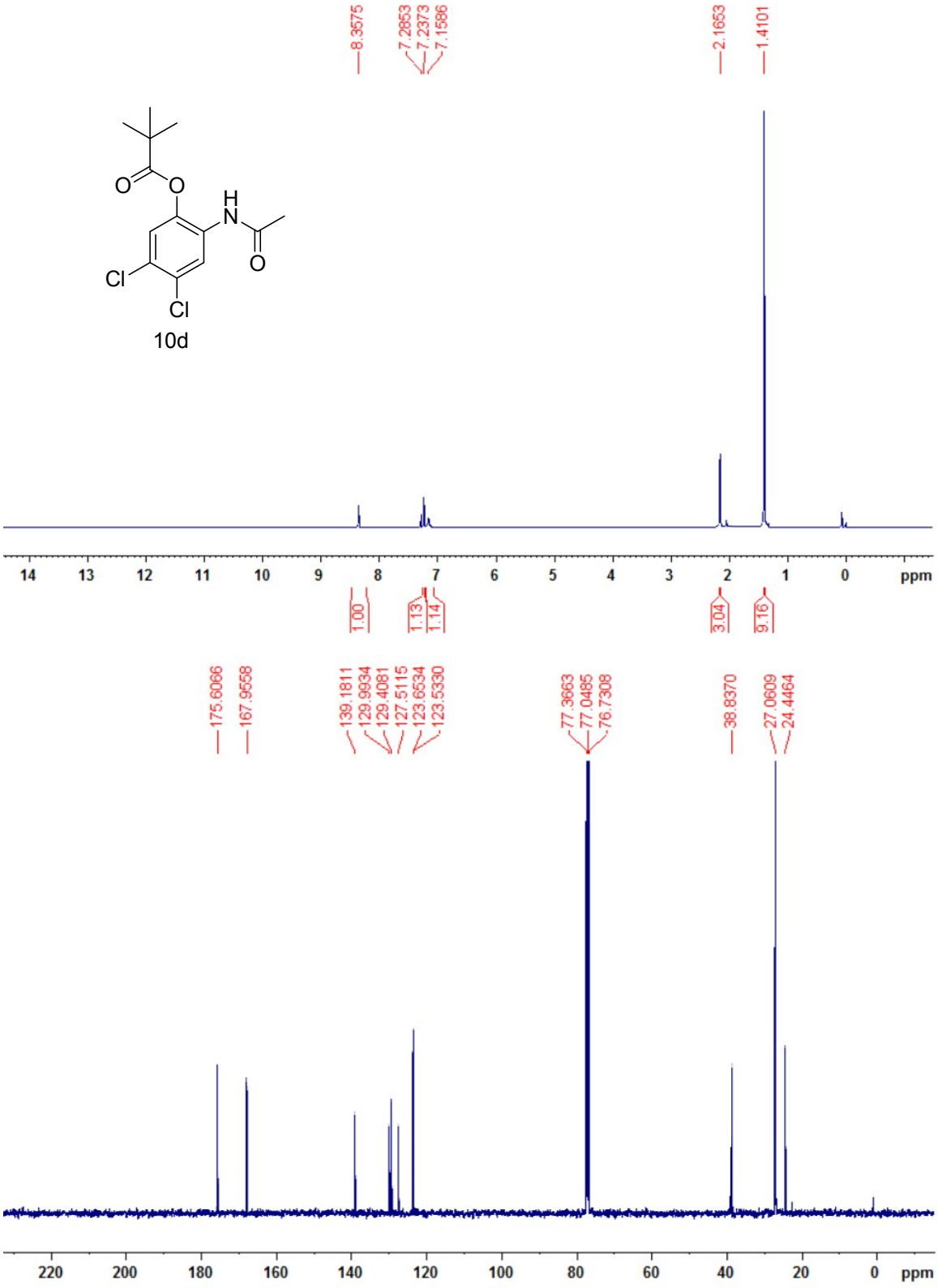
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O
O
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Cl
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1.13
1.14
3.04
9.16
175.6066
167.9558
139.1811
129.9934
129.4081
127.5115
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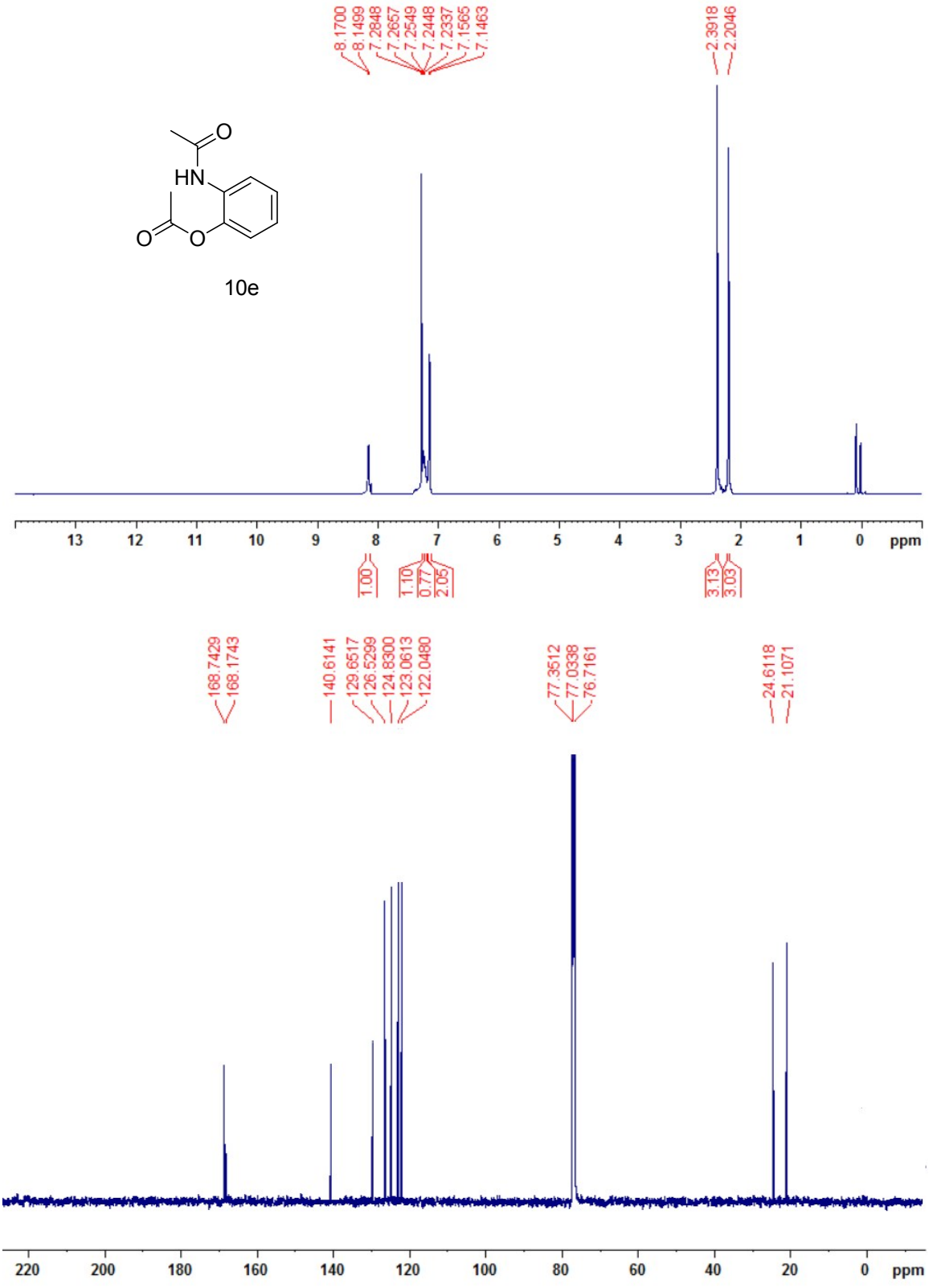
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2.2046
O
HN
O
O
10e
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.10
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3.03
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120
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40
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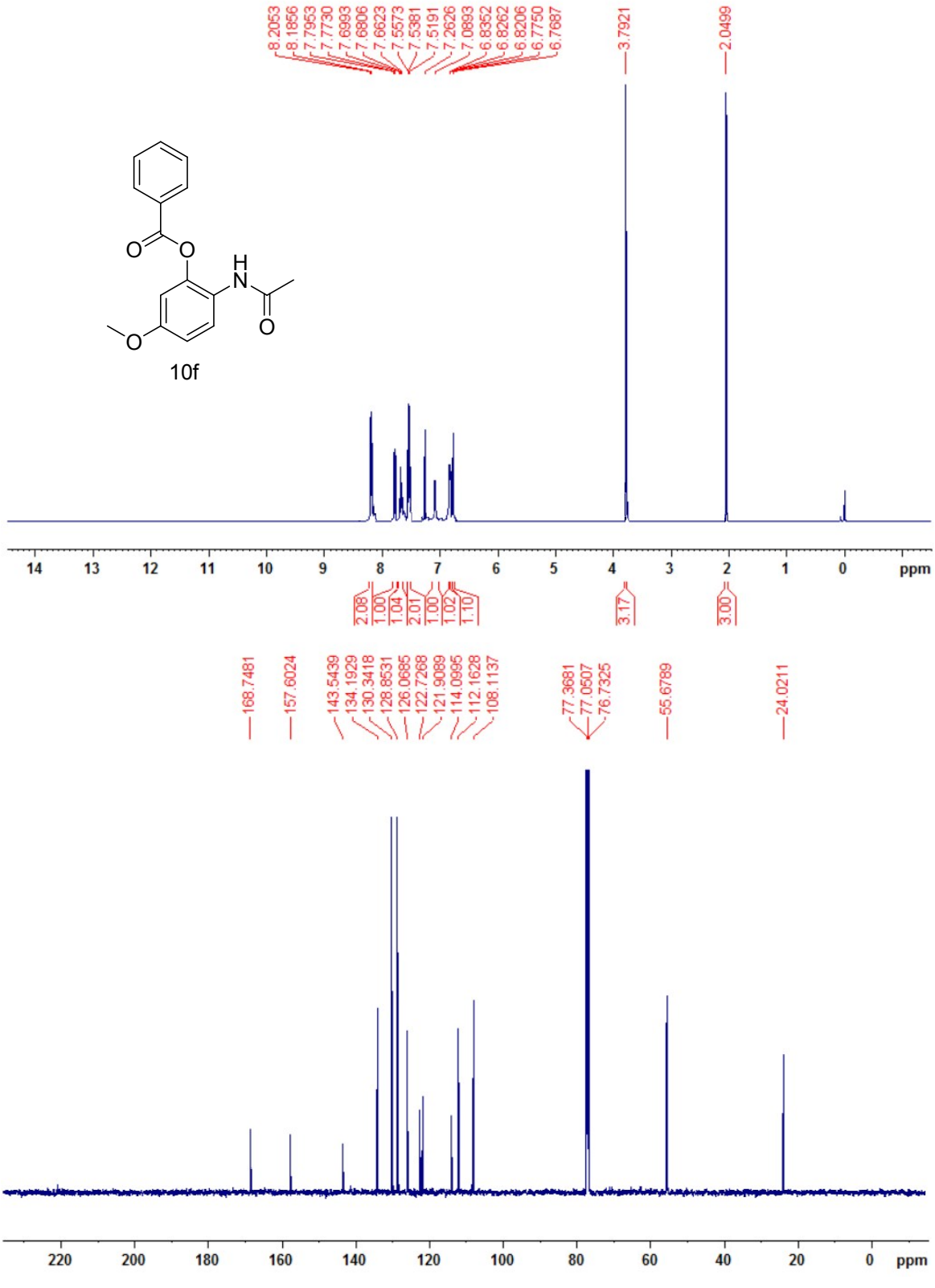
ppm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O
O
H
N
O
O
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2.08 1.00 1.04 2.01 1.00 1.02 1.10
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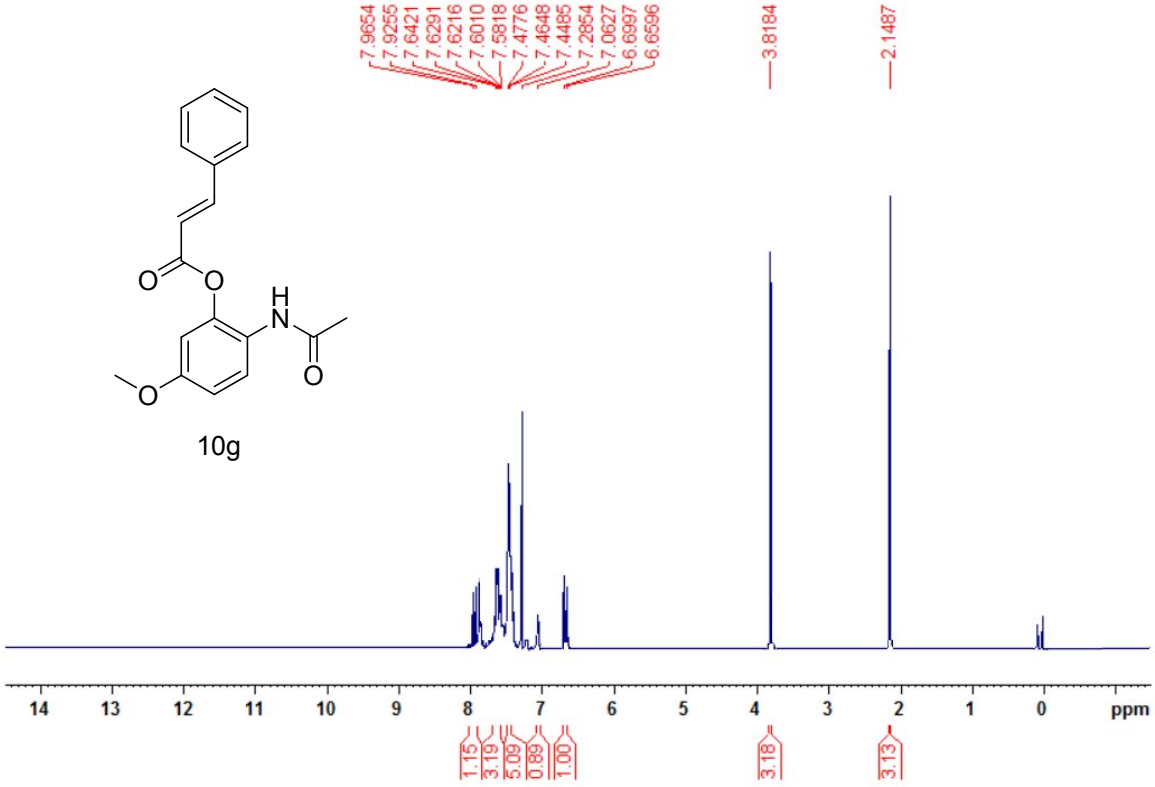
10f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O
O
H
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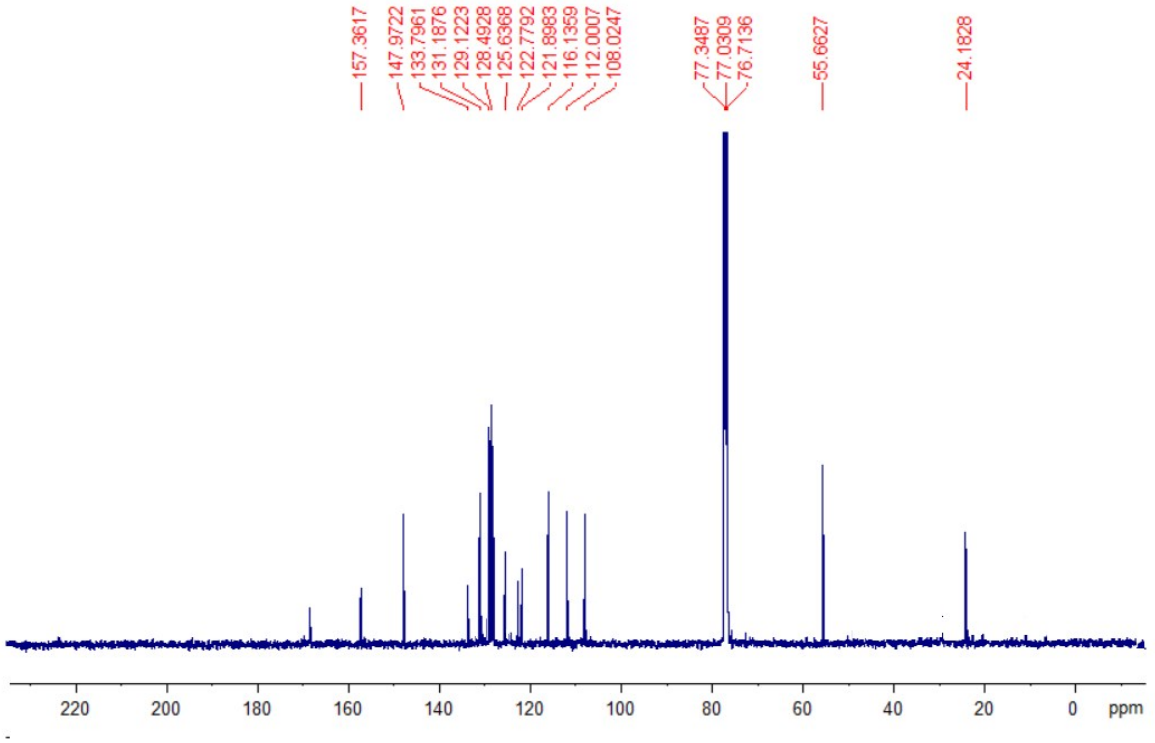
3.18
3.13

10g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77.0309
76.7136
55.6627
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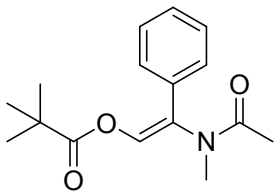
O
O
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O

11a

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7.4149
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7.3972
7.3958
7.3922
7.2848
3.1001
1.9904
1.3148
13
12
11
10
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6
5
4
3
2
1
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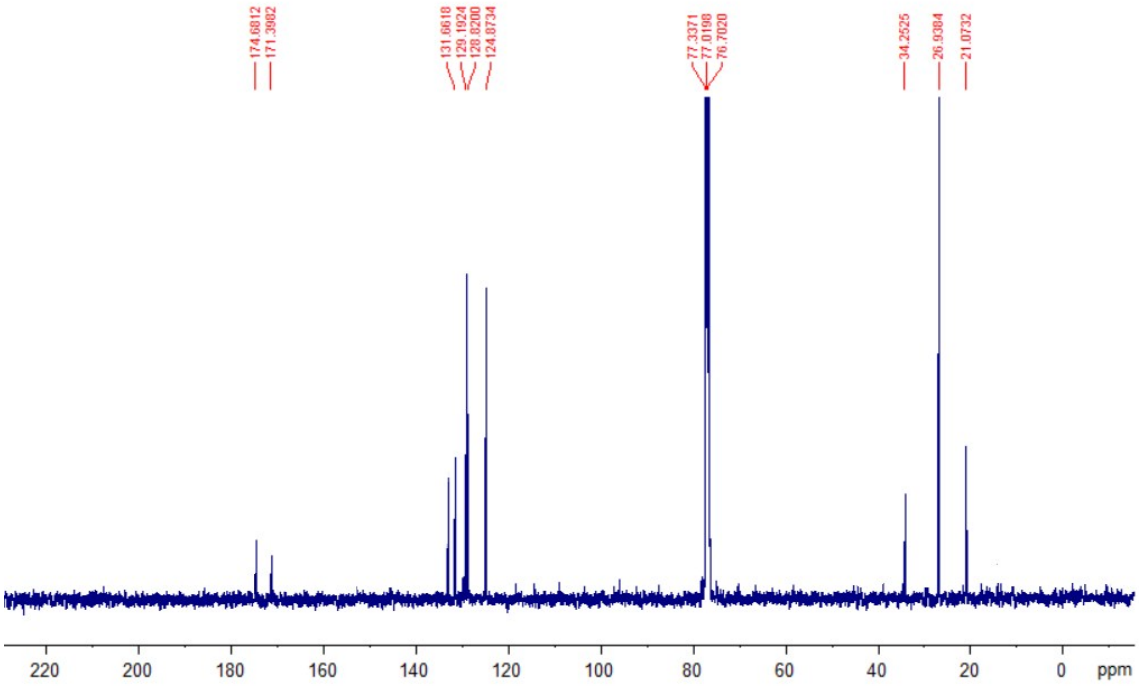
ppm
1.00
5.02
3.11
3.13
9.03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128.8200
124.8734
77.3371
77.0198
76.7020
34.2525
26.9384
21.0732
220
200
180
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140
120
100
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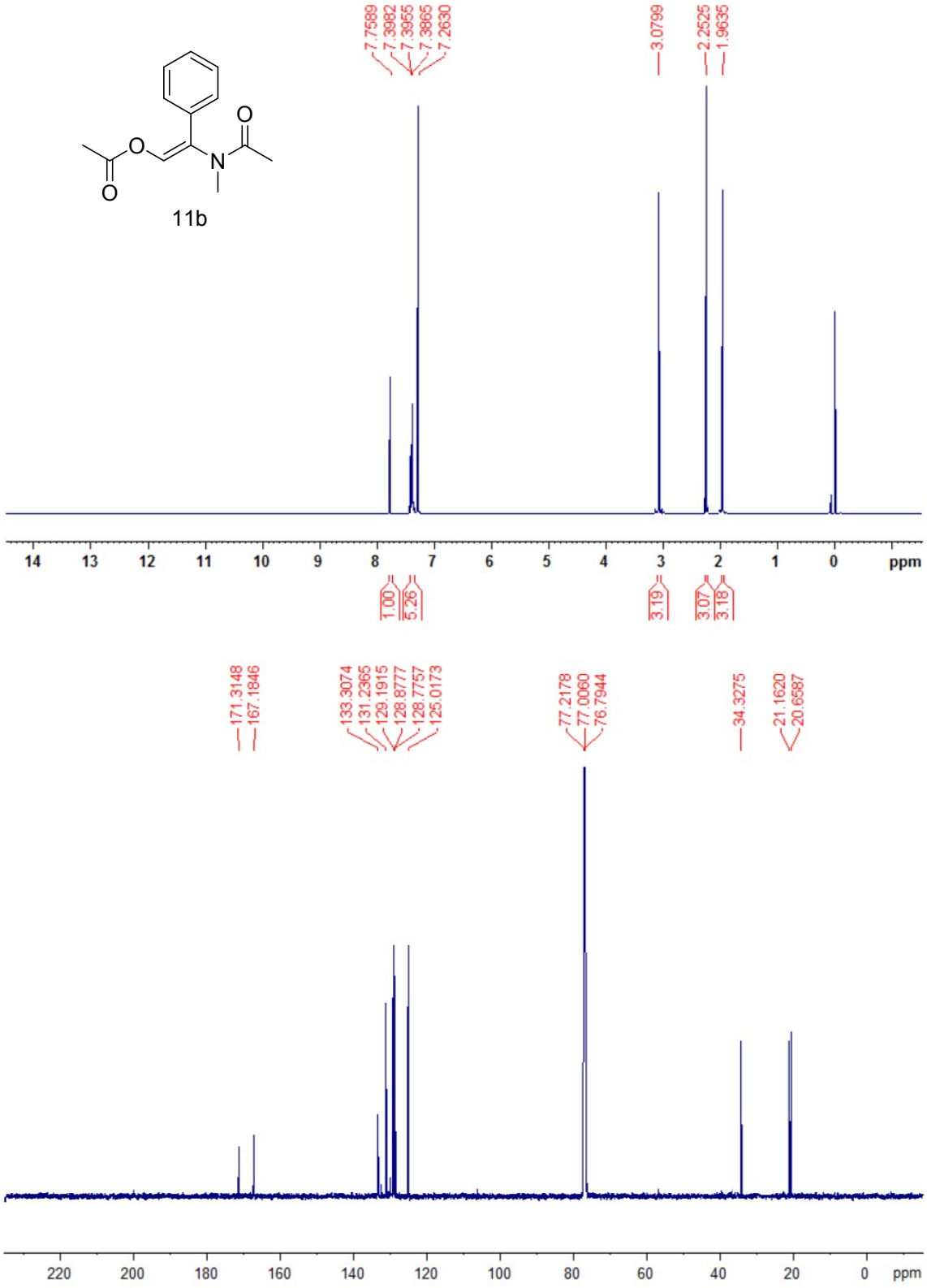
60
40
20
0
ppm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1.9635
ppm
1.00
5.26
3.19
3.07
3.18
171.3148
167.1846
133.3074
131.2365
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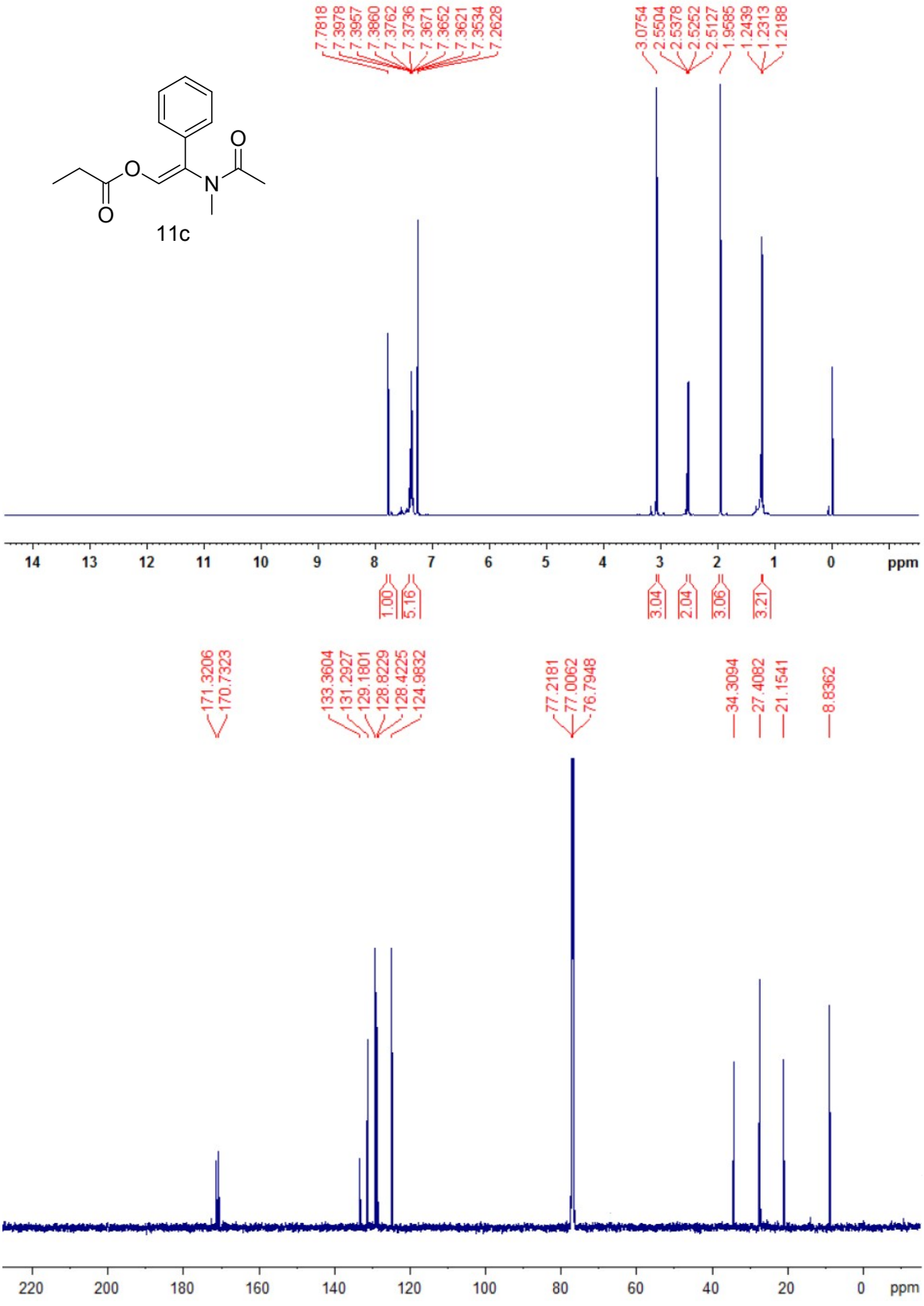
20.6587
ppm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7.3957
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7.3762
7.3736
7.3671
7.3652
7.3621
7.3534
7.2628
3.0754
2.5504
2.5378
2.5252
2.5127
1.9585
1.2439
1.2313
1.2188
O
O
N
O
11c
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
5.16
3.04
2.04
3.06
3.21
171.3206
170.7323
133.3604
131.2927
129.1801
128.8229
128.4225
124.9832
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77.0062
76.7948
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27.4082
21.1541
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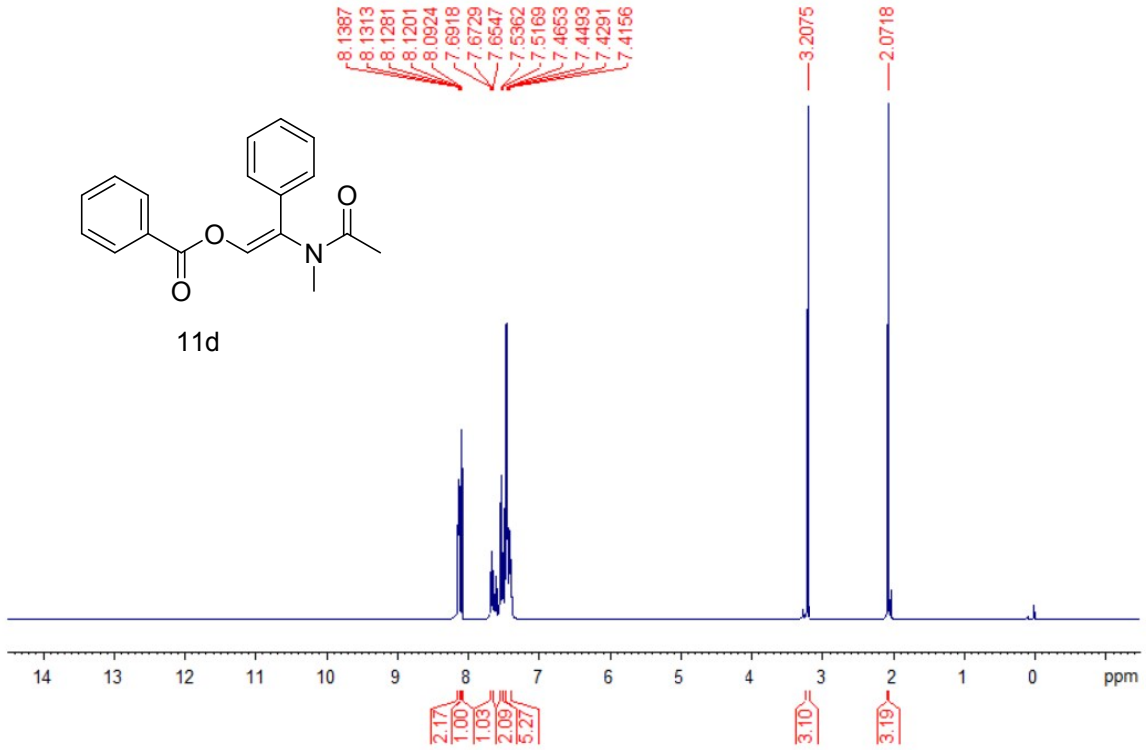
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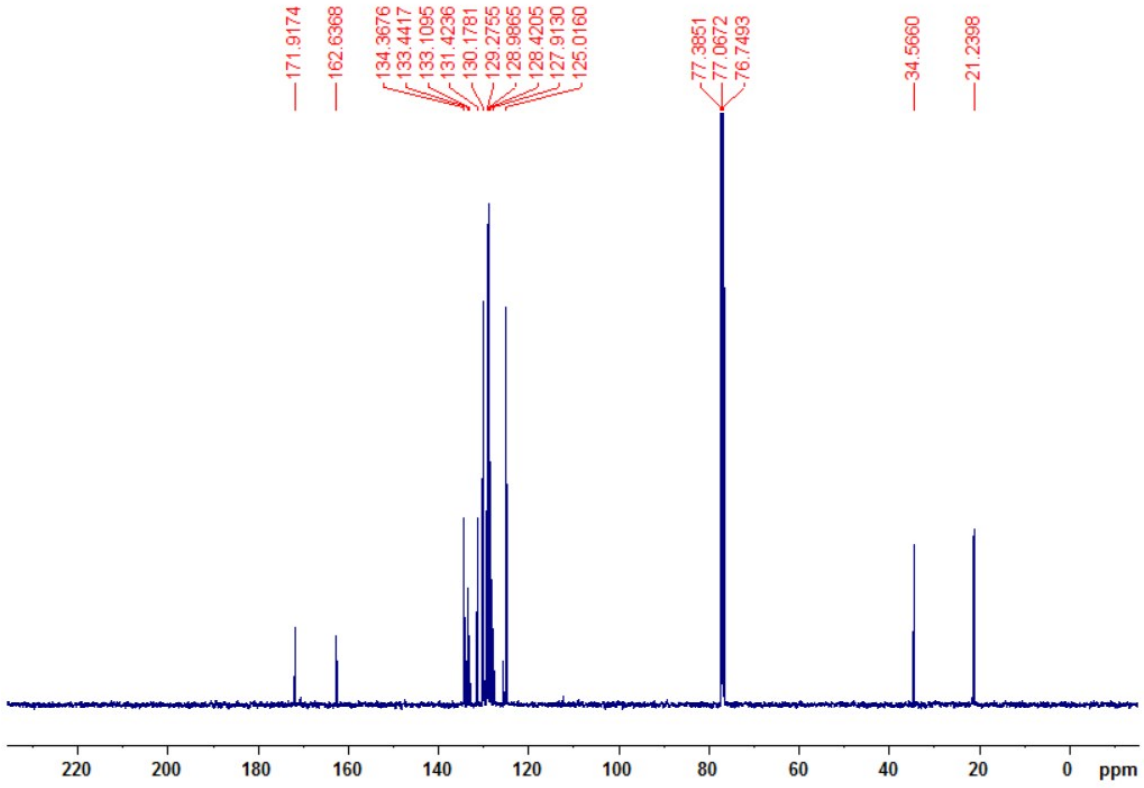
8.1201
8.0924
7.6918
7.6729
7.6547
7.5362
7.5169
7.4653
7.4493
7.4291
7.4156
3.2075
2.0718
O
O
O
N
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
2.17
1.00
1.03
2.09
5.27
3.10
3.19

11d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133.1095
131.4236
130.1781
129.2755
128.9865
128.4205
127.9130
125.0160
77.3851
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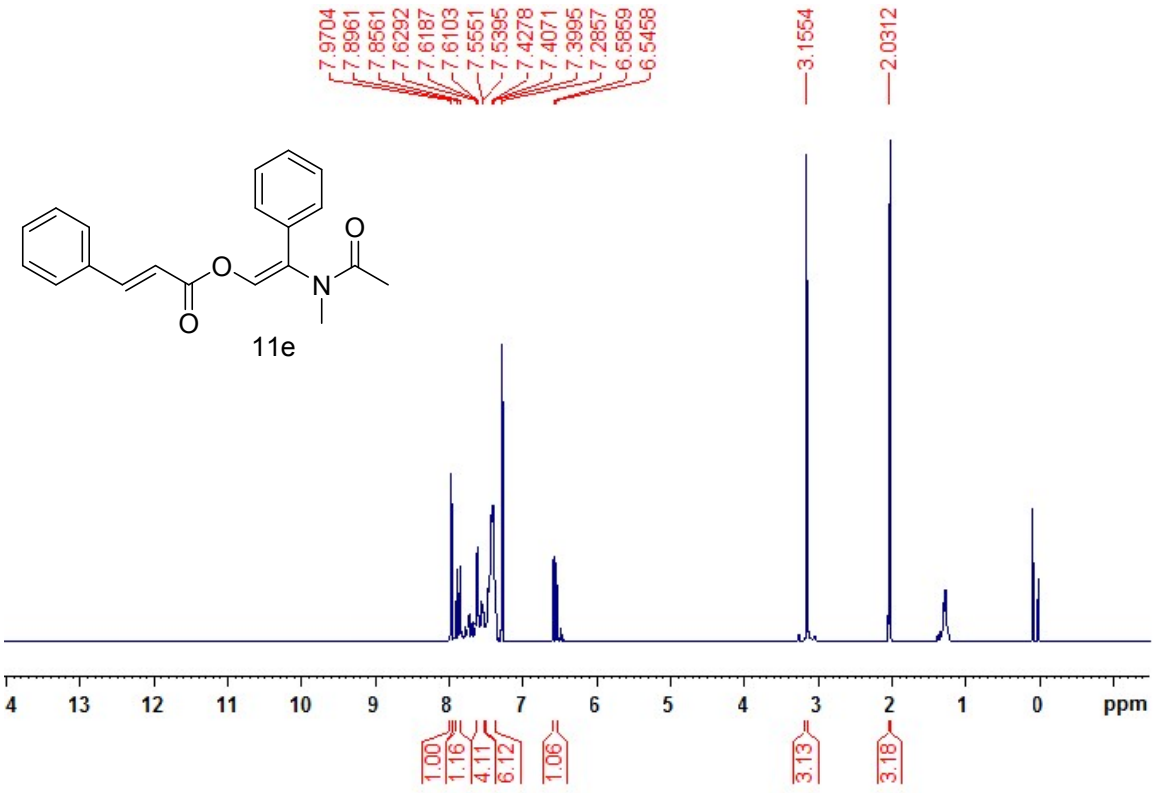
76.7493
34.5660
21.2398
220 200 180 160 140 120 100 80 60 40 20 0 ppm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7.8561
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7.6187
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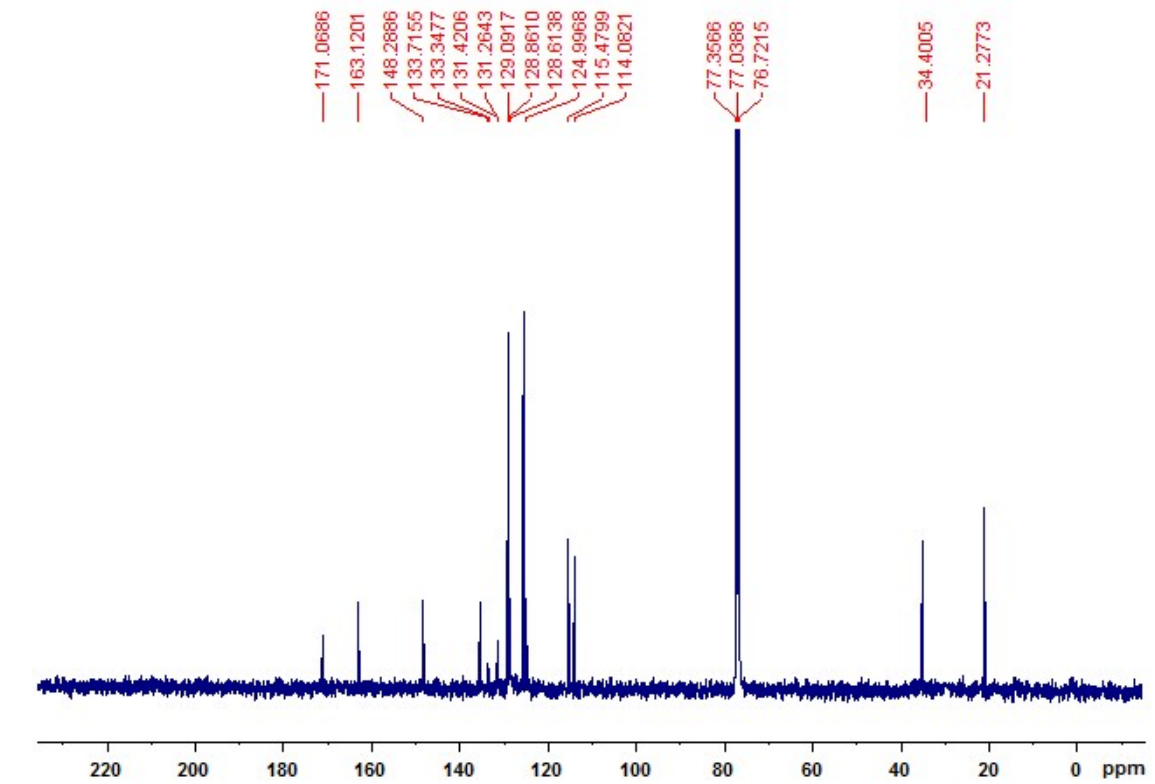
7.5551
7.5395
7.4278
7.4071
7.3995
7.2857
6.5859
6.5458
3.1554
2.0312
O
O
O
N
11e
4
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.16
4.11
6.12
1.06
3.13
3.18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133.3477
131.4206
131.2643
129.0917
128.8610
128.6138
124.9968
115.4799
114.0821
77.3566
77.0388
76.7215
34.4005
21.2773
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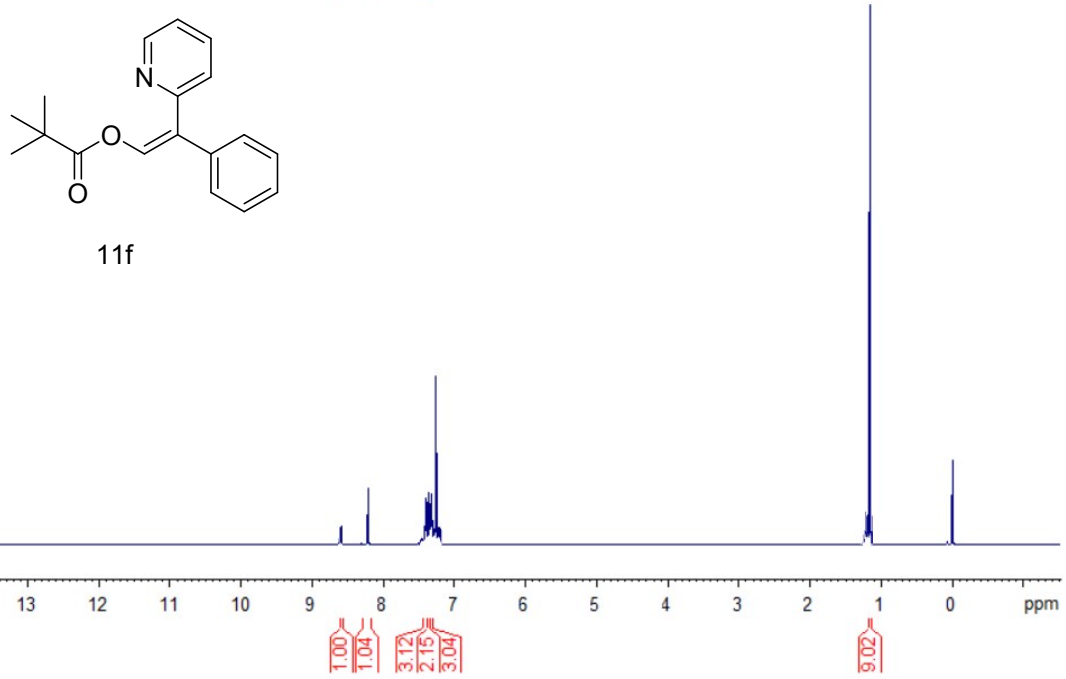
200
180
160
140
120
100
80
60
40
20
0
ppm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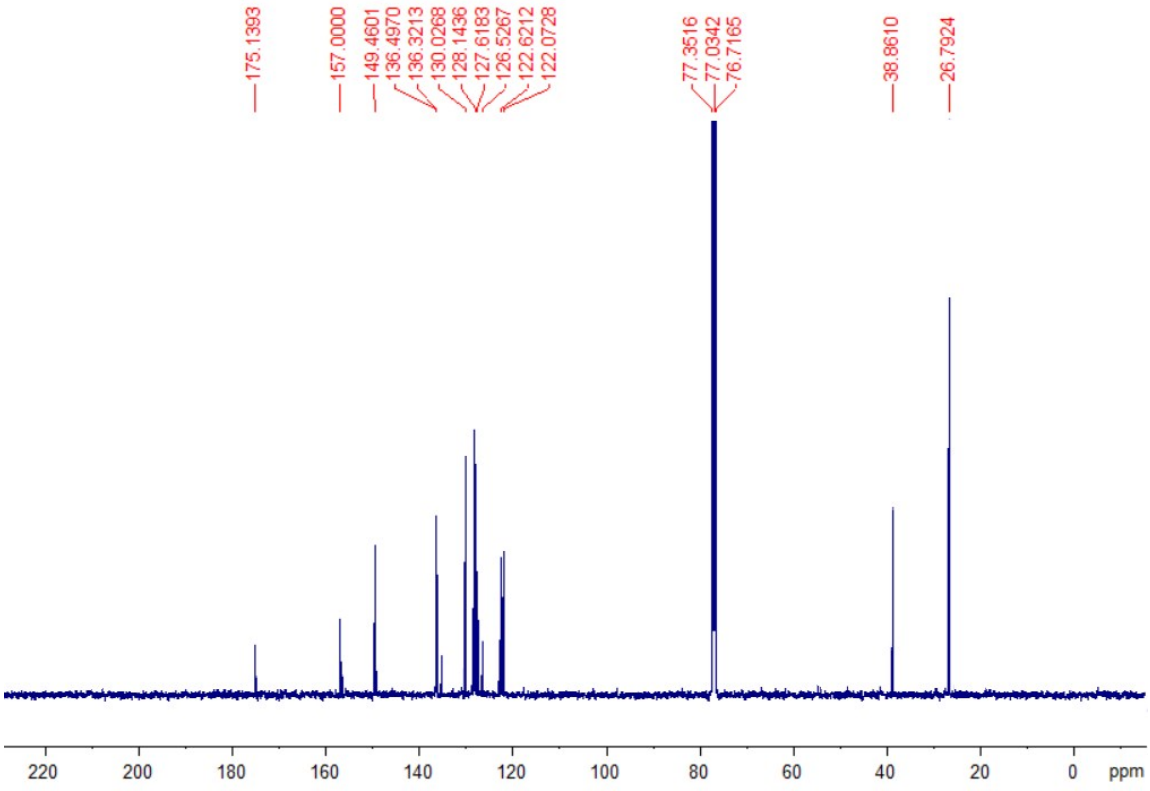
8.5945
8.5894
8.5880
8.2147
7.3871
7.3584
7.3499
7.3381
7.3293
7.3274
7.3158
1.1627
N
O
O
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.04
3.12
2.15
3.04
9.02

11f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136.3213
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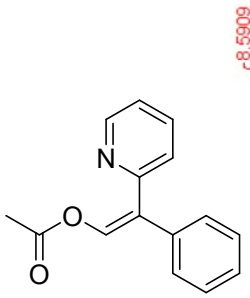
128.1436
127.6183
126.5267
122.6212
122.0728
77.3516
77.0342
76.7165
38.8610
26.7924
220
200
180
160
140
120
100
80
60
40
20
0
ppm


N
O
O

11g

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7.7217
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7.6830
7.5450
7.5254
7.4142
7.3944
7.3787
7.3603
7.2857
7.2529
7.2351
5.7091
1.9905
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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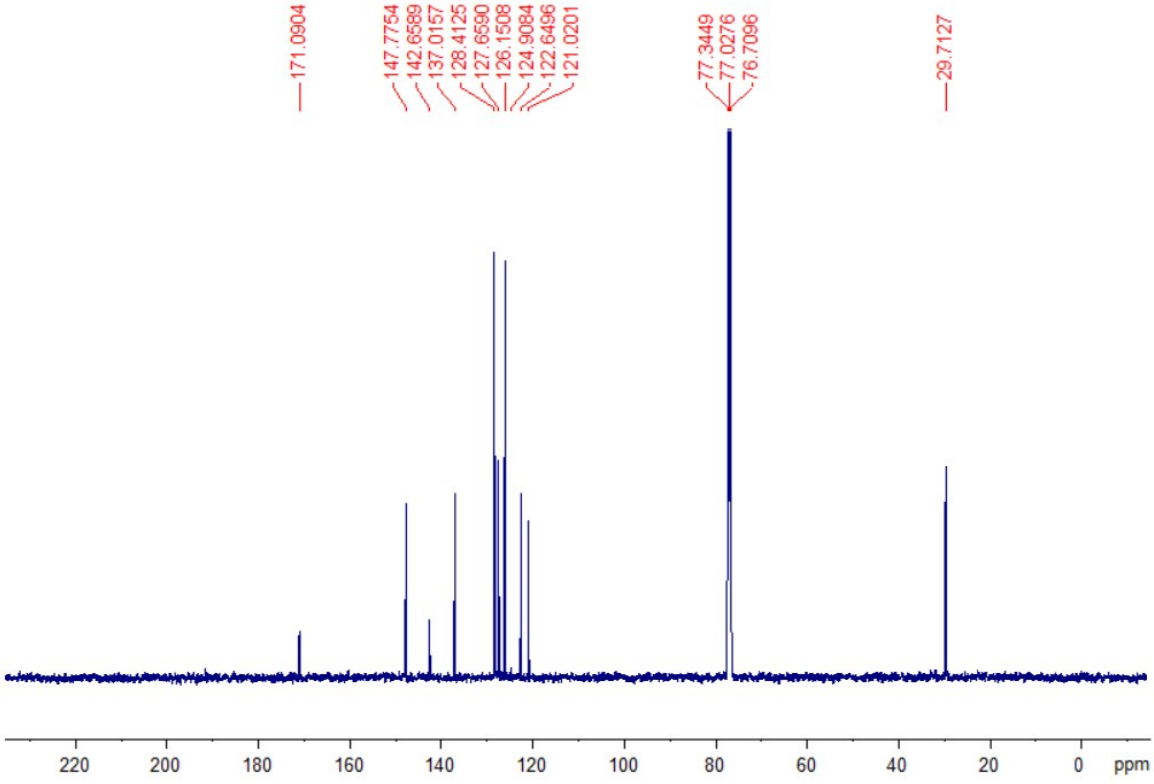
1.08
2.03
3.22
2.00
1.00
3.01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128.4125
127.6590
126.1508
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29.7127
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200
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140
120
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40
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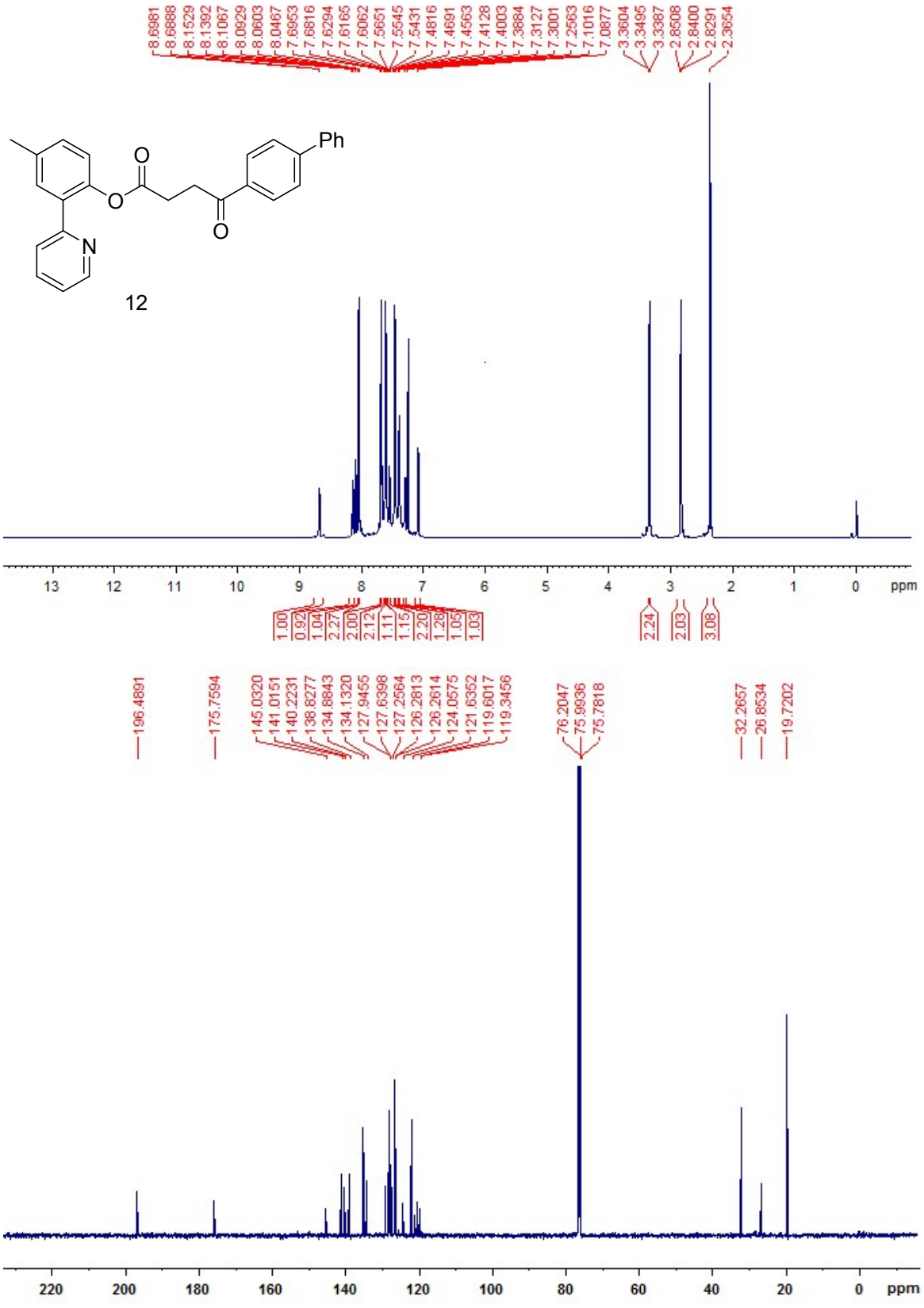
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7.6294
7.6165
7.6062
7.5651
7.5545
7.5431
7.4816
7.4691
7.4563
7.4128
7.4003
7.3884
7.3127
7.3001
7.2563
7.1016
7.0877
3.3604
3.3495
3.3387
2.8508
2.8400
2.8291
2.3654
Ph
O
O
O
N
12
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
0.92
1.04
2.27
2.00
2.12
1.11
1.15
2.20
1.28
1.05
1.03
2.24
2.03
3.08
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175.7594
145.0320
141.0151
140.2231
138.8277
134.8843
134.1320
127.9455
127.6396
127.2564
126.2813
126.2614
124.0575
121.6352
119.6017
119.3456
76.2047
75.9936
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19.7202
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120
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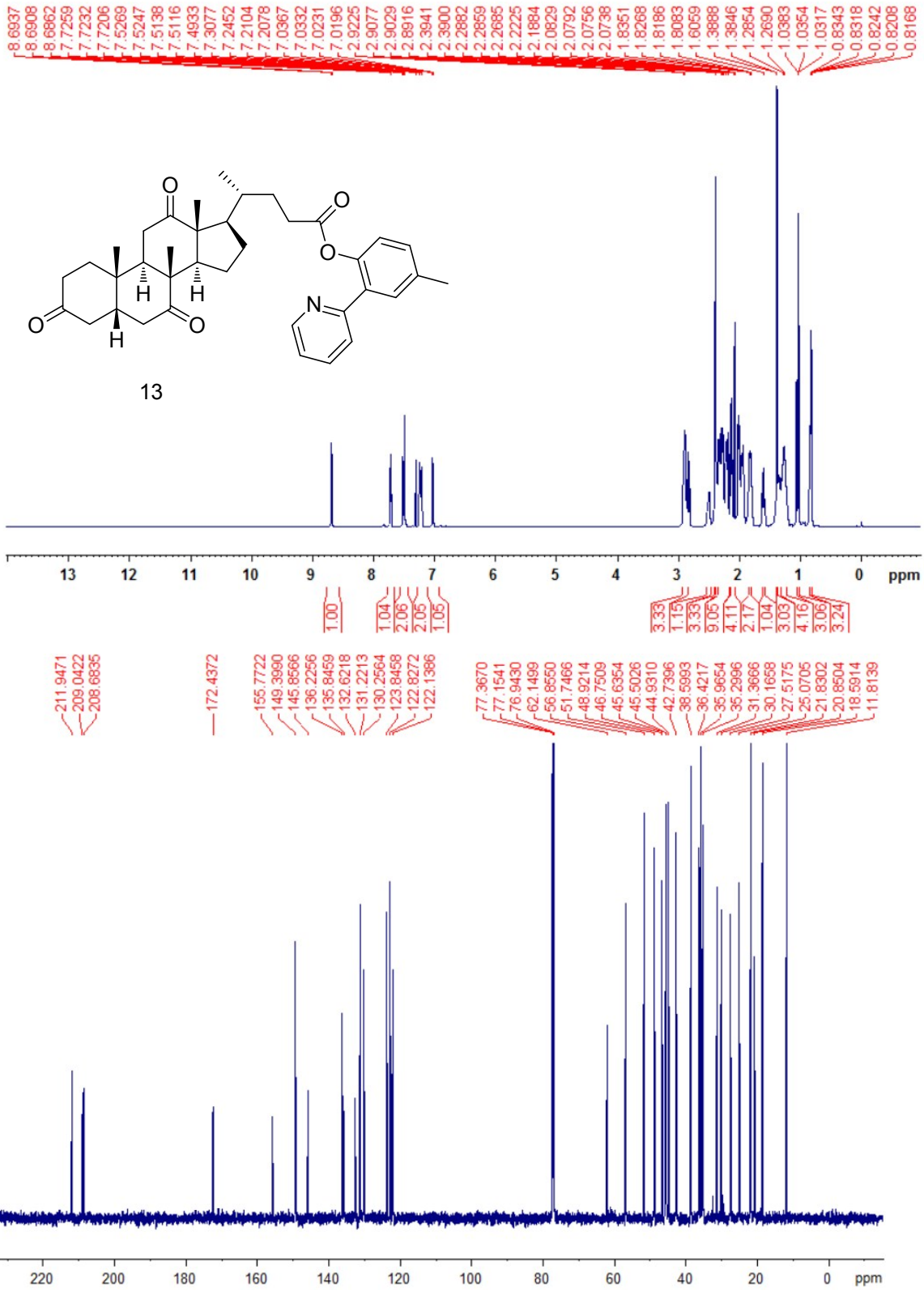
20
0
ppm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7.4933
7.3077
7.2452
7.2104
7.2078
7.0367
7.0332
7.0231
7.0196
2.9225
2.9077
2.9029
2.8916
2.3941
2.3900
2.2882
2.2859
2.2685
2.2225
2.1884
2.0829
2.0792
2.0756
2.0738
1.8351
1.8268
1.8186
1.8083
1.6059
1.3888
1.3846
1.2854
1.2690
1.0383
1.0354
1.0317
0.8343
0.8318
0.8242
0.8208
0.8168
O
O
O
O
H
H
H
O
N
13
13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.04
2.06
2.05
1.05
3.33
1.15
3.33
9.05
4.11
2.17
1.04
3.03
4.16
3.06
3.24
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209.0422
208.6835
172.4372
155.7722
149.3990
145.8566
136.2256
135.8459
132.6218
131.2213
130.2564
123.8458
122.8272
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77.3670
77.1541
76.9430
62.1499
56.8550
51.7466
48.9214
46.7509
45.6354
45.5026
44.9310
42.7396
38.5993
36.4217
35.9654
35.2996
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25.0705
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20.8504
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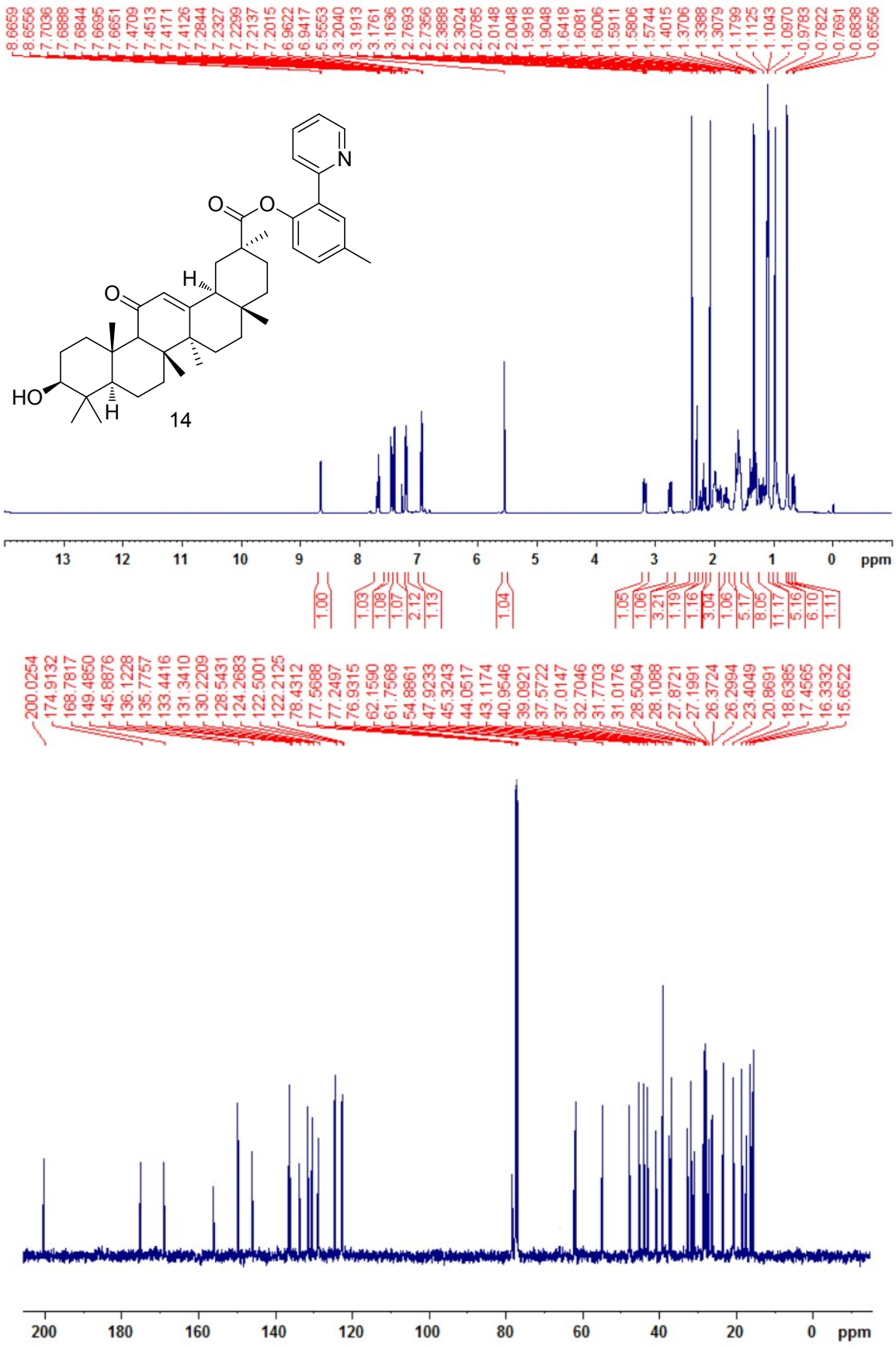
220 200 180 160 140 120 100 80 60 40 20 0 ppm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7.2844
7.2327
7.2299
7.2137
7.2015
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6.9417
5.5553
3.2040
3.1913
3.1761
3.1636
2.7693
2.7356
2.3888
2.3024
2.0785
2.0148
2.0048
1.9918
1.9048
1.6418
1.6081
1.6006
1.5911
1.5806
1.5744
1.4015
1.3706
1.3388
1.3079
1.1799
1.1125
1.1043
1.0970
0.9783
0.7822
0.7691
0.6838
0.6556
N
O
O
H
O
HO
H
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.03
1.08
1.07
2.12
1.13
1.04
1.05
1.06
3.21
1.19
1.16
3.04
1.06
5.17
8.05
11.17
5.16
6.10
1.11
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135.7757
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43.1174
40.9546
39.0921
37.5722
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32.7046
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28.5094
28.1088
27.8721
27.1991
26.3724
26.2994
23.4049
20.8691
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200
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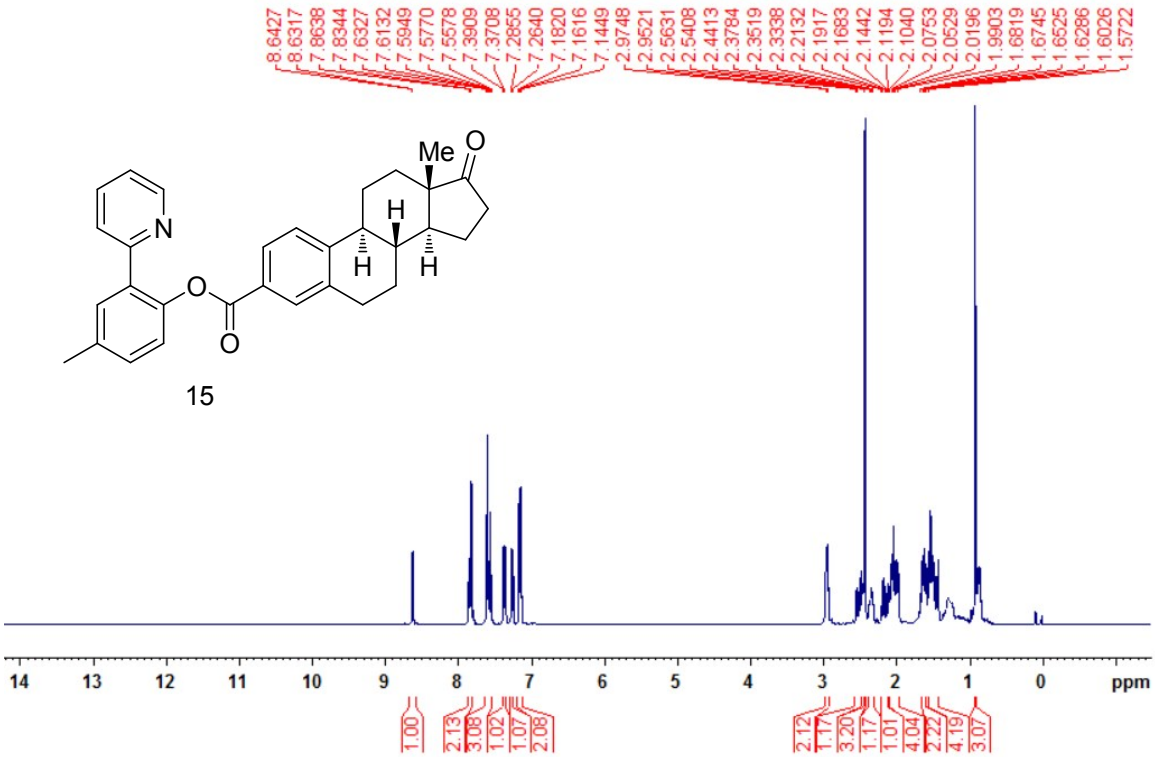
40
20
0
ppm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7.3708
7.2855
7.2640
7.1820
7.1616
7.1449
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2.9521
2.5631
2.5408
2.4413
2.3784
2.3519
2.3338
2.2132
2.1917
2.1683
2.1442
2.1194
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2.0753
2.0529
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1.9903
1.6819
1.6745
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1.6286
1.6026
1.5722
Me
O
N
H
H
H
O
O
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.13
3.08
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2.12
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3.20
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1.01
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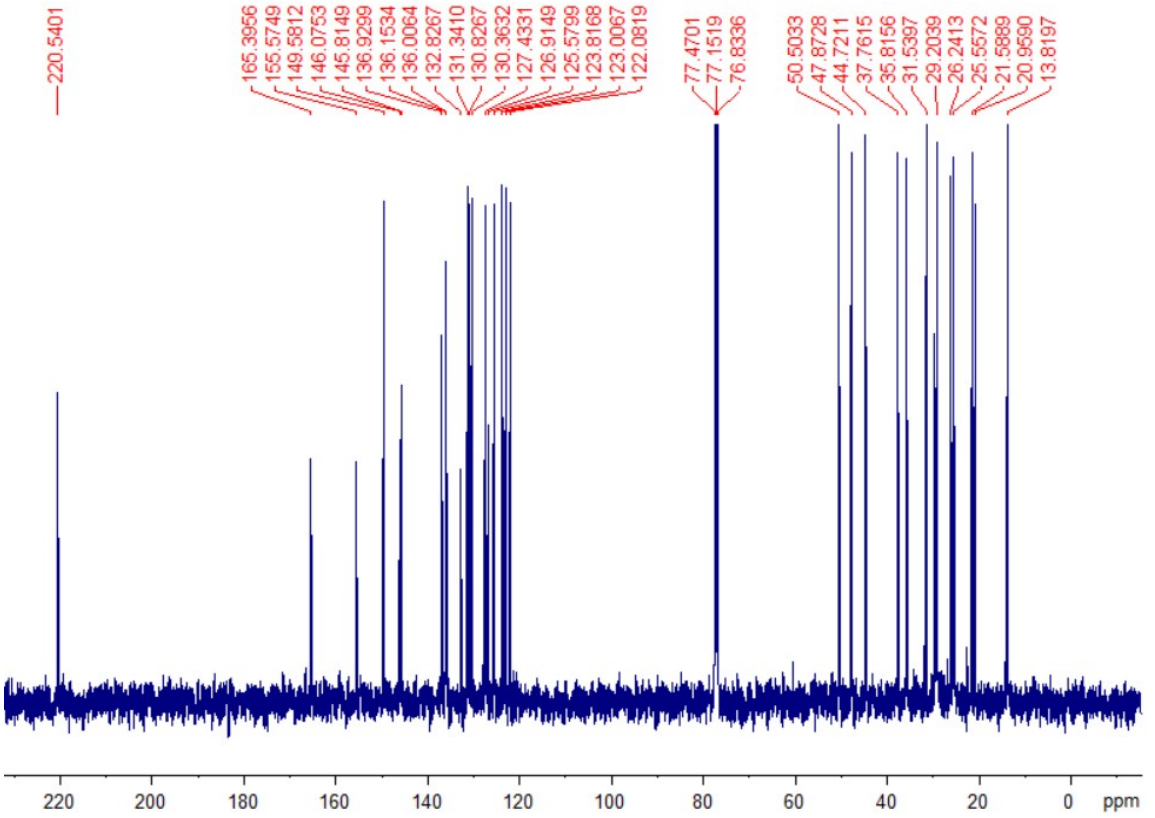
2.22
4.19
3.07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126.9149
125.5799
123.8168
123.0067
122.0819
77.4701
77.1519
76.8336
50.5033
47.8728
44.7211
37.7615
35.8156
31.5397
29.2039
26.2413
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13.8197
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200
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120
100
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40
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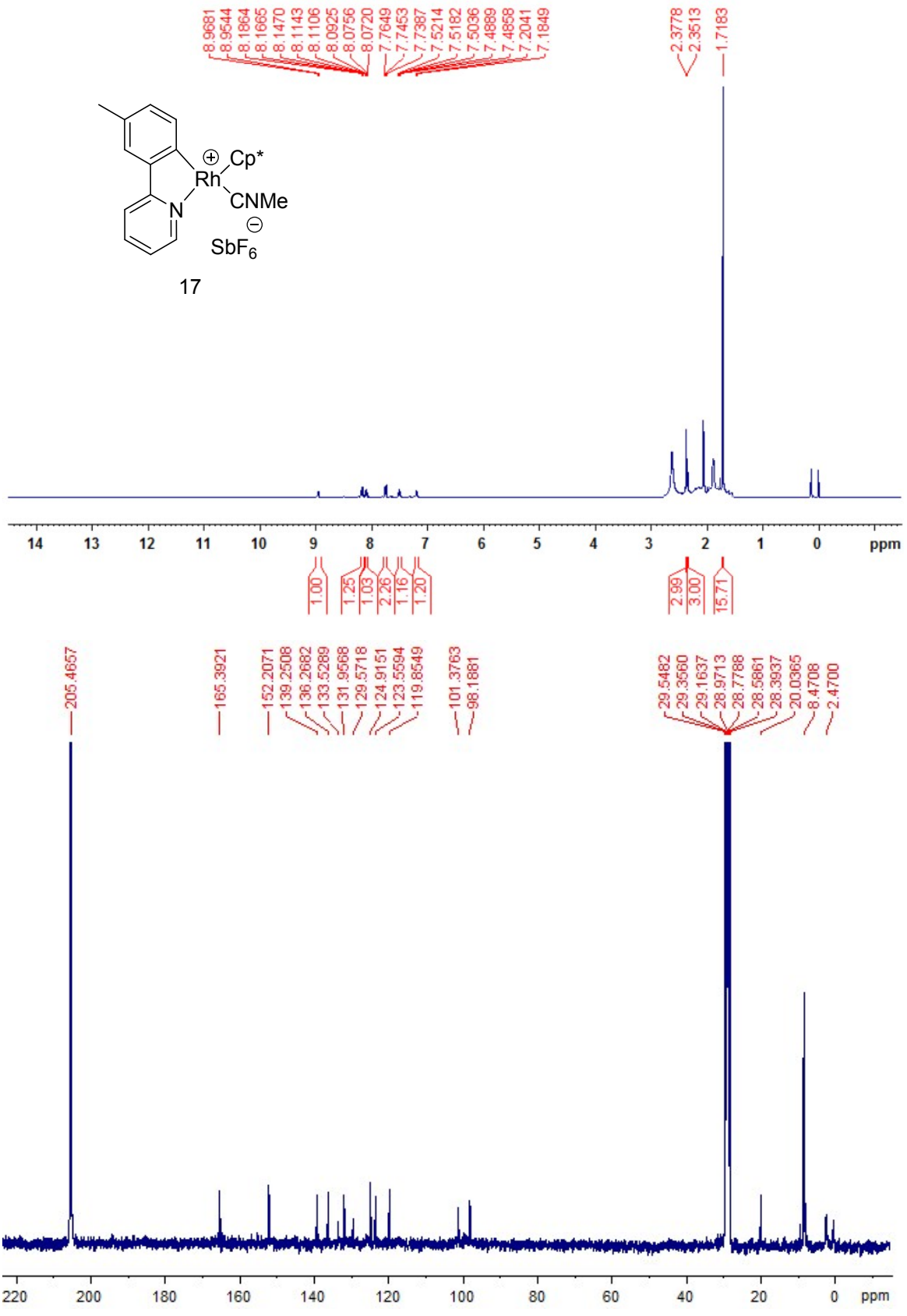
ppm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8.0756
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7.7649
7.7453
7.7387
7.5214
7.5182
7.5036
7.4889
7.4858
7.2041
7.1849
2.3778
2.3513
1.7183
Cp*
Rh
CNMe
N
SbF6
17
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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1.25
1.03
2.26
1.16
1.20
2.99
3.00
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165.3921
152.2071
139.2508
136.2682
133.5289
131.9568
129.5718
124.9151
123.5594
119.8549
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29.1637
28.9713
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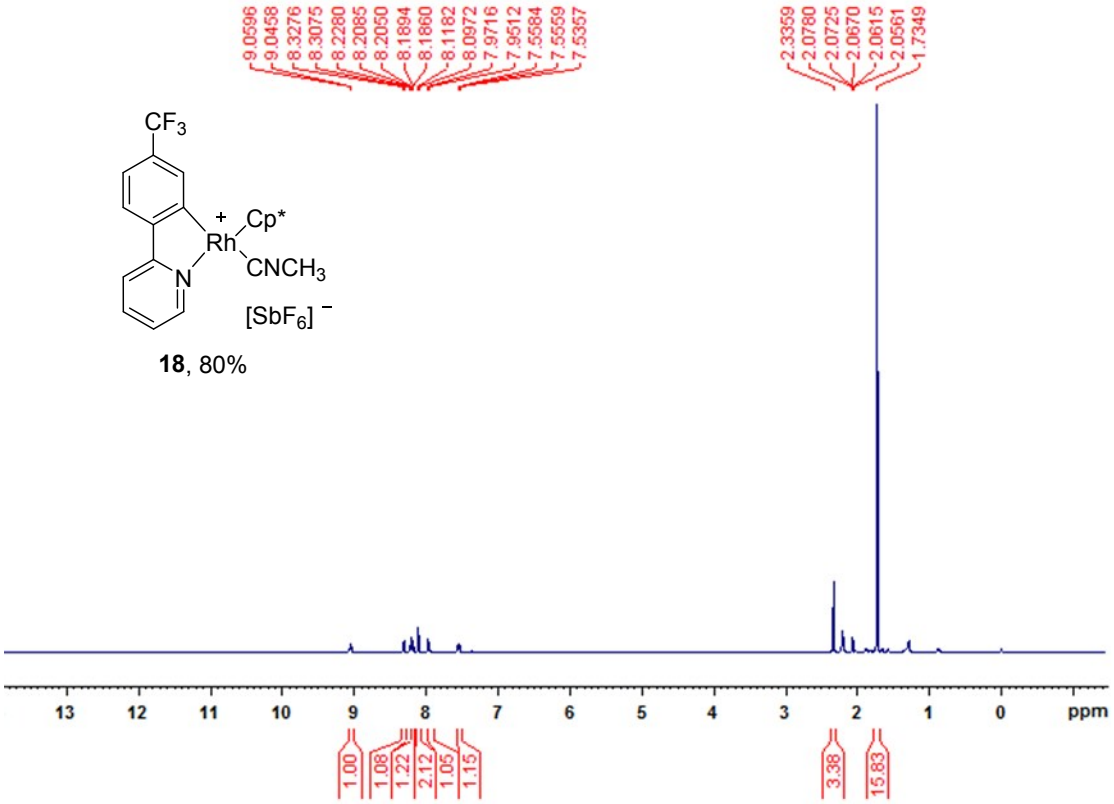
ppm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8.2050
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8.1860
8.1182
8.0972
7.9716
7.9512
7.5584
7.5559
7.5357
2.3359
2.0780
2.0725
2.0670
2.0615
2.0561
1.7349
CF3
Rh
Cp*
CNCH3
N
[SbF6] −
13
12
11
10
9
8
7
6
5
4
3
2
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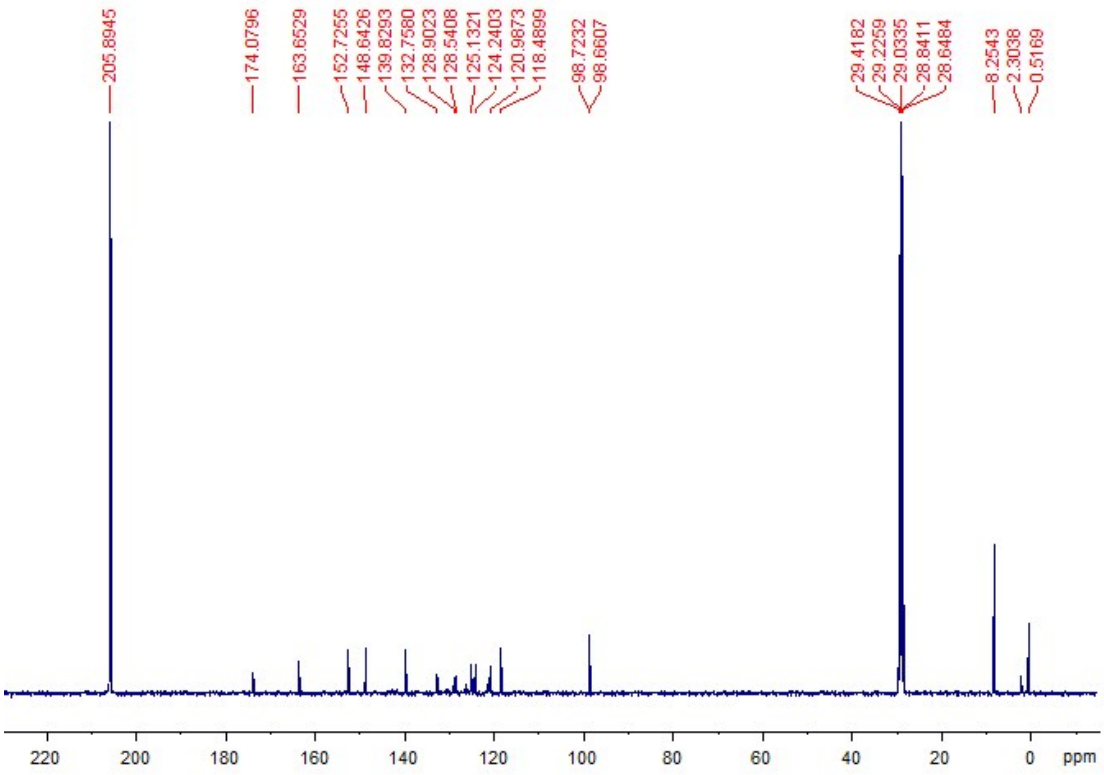
ppm
1.00
1.08
1.22
2.12
1.05
1.15
3.38
15.83

18, 80%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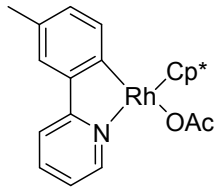
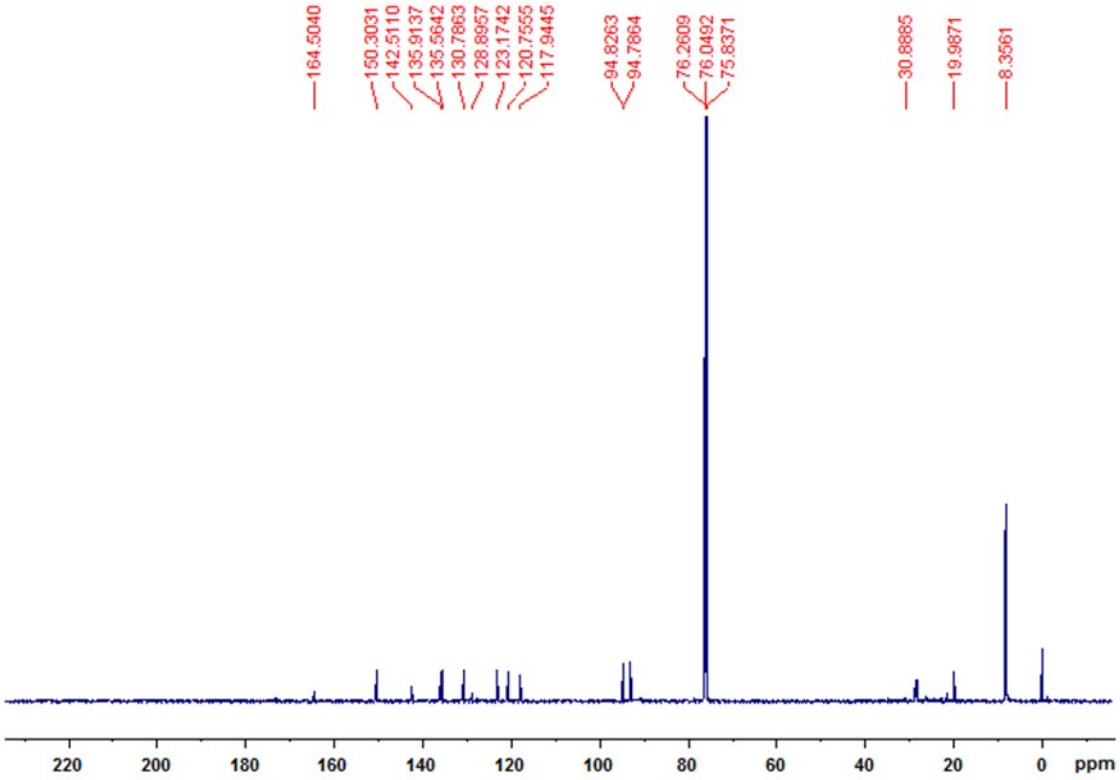
125.1321
124.2403
120.9873
118.4899
98.7232
98.6607
29.4182
29.2259
29.0335
28.8411
28.6484
8.2543
2.3038
0.5169
220
200
180
160
140
120
100
80
60
40
20
0
ppm


Cp*
Rh
OAc
N

19, 88%

8.7640
8.7501
7.8708
7.8546
7.7876
7.7676
7.4528
7.2858
7.1470
7.1286
7.1048
2.3607
1.6686
1.6499
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.01
1.14
2.20
1.00
2.00
3.06
3.35
15.16


164.5040
150.3031
142.5110
135.9137
135.5642
130.7863
128.8957
123.1742
120.7555
117.9445
94.8263
94.7864
76.2609
76.0492
75.8371
30.8885
19.9871
8.3561
220 200 180 160 140 120 100 80 60 40 20 0 ppm

8. X-ray Data

Table 1. Crystal data and structure refinement for zzyccj5.

Identification code	1	
Empirical formula	C2.44 H1.78 N0.22 O0.22	
Formula weight	37.82	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.1832(10) Å	α= 99.499(6)°.
	b = 10.3531(16) Å	β= 102.356(6)°.
	c = 12.7041(18) Å	γ = 98.881(5)°.
Volume	892.4(2) $Å^3$	
Z	18	
Density (calculated)	1.267 mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	356	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.89 to 26.43°.	
Index ranges	-8<=h<=8, -12<=k<=12, -15<=l<=15	
Reflections collected	15137	
Independent reflections	3627 [R(int) = 0.0323]	
Completeness to theta = 26.43°	99.2 %;	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9837 and 0.9837	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3627 / 0 / 236	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0369, wR2 = 0.0949	
R indices (all data)	R1 = 0.0429, wR2 = 0.0987	
Largest diff. peak and hole	0.234 and -0.187 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1160(1)	2998(1)	7601(1)	22(1)
O(2)	1290(1)	1594(1)	6070(1)	24(1)
C(1)	-9615(2)	-3222(1)	5808(1)	23(1)
N(1)	-11076(2)	-3890(1)	5754(1)	30(1)
C(2)	-7340(2)	-1076(1)	6506(1)	22(1)
C(3)	-4699(2)	-2034(1)	5419(1)	22(1)
C(4)	4478(2)	3274(1)	8610(1)	22(1)
C(5)	-5578(2)	-262(1)	6587(1)	21(1)
C(6)	-4226(2)	-733(1)	6053(1)	19(1)
C(7)	3134(2)	3556(1)	7755(1)	21(1)
C(8)	-7774(2)	-2379(1)	5888(1)	20(1)
C(9)	6410(2)	3934(1)	8810(1)	25(1)
C(10)	-2333(2)	88(1)	6116(1)	19(1)
N(2)	2729(2)	1158(1)	8786(1)	28(1)
C(11)	-6456(2)	-2860(1)	5334(1)	23(1)
C(12)	3680(2)	4420(1)	7104(1)	24(1)
C(13)	420(2)	1926(1)	6746(1)	19(1)
C(14)	-1524(2)	1267(1)	6785(1)	21(1)
C(15)	7004(2)	4821(1)	8179(1)	26(1)
C(16)	5619(2)	5042(1)	7311(1)	26(1)
C(17)	9088(2)	5561(2)	8456(1)	37(1)
C(18)	4656(2)	2654(1)	10444(1)	30(1)
C(19)	2267(2)	300(1)	9413(1)	35(1)
C(20)	3927(2)	2328(1)	9306(1)	23(1)
C(21)	4133(2)	1751(2)	11070(1)	38(1)
C(22)	2920(2)	547(2)	10547(1)	39(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

O(1)-C(13)	1.3664(14)
O(1)-C(7)	1.4048(14)
O(2)-C(13)	1.2014(15)
C(1)-N(1)	1.1462(16)
C(1)-C(8)	1.4417(16)
C(2)-C(5)	1.3818(16)
C(2)-C(8)	1.3964(17)
C(3)-C(11)	1.3832(17)
C(3)-C(6)	1.4004(17)
C(4)-C(7)	1.3923(17)
C(4)-C(9)	1.3987(17)
C(4)-C(20)	1.4885(17)
C(5)-C(6)	1.4001(16)
C(6)-C(10)	1.4675(16)
C(7)-C(12)	1.3833(17)
C(8)-C(11)	1.3975(17)
C(9)-C(15)	1.3913(19)
C(10)-C(14)	1.3322(17)
N(2)-C(19)	1.3373(18)
N(2)-C(20)	1.3471(16)
C(12)-C(16)	1.3909(18)
C(13)-C(14)	1.4711(16)
C(15)-C(16)	1.3941(19)
C(15)-C(17)	1.5109(18)
C(18)-C(21)	1.383(2)
C(18)-C(20)	1.3923(18)
C(19)-C(22)	1.383(2)
C(21)-C(22)	1.378(2)

C(13)-O(1)-C(7)	115.47(9)
N(1)-C(1)-C(8)	179.35(13)
C(5)-C(2)-C(8)	119.69(11)
C(11)-C(3)-C(6)	120.96(11)
C(7)-C(4)-C(9)	117.27(11)
C(7)-C(4)-C(20)	122.69(11)
C(9)-C(4)-C(20)	120.04(11)

C(2)-C(5)-C(6)	120.52(11)
C(5)-C(6)-C(3)	119.05(11)
C(5)-C(6)-C(10)	122.66(11)
C(3)-C(6)-C(10)	118.28(11)
C(12)-C(7)-C(4)	121.86(11)
C(12)-C(7)-O(1)	119.71(11)
C(4)-C(7)-O(1)	118.32(11)
C(2)-C(8)-C(11)	120.61(11)
C(2)-C(8)-C(1)	119.33(11)
C(11)-C(8)-C(1)	120.05(11)
C(15)-C(9)-C(4)	122.34(12)
C(14)-C(10)-C(6)	126.80(11)
C(19)-N(2)-C(20)	116.97(12)
C(3)-C(11)-C(8)	119.15(11)
C(7)-C(12)-C(16)	119.48(12)
O(2)-C(13)-O(1)	122.79(10)
O(2)-C(13)-C(14)	126.26(11)
O(1)-C(13)-C(14)	110.95(10)
C(10)-C(14)-C(13)	118.81(11)
C(9)-C(15)-C(16)	118.40(12)
C(9)-C(15)-C(17)	120.60(12)
C(16)-C(15)-C(17)	120.97(12)
C(12)-C(16)-C(15)	120.61(12)
C(21)-C(18)-C(20)	119.11(13)
N(2)-C(19)-C(22)	124.28(14)
N(2)-C(20)-C(18)	122.46(12)
N(2)-C(20)-C(4)	117.17(11)
C(18)-C(20)-C(4)	120.36(11)
C(22)-C(21)-C(18)	118.99(13)
C(21)-C(22)-C(19)	118.18(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	17(1)	21(1)	23(1)	-1(1)	4(1)	-1(1)
O(2)	21(1)	25(1)	24(1)	0(1)	8(1)	-1(1)
C(1)	23(1)	22(1)	24(1)	6(1)	6(1)	4(1)
N(1)	24(1)	29(1)	37(1)	6(1)	10(1)	-2(1)
C(2)	19(1)	24(1)	23(1)	6(1)	6(1)	4(1)
C(3)	19(1)	22(1)	26(1)	4(1)	7(1)	4(1)
C(4)	23(1)	20(1)	19(1)	-1(1)	5(1)	2(1)
C(5)	20(1)	19(1)	21(1)	3(1)	4(1)	3(1)
C(6)	17(1)	20(1)	19(1)	6(1)	2(1)	3(1)
C(7)	18(1)	19(1)	21(1)	-2(1)	4(1)	-1(1)
C(8)	17(1)	21(1)	22(1)	8(1)	3(1)	1(1)
C(9)	22(1)	28(1)	22(1)	2(1)	2(1)	3(1)
C(10)	17(1)	22(1)	20(1)	7(1)	4(1)	4(1)
N(2)	31(1)	25(1)	28(1)	4(1)	9(1)	1(1)
C(11)	22(1)	18(1)	27(1)	3(1)	5(1)	1(1)
C(12)	25(1)	24(1)	20(1)	2(1)	2(1)	1(1)
C(13)	19(1)	18(1)	19(1)	4(1)	2(1)	3(1)
C(14)	18(1)	23(1)	22(1)	4(1)	6(1)	3(1)
C(15)	22(1)	27(1)	26(1)	-1(1)	6(1)	-1(1)
C(16)	28(1)	25(1)	24(1)	4(1)	8(1)	-2(1)
C(17)	24(1)	42(1)	40(1)	6(1)	5(1)	-6(1)
C(18)	33(1)	30(1)	24(1)	5(1)	4(1)	9(1)
C(19)	38(1)	28(1)	42(1)	10(1)	15(1)	3(1)
C(20)	22(1)	24(1)	24(1)	4(1)	7(1)	7(1)
C(21)	47(1)	44(1)	27(1)	13(1)	9(1)	16(1)
C(22)	47(1)	39(1)	42(1)	23(1)	20(1)	14(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for 1.

	x	y	z	U(eq)
H(2)	-8252	-751	6870	26
H(3)	-3801	-2353	5041	26
H(5)	-5283	625	7007	25
H(9)	7350	3771	9397	30
H(10)	-1608	-255	5629	23
H(11)	-6762	-3742	4905	27
H(12)	2737	4587	6520	29
H(14)	-2190	1674	7278	25
H(16)	6002	5623	6856	32
H(17A)	9222	6427	8943	56
H(17B)	9454	5702	7777	56
H(17C)	9941	5034	8827	56
H(18)	5502	3487	10786	35
H(19)	1436	-533	9056	42
H(21)	4602	1957	11848	45
H(22)	2543	-97	10954	47

Table 6. Torsion angles [°] for zzycc*J*5.

Table 1. Crystal data and structure refinement for zzyccj4

Identification code	1	
Empirical formula	C3.80 H2.80 Br0.20 N0.20 O0.40	
Formula weight	73.64	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.1209(10) Å	α= 90°.
	b = 6.8257(5) Å	β= 100.200(3)°.
	c = 14.2218(10) Å	γ = 90°.
Volume	1635.72(19) $Å^3$	
Z	20	
Density (calculated)	1.495 mg/m^3	
Absorption coefficient	2.522 mm^{-1}	
F(000)	744	
Crystal size	0.35 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.91 to 26.38°.	
Index ranges	-21<=h<=21, -7<=k<=8, -17<=l<=17	
Reflections collected	12488	
Independent reflections	3326 [R(int) = 0.0370]	
Completeness to theta = 26.38°	98.9 %;	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6325 and 0.4723	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3326 / 0 / 209	
Goodness-of-fit on F^2	1.016	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0917	
R indices (all data)	R1 = 0.0480, wR2 = 0.0987	
Largest diff. peak and hole	0.332 and -0.708 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	11282(1)	3567(1)	4424(1)	65(1)
O(1)	7660(1)	-456(2)	2897(1)	40(1)
O(2)	8377(1)	-3212(3)	2857(2)	56(1)
C(7)	8349(1)	-1493(3)	3007(2)	38(1)
C(14)	6561(1)	-850(3)	1607(2)	37(1)
C(15)	6848(1)	800(3)	1074(2)	34(1)
C(8)	6953(1)	-1432(3)	2504(2)	37(1)
N(1)	6876(1)	496(3)	152(1)	46(1)
C(4)	9040(1)	-213(3)	3344(2)	38(1)
C(12)	5863(1)	-1841(4)	1228(2)	48(1)
C(9)	6652(2)	-2864(4)	3028(2)	47(1)
C(16)	7048(2)	2589(3)	1516(2)	44(1)
C(2)	10456(2)	56(4)	3825(2)	54(1)
C(3)	9794(2)	-1057(4)	3505(2)	50(1)
C(5)	8970(2)	1777(4)	3493(2)	50(1)
C(10)	5955(2)	-3776(4)	2634(2)	55(1)
C(1)	10370(1)	2027(4)	3981(2)	45(1)
C(11)	5551(2)	-3296(4)	1726(2)	56(1)
C(19)	7122(2)	1987(4)	-328(2)	55(1)
C(17)	7289(2)	4105(4)	997(2)	50(1)
C(18)	7333(2)	3803(4)	60(2)	52(1)
C(6)	9636(2)	2902(4)	3818(2)	56(1)
C(13)	4793(2)	-4333(6)	1301(3)	93(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

Br(1)-C(1)	1.897(2)
O(1)-C(7)	1.361(3)
O(1)-C(8)	1.407(3)
O(2)-C(7)	1.195(3)
C(7)-C(4)	1.481(3)
C(14)-C(8)	1.390(3)
C(14)-C(12)	1.396(3)
C(14)-C(15)	1.489(3)
C(15)-N(1)	1.336(3)
C(15)-C(16)	1.389(3)
C(8)-C(9)	1.383(3)
N(1)-C(19)	1.335(3)
C(4)-C(5)	1.383(3)
C(4)-C(3)	1.395(3)
C(12)-C(11)	1.381(4)
C(12)-H(12)	0.9500
C(9)-C(10)	1.375(4)
C(9)-H(9)	0.9500
C(16)-C(17)	1.376(3)
C(16)-H(16)	0.9500
C(2)-C(3)	1.372(4)
C(2)-C(1)	1.376(4)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(5)-C(6)	1.385(4)
C(5)-H(5)	0.9500
C(10)-C(11)	1.392(4)
C(10)-H(10)	0.9500
C(1)-C(6)	1.372(4)
C(11)-C(13)	1.508(4)
C(19)-C(18)	1.379(4)
C(19)-H(19)	0.9500
C(17)-C(18)	1.364(4)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(6)-H(6)	0.9500

C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(7)-O(1)-C(8)	117.78(17)
O(2)-C(7)-O(1)	123.5(2)
O(2)-C(7)-C(4)	125.6(2)
O(1)-C(7)-C(4)	110.93(18)
C(8)-C(14)-C(12)	117.2(2)
C(8)-C(14)-C(15)	122.3(2)
C(12)-C(14)-C(15)	120.4(2)
N(1)-C(15)-C(16)	122.2(2)
N(1)-C(15)-C(14)	117.02(19)
C(16)-C(15)-C(14)	120.77(19)
C(9)-C(8)-C(14)	122.1(2)
C(9)-C(8)-O(1)	119.8(2)
C(14)-C(8)-O(1)	118.04(19)
C(19)-N(1)-C(15)	116.9(2)
C(5)-C(4)-C(3)	118.9(2)
C(5)-C(4)-C(7)	122.9(2)
C(3)-C(4)-C(7)	118.2(2)
C(11)-C(12)-C(14)	122.2(2)
C(11)-C(12)-H(12)	118.9
C(14)-C(12)-H(12)	118.9
C(10)-C(9)-C(8)	118.7(2)
C(10)-C(9)-H(9)	120.7
C(8)-C(9)-H(9)	120.7
C(17)-C(16)-C(15)	119.4(2)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(3)-C(2)-C(1)	119.2(2)
C(3)-C(2)-H(2)	120.4
C(1)-C(2)-H(2)	120.4
C(2)-C(3)-C(4)	120.8(2)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(4)-C(5)-C(6)	120.5(2)
C(4)-C(5)-H(5)	119.8

C(6)-C(5)-H(5)	119.8
C(9)-C(10)-C(11)	121.6(2)
C(9)-C(10)-H(10)	119.2
C(11)-C(10)-H(10)	119.2
C(6)-C(1)-C(2)	121.3(2)
C(6)-C(1)-Br(1)	119.4(2)
C(2)-C(1)-Br(1)	119.35(19)
C(12)-C(11)-C(10)	118.2(2)
C(12)-C(11)-C(13)	121.0(3)
C(10)-C(11)-C(13)	120.8(3)
N(1)-C(19)-C(18)	124.4(2)
N(1)-C(19)-H(19)	117.8
C(18)-C(19)-H(19)	117.8
C(18)-C(17)-C(16)	118.9(2)
C(18)-C(17)-H(17)	120.5
C(16)-C(17)-H(17)	120.5
C(17)-C(18)-C(19)	118.1(2)
C(17)-C(18)-H(18)	120.9
C(19)-C(18)-H(18)	120.9
C(1)-C(6)-C(5)	119.3(2)
C(1)-C(6)-H(6)	120.3
C(5)-C(6)-H(6)	120.3
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	57(1)	70(1)	66(1)	-14(1)	9(1)	-19(1)
O(1)	40(1)	37(1)	42(1)	-2(1)	2(1)	3(1)
O(2)	51(1)	40(1)	75(1)	-12(1)	5(1)	4(1)
C(7)	43(1)	40(1)	32(1)	0(1)	6(1)	5(1)
C(14)	36(1)	35(1)	41(1)	0(1)	9(1)	2(1)
C(15)	29(1)	38(1)	35(1)	1(1)	4(1)	2(1)
C(8)	38(1)	35(1)	40(1)	-2(1)	10(1)	3(1)
N(1)	55(1)	48(1)	34(1)	-3(1)	5(1)	-9(1)
C(4)	41(1)	39(1)	32(1)	1(1)	6(1)	3(1)
C(12)	39(1)	48(1)	55(2)	3(1)	2(1)	-4(1)
C(9)	54(1)	41(1)	49(1)	7(1)	16(1)	5(1)
C(16)	58(1)	39(1)	38(1)	-4(1)	13(1)	2(1)
C(2)	42(1)	54(2)	65(2)	-4(1)	5(1)	5(1)
C(3)	46(1)	41(1)	62(2)	-4(1)	4(1)	6(1)
C(5)	45(1)	42(1)	62(2)	-1(1)	8(1)	6(1)
C(10)	55(2)	43(1)	72(2)	10(1)	27(1)	-2(1)
C(1)	46(1)	51(1)	40(1)	-4(1)	9(1)	-7(1)
C(11)	41(1)	49(2)	78(2)	2(1)	14(1)	-6(1)
C(19)	68(2)	64(2)	33(1)	2(1)	8(1)	-12(1)
C(17)	60(2)	34(1)	56(2)	-1(1)	7(1)	-4(1)
C(18)	56(1)	49(2)	48(1)	13(1)	6(1)	-10(1)
C(6)	55(2)	39(1)	73(2)	-7(1)	14(1)	-3(1)
C(13)	63(2)	90(3)	122(3)	11(2)	4(2)	-34(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for 1.

	x	y	z	U(eq)
H(12)	5593	-1502	607	57
H(9)	6922	-3211	3648	56
H(16)	7020	2765	2172	53
H(2)	10968	-529	3936	65
H(3)	9850	-2417	3393	60
H(5)	8461	2376	3373	60
H(10)	5743	-4758	2991	66
H(19)	7154	1783	-981	66
H(17)	7422	5343	1287	60
H(18)	7505	4814	-315	62
H(6)	9587	4265	3927	67
H(13A)	4516	-3582	755	140
H(13B)	4452	-4447	1784	140
H(13C)	4917	-5643	1088	140

Table 6. Torsion angles [°] for 1.

C(8)-O(1)-C(7)-O(2)	-5.8(3)
C(8)-O(1)-C(7)-C(4)	174.78(17)
C(8)-C(14)-C(15)-N(1)	133.4(2)
C(12)-C(14)-C(15)-N(1)	-48.7(3)
C(8)-C(14)-C(15)-C(16)	-48.7(3)
C(12)-C(14)-C(15)-C(16)	129.1(2)
C(12)-C(14)-C(8)-C(9)	-3.0(3)
C(15)-C(14)-C(8)-C(9)	174.9(2)
C(12)-C(14)-C(8)-O(1)	179.80(19)
C(15)-C(14)-C(8)-O(1)	-2.3(3)
C(7)-O(1)-C(8)-C(9)	69.9(3)
C(7)-O(1)-C(8)-C(14)	-112.8(2)
C(16)-C(15)-N(1)-C(19)	1.2(3)
C(14)-C(15)-N(1)-C(19)	179.0(2)
O(2)-C(7)-C(4)-C(5)	179.1(2)
O(1)-C(7)-C(4)-C(5)	-1.5(3)
O(2)-C(7)-C(4)-C(3)	-0.2(4)
O(1)-C(7)-C(4)-C(3)	179.2(2)
C(8)-C(14)-C(12)-C(11)	2.1(4)
C(15)-C(14)-C(12)-C(11)	-175.9(2)
C(14)-C(8)-C(9)-C(10)	1.9(3)
O(1)-C(8)-C(9)-C(10)	179.0(2)
N(1)-C(15)-C(16)-C(17)	-0.4(4)
C(14)-C(15)-C(16)-C(17)	-178.1(2)
C(1)-C(2)-C(3)-C(4)	-0.3(4)
C(5)-C(4)-C(3)-C(2)	1.2(4)
C(7)-C(4)-C(3)-C(2)	-179.5(2)
C(3)-C(4)-C(5)-C(6)	-1.4(4)
C(7)-C(4)-C(5)-C(6)	179.3(2)
C(8)-C(9)-C(10)-C(11)	0.2(4)
C(3)-C(2)-C(1)-C(6)	-0.4(4)
C(3)-C(2)-C(1)-Br(1)	179.9(2)
C(14)-C(12)-C(11)-C(10)	-0.1(4)
C(14)-C(12)-C(11)-C(13)	179.6(3)
C(9)-C(10)-C(11)-C(12)	-1.1(4)
C(9)-C(10)-C(11)-C(13)	179.2(3)

C(15)-N(1)-C(19)-C(18)	-1.1(4)
C(15)-C(16)-C(17)-C(18)	-0.8(4)
C(16)-C(17)-C(18)-C(19)	0.9(4)
N(1)-C(19)-C(18)-C(17)	0.0(4)
C(2)-C(1)-C(6)-C(5)	0.2(4)
Br(1)-C(1)-C(6)-C(5)	179.9(2)
C(4)-C(5)-C(6)-C(1)	0.7(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

Table 1. Crystal data and structure refinement for cc*J*-OMeRh.

Identification code	1	
Empirical formula	C24 H28 N O2 Rh	
Formula weight	465.38	
Temperature	194(2) K	
Wavelength	0.72010 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5810(17) Å	α= 93.19(3)°.
	b = 10.888(2) Å	β= 106.92(3)°.
	c = 11.352(2) Å	γ = 90.49(3)°.
Volume	1012.8(3) $Å^3$	
Z	2	
Density (calculated)	1.526 mg/m^3	
Absorption coefficient	0.863 mm^{-1}	
F(000)	480	
Crystal size	0.15 x 0.12 x 0.10 mm^3	
Theta range for data collection	1.90 to 25.00°.	
Index ranges	-9<=h<=0, -12<=k<=12, -12<=l<=13	
Reflections collected	3146	
Independent reflections	3146 [R(int) = 0.0000]	
Completeness to theta = 25.00°	91.7 %;	
Max. and min. transmission	0.9187 and 0.8815	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3146 / 0 / 260	
Goodness-of-fit on F^2	1.105	
Final R indices [I>2sigma(I)]	R1 = 0.0601, wR2 = 0.1666	
R indices (all data)	R1 = 0.0697, wR2 = 0.1888	
Largest diff. peak and hole	1.193 and -1.693 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-352(9)	1688(6)	2673(6)	14(1)
C(2)	-1906(9)	1201(6)	2439(6)	15(1)
C(3)	-2805(9)	882(6)	1200(6)	18(2)
C(4)	-2094(8)	1075(6)	284(6)	17(2)
C(5)	-514(8)	1601(5)	569(6)	11(1)
C(6)	399(8)	1839(5)	-306(6)	13(1)
C(7)	1947(8)	2419(6)	201(6)	11(1)
C(8)	2886(9)	2645(6)	-611(6)	16(2)
C(9)	2254(8)	2316(5)	-1877(6)	14(2)
C(10)	719(9)	1768(5)	-2375(5)	13(1)
C(11)	-190(8)	1522(6)	-1574(6)	15(2)
C(12)	53(9)	1434(6)	-3750(6)	18(2)
C(13)	4505(8)	4240(6)	2458(5)	11(1)
C(14)	2954(8)	4783(5)	2013(6)	11(1)
C(15)	2049(8)	4546(6)	2885(6)	13(1)
C(16)	3107(8)	3926(6)	3896(5)	11(1)
C(17)	4585(8)	3735(6)	3626(6)	12(1)
C(18)	5894(8)	4330(6)	1906(6)	14(1)
C(19)	2399(9)	5552(6)	917(6)	19(2)
C(20)	363(9)	4965(6)	2795(7)	20(2)
C(21)	2758(10)	3567(7)	5059(6)	21(2)
C(22)	6028(8)	3096(6)	4442(6)	15(2)
C(23)	3778(9)	470(7)	3093(6)	20(2)
C(24)	4738(11)	-720(7)	3183(8)	32(2)
N(1)	327(7)	1919(5)	1765(5)	11(1)
O(1)	3755(5)	1056(4)	2196(4)	14(1)
O(2)	3072(7)	748(5)	3896(5)	29(1)
Rh(1)	2605(1)	2811(1)	2065(1)	8(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

C(1)-N(1)	1.356(8)
C(1)-C(2)	1.377(10)
C(1)-H(1)	0.9500
C(2)-C(3)	1.415(9)
C(2)-H(2)	0.9500
C(3)-C(4)	1.375(10)
C(3)-H(3)	0.9500
C(4)-C(5)	1.408(10)
C(4)-H(4)	0.9500
C(5)-N(1)	1.363(8)
C(5)-C(6)	1.465(9)
C(6)-C(11)	1.402(9)
C(6)-C(7)	1.412(9)
C(7)-C(8)	1.418(9)
C(7)-Rh(1)	2.044(6)
C(8)-C(9)	1.404(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.388(9)
C(9)-H(9)	0.9500
C(10)-C(11)	1.394(10)
C(10)-C(12)	1.519(8)
C(11)-H(11)	0.9500
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.426(9)
C(13)-C(17)	1.447(9)
C(13)-C(18)	1.505(9)
C(13)-Rh(1)	2.176(6)
C(14)-C(15)	1.457(9)
C(14)-C(19)	1.501(9)
C(14)-Rh(1)	2.172(6)
C(15)-C(16)	1.445(9)
C(15)-C(20)	1.498(10)
C(15)-Rh(1)	2.178(6)
C(16)-C(17)	1.403(10)

C(16)-C(21)	1.507(8)
C(16)-Rh(1)	2.274(6)
C(17)-C(22)	1.515(9)
C(17)-Rh(1)	2.249(6)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-O(1)	1.227(9)
C(23)-O(2)	1.259(9)
C(23)-C(24)	1.533(11)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
N(1)-Rh(1)	2.103(6)
O(1)-Rh(1)	2.150(4)

N(1)-C(1)-C(2)	122.8(6)
N(1)-C(1)-H(1)	118.6
C(2)-C(1)-H(1)	118.6
C(1)-C(2)-C(3)	118.4(6)
C(1)-C(2)-H(2)	120.8
C(3)-C(2)-H(2)	120.8
C(4)-C(3)-C(2)	118.7(6)
C(4)-C(3)-H(3)	120.7
C(2)-C(3)-H(3)	120.7
C(3)-C(4)-C(5)	120.7(6)

C(3)-C(4)-H(4)	119.7
C(5)-C(4)-H(4)	119.7
N(1)-C(5)-C(4)	119.8(6)
N(1)-C(5)-C(6)	113.6(6)
C(4)-C(5)-C(6)	126.5(6)
C(11)-C(6)-C(7)	120.6(6)
C(11)-C(6)-C(5)	123.4(6)
C(7)-C(6)-C(5)	115.9(5)
C(6)-C(7)-C(8)	117.8(6)
C(6)-C(7)-Rh(1)	115.2(4)
C(8)-C(7)-Rh(1)	127.0(5)
C(9)-C(8)-C(7)	120.0(6)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0
C(10)-C(9)-C(8)	122.0(6)
C(10)-C(9)-H(9)	119.0
C(8)-C(9)-H(9)	119.0
C(9)-C(10)-C(11)	118.0(6)
C(9)-C(10)-C(12)	121.1(6)
C(11)-C(10)-C(12)	120.9(6)
C(10)-C(11)-C(6)	121.6(6)
C(10)-C(11)-H(11)	119.2
C(6)-C(11)-H(11)	119.2
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(17)	107.7(6)
C(14)-C(13)-C(18)	126.0(6)
C(17)-C(13)-C(18)	125.8(6)
C(14)-C(13)-Rh(1)	70.7(3)
C(17)-C(13)-Rh(1)	73.7(4)
C(18)-C(13)-Rh(1)	127.5(4)
C(13)-C(14)-C(15)	107.1(5)
C(13)-C(14)-C(19)	126.8(6)
C(15)-C(14)-C(19)	125.9(6)

C(13)-C(14)-Rh(1)	71.0(3)
C(15)-C(14)-Rh(1)	70.6(3)
C(19)-C(14)-Rh(1)	127.5(4)
C(16)-C(15)-C(14)	108.1(6)
C(16)-C(15)-C(20)	126.0(6)
C(14)-C(15)-C(20)	125.7(6)
C(16)-C(15)-Rh(1)	74.7(3)
C(14)-C(15)-Rh(1)	70.2(3)
C(20)-C(15)-Rh(1)	124.5(5)
C(17)-C(16)-C(15)	107.4(5)
C(17)-C(16)-C(21)	124.8(6)
C(15)-C(16)-C(21)	127.8(6)
C(17)-C(16)-Rh(1)	71.0(3)
C(15)-C(16)-Rh(1)	67.5(3)
C(21)-C(16)-Rh(1)	128.2(4)
C(16)-C(17)-C(13)	109.5(6)
C(16)-C(17)-C(22)	124.6(6)
C(13)-C(17)-C(22)	125.9(6)
C(16)-C(17)-Rh(1)	72.9(4)
C(13)-C(17)-Rh(1)	68.2(3)
C(22)-C(17)-Rh(1)	125.3(4)
C(13)-C(18)-H(18A)	109.5
C(13)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(13)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(15)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5

H(20B)-C(20)-H(20C)	109.5
C(16)-C(21)-H(21A)	109.5
C(16)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(16)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(17)-C(22)-H(22A)	109.5
C(17)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(17)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
O(1)-C(23)-O(2)	126.1(7)
O(1)-C(23)-C(24)	114.7(7)
O(2)-C(23)-C(24)	119.2(7)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(1)-N(1)-C(5)	119.4(6)
C(1)-N(1)-Rh(1)	124.2(4)
C(5)-N(1)-Rh(1)	116.3(4)
C(23)-O(1)-Rh(1)	117.5(4)
C(7)-Rh(1)-N(1)	78.7(2)
C(7)-Rh(1)-O(1)	85.5(2)
N(1)-Rh(1)-O(1)	89.92(18)
C(7)-Rh(1)-C(14)	96.7(2)
N(1)-Rh(1)-C(14)	124.4(2)
O(1)-Rh(1)-C(14)	145.5(2)
C(7)-Rh(1)-C(13)	106.2(2)
N(1)-Rh(1)-C(13)	161.6(2)
O(1)-Rh(1)-C(13)	108.0(2)
C(14)-Rh(1)-C(13)	38.3(2)
C(7)-Rh(1)-C(15)	122.5(2)
N(1)-Rh(1)-C(15)	97.8(2)

O(1)-Rh(1)-C(15)	151.9(2)
C(14)-Rh(1)-C(15)	39.1(2)
C(13)-Rh(1)-C(15)	64.4(2)
C(7)-Rh(1)-C(17)	142.1(3)
N(1)-Rh(1)-C(17)	139.2(2)
O(1)-Rh(1)-C(17)	94.3(2)
C(14)-Rh(1)-C(17)	63.3(2)
C(13)-Rh(1)-C(17)	38.1(2)
C(15)-Rh(1)-C(17)	62.5(2)
C(7)-Rh(1)-C(16)	159.5(2)
N(1)-Rh(1)-C(16)	106.3(2)
O(1)-Rh(1)-C(16)	114.1(2)
C(14)-Rh(1)-C(16)	63.8(2)
C(13)-Rh(1)-C(16)	63.0(2)
C(15)-Rh(1)-C(16)	37.8(2)
C(17)-Rh(1)-C(16)	36.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(4)	16(3)	7(3)	-4(2)	5(3)	2(3)
C(2)	15(4)	14(3)	20(3)	-7(3)	12(3)	-2(3)
C(3)	12(4)	15(3)	27(4)	-3(3)	5(3)	-5(3)
C(4)	9(4)	17(3)	22(3)	-9(3)	2(3)	-7(3)
C(5)	13(4)	5(3)	16(3)	0(2)	5(3)	-2(2)
C(6)	17(4)	8(3)	16(3)	-5(2)	8(3)	2(3)
C(7)	14(4)	10(3)	11(3)	3(2)	8(3)	-2(3)
C(8)	15(4)	18(3)	16(3)	0(3)	7(3)	-7(3)
C(9)	25(5)	7(3)	15(3)	-1(2)	15(3)	0(3)
C(10)	24(4)	8(3)	10(3)	2(2)	6(3)	3(3)
C(11)	10(4)	13(3)	22(3)	-4(3)	3(3)	-2(3)
C(12)	21(4)	14(3)	18(3)	-2(3)	6(3)	-4(3)
C(13)	11(4)	12(3)	10(3)	-2(2)	1(3)	-3(3)
C(14)	11(4)	7(3)	16(3)	-4(2)	5(3)	-6(2)
C(15)	11(4)	12(3)	18(3)	-6(2)	9(3)	-5(3)
C(16)	11(4)	12(3)	11(3)	-5(2)	7(3)	-2(3)
C(17)	6(4)	17(3)	11(3)	-2(2)	-1(3)	-4(2)
C(18)	9(4)	20(3)	17(3)	1(3)	7(3)	-8(3)
C(19)	22(5)	18(3)	17(3)	0(3)	6(3)	-3(3)
C(20)	18(5)	17(4)	26(4)	-1(3)	10(3)	0(3)
C(21)	29(5)	27(4)	11(3)	-4(3)	11(3)	-11(3)
C(22)	12(4)	16(3)	18(3)	4(3)	2(3)	2(3)
C(23)	7(4)	24(4)	26(4)	-8(3)	2(3)	-8(3)
C(24)	39(6)	20(4)	34(4)	9(3)	4(4)	5(4)
N(1)	13(3)	8(3)	13(3)	2(2)	5(2)	2(2)
O(1)	4(3)	14(2)	20(2)	-11(2)	4(2)	-3(2)
O(2)	31(4)	28(3)	29(3)	6(2)	9(2)	1(2)
Rh(1)	7(1)	10(1)	10(1)	-1(1)	4(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for 1.

	x	y	z	U(eq)
H(1)	272	1871	3506	16
H(2)	-2363	1082	3093	18
H(3)	-3880	542	1006	22
H(4)	-2675	851	-550	20
H(8)	3942	3018	-298	19
H(9)	2898	2474	-2408	17
H(11)	-1233	1130	-1895	18
H(12A)	-282	2182	-4189	26
H(12B)	-888	868	-3902	26
H(12C)	900	1036	-4046	26
H(18A)	6663	4985	2358	22
H(18B)	5471	4520	1038	22
H(18C)	6453	3545	1961	22
H(19A)	1211	5611	682	29
H(19B)	2724	5168	226	29
H(19C)	2901	6377	1127	29
H(20A)	425	5750	3275	30
H(20B)	-210	4347	3123	30
H(20C)	-230	5071	1930	30
H(21A)	2949	2687	5159	32
H(21B)	1620	3735	5005	32
H(21C)	3478	4044	5770	32
H(22A)	6619	3667	5128	23
H(22B)	6757	2833	3959	23
H(22C)	5642	2376	4768	23
H(24A)	5178	-822	2479	48
H(24B)	4013	-1423	3176	48
H(24C)	5635	-676	3952	48

Table 6. Torsion angles [°] for 1.

N(1)-C(1)-C(2)-C(3)	2.6(10)
C(1)-C(2)-C(3)-C(4)	-0.2(10)
C(2)-C(3)-C(4)-C(5)	-1.2(10)
C(3)-C(4)-C(5)-N(1)	0.3(10)
C(3)-C(4)-C(5)-C(6)	178.9(6)
N(1)-C(5)-C(6)-C(11)	176.4(6)
C(4)-C(5)-C(6)-C(11)	-2.3(10)
N(1)-C(5)-C(6)-C(7)	-3.6(8)
C(4)-C(5)-C(6)-C(7)	177.7(6)
C(11)-C(6)-C(7)-C(8)	-1.2(9)
C(5)-C(6)-C(7)-C(8)	178.8(6)
C(11)-C(6)-C(7)-Rh(1)	-179.9(5)
C(5)-C(6)-C(7)-Rh(1)	0.1(7)
C(6)-C(7)-C(8)-C(9)	1.3(9)
Rh(1)-C(7)-C(8)-C(9)	179.9(5)
C(7)-C(8)-C(9)-C(10)	-0.1(10)
C(8)-C(9)-C(10)-C(11)	-1.3(9)
C(8)-C(9)-C(10)-C(12)	179.3(6)
C(9)-C(10)-C(11)-C(6)	1.4(9)
C(12)-C(10)-C(11)-C(6)	-179.2(6)
C(7)-C(6)-C(11)-C(10)	-0.2(9)
C(5)-C(6)-C(11)-C(10)	179.9(6)
C(17)-C(13)-C(14)-C(15)	-3.1(7)
C(18)-C(13)-C(14)-C(15)	-175.3(6)
Rh(1)-C(13)-C(14)-C(15)	61.8(4)
C(17)-C(13)-C(14)-C(19)	172.0(6)
C(18)-C(13)-C(14)-C(19)	-0.2(10)
Rh(1)-C(13)-C(14)-C(19)	-123.2(6)
C(17)-C(13)-C(14)-Rh(1)	-64.9(4)
C(18)-C(13)-C(14)-Rh(1)	122.9(6)
C(13)-C(14)-C(15)-C(16)	3.6(7)
C(19)-C(14)-C(15)-C(16)	-171.5(6)
Rh(1)-C(14)-C(15)-C(16)	65.6(4)
C(13)-C(14)-C(15)-C(20)	179.1(6)
C(19)-C(14)-C(15)-C(20)	4.0(10)
Rh(1)-C(14)-C(15)-C(20)	-118.9(6)

C(13)-C(14)-C(15)-Rh(1)	-62.0(4)
C(19)-C(14)-C(15)-Rh(1)	122.9(6)
C(14)-C(15)-C(16)-C(17)	-2.7(7)
C(20)-C(15)-C(16)-C(17)	-178.2(6)
Rh(1)-C(15)-C(16)-C(17)	60.0(4)
C(14)-C(15)-C(16)-C(21)	175.6(6)
C(20)-C(15)-C(16)-C(21)	0.2(10)
Rh(1)-C(15)-C(16)-C(21)	-121.6(6)
C(14)-C(15)-C(16)-Rh(1)	-62.7(4)
C(20)-C(15)-C(16)-Rh(1)	121.8(6)
C(15)-C(16)-C(17)-C(13)	0.8(7)
C(21)-C(16)-C(17)-C(13)	-177.6(6)
Rh(1)-C(16)-C(17)-C(13)	58.6(4)
C(15)-C(16)-C(17)-C(22)	-179.2(6)
C(21)-C(16)-C(17)-C(22)	2.3(10)
Rh(1)-C(16)-C(17)-C(22)	-121.4(6)
C(15)-C(16)-C(17)-Rh(1)	-57.8(4)
C(21)-C(16)-C(17)-Rh(1)	123.8(6)
C(14)-C(13)-C(17)-C(16)	1.5(7)
C(18)-C(13)-C(17)-C(16)	173.7(6)
Rh(1)-C(13)-C(17)-C(16)	-61.5(4)
C(14)-C(13)-C(17)-C(22)	-178.5(6)
C(18)-C(13)-C(17)-C(22)	-6.3(10)
Rh(1)-C(13)-C(17)-C(22)	118.6(6)
C(14)-C(13)-C(17)-Rh(1)	62.9(4)
C(18)-C(13)-C(17)-Rh(1)	-124.8(6)
C(2)-C(1)-N(1)-C(5)	-3.6(9)
C(2)-C(1)-N(1)-Rh(1)	174.1(5)
C(4)-C(5)-N(1)-C(1)	2.0(9)
C(6)-C(5)-N(1)-C(1)	-176.7(5)
C(4)-C(5)-N(1)-Rh(1)	-175.8(4)
C(6)-C(5)-N(1)-Rh(1)	5.4(7)
O(2)-C(23)-O(1)-Rh(1)	6.4(9)
C(24)-C(23)-O(1)-Rh(1)	-175.2(5)
C(6)-C(7)-Rh(1)-N(1)	2.1(4)
C(8)-C(7)-Rh(1)-N(1)	-176.5(6)
C(6)-C(7)-Rh(1)-O(1)	92.9(5)
C(8)-C(7)-Rh(1)-O(1)	-85.6(6)

C(6)-C(7)-Rh(1)-C(14)	-121.7(5)
C(8)-C(7)-Rh(1)-C(14)	59.8(6)
C(6)-C(7)-Rh(1)-C(13)	-159.6(4)
C(8)-C(7)-Rh(1)-C(13)	21.8(6)
C(6)-C(7)-Rh(1)-C(15)	-90.0(5)
C(8)-C(7)-Rh(1)-C(15)	91.4(6)
C(6)-C(7)-Rh(1)-C(17)	-175.8(4)
C(8)-C(7)-Rh(1)-C(17)	5.6(8)
C(6)-C(7)-Rh(1)-C(16)	-104.3(8)
C(8)-C(7)-Rh(1)-C(16)	77.1(10)
C(1)-N(1)-Rh(1)-C(7)	178.0(5)
C(5)-N(1)-Rh(1)-C(7)	-4.3(4)
C(1)-N(1)-Rh(1)-O(1)	92.6(5)
C(5)-N(1)-Rh(1)-O(1)	-89.7(4)
C(1)-N(1)-Rh(1)-C(14)	-91.5(5)
C(5)-N(1)-Rh(1)-C(14)	86.2(5)
C(1)-N(1)-Rh(1)-C(13)	-74.4(8)
C(5)-N(1)-Rh(1)-C(13)	103.3(7)
C(1)-N(1)-Rh(1)-C(15)	-60.2(5)
C(5)-N(1)-Rh(1)-C(15)	117.5(4)
C(1)-N(1)-Rh(1)-C(17)	-3.9(7)
C(5)-N(1)-Rh(1)-C(17)	173.8(4)
C(1)-N(1)-Rh(1)-C(16)	-22.5(5)
C(5)-N(1)-Rh(1)-C(16)	155.2(4)
C(23)-O(1)-Rh(1)-C(7)	-147.0(5)
C(23)-O(1)-Rh(1)-N(1)	-68.3(5)
C(23)-O(1)-Rh(1)-C(14)	117.7(5)
C(23)-O(1)-Rh(1)-C(13)	107.4(5)
C(23)-O(1)-Rh(1)-C(15)	38.3(7)
C(23)-O(1)-Rh(1)-C(17)	71.0(5)
C(23)-O(1)-Rh(1)-C(16)	39.6(5)
C(13)-C(14)-Rh(1)-C(7)	-107.7(4)
C(15)-C(14)-Rh(1)-C(7)	135.5(4)
C(19)-C(14)-Rh(1)-C(7)	14.6(6)
C(13)-C(14)-Rh(1)-N(1)	171.4(3)
C(15)-C(14)-Rh(1)-N(1)	54.6(4)
C(19)-C(14)-Rh(1)-N(1)	-66.3(7)
C(13)-C(14)-Rh(1)-O(1)	-15.9(5)

C(15)-C(14)-Rh(1)-O(1)	-132.7(4)
C(19)-C(14)-Rh(1)-O(1)	106.4(6)
C(15)-C(14)-Rh(1)-C(13)	-116.8(5)
C(19)-C(14)-Rh(1)-C(13)	122.3(7)
C(13)-C(14)-Rh(1)-C(15)	116.8(5)
C(19)-C(14)-Rh(1)-C(15)	-120.9(8)
C(13)-C(14)-Rh(1)-C(17)	38.4(4)
C(15)-C(14)-Rh(1)-C(17)	-78.4(4)
C(19)-C(14)-Rh(1)-C(17)	160.7(7)
C(13)-C(14)-Rh(1)-C(16)	79.0(4)
C(15)-C(14)-Rh(1)-C(16)	-37.8(4)
C(19)-C(14)-Rh(1)-C(16)	-158.7(7)
C(14)-C(13)-Rh(1)-C(7)	80.1(4)
C(17)-C(13)-Rh(1)-C(7)	-163.9(4)
C(18)-C(13)-Rh(1)-C(7)	-41.0(6)
C(14)-C(13)-Rh(1)-N(1)	-23.1(8)
C(17)-C(13)-Rh(1)-N(1)	93.0(7)
C(18)-C(13)-Rh(1)-N(1)	-144.1(6)
C(14)-C(13)-Rh(1)-O(1)	170.6(3)
C(17)-C(13)-Rh(1)-O(1)	-73.4(4)
C(18)-C(13)-Rh(1)-O(1)	49.5(6)
C(17)-C(13)-Rh(1)-C(14)	116.0(5)
C(18)-C(13)-Rh(1)-C(14)	-121.1(7)
C(14)-C(13)-Rh(1)-C(15)	-38.7(4)
C(17)-C(13)-Rh(1)-C(15)	77.4(4)
C(18)-C(13)-Rh(1)-C(15)	-159.7(6)
C(14)-C(13)-Rh(1)-C(17)	-116.0(5)
C(18)-C(13)-Rh(1)-C(17)	122.9(7)
C(14)-C(13)-Rh(1)-C(16)	-81.0(4)
C(17)-C(13)-Rh(1)-C(16)	35.0(4)
C(18)-C(13)-Rh(1)-C(16)	157.9(6)
C(16)-C(15)-Rh(1)-C(7)	-171.9(4)
C(14)-C(15)-Rh(1)-C(7)	-55.7(5)
C(20)-C(15)-Rh(1)-C(7)	64.7(6)
C(16)-C(15)-Rh(1)-N(1)	106.6(4)
C(14)-C(15)-Rh(1)-N(1)	-137.2(4)
C(20)-C(15)-Rh(1)-N(1)	-16.9(6)
C(16)-C(15)-Rh(1)-O(1)	1.9(7)

C(14)-C(15)-Rh(1)-O(1)	118.1(5)
C(20)-C(15)-Rh(1)-O(1)	-121.6(6)
C(16)-C(15)-Rh(1)-C(14)	-116.2(6)
C(20)-C(15)-Rh(1)-C(14)	120.4(7)
C(16)-C(15)-Rh(1)-C(13)	-78.3(4)
C(14)-C(15)-Rh(1)-C(13)	37.8(4)
C(20)-C(15)-Rh(1)-C(13)	158.2(6)
C(16)-C(15)-Rh(1)-C(17)	-35.6(4)
C(14)-C(15)-Rh(1)-C(17)	80.6(4)
C(20)-C(15)-Rh(1)-C(17)	-159.0(6)
C(14)-C(15)-Rh(1)-C(16)	116.2(6)
C(20)-C(15)-Rh(1)-C(16)	-123.5(7)
C(16)-C(17)-Rh(1)-C(7)	145.7(4)
C(13)-C(17)-Rh(1)-C(7)	25.8(6)
C(22)-C(17)-Rh(1)-C(7)	-93.6(7)
C(16)-C(17)-Rh(1)-N(1)	-31.2(5)
C(13)-C(17)-Rh(1)-N(1)	-151.1(4)
C(22)-C(17)-Rh(1)-N(1)	89.5(6)
C(16)-C(17)-Rh(1)-O(1)	-126.1(4)
C(13)-C(17)-Rh(1)-O(1)	114.0(4)
C(22)-C(17)-Rh(1)-O(1)	-5.4(6)
C(16)-C(17)-Rh(1)-C(14)	81.4(4)
C(13)-C(17)-Rh(1)-C(14)	-38.6(4)
C(22)-C(17)-Rh(1)-C(14)	-157.9(7)
C(16)-C(17)-Rh(1)-C(13)	119.9(5)
C(22)-C(17)-Rh(1)-C(13)	-119.4(7)
C(16)-C(17)-Rh(1)-C(15)	37.2(4)
C(13)-C(17)-Rh(1)-C(15)	-82.8(4)
C(22)-C(17)-Rh(1)-C(15)	157.9(7)
C(13)-C(17)-Rh(1)-C(16)	-119.9(5)
C(22)-C(17)-Rh(1)-C(16)	120.7(7)
C(17)-C(16)-Rh(1)-C(7)	-99.2(8)
C(15)-C(16)-Rh(1)-C(7)	19.9(9)
C(21)-C(16)-Rh(1)-C(7)	141.1(7)
C(17)-C(16)-Rh(1)-N(1)	159.3(4)
C(15)-C(16)-Rh(1)-N(1)	-81.6(4)
C(21)-C(16)-Rh(1)-N(1)	39.6(7)
C(17)-C(16)-Rh(1)-O(1)	61.9(4)

C(15)-C(16)-Rh(1)-O(1)	-179.0(4)
C(21)-C(16)-Rh(1)-O(1)	-57.8(7)
C(17)-C(16)-Rh(1)-C(14)	-79.9(4)
C(15)-C(16)-Rh(1)-C(14)	39.2(4)
C(21)-C(16)-Rh(1)-C(14)	160.4(7)
C(17)-C(16)-Rh(1)-C(13)	-36.9(4)
C(15)-C(16)-Rh(1)-C(13)	82.2(4)
C(21)-C(16)-Rh(1)-C(13)	-156.6(7)
C(17)-C(16)-Rh(1)-C(15)	-119.1(6)
C(21)-C(16)-Rh(1)-C(15)	121.2(8)
C(15)-C(16)-Rh(1)-C(17)	119.1(6)
C(21)-C(16)-Rh(1)-C(17)	-119.7(8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)