Transition metal-free [3+3] annulation of cyclopropanols with β-enamine esters to assemble nicotinate derivatives

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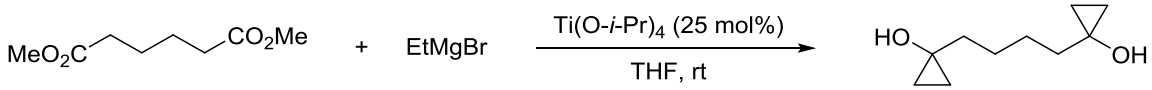
Supporting Information

General:

All reagents were purchased from Adamas, 3A Materials, TCI or Energy-Chemical and used without further purification. Flash chromatography was carried out with silica gel (200-300 mesh). Analytical TLC was performed with silica gel GF254 plates, and the products were visualized by UV detection. ^{1}H NMR（400 MHz），^{13}C NMR (100 MHz) spectra were recorded in $CDCl_3$. Chemical shifts (δ) are reported in ppm using TMS as internal standard and spin-spin coupling constants (J) are given in Hz. Proton and carbon multiplicity are recorded as singlet (s), doublet (d), triplet (t), quartet (q), quintet (quin), sextet (sex) septet (sep) multiplet (m) and broad (brs). Melting points were obtained with a micro melting point XT4A Beijing Keyi electrooptic apparatus and uncorrected. The high-resolution mass spectra (HRMS) were measured on a Waters LCT Premierxe^{TM} spectrometer by ESI.

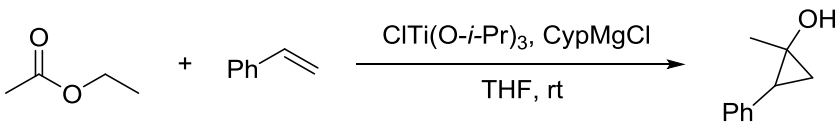
Substrates preparation:

The procedure for the synthesis of the cyclopropanol 1n.



In a fume hood, 44 mmol of ethylmagnesium bromide in THF (2M) was added dropwise over 30 minutes at room temperature to a solution of 10 mmol of dimethyl adipate and 2.5 mmol of titanium tetraisopropoxide in 50 mL THF. The reacton mixture was stirred overnight. Then, the solution was quenched with 20 mL H_2SO_4 (1 M) and stirred while still in the fume hood. The solution was extracted with 3 x 30 mL of ethyl acetate, washed with distilled water, and dried over Na_2SO_4 followed by filtration and concentration. The mixture was subjected to column chromatography to afford the corresponding alkylcyclopropanol **1n**.[1]

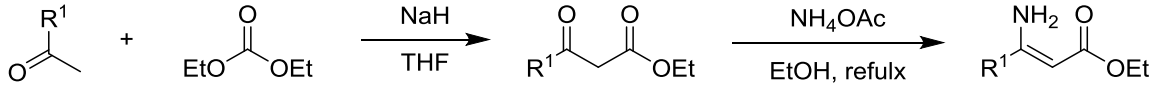
The procedure for the synthesis of the cyclopropanol 1o.



To a solution of ethyl acetate (10.0 mmol) and styrene (11.0 mmol) in anhydrous

THF (80 mL), a solution of chlorotriisopropoxytitanium ($ClTi(O\text{-}i\text{-}Pr)_3$ 1 M in hexane, 10.0 mmol) was added under argon atmosphere. Cyclopentylmagnesium chloride (CypMgCl, 2 M in Et_2O, 40 mmol) was then added over a period of 2.5 h. After the addition is complete, the resulting black reaction mixture is stirred for another 30 min at room temperature. The reaction was quenched with 1M aqueous H_2SO_4 (40 mL) at 0 °C and extracted with ethyl acetate (30 mL x 2). The organic phase was washed with saturated $NaHCO_3$ (200 mL) and dried over Na_2SO_4 and concentrated *in vacuo*. The residue was purified by column chromatography on silica gel to give the desired product. [2]

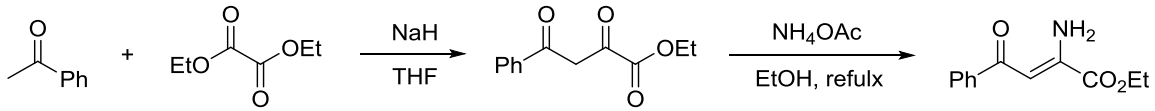
General procedure for the synthesis of enamines 2b-m and 2p-q.



To a suspension of ketone (20 mmol) in THF (80 mL) was added NaH (40 mmol, 60%). After the reaction mixture was stirred at 0 °C for about 10 minites, the ester was added dropwise at the same temperature. Then the mixture was stirred at room temperature until TLC indicated the total consumption of the ketone. The reaction mixture was poured into ice-water (100 mL), acidified with aqueous HCl (3 M) to pH 2~3 and extracted with EtOAc (100 mL x 3). The combined organic layer was dried over sodium sulfate and evaporated under reduced pressure. The β-keto ester obtained was used for the next step without further purification.

A round-bottom flask was charged with *β*-keto ester (20 mmol), NH_4OAc (100 mmol) and EtOH (40 mL). The mixture was refluxed for 12 h. After removal of the solvent, the residue was dissolved into 60 mL water, extracted with ethyl acetate, dried with anhydrous Na_2SO_4 and concentrated under vacuum. The mixture was subjected to column chromatography to afford the product. [3]

The procedure for the synthesis of the enamine 2n.

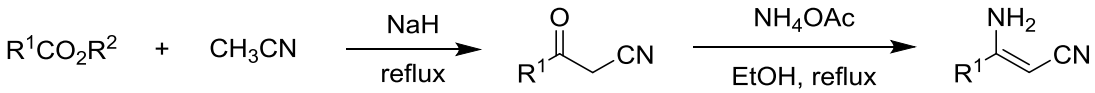


To a suspension of ketone (20 mmol) in THF (80 mL) was added NaH (40 mmol, 60%). After the reaction mixture was stirred at 0 °C for about 10 minites, the ester was added dropwise at the same temperature. Then the mixture was stirred at room temperature

until TLC indicated the total consumption of the ketone. The reaction mixture was poured into ice-water (100 mL), acidified with aqueous HCl (3 M) to pH 2~3 and extracted with EtOAc (100 mL x 3). The combined organic layer was dried over sodium sulfate and evaporated under reduced pressure. The *β*-keto ester obtained was used for the next step without further purification. [4]

The enamine was obtained in the same method as above.

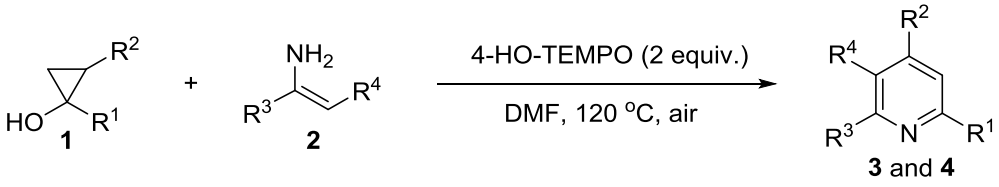
The procedure for the synthesis of the enamine 2o.



A solution of acetonitrile (90 mmol) in toluene (100 mL) was treated with substituted ester (30 mmol), then sodium hydride (90 mmol, 60%) was added. The reaction mixture was refluxed until TLC indicated the total consumption of the ester. After cooling, the mixture was treated with ice-water (100 mL), acidified with 2 N HCl (to pH 2~3) and extracted with EA (100 mL x 3). The combined organic layer was dried over sodium sulfate and evaporated under reduced pressure to remove the solvent. The given residue was purified by column chromatography using a mixture of PE and EA as eluent to afford corresponding ketone in 44-89% yield. [5]

The enamine was obtained in the same method as above.

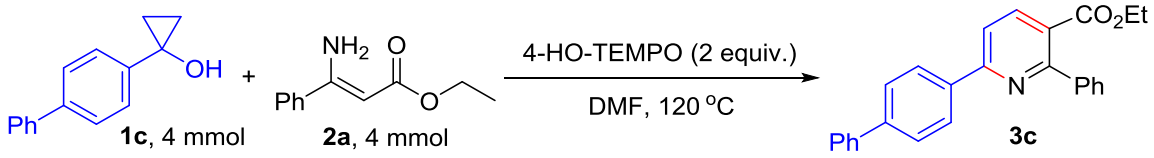
General experimental procedure:



A 25 mL oven-dried reaction pressure tube were charged with cyclopropanols **1** (0.3 mmol), enamines **2**, (0.3 mmol, 1 equiv.), 4-HO-TEMPO (0.6 mmol, 2 equiv.) and DMF (2 mL). The tube was then sealed and the mixture was stirred for 48 h at 120 °C under air. Upon completion of the reaction, the mixture was extracted with EA and washed with brines. Then, the solvent was removed under vacuo and the residue was purified with chromatography column on silica gel (gradient eluent of EtOAc/petroleum ether: 1⁄40 to 1⁄10) to give the corresponding products **3 and 4**. The identity and purity of the product

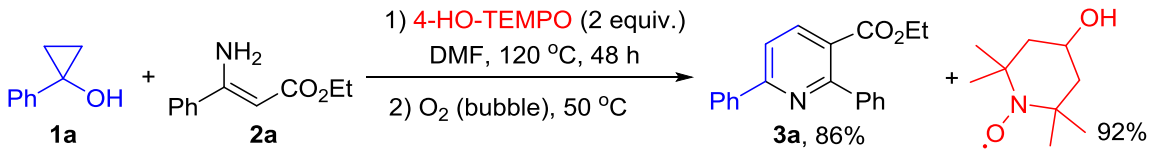
was confirmed by ^{1}H and ^{13}C spectroscopic analysis.

Gram-scale synthesis of 3c:



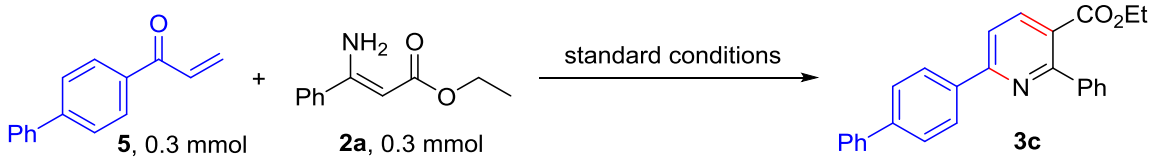
A 100 mL oven-dried reaction pressure tube were charged with cyclopropanol **1c** (4.0 mmol), enamine **2a**, (4.0 mmol), 4-HO-TEMPO (8.0 mmol, 2 equiv.) and DMF (30 mL) The tube was then sealed and the mixture was stirred for 48 h at 120 °C under air. Upon completion of the reaction, the mixture was extracted with EA and washed with brines. Then, the solvent was removed under vacuo and the residue was purified with chromatography column on silica gel to give the corresponding products **3c** in 80% yield.

The regeneration of 4-HO-TEMPO:



A 25 mL oven-dried reaction pressure tube were charged with cyclopropanol **1a** (0.3 mmol), enamine **2a**, (0.3 mmol, 1 equiv.), 4-HO-TEMPO (0.6 mmol, 2 equiv.) and DMF (2 mL) The tube was then sealed and the mixture was stirred for 48 h at 120 °C under air. After completion of the reaction, the mixture was stirred under an oxygen atmosphere at 50 °C for 12 h. Subsequently, the mixture was extracted with EA and washed with brines. Next, the solvent was removed under vacuo and the residue was purified with chromatography column on silica gel to give a yellow solid 4-HO-TEMPO in 92% yield.

Control experiments:

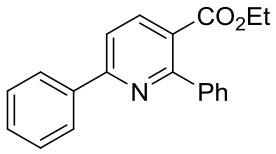


A 25 mL oven-dried reaction pressure tube were charged with enone **5** (0.3 mmol), enamine **2a**, (0.3 mmol, 1 equiv.), 4-HO-TEMPO (0.6 mmol, 2 equiv.) and DMF (2 mL). The tube was then sealed and the mixture was stirred for 48 h at 120 °C under air. Upon completion of the reaction, the mixture was extracted with EA and washed with brines.

Then, the solvent was removed under vacuo and the residue was purified with chromatography column on silica gel to give the corresponding products **3c** in 86% yield.

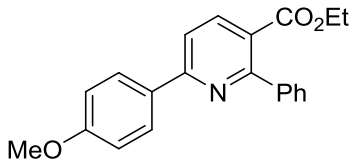
Analytical Data for Products:

Ethyl 2,6-diphenylnicotinate (3a)



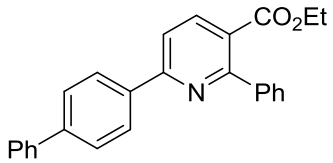
Yellow oil; (78 mg, 86%); R_f = 0.36 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, *J* = 8.0 Hz, 1H), 8.16–8.14 (m, 2H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.68 (dd, *J* = 1.2 Hz, *J* = 6.4 Hz, 2H), 7.52–7.44 (m, 6H), 4.20 (q, *J* = 7.2 Hz, 2H), 1.10 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 158.7, 158.3, 140.5, 138.8, 138.2, 129.7, 128.8, 128.7, 128.5, 127.9, 127.3, 125.3, 117.7, 61.3, 13.6; ESI-HRMS: m/z Calcd for $C_{20}H_{18}NO_2$, $[M + H]^+$: 304.1332, found 304.1335. [6]

Ethyl 6-(4-methoxyphenyl)-2-phenylnicotinate (3b)



White solid; (84 mg, 84%); mp: 106–109 °C; R_f = 0.23 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, *J* = 8.0 Hz, 1H), 8.09 (d, *J* = 8.8 Hz, 2H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.64–7.62 (m, 2H), 7.46–7.42 (m, 3H), 6.99 (d, *J* = 8.8 Hz, 2H), 4.16 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 1.06 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 161.1, 158.7, 158.0, 140.7, 138.8, 130.9, 128.8, 128.7, 128.4, 127.9, 124.5, 116.9, 114.1, 61.2, 55.3, 13.7; ESI-HRMS: m/z Calcd for $C_{21}H_{20}NO_3$, $[M + H]^+$: 334.1438, found 334.1445. [7]

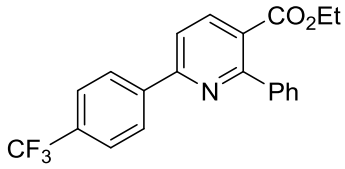
Ethyl 6-([1,1'-biphenyl]-4-yl)-2-phenylnicotinate (3c)



White solid; (107 mg, 94%); mp: 143–145 °C; R_f = 0.23 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21–8.16 (m, 3H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 2H), 7.67–7.63 (m, 4H), 7.47–7.41 (m, 5H), 7.36 (t, *J* = 7.2 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H),

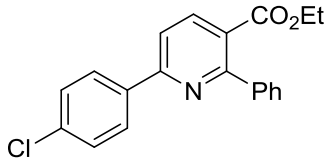
1.06 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 158.8, 157.9, 142.4, 140.6, 140.4, 138.9, 137.1, 128.83, 128.81, 128.5, 128.0, 127.7, 127.6, 127.4, 127.1, 125.3, 117.6, 61.3, 13.6; ESI-HRMS: m/z Calcd for $C_{26}H_{21}NO_2$, $[M + H]^+$: 380.1645, found 380.1648.

Ethyl 2-phenyl-6-(4-(trifluoromethyl)phenyl)nicotinate (3d)



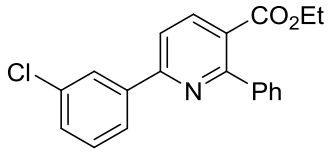
Yellow oil; (90 mg, 81%); R_f = 0.36 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (dd, *J* = 8.4 Hz, *J* = 10.0 Hz, 3H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.65–7.62 (m, 2H), 7.48–7.45 (m, 3H), 4.18 (q, *J* = 7.2 Hz, 2H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 158.9, 156.8, 141.6, 140.2, 139.1, 131.4 (q, $^{C,F}J_2$ = 32.0 Hz), 128.8, 128.1, 127.6, 126.3, 125.7 (q, $^{C,F}J_3$ = 3.0 Hz), 124.1 (q, $^{C,F}J_1$ = 271.0 Hz), 118.2, 61.5, 13.6; ESI-HRMS: m/z Calcd for $C_{21}H_{17}F_3NO_2$, $[M + H]^+$: 372.1206, found 372.1210. [7]

Ethyl 6-(4-chlorophenyl)-2-phenylnicotinate (3e)



Yellow oil; (81 mg, 80%); R_f = 0.33 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 8.4 Hz, 1H), 8.05 (dd, *J* = 2.0 Hz, *J* = 6.8 Hz, 2H), 7.70 (d, *J* = 8.0 Hz, 1H), 7.63–7.61 (m, 2H), 7.47–7.40 (m, 5H), 4.16 (q, *J* = 7.2 Hz, 2H), 1.06 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 158.7, 157.0, 140.3, 138.9, 136.6, 135.9, 128.9, 128.8, 128.6, 128.5, 128.0, 125.6, 117.5, 61.4, 13.6; ESI-HRMS: m/z Calcd for $C_{20}H_{16}ClNO_2$, $[M + H]^+$: 338.0942, found 338.0945. [8]

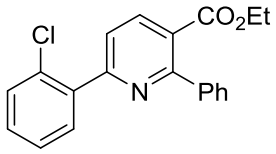
Ethyl 6-(3-chlorophenyl)-2-phenylnicotinate (3f)



White solid; (82 mg, 81%); mp: 59–61 °C; R_f = 0.35 (hexanes/ethyl acetate 10:1); ^{1}H NMR

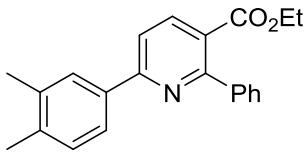
(400 MHz, $CDCl_3$): δ 8.17 (d, J = 8.4 Hz, 1H), 8.14–8.13 (m, 1H), 7.99–7.95 (m, 1H), 7.72 (d, J = 8.4 Hz, 1H), 7.64–7.60 (m, 2H), 7.48–7.41 (m, 3H), 7.40–7.37 (m, 2H), 4.17 (q, J = 7.2 Hz, 2H), 1.06 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 158.8, 156.8, 140.2, 140.0, 139.0, 134.9, 130.0, 129.6, 128.8, 128.7, 128.0, 127.4, 125.9, 125.3, 117.8, 61.4, 13.6; ESI-HRMS: m/z Calcd for $C_{20}H_{16}ClNO_2$, $[M + H]^+$: 338.0942, found 338.0945.

Ethyl 6-(2-chlorophenyl)-2-phenylnicotinate (3g)



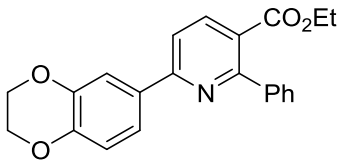
Yellow oil; (51 mg, 50%); R_f = 0.36 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (d, J = 8.0 Hz, 1H), 7.72–7.67 (m, 2H), 7.63–7.60 (m, 2H), 7.49–7.47 (m, 1H), 7.46–7.40 (m, 3H), 7.38–7.32 (m, 2H), 4.18 (q, J = 7.2 Hz, 2H), 1.08 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 158.6, 158.2, 140.2, 138.4, 137.8, 132.3, 131.8, 130.2, 130.0, 128.8, 128.6, 128.0, 127.0, 125.8, 122.6, 61.5, 13.6; ESI-HRMS: m/z Calcd for $C_{20}H_{17}ClNO_2$, $[M + H]^+$: 338.0942, found 338.0945.

Ethyl 6-(3,4-dimethylphenyl)-2-phenylnicotinate (3h)



Yellow oil; (93 mg, 76%); R_f = 0.38 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (d, J = 8.0 Hz, 1H), 7.91 (s, 1H), 7.83 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 7.63 (dd, J = 2.0 Hz, J = 7.6 Hz, 2H), 7.46–7.42 (m, 3H), 7.22 (d, J = 8.0 Hz, 1H), 4.16 (q, J = 7.2 Hz, 2H), 2.34 (s, 3H), 2.31 (s, 3H), 1.06 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 158.7, 158.6, 140.7, 138.7, 138.6, 137.0, 135.9, 130.0, 128.8, 128.45, 128.43, 127.9, 124.9, 124.7, 117.5, 61.2, 19.9, 19.6, 13.6; ESI-HRMS: m/z Calcd for $C_{28}H_{26}NO_2$, $[M + H]^+$: 408.1958, found 408.1962.

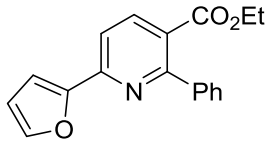
Ethyl 6-(2,3-dihydrobenzo[b][1,4]dioxin-5-yl)-2-phenylnicotinate (3i)



Colorless oil; (87 mg, 80%); R_f = 0.34 (hexanes/ethyl acetate 5:1); ^{1}H NMR (400 MHz,

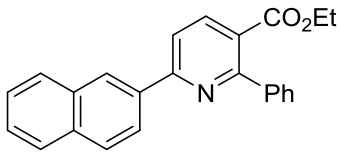
$CDCl_3$): δ 8.12 (d, J = 8.4 Hz, 1H), 7.70 (d, J = 2.0 Hz, 1H), 7.66–7.61 (m, 4H), 7.45–7.41 (m, 3H), 6.94 (d, J = 8.4 Hz, 1H), 4.27 (s, 4H), 4.16 (q, J = 7.2 Hz, 2H), 1.06 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 158.5, 157.6, 145.2, 143.7, 140.5, 138.7, 131.8, 128.8, 128.4, 127.8, 124.6, 120.5, 117.4, 116.9, 116.3, 64.5, 64.2, 61.2, 13.6; ESI-HRMS: m/z Calcd for $C_{22}H_{20}NO_4$, $[M + H]^+$: 362.1387, found 362.1390.

Ethyl 6-(furan-2-yl)-2-phenylnicotinate (3j)



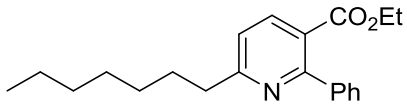
Yellow oil; (40 mg, 45%); R_f = 0.42 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, J = 8.0 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.59–7.57 (m, 3H), 7.45–7.42 (m, 3H), 7.21 (dd, J = 0.4 Hz, J = 3.6 Hz, 1H), 6.54 (dd, J = 1.6 Hz, J = 3.6 Hz, 1H), 4.15 (q, J = 7.2 Hz, 2H), 1.05 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.0, 159.1, 153.2, 150.4, 144.1, 140.4, 138.8, 128.8, 128.6, 128.0, 124.9, 115.9, 112.3, 110.8, 61.3, 13.6; ESI-HRMS: m/z Calcd for $C_{18}H_{16}NO_3$, $[M + H]^+$: 294.1125, found 294.1128.

N-Methyl-N-(3-oxo-3-phenylpropyl)octane-1-sulfonamide (3k)



White solid; (86 mg, 81%); mp: 95–98 °C; R_f = 0.33 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.59 (s, 1H), 8.24 (dd, J = 1.6 Hz, J = 8.4 Hz, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.94–7.90 (m, 2H), 7.88–7.83 (m, 2H), 7.68 (dd, J = 1.6 Hz, J = 7.6 Hz, 2H), 7.50–7.43 (m, 5H), 4.17 (q, J = 7.2 Hz, 2H), 1.06 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 158.8, 158.2, 140.6, 138.8, 135.5, 134.0, 133.3, 128.8, 128.6, 128.4, 128.0, 127.6, 127.0, 126.8, 126.3, 125.3, 124.6, 118.0, 61.3, 13.6; ESI-HRMS: m/z Calcd for $C_{24}H_{20}NO_2$, $[M + H]^+$: 354.1489, found 354.1494.

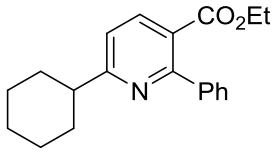
Ethyl 6-heptyl-2-phenylnicotinate (3l)



Colorless oil; (49 mg, 50%); R_f = 0.53 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz,

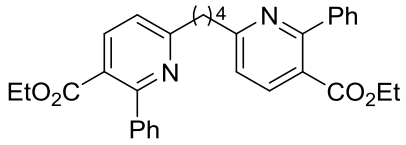
$CDCl_3$): 8.02 (d, *J* = 8.0 Hz, 1H), 7.53–7.50 (m, 2H), 7.44–7.38 (m, 3H), 7.17 (d, *J* = 8.4 Hz, 1H), 4.12 (q, *J* = 7.2 Hz, 2H), 2.87 (t, *J* = 8.0 Hz, 2H), 1.80–1.72 (m, 2H), 1.39–1.24 (m, 8H), 1.03 (t, *J* = 7.2 Hz, 3H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 168.3, 164.8, 158.5, 140.7, 138.1, 128.6, 128.3, 128.0, 124.5, 120.5, 61.2, 38.5, 31.7, 29.6, 29.3, 29.1, 22.6, 14.0, 13.6; ESI-HRMS: m/z Calcd for $C_{21}H_{28}NO_2$, $[M + H]^+$: 326.2115, found 326.2117.

Ethyl 6-cyclohexyl-2-phenylnicotinate (3m)



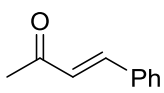
Colorless oil; (52 mg, 56%); R_f = 0.55 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.02 (d, *J* = 8.4 Hz, 1H), 7.54 (dd, *J* = 1.6 Hz, *J* =7.2 Hz, 2H), 7.43–7.36 (m, 3H), 7.18 (d, *J* = 8.0 Hz, 1H), 4.12 (q, *J* = 7.2 Hz, 2H), 2.86–2.78 (m, 1H), 2.00 (d, *J* = 11.6 Hz, 2H), 1.85 (d, *J* = 12.8 Hz, 2H), 1.75 (d, *J* = 12.4 Hz, 1H), 1.47–1.37 (m, 2H), 1.33–1.29 (m, 1H), 1.06 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 168.6, 168.4, 158.1, 140.8, 138.2, 128.7, 128.3, 127.9, 124.6, 118.5, 61.2, 46.6, 32.7, 26.4, 26.0, 13.6; ESI-HRMS: m/z Calcd for $C_{20}H_{24}NO_2$, $[M + H]^+$: 310.1802, found 310.1804.[9]

Diethyl 6,6'-(butane-1,4-diyl)bis(2-phenylnicotinate) (3n)



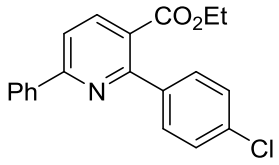
Yellow oil; (81 mg, 53%); R_f = 0.27 (hexanes/ethyl acetate 5:1); ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.00 (d, *J* = 8.0 Hz, 2H), 7.52–7.49 (m, 4H), 7.43–7.38 (m, 6H), 7.16 (d, *J* = 8.0 Hz, 2H), 4.12 (q, *J* = 7.2 Hz, 4H), 2.95–2.91 (m, 4H), 1.89–1.85 (m, 4H), 1.03 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ* 168.1, 164.1, 158.4, 140.5, 138.1, 128.5, 128.2, 127.9, 124.5, 120.4, 61.1, 38.0, 29.0, 13.5; ESI-HRMS: m/z Calcd for $C_{32}H_{33}N_2O_4$, $[M + H]^+$: 509.2435, found 509.2439.

(E)-4-Phenylbut-3-en-2-one (3o')



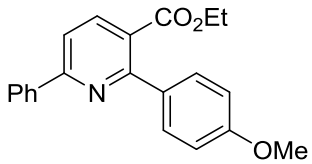
White solid; (40 mg, 92%); mp: 72-74 °C; R_f = 0.18 (hexanes/ethyl acetate 20:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53–7.49 (m, 3H), 7.40–7.38 (m, 3H), 6.71 (d, *J* = 16.0 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 198.2, 143.3, 134.3, 130.4, 128.8, 128.1, 127.0, 27.4; ESI-HRMS: m/z Calcd for $C_{10}H_{11}O$, $[M + H]^+$: 147.0804, found 147.0799. [10]

Ethyl 2-(4-chlorophenyl)-6-phenylnicotinate (4b)



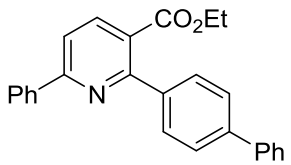
Yellow oil; (81 mg, 80%); R_f = 0.44 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17(d, *J* = 8.0 Hz, 1H), 8.10–8.08 (m, 2H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.59–7.56 (m, 2H), 7.49–7.40 (m, 5H), 4.20 (q, *J* = 7.2 Hz, 2H), 1H), 1.13 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 158.5, 157.6, 139.1, 139.0, 138.0, 134.7, 130.2, 129.8, 128.8, 128.1, 127.2, 125.0, 118.0, 61.4, 13.7; ESI-HRMS: m/z Calcd for $C_{20}H_{17}ClNO_2$, $[M + H]^+$: 338.0942, found 338.0945. [9]

Ethyl 2-(4-methoxyphenyl)-6-phenylnicotinate (4c)



Colorless oil; (76 mg, 76%); R_f = 0.26 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13–8.11 (m, 3H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.64–7.60 (m, 2H), 7.49–7.41 (m, 3H), 6.98 (d, *J* = 8.8 Hz, 2H), 4.22 (q, *J* = 7.2 Hz, 2H), 3.85 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.5, 160.2, 158.2, 158.0, 138.8, 138.4, 132.9, 130.3, 129.6, 128.7, 127.2, 124.9, 117.2, 113.4, 61.3, 55.3, 13.8; ESI-HRMS: m/z Calcd for $C_{21}H_{20}F_3NO_3$, $[M + H]^+$: 334.1438, found 334.1439. [6]

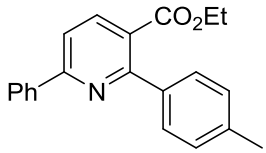
Ethyl 2-([1,1'-biphenyl]-4-yl)-6-phenylnicotinate (4d)



Yellow oil; (83 mg, 73%); R_f = 0.31 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17–8.12 (m, 3H), 7.74–7.72 (m, 3H), 7.68–7.64 (m, 4H), 7.48–7.40 (m, 5H), 7.36–7.32 (m, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 1.09 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz,

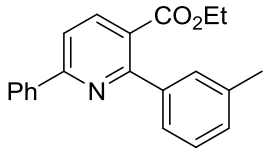
$CDCl_3$): δ 168.2, 158.4, 158.3, 141.4, 140.7, 139.4, 138.9, 138.2, 129.7, 129.3, 128.74, 128.71, 127.4, 127.3, 127.1, 126.7, 125.2, 117.7, 61.3, 13.7; ESI-HRMS: m/z Calcd for $C_{26}H_{22}NO_2$, $[M + H]^+$: 380.1645, found 380.1646.

Ethyl 6-phenyl-2-(p-tolyl)nicotinate (4e)



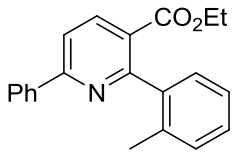
Yellow oil; (78 mg, 82%); R_f = 0.39 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13–8.10 (m, 3H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.48–7.39 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.19 (q, *J* = 7.2 Hz, 2H), 2.40 (s, 3H), 1.11 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 158.6, 158.2, 138.7, 138.4, 138.3, 137.6, 129.6, 128.74, 128.67, 128.6, 127.2, 125.1, 117.4, 61.3, 21.3, 13.7; ESI-HRMS: m/z Calcd for $C_{21}H_{20}NO_2$, $[M + H]^+$: 318.1489, found 318.1490. [9]

Ethyl 6-phenyl-2-(m-tolyl)nicotinate (4f)



Colorless oil; (67 mg, 70%); R_f = 0.44 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14–8.10 (m, 3H), 7.73 (d, *J* = 8.0 Hz, 1H), 7.48–7.40 (m, 5H), 7.32(t, *J* = 7.2 Hz, 1H), 7.23 (d, *J* = 6.0 Hz, 1H), 4.17 (q, *J* = 7.2 Hz, 2H), 2.41 (s, 3H), 1.07 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 158.8, 158.3, 140.4, 138.7, 138.3, 137.5, 129.6, 129.4, 129.3, 128.7, 127.8, 127.3, 125.9, 125.4, 117.7, 61.2, 21.4, 13.6; ESI-HRMS: m/z Calcd for $C_{21}H_{20}NO_2$, $[M + H]^+$: 318.1489, found 318.1490.

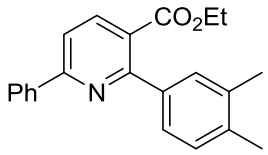
Ethyl 6-phenyl-2-(o-tolyl)nicotinate (4g)



Colorless oil; (60 mg, 63%); R_f = 0.53 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.30 (d, *J* = 8.0 Hz, 1H), 8.10–8.08 (m, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.48–7.40 (m, 3H), 7.32–7.19 (m, 4H), 4.08 (q, *J* = 7.2 Hz, 2H), 2.22 (s, 3H), 0.97 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.0, 160.2, 158.7, 141.0, 138.9, 138.3, 135.5, 129.8, 129.7,

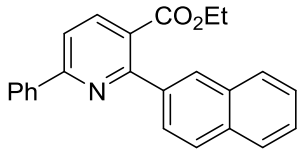
128.7, 128.5, 128.0, 127.4, 125.5, 125.3, 118.1, 61.1, 19.8, 13.5; ESI-HRMS: m/z Calcd for $C_{21}H_{20}NO_2$, $[M + H]^+$: 318.1489, found 318.1490.

Ethyl 2-(3,4-dimethylphenyl)-6-phenylnicotinate (4h)



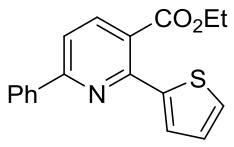
Yellow oil; (84 mg, 85%); R_f = 0.38 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.11 (dd, *J* = 1.2 Hz, *J* = 8.4 Hz, 3H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.48–7.39 (m, 4H), 7.36 (dd, *J* = 1.2 Hz, *J* = 8.0 Hz, 1H), 7.20 (t, *J* = 8.0 Hz, 1H), 4.20 (q, *J* = 7.2 Hz, 2H), 2.32 (s, 3H), 2.31 (s, 3H), 1.12 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 158.7, 158.2, 138.6, 138.4, 137.9, 137.1, 136.1, 130.0, 129.6, 129.2, 128.7, 127.3, 126.3, 125.2, 117.4, 61.2, 19.8, 19.6, 13.7; ESI-HRMS: m/z Calcd for $C_{22}H_{22}NO_2$, $[M + H]^+$: 332.1645, found 332.1647.

Ethyl 2-(naphthalen-2-yl)-6-phenylnicotinate (4i)



Yellow oil; (42 mg, 40%); R_f = 0.32 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 8.4 Hz, 1H), 8.16–8.13 (m, 3H), 7.92–7.87 (m, 3H), 7.80–7.76 (m, 2H), 7.53–7.42 (m, 5H), 4.15 (q, *J* = 7.2 Hz, 2H), 0.98 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 158.6, 158.5, 139.0, 138.3, 137.9, 133.3, 133.1, 129.8, 128.8, 128.5, 128.3, 127.7, 127.5, 127.4, 126.7, 126.4, 126.1, 125.6, 117.8, 61.4, 13.7; ESI-HRMS: m/z Calcd for $C_{24}H_{20}NO_2$, $[M + H]^+$: 354.1489, found 354.1490.

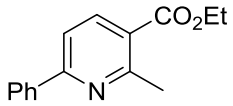
Ethyl 6-phenyl-2-(thiophen-2-yl)nicotinate (4j)



Yellow oil; (51 mg, 55%); R_f = 0.33 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13–8.11 (m, 2H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.51–7.42 (m, 5H), 7.08 (dd, *J* = 3.6 Hz, *J* = 5.2 Hz, 1H), 4.36 (q, *J* = 7.2 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.4, 157.9, 150.4, 143.4, 138.5, 137.8, 129.8, 128.8,

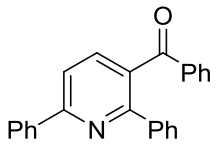
128.5, 127.8, 127.5, 127.2, 124.0, 117.2, 61.7, 13.9; ESI-HRMS: m/z Calcd for $C_{18}H_{16}NO_2S$, $[M + H]^+$: 310.0896, found 310.0899. [6]

Ethyl 2-methyl-6-phenylnicotinate (4k)



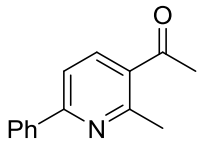
Yellow oil; (64 mg, 88%); R_f = 0.56 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.24 (d, J = 8.0 Hz, 1H), 8.06–8.04 (m, 2H), 7.60 (d, J = 8.0 Hz, 1H), 7.49–7.40 (m, 3H), 4.38 (q, J = 7.2 Hz, 2H), 2.91 (s, 3H), 1.40 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 166.6, 159.9, 159.0, 139.2, 138.4, 129.6, 128.7, 127.2, 123.6, 117.2, 61.0, 25.2, 14.2; ESI-HRMS: m/z Calcd for $C_{15}H_{16}NO_2$, $[M + H]^+$: 242.1176, found 242.1178. [6]

(2,6-Diphenylpyridin-3-yl)(phenyl)methanone (4l)



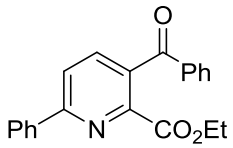
White solid; (63 mg, 63%); mp: 98–102 ^{o}C; R_f = 0.35 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20–8.18 (m, 2H), 7.91 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.62 (dd, J = 1.6 Hz, J = 8.0 Hz, 2H), 7.52–7.43 (m, 3H), 7.41 (t, J = 7.6 Hz, 1H), 7.29–7.21 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.4, 158.0, 157.2, 139.5, 138.4, 138.2, 136.8, 133.1, 132.5, 129.8, 129.6, 129.4, 128.8, 128.3, 128.2, 127.2, 117.7; ESI-HRMS: m/z Calcd for $C_{24}H_{18}NO$, $[M + H]^+$: 336.1383, found 336.1384. [9]

1-(2-Methyl-6-phenylpyridin-3-yl)ethan-1-one (4m)



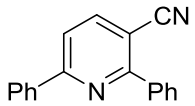
White solid; (35 mg, 56%); mp: 85–88 ^{o}C; R_f = 0.23 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.07–8.03 (m, 3H), 7.63 (d, J = 8.0 Hz, 1H), 7.50–7.42 (m, 3H), 2.84 (s, 3H), 2.61 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 199.9, 158.6, 158.5, 138.4, 137.9, 130.7, 129.6, 128.8, 127.2, 117.2, 29.2, 25.3; ESI-HRMS: m/z Calcd for $C_{14}H_{14}NO$, $[M + H]^+$: 212.1070, found 212.1073. [9]

Ethyl 3-benzoyl-6-phenylpicolinate (4n)



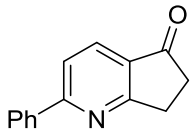
Yellow oil; (50 mg, 50%); R_f = 0.39 (hexanes/ethyl acetate 5:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14–8.12 (m, 2H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.82–7.80 (m, 2H), 7.60 (t, *J* = 7.2 Hz, 1H), 7.55–7.45 (m, 5H), 4.18 (q, *J* = 7.2 Hz, 2H), 1.16 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 194.8, 165.1, 158.4, 147.6, 137.6, 137.5, 136.9, 134.8, 133.4, 130.1, 129.4, 128.9, 128.7, 127.4, 122.0, 62.2, 13.7; ESI-HRMS: m/z Calcd for $C_{21}H_{18}NO_3$, $[M + H]^+$: 332.1281, found 332.1284.

2,6-Diphenylnicotinonitrile (4o)



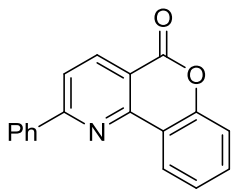
White solid; (41 mg, 54%); mp: 146–149 °C; R_f = 0.28 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15–8.12 (m, 2H), 8.09–8.04 (m, 3H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.57–7.48 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 159.6, 142.5, 137.5, 137.4, 130.5, 130.2, 129.0, 128.9, 128.6, 127.4, 118.2, 117.7, 105.1; ESI-HRMS: m/z Calcd for $C_{18}H_{13}N_2$, $[M + H]^+$: 257.1073, found 257.1078. [11]

2-Phenyl-6,7-dihydro-5H-cyclopenta[b]pyridin-5-one (4p)



Yellow solid; (48 mg, 76%); mp: 174–176 °C; R_f = 0.20 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.09–8.07 (m, 3H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.54–7.50 (m, 3H), 3.34 (t, *J* = 6.0 Hz, 2H), 2.84–2.82 (m, 2H) ; ^{13}C NMR (100 MHz, $CDCl_3$): δ 204.8, 174.9, 163.6, 138.4, 132.6, 130.3, 129.0, 128.7, 127.7, 119.7, 36.0, 29.0; ESI-HRMS: m/z Calcd for $C_{14}H_{12}NO$, $[M +H]^+$: 210.0913, found 210.0917.

2-Phenyl-5H-chromeno[4,3-b]pyridin-5-one (4q)



White solid; (50 mg, 60%); mp: 213–217 ^{o}C; R_f = 0.47 (hexanes/ethyl acetate 10:1); ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.76 (dd, J = 1.6 Hz, J = 8.0 Hz,1H), 8.65 (d, J = 8.4 Hz, 1H), 8.27–8.24 (m, 2H), 7.96 (d, J = 8.4 Hz, 1H), 7.62–7.52 (m, 4H), 7.45–7.39 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.5, 161.2, 152.9, 151.7, 138.9, 137.8, 132.1, 130.8, 129.0, 127.7, 124.9, 124.8, 120.3, 119.6, 117.2, 115.6; ESI-HRMS: m/z Calcd for $C_{18}H_{12}NO_2$, $[M + H]^+$: 274.0863, found 274.0865. [12]

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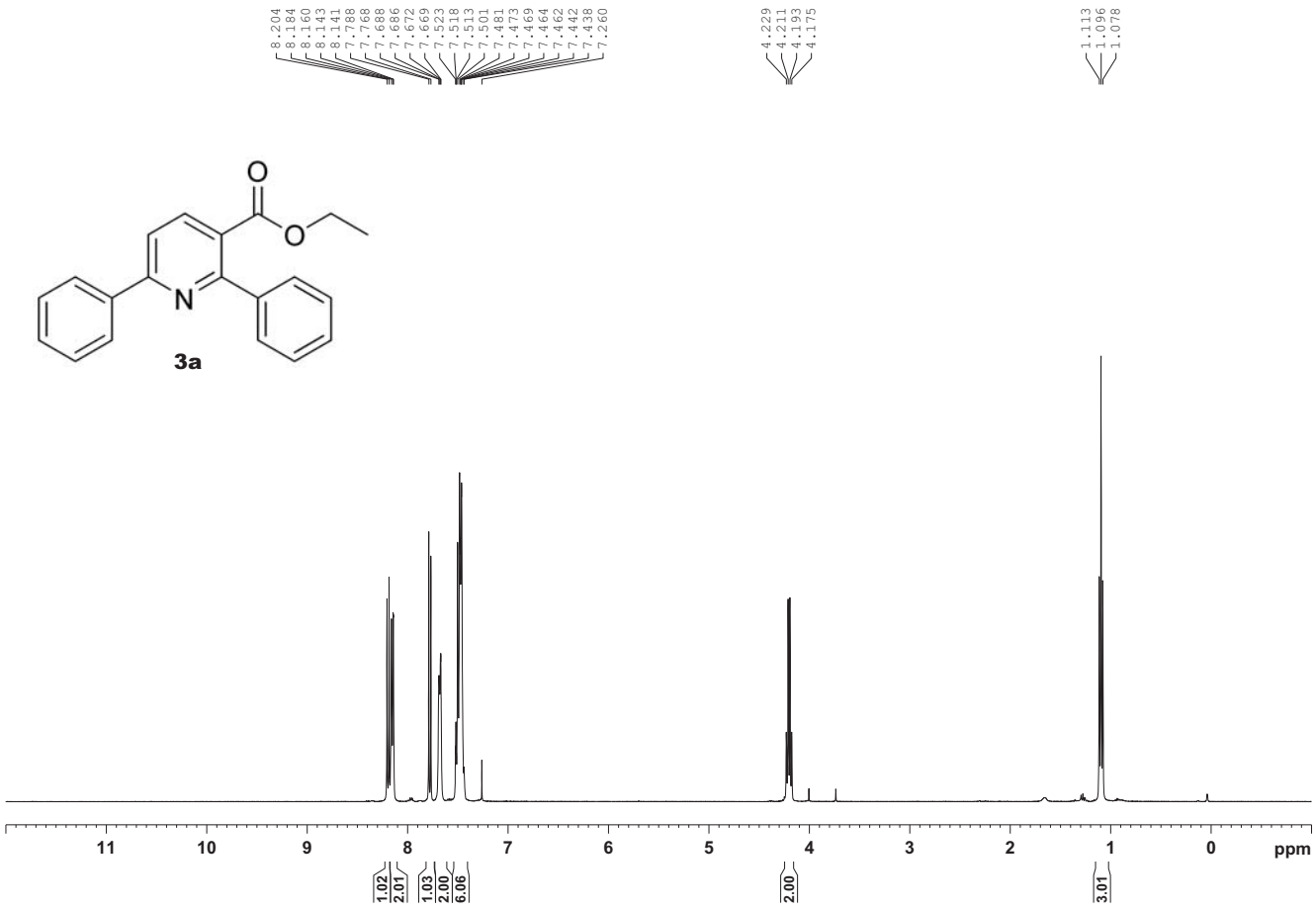
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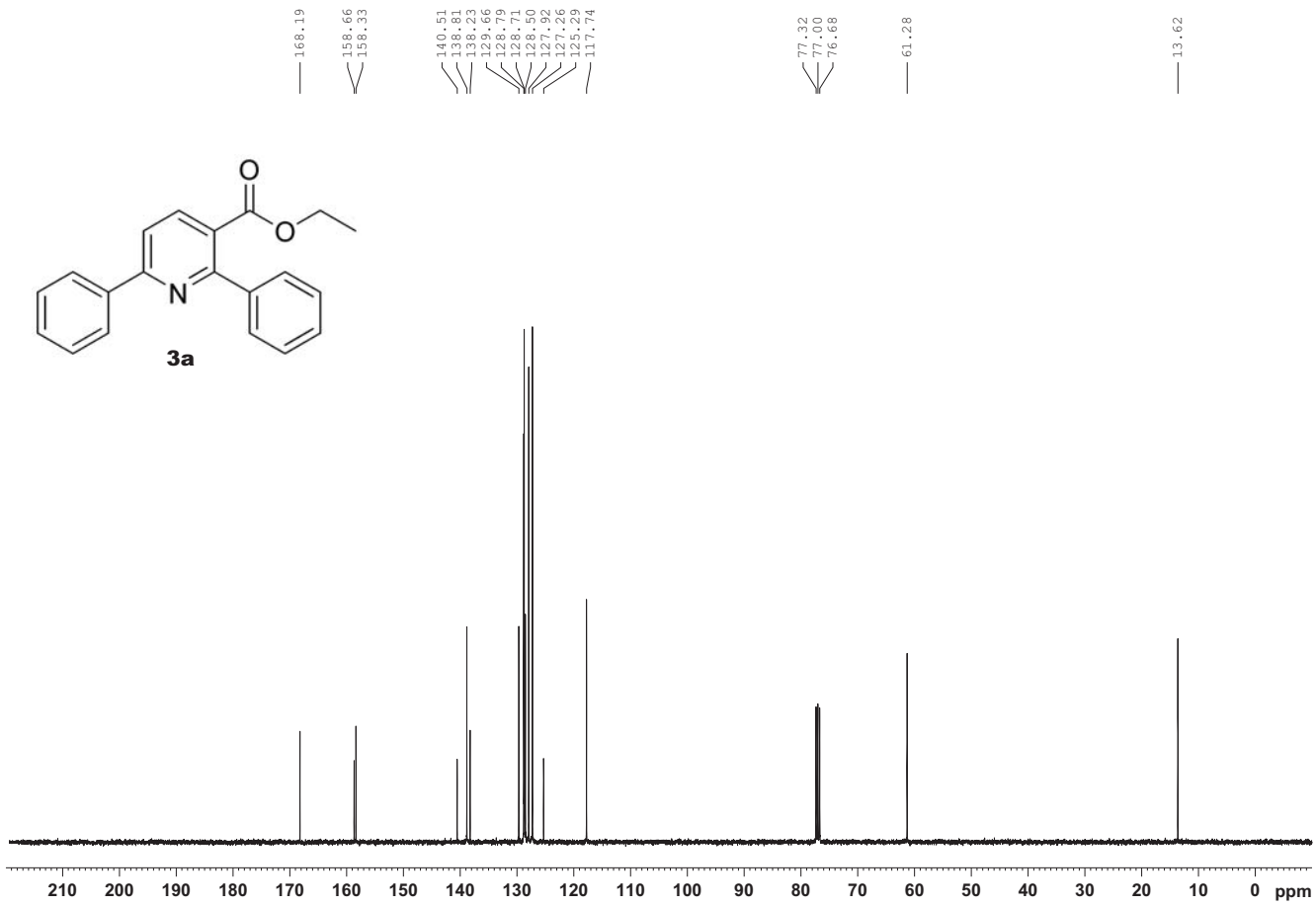
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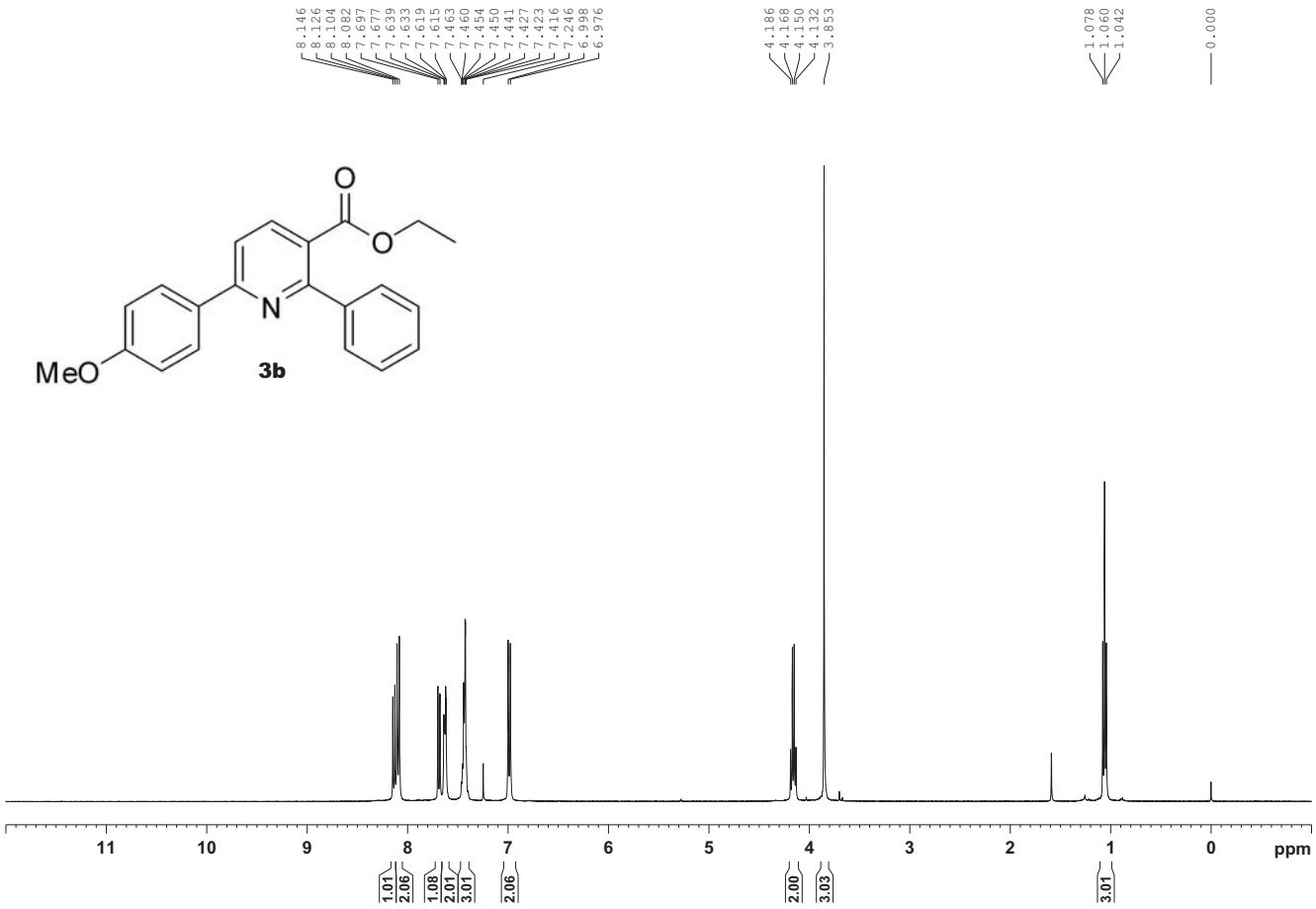
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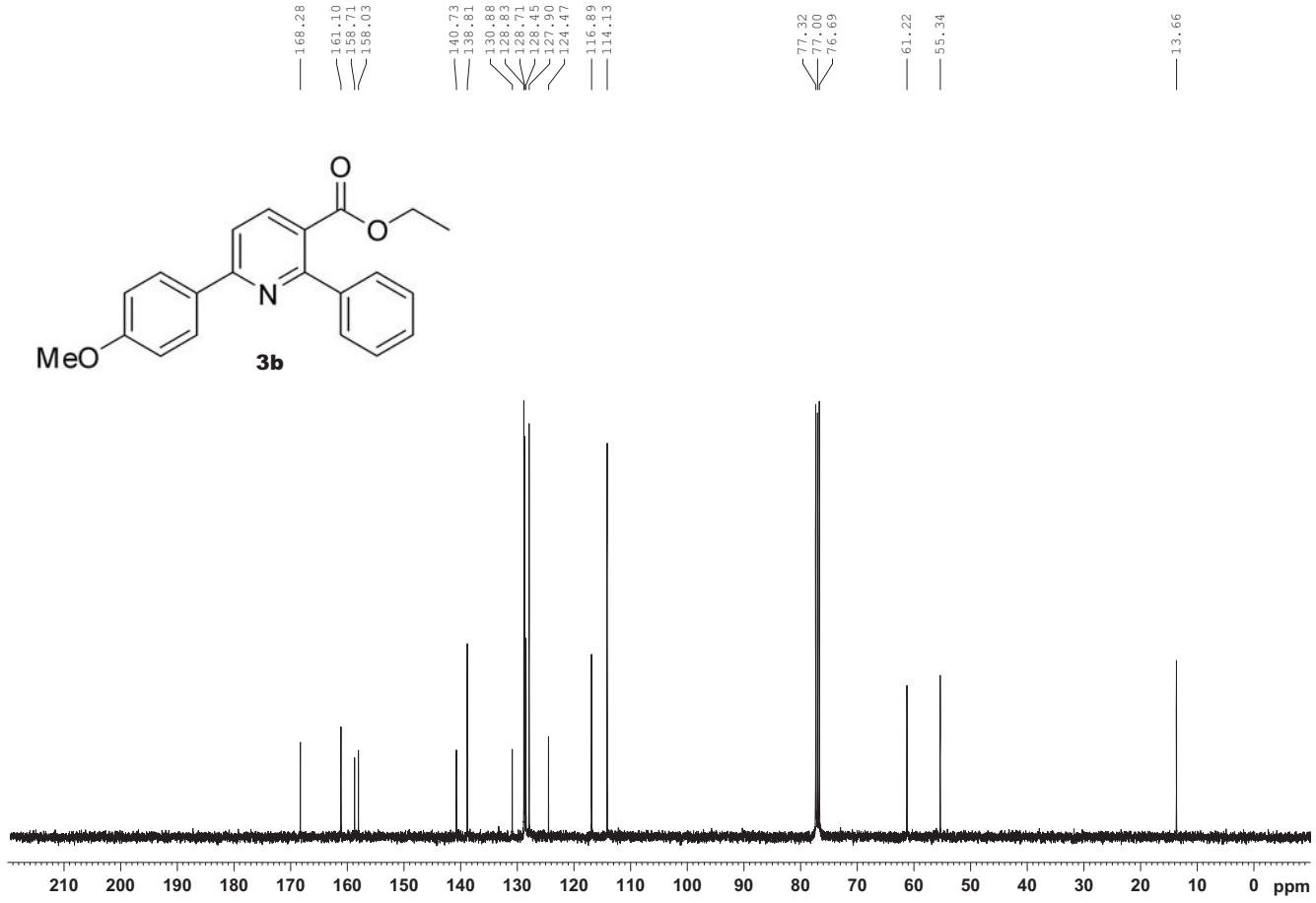
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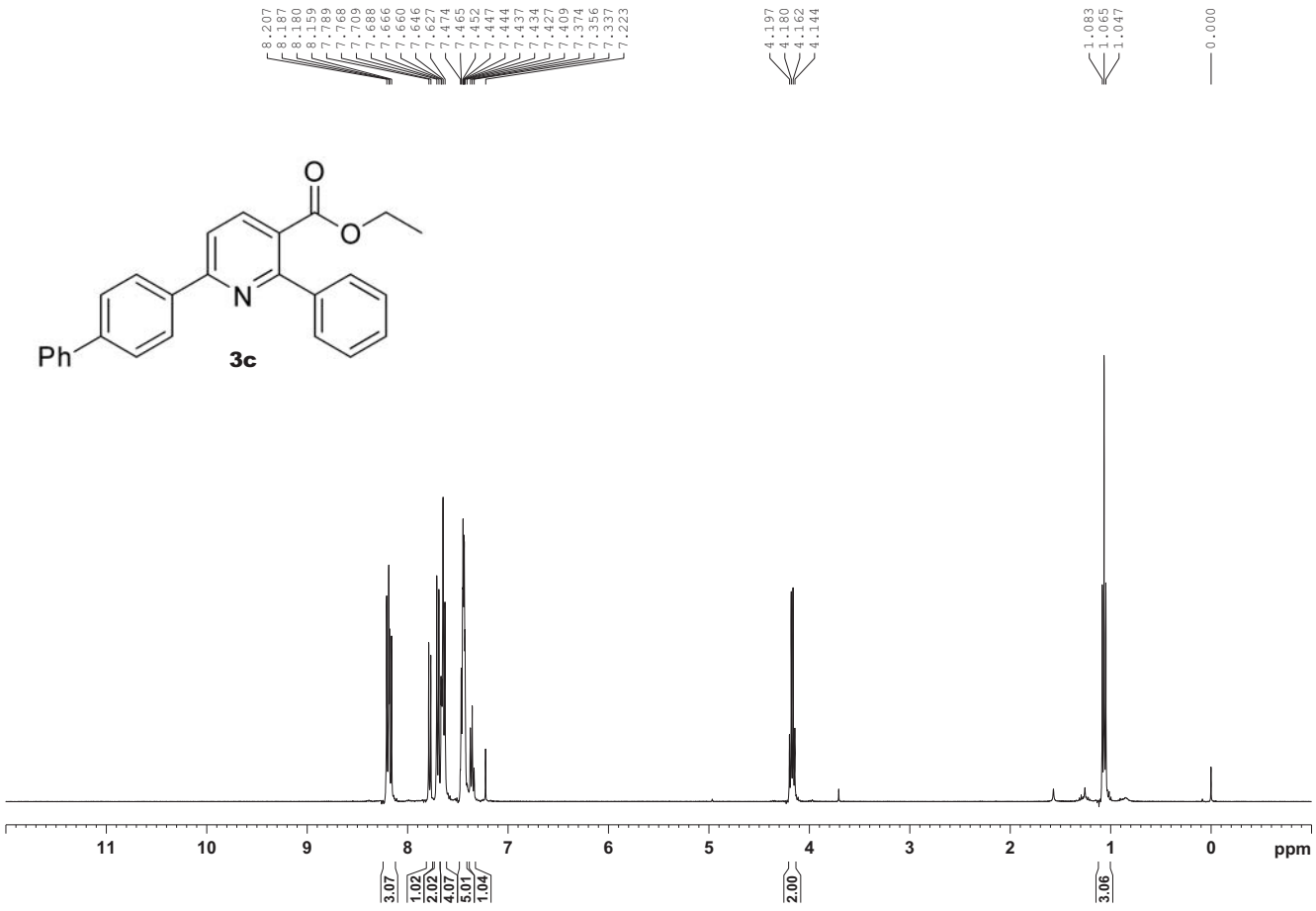
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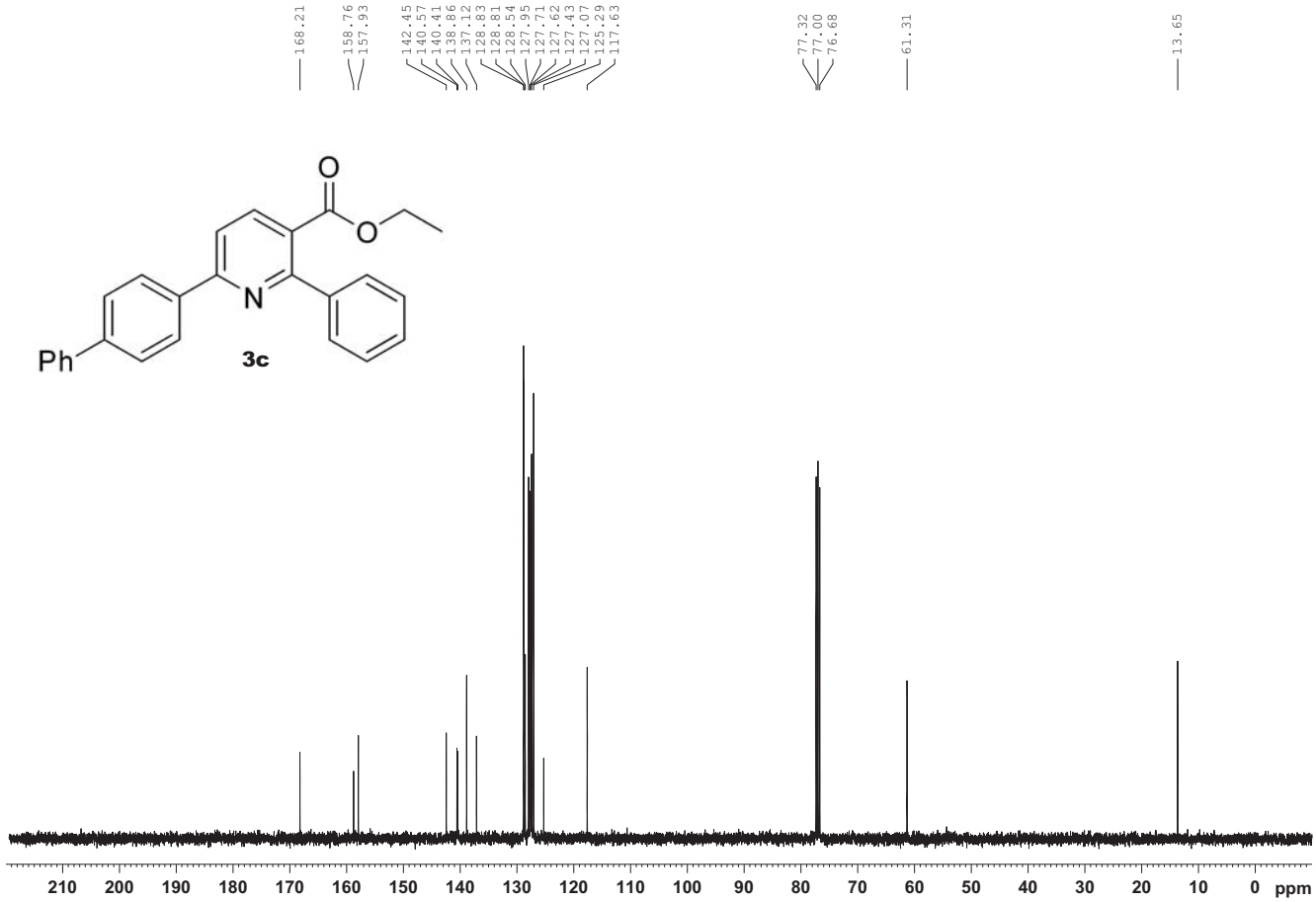
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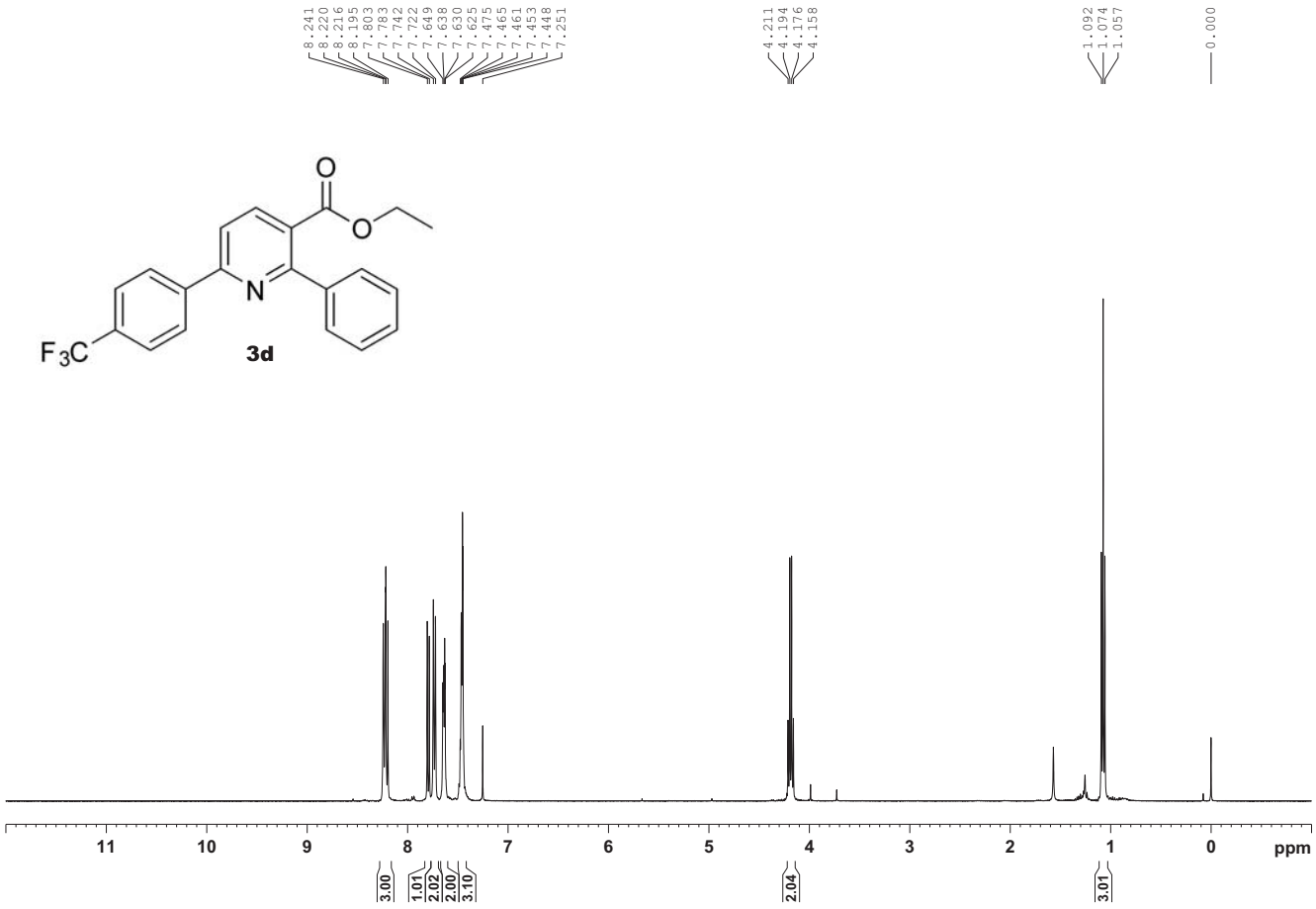
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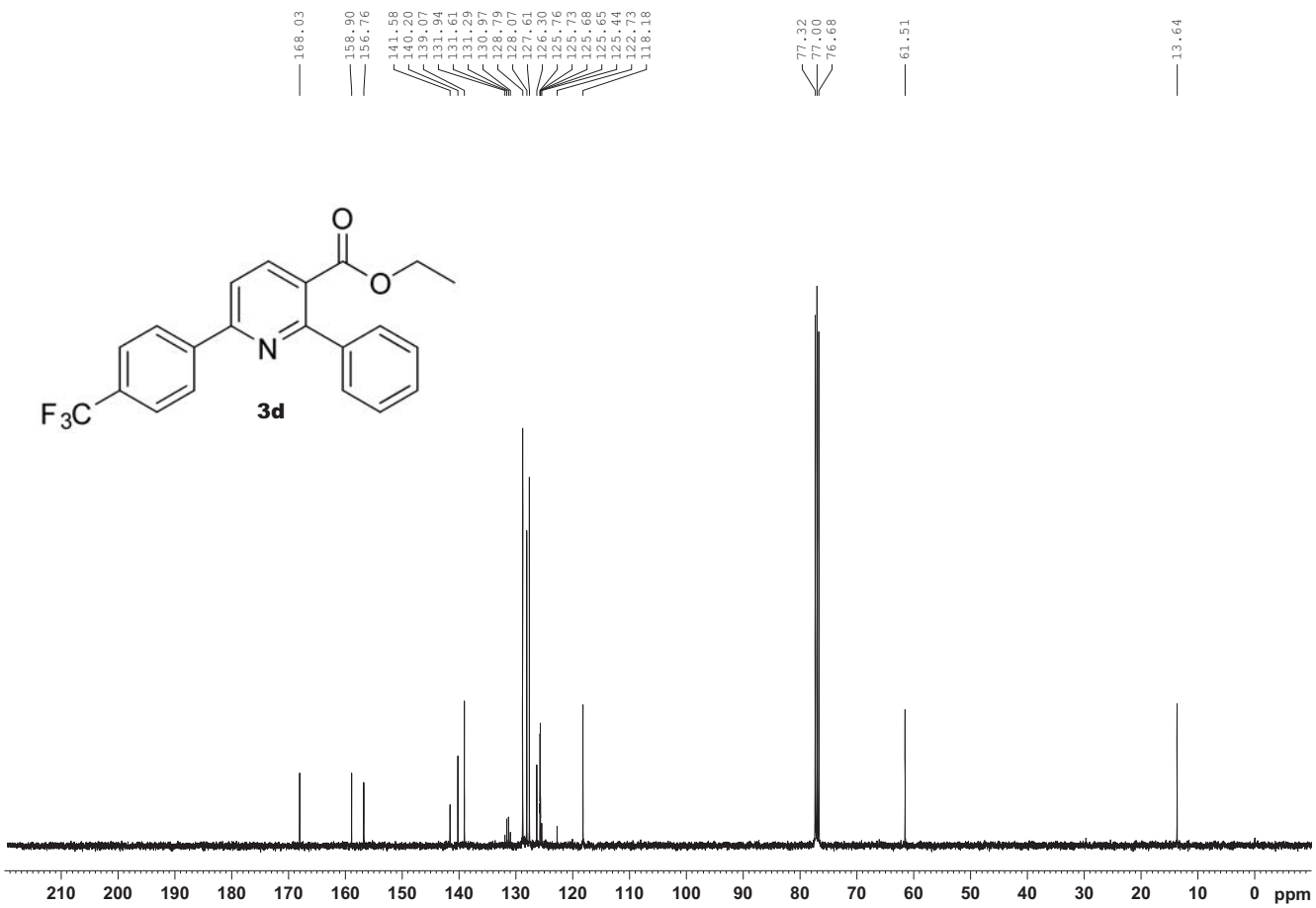
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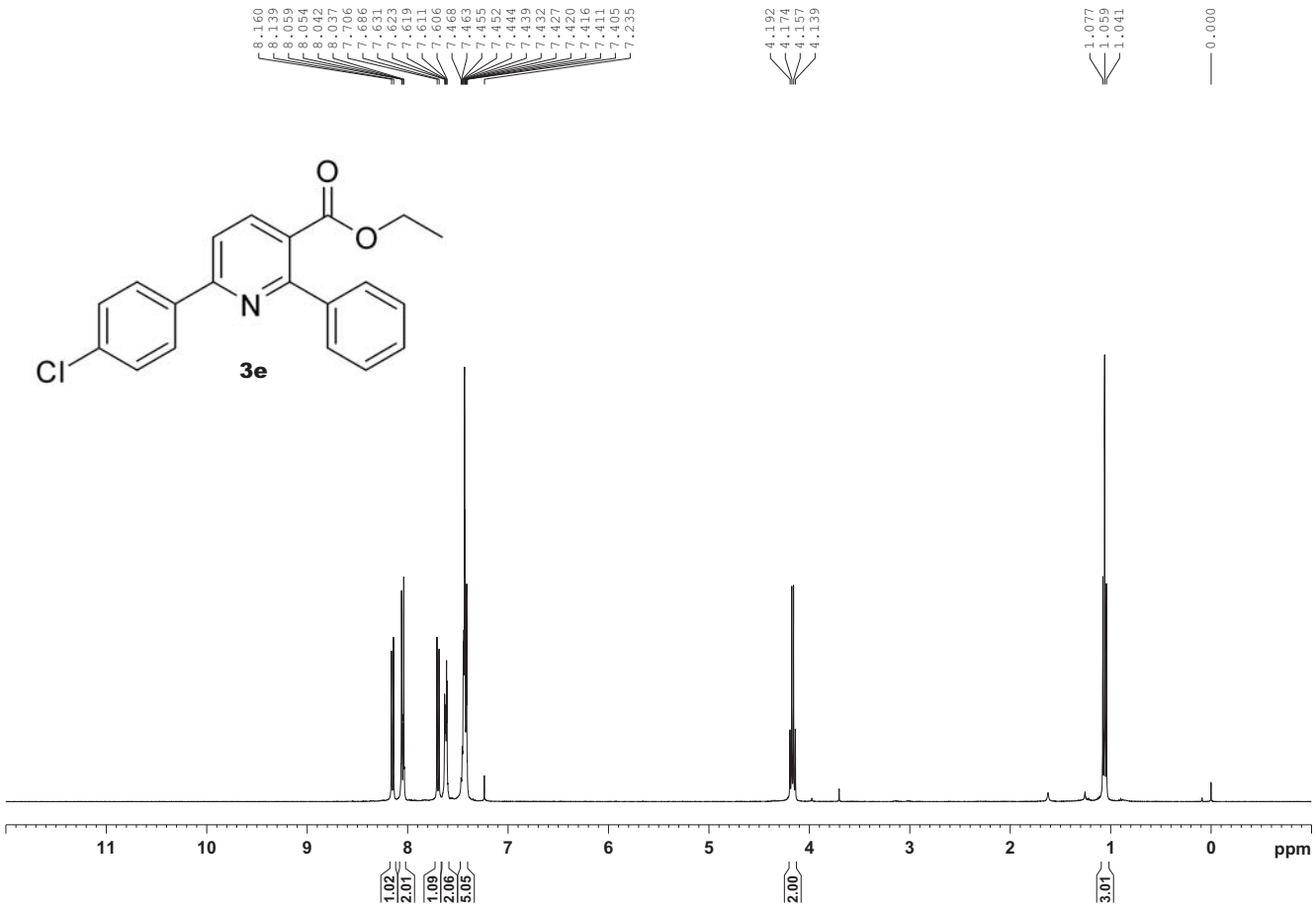
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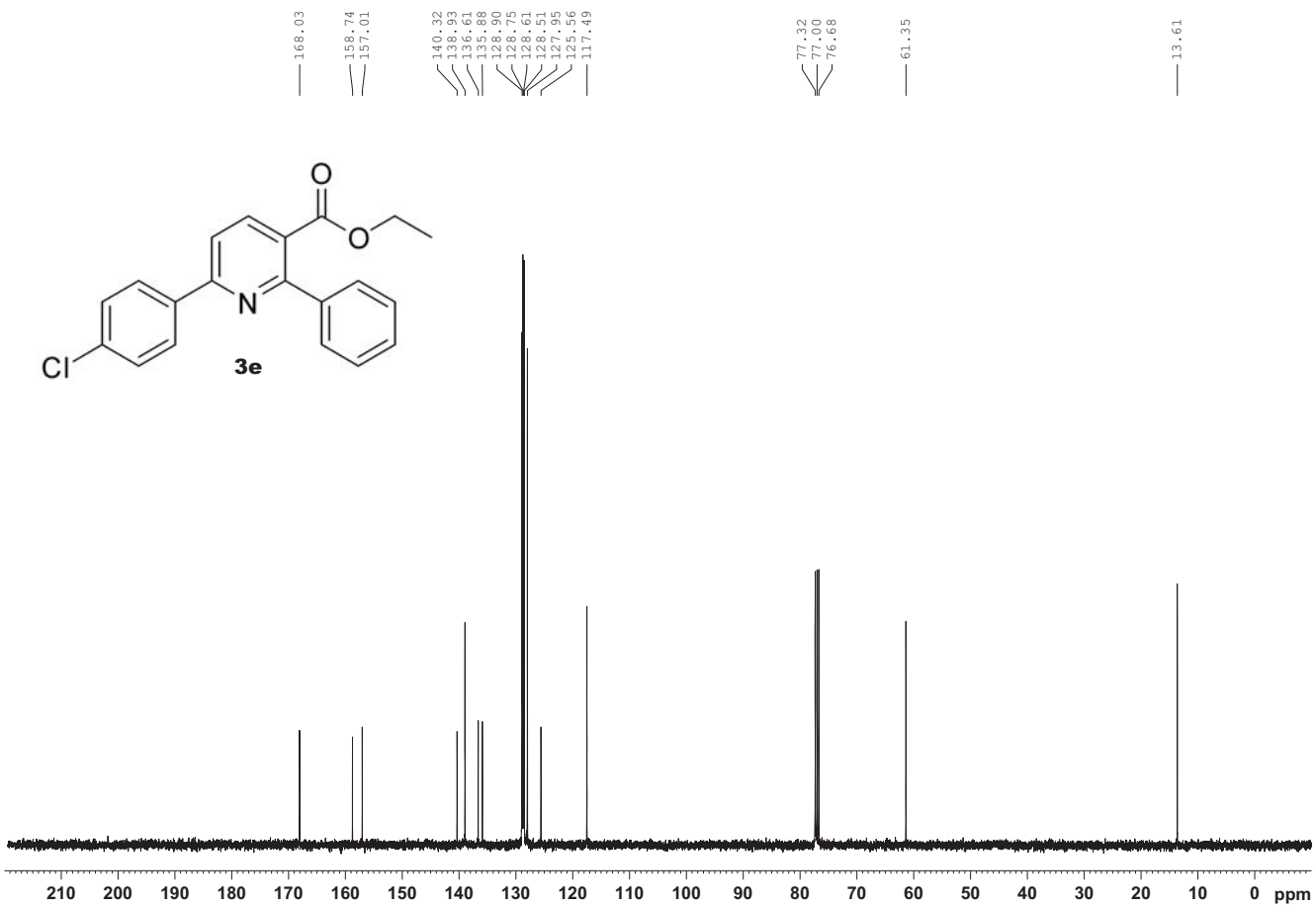
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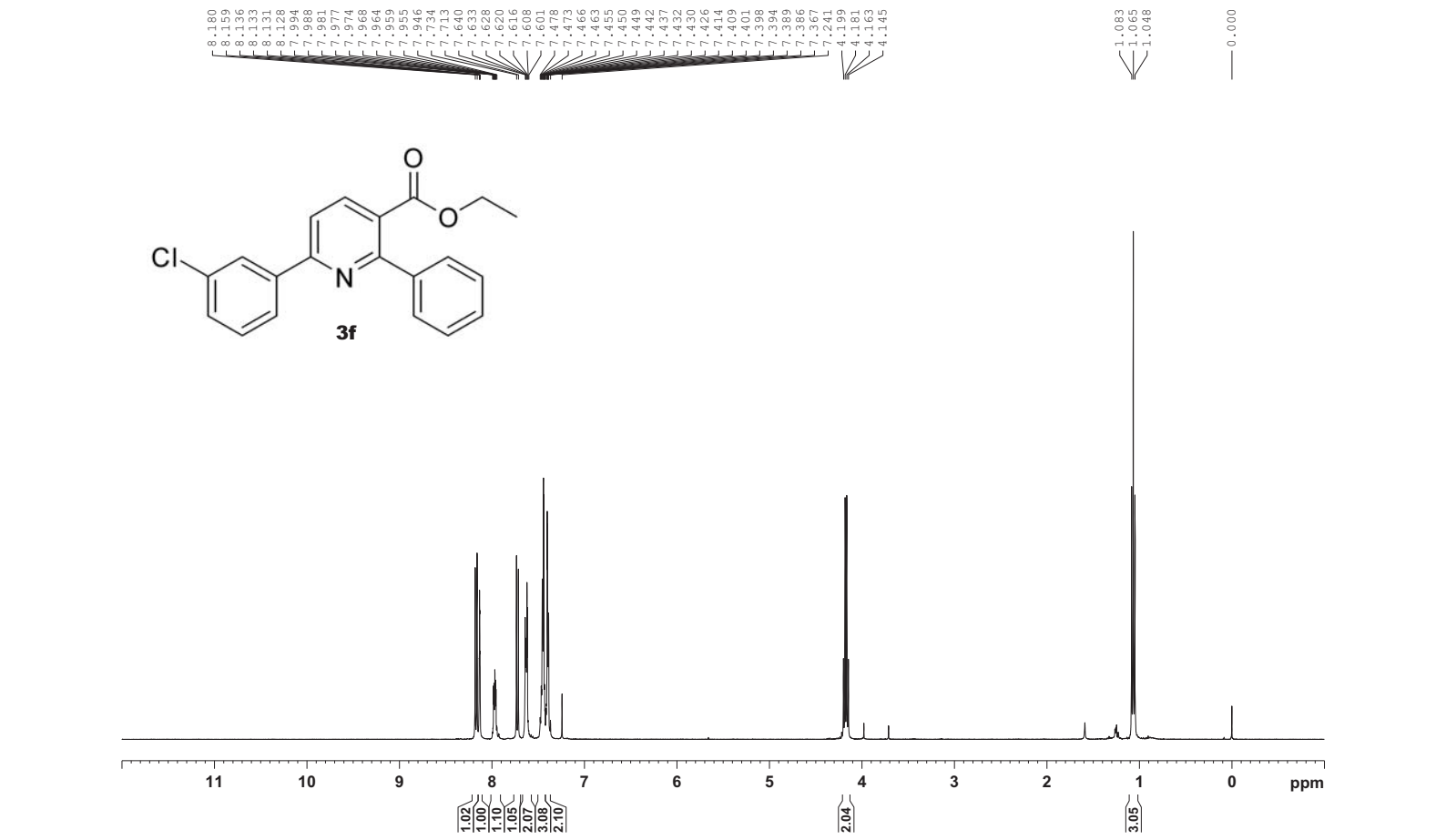
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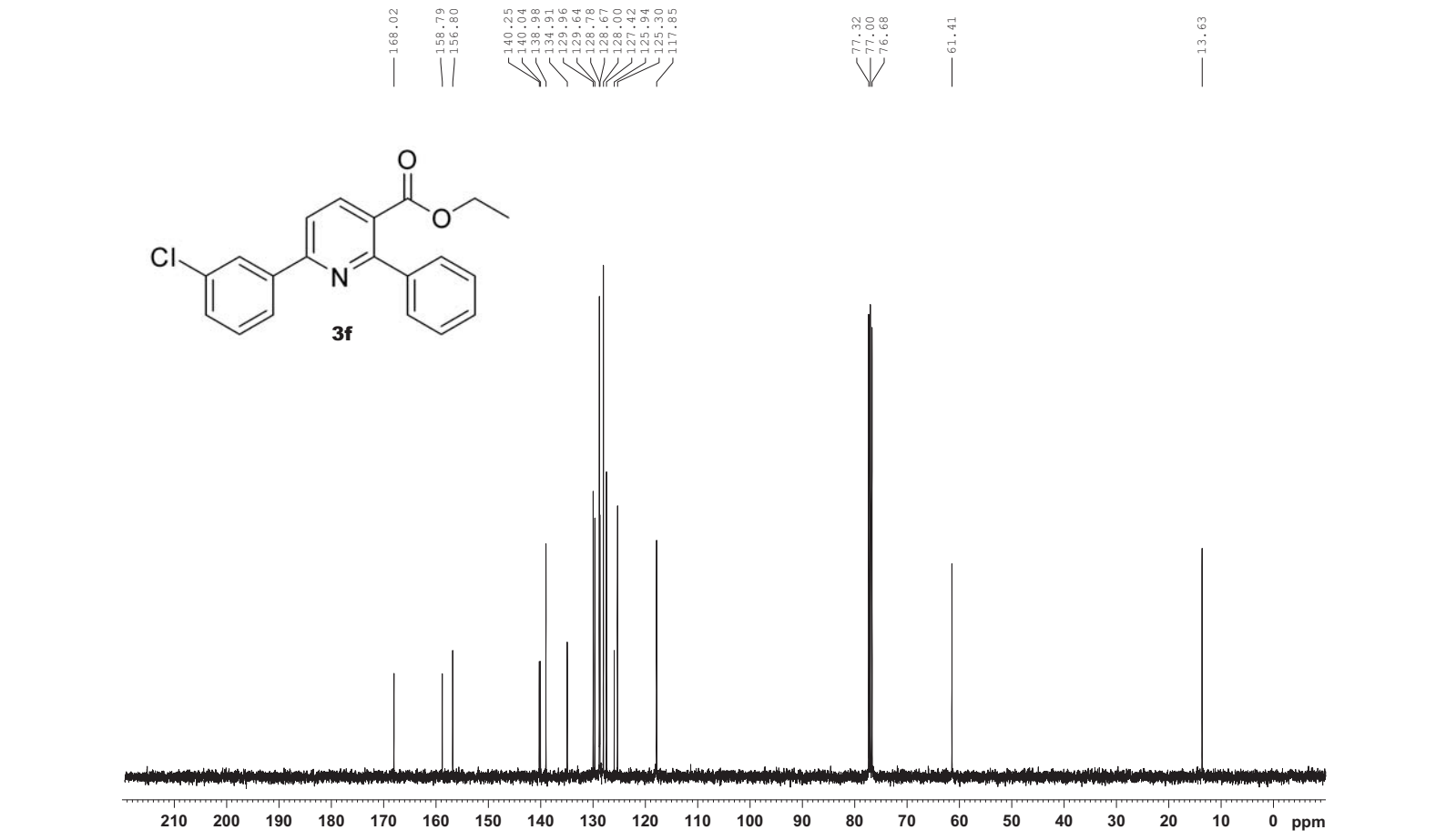
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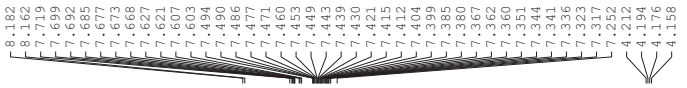
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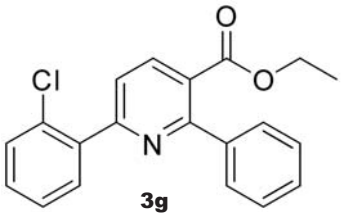
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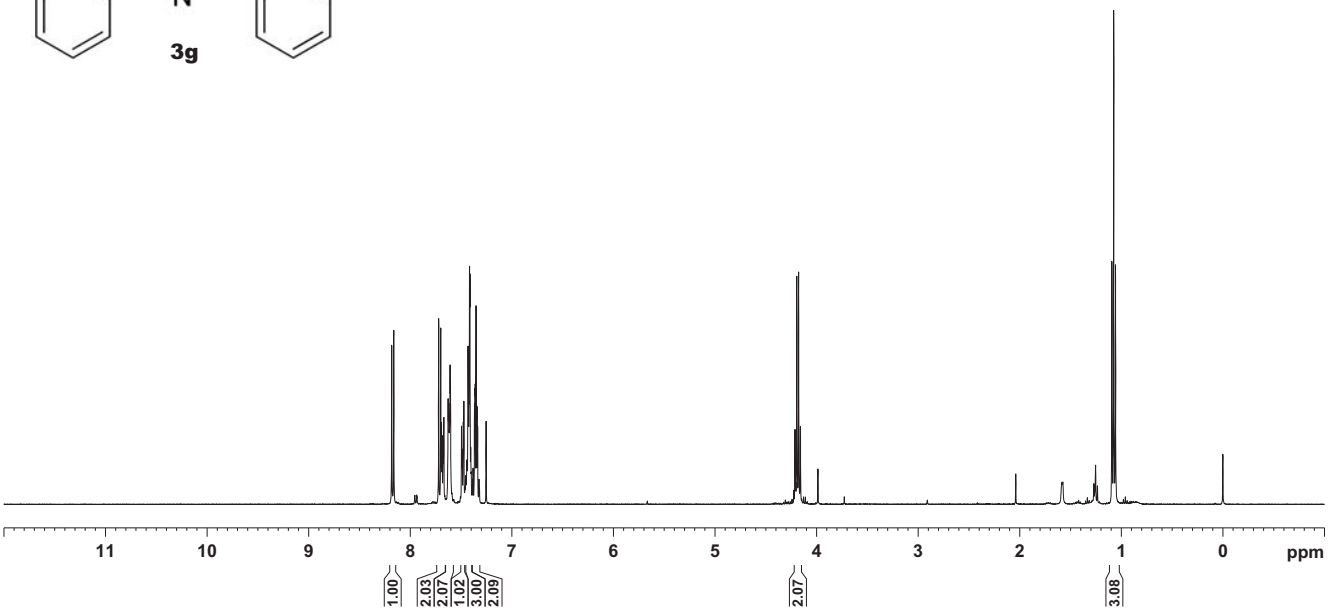
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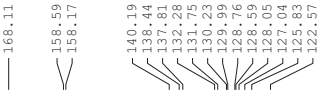
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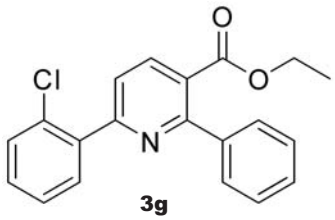
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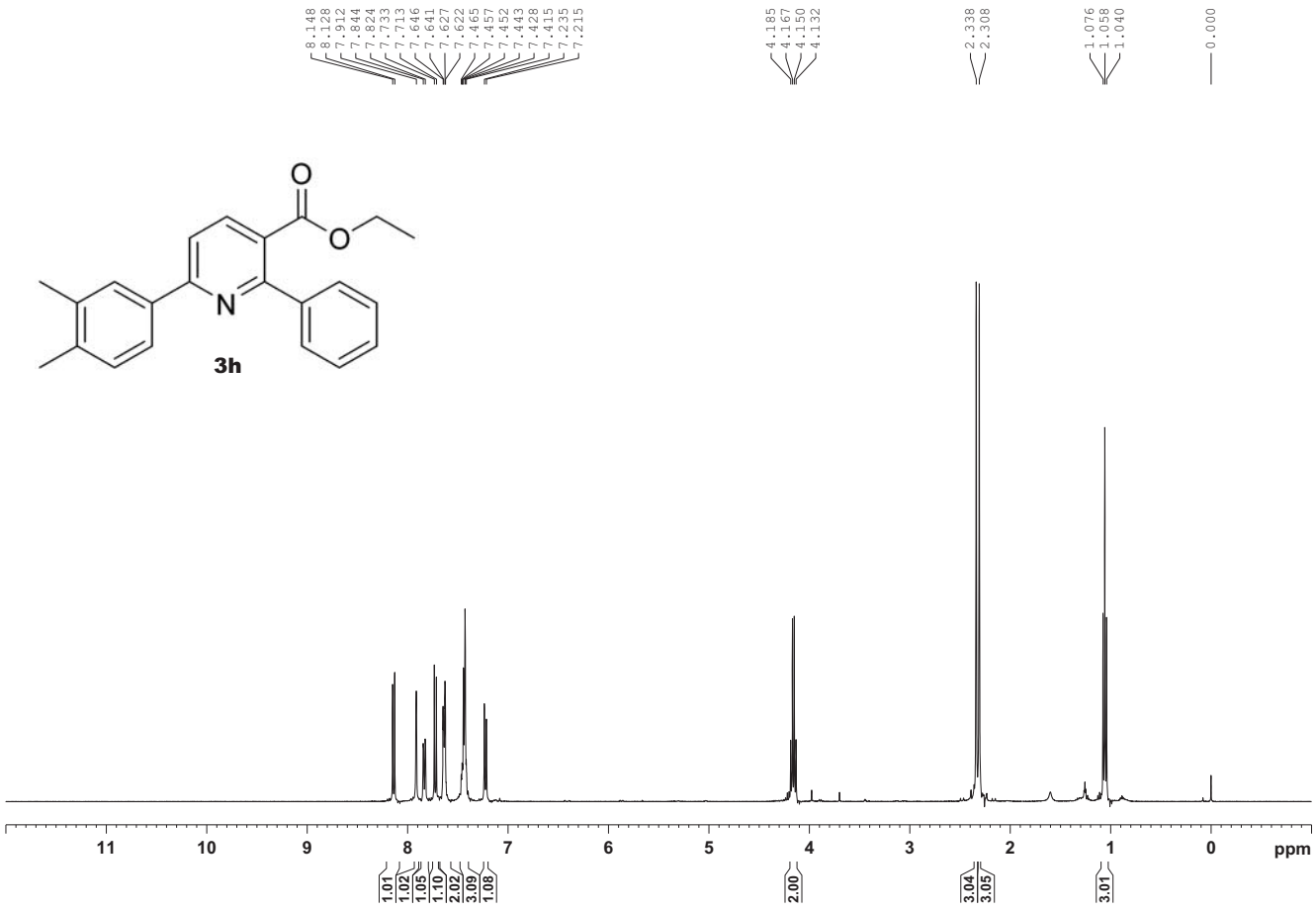
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7.215
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O
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3h
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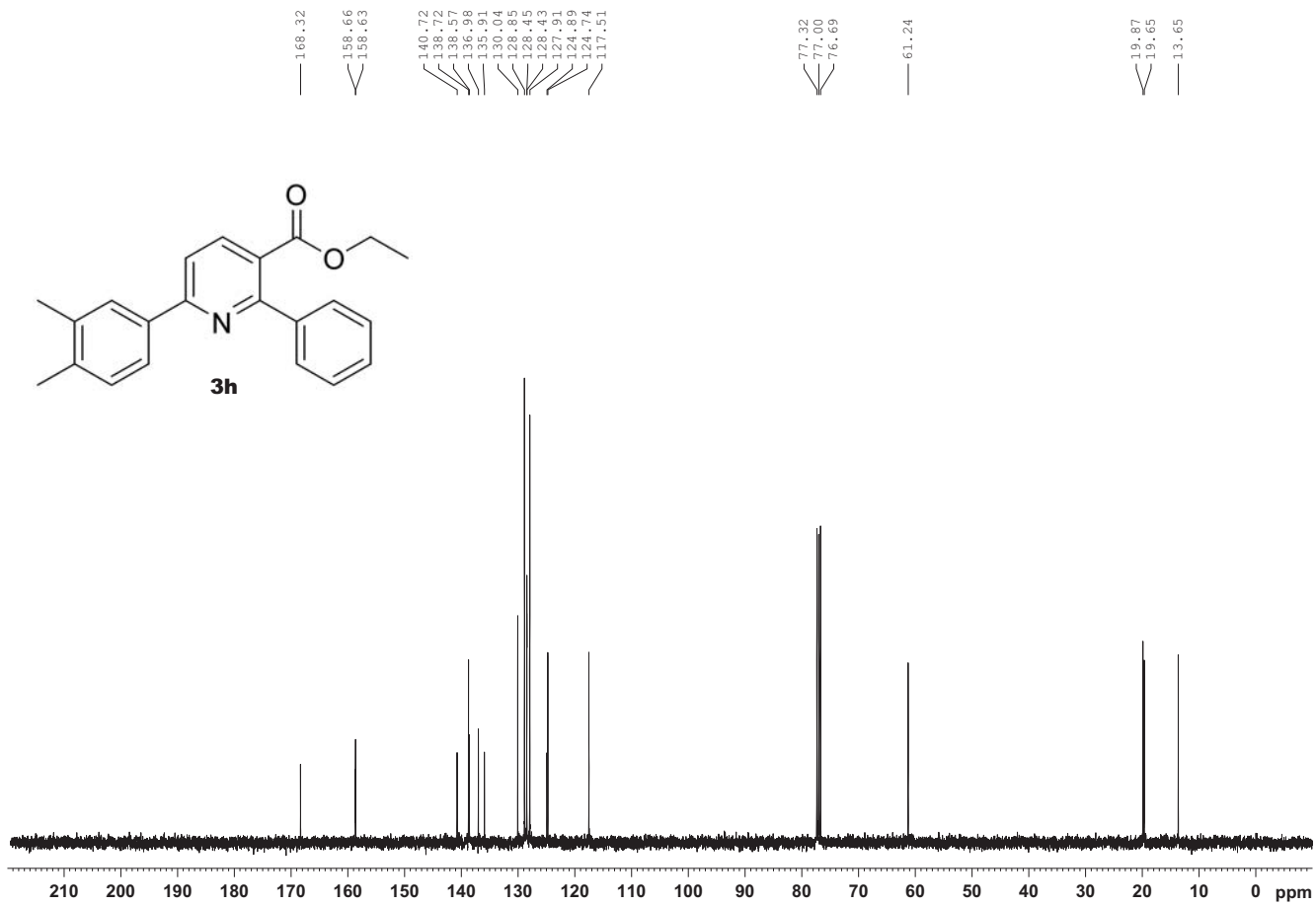
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76.69
61.24
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19.65
13.65
O
O
N
3h
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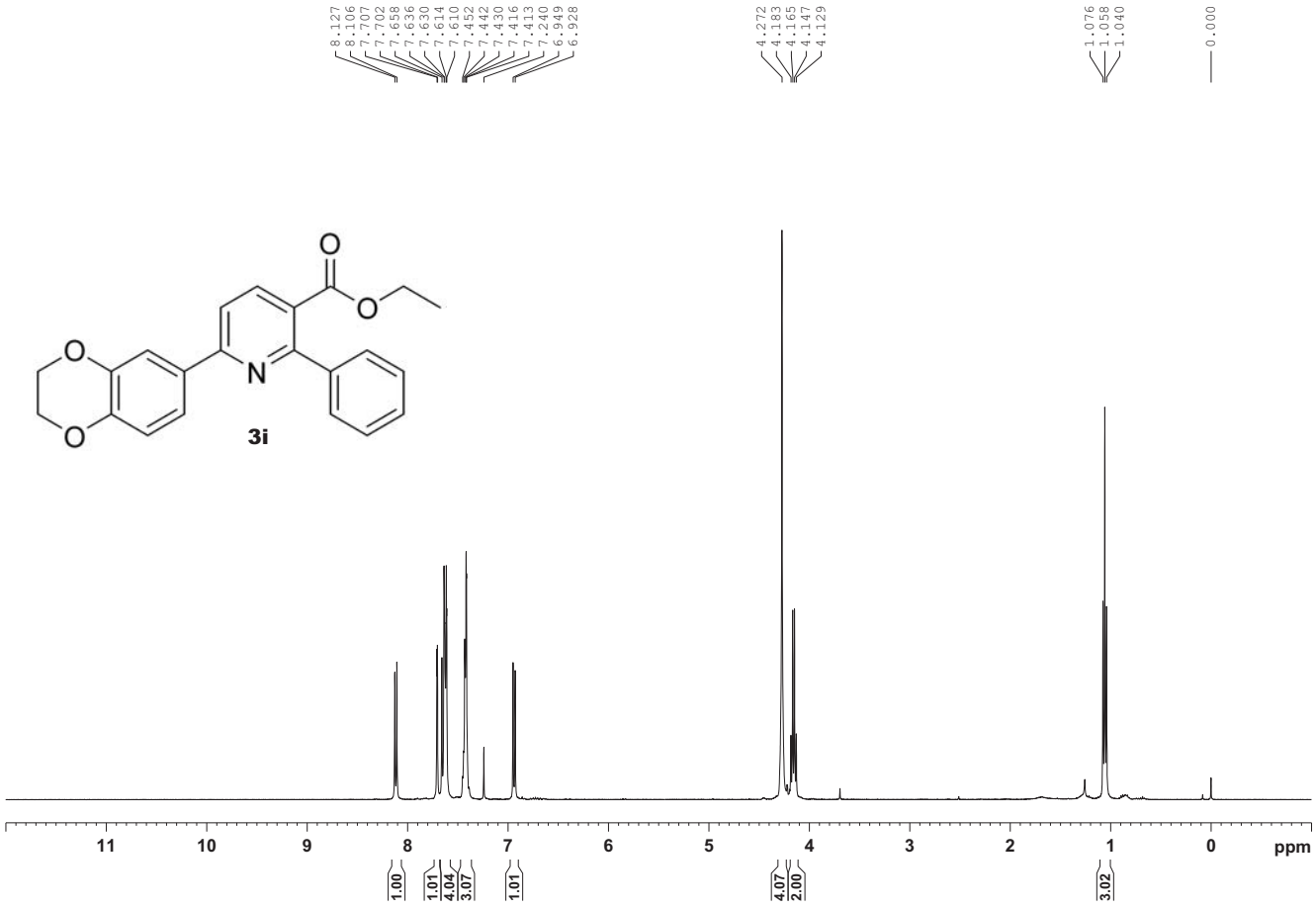
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7.413
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1.058
1.040
0.000
O
O
N
O
O
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10
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7
6
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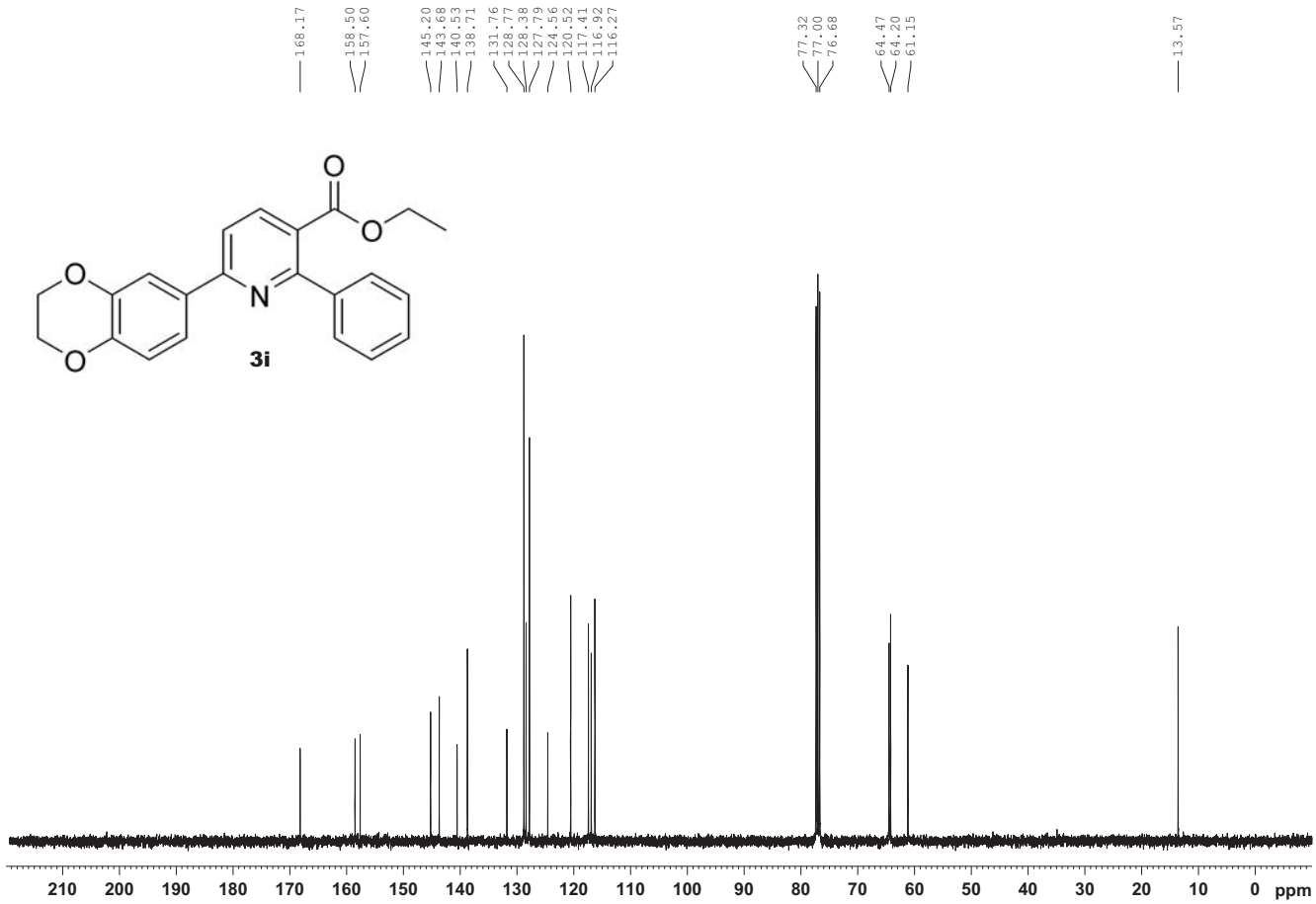
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64.20
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13.57
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O
N
O
O
3i
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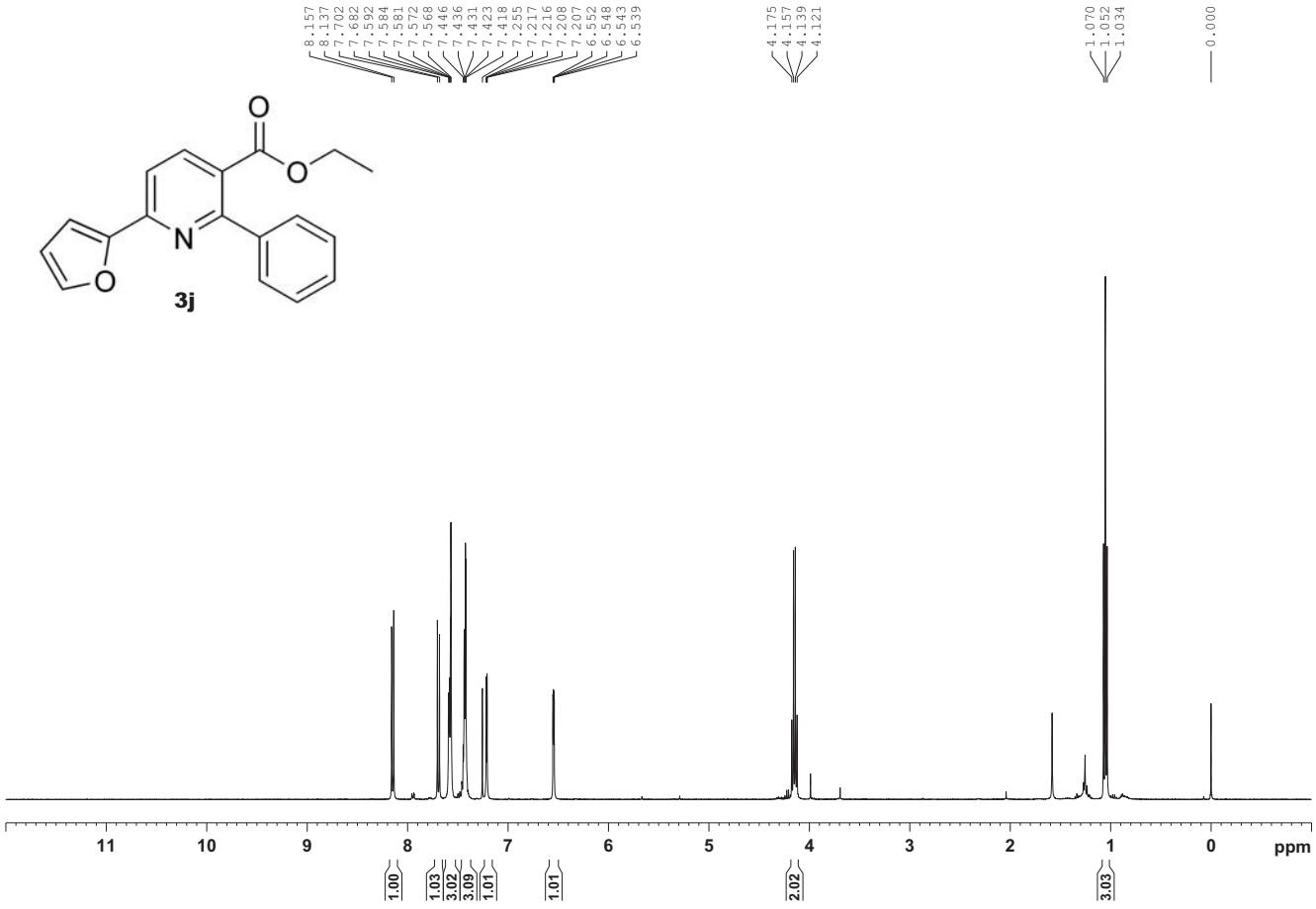
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7.418
7.255
7.217
7.216
7.208
7.207
6.552
6.548
6.543
6.539
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4.139
4.121
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1.052
1.034
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1.03
3.02
3.09
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1.01
2.02
3.03


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O
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O
3j
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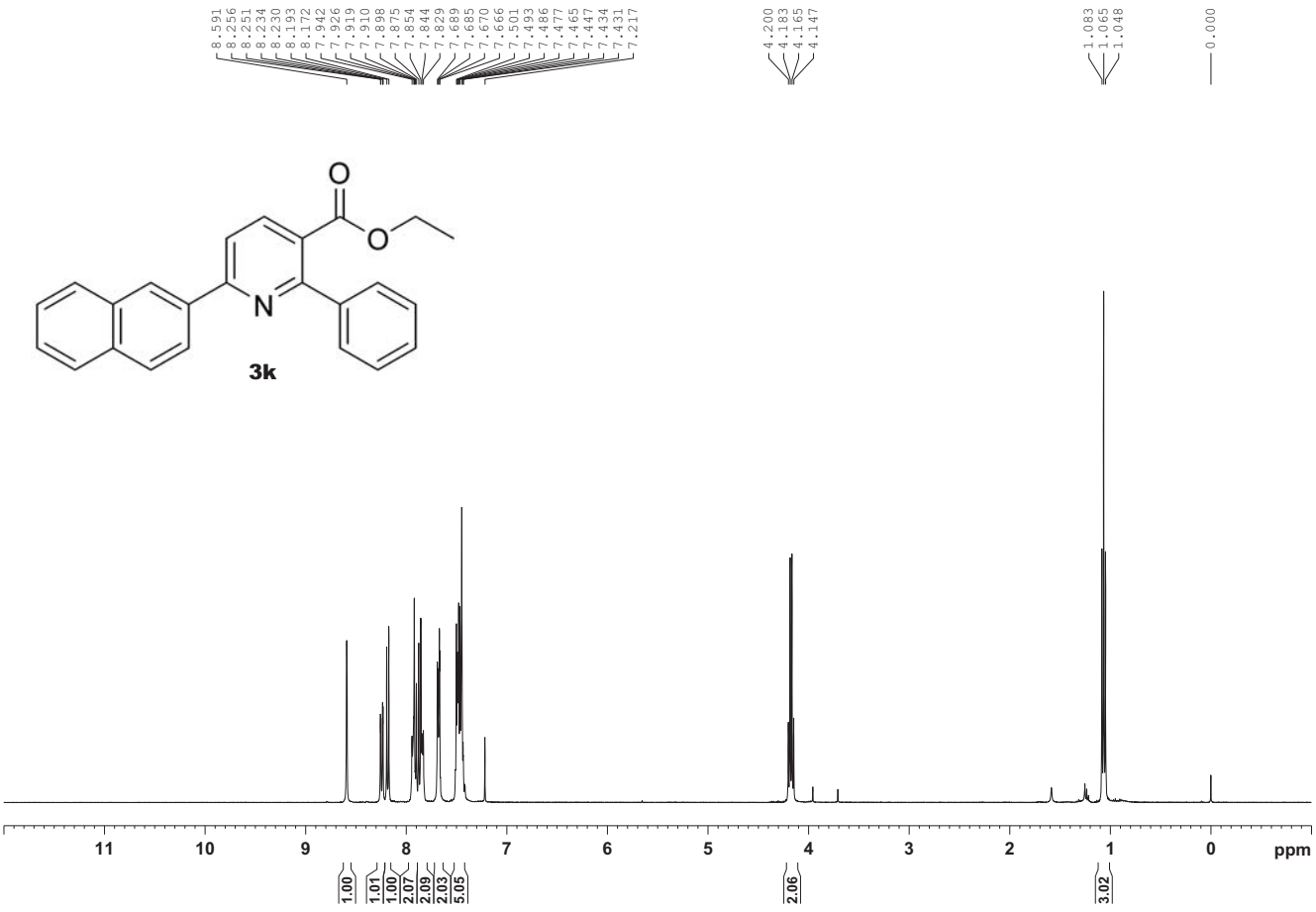
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7.670
7.666
7.501
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7.477
7.465
7.447
7.434
7.431
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1.048
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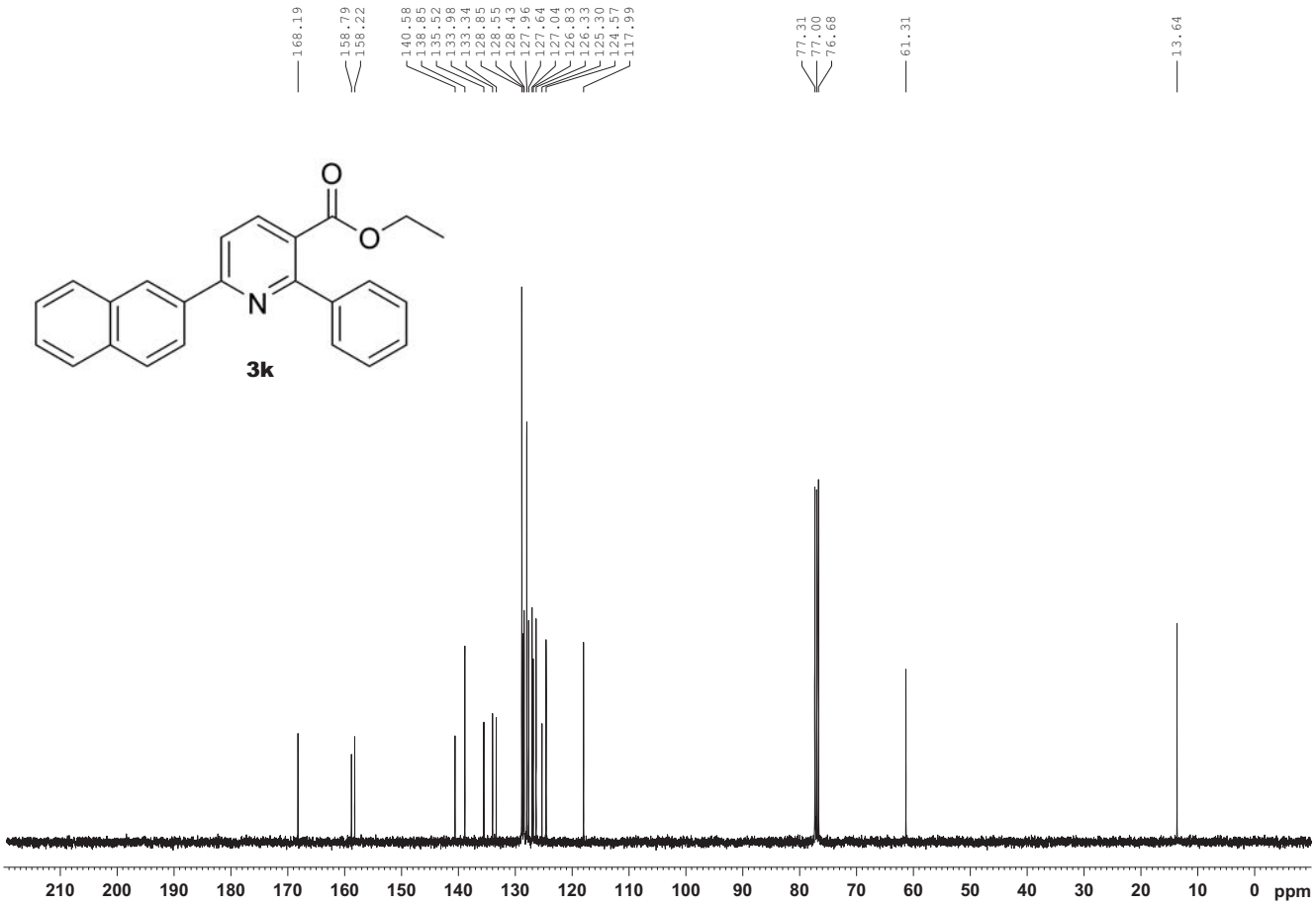
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126.33
125.30
124.57
117.99
77.31
77.00
76.68
61.31
13.64
O
O
N
3k
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200
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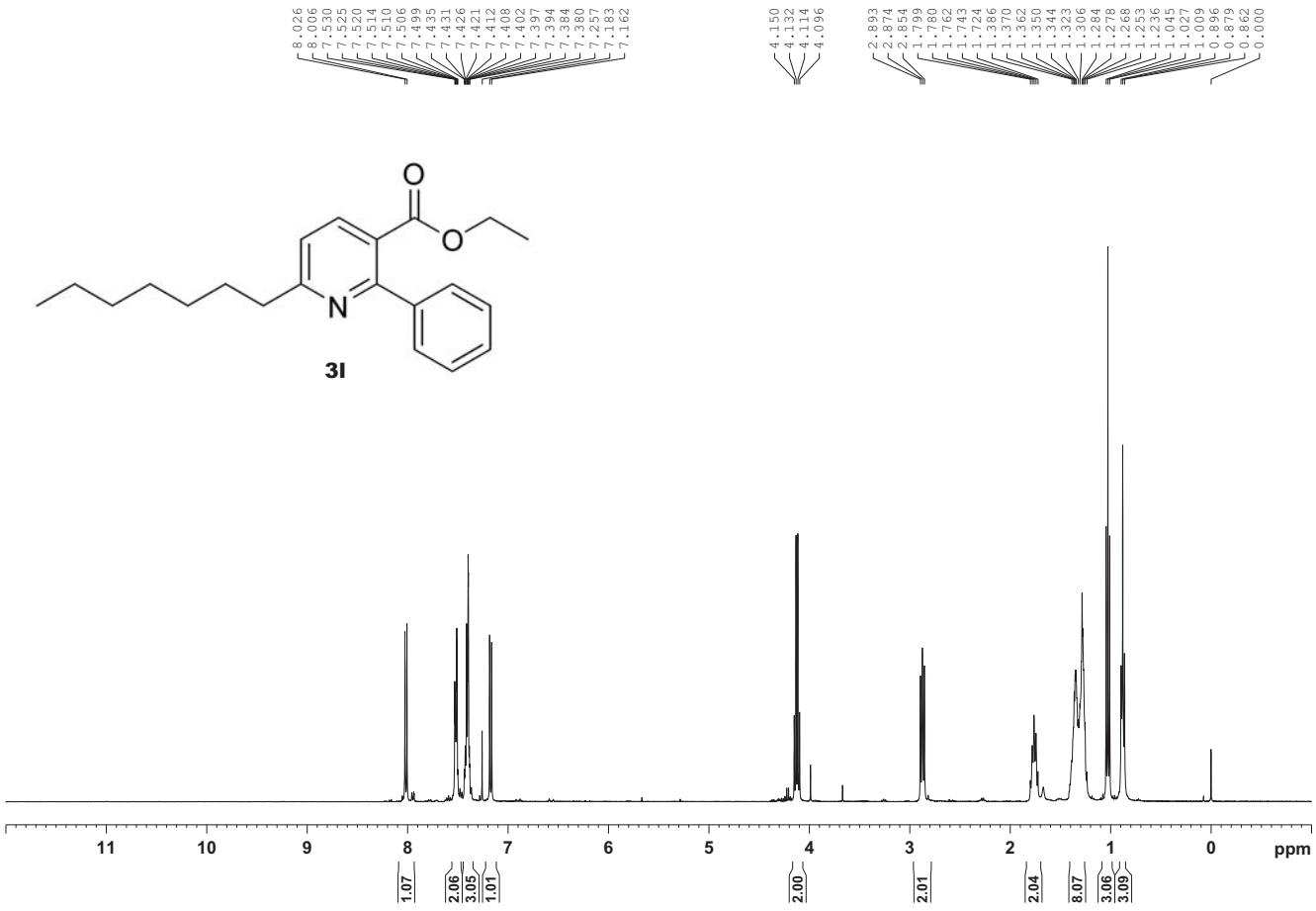
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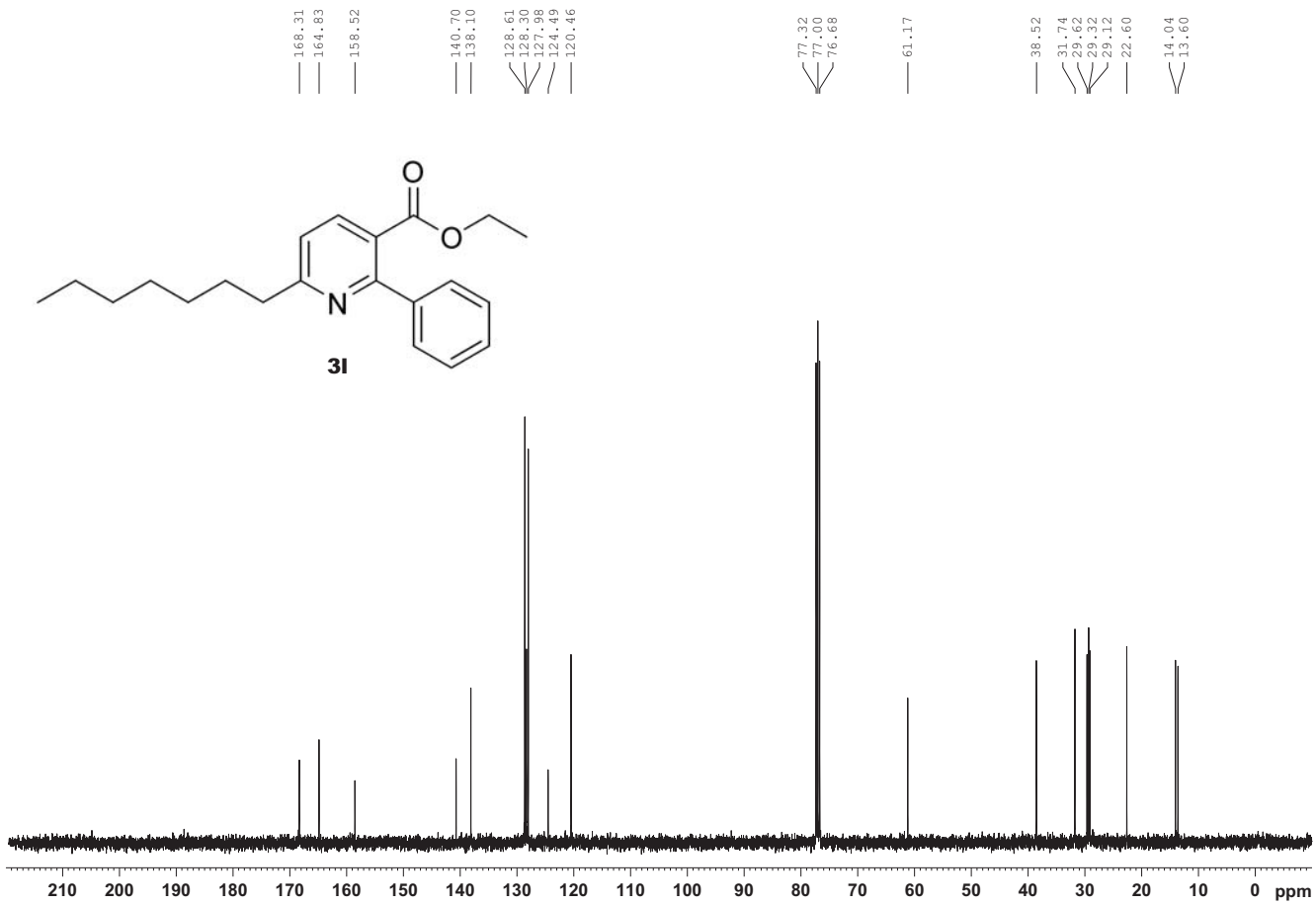
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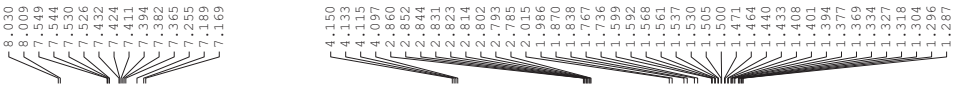
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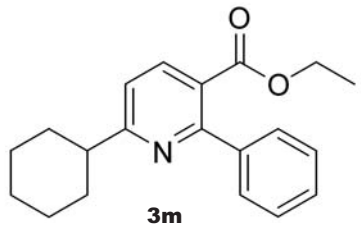
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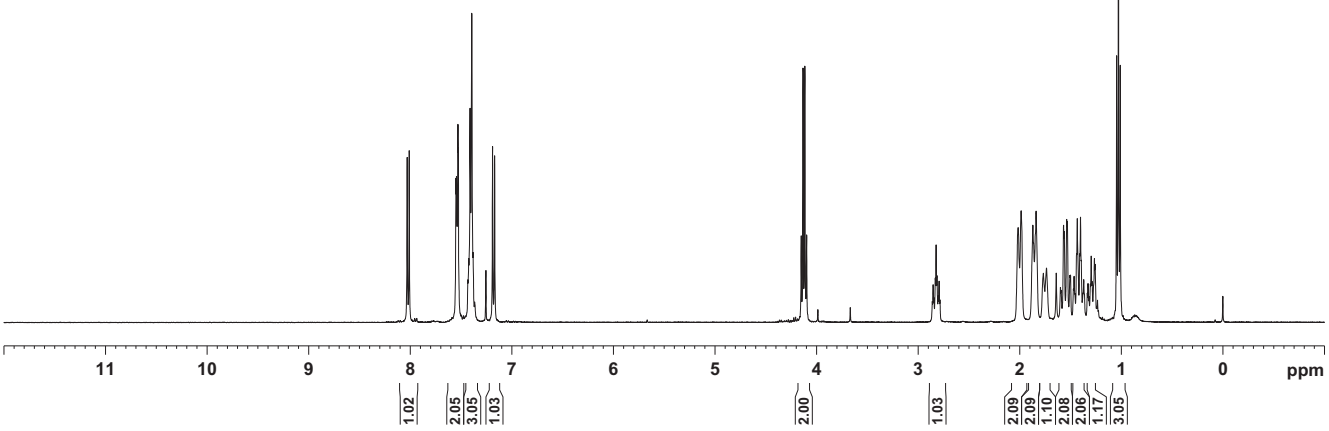
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2.05
3.05
1.03
2.00
1.03
2.09
2.09
1.10
2.08
2.06
1.17
3.05


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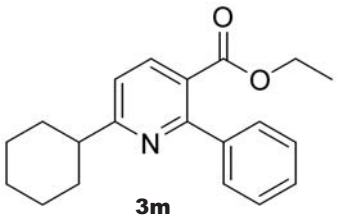
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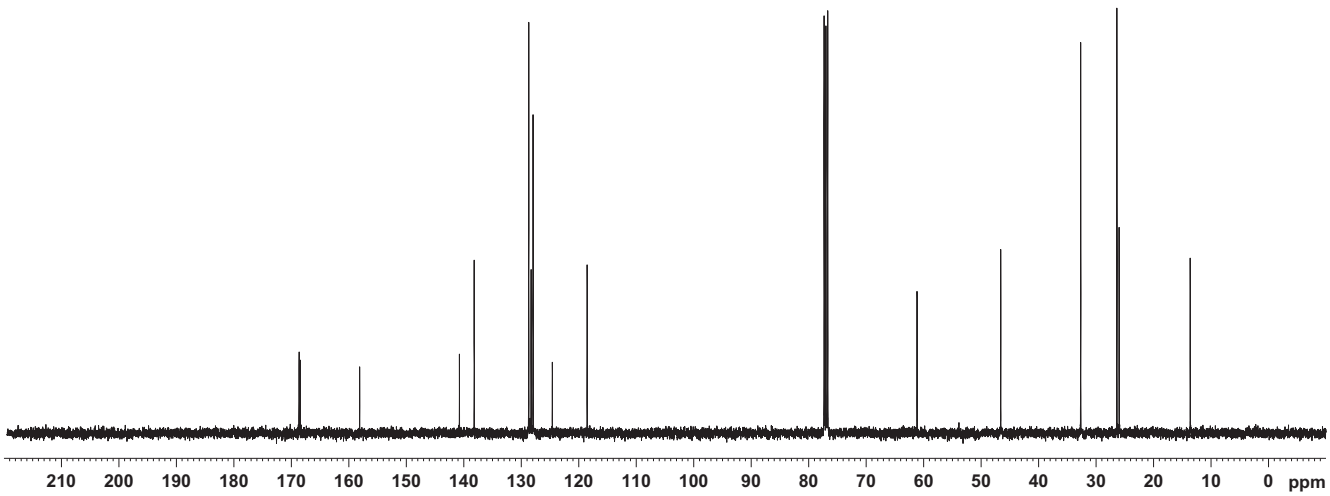
3m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200
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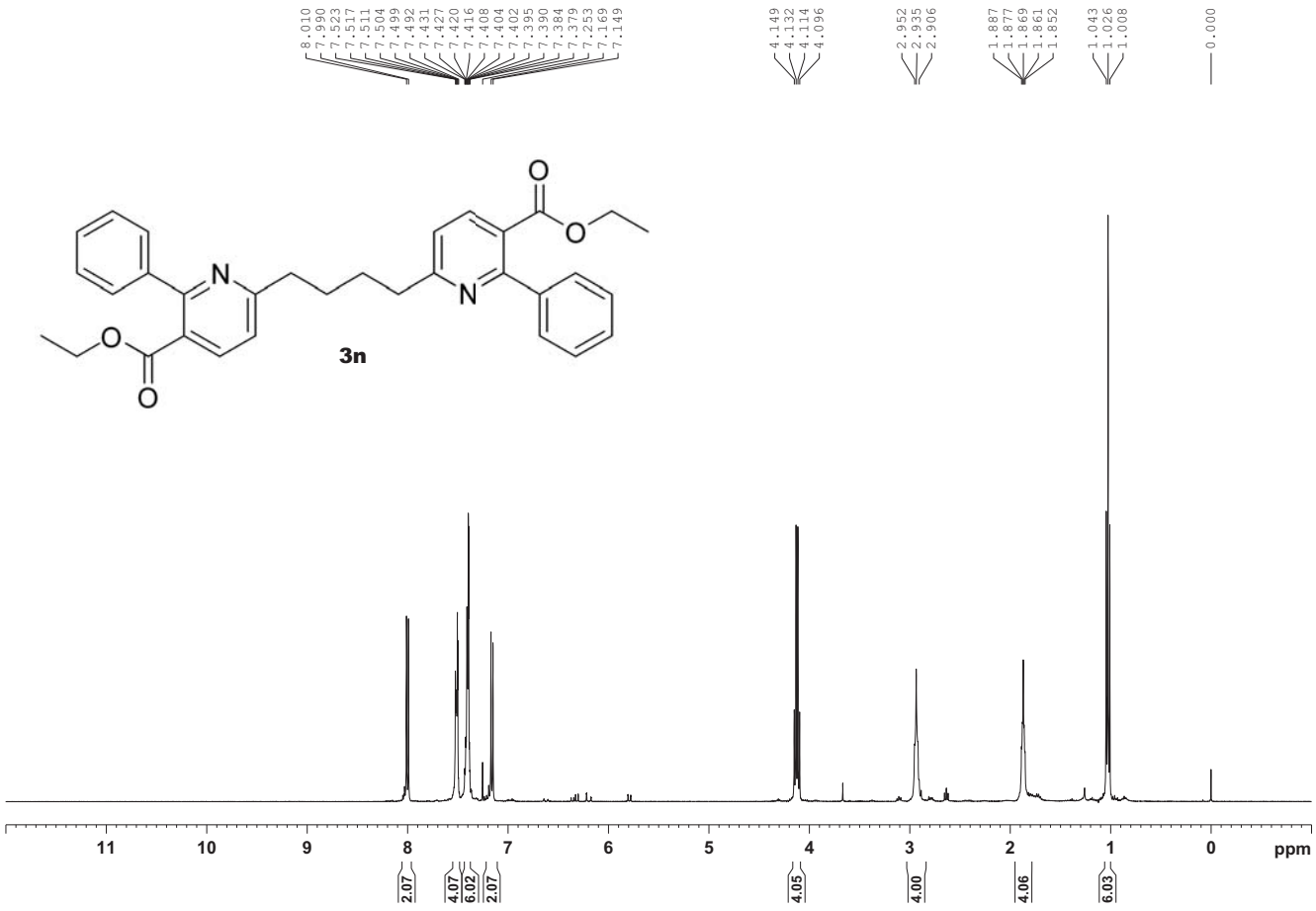
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7.404
7.402
7.395
7.390
7.384
7.379
7.253
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1.852
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1.008
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4.07
6.02
2.07
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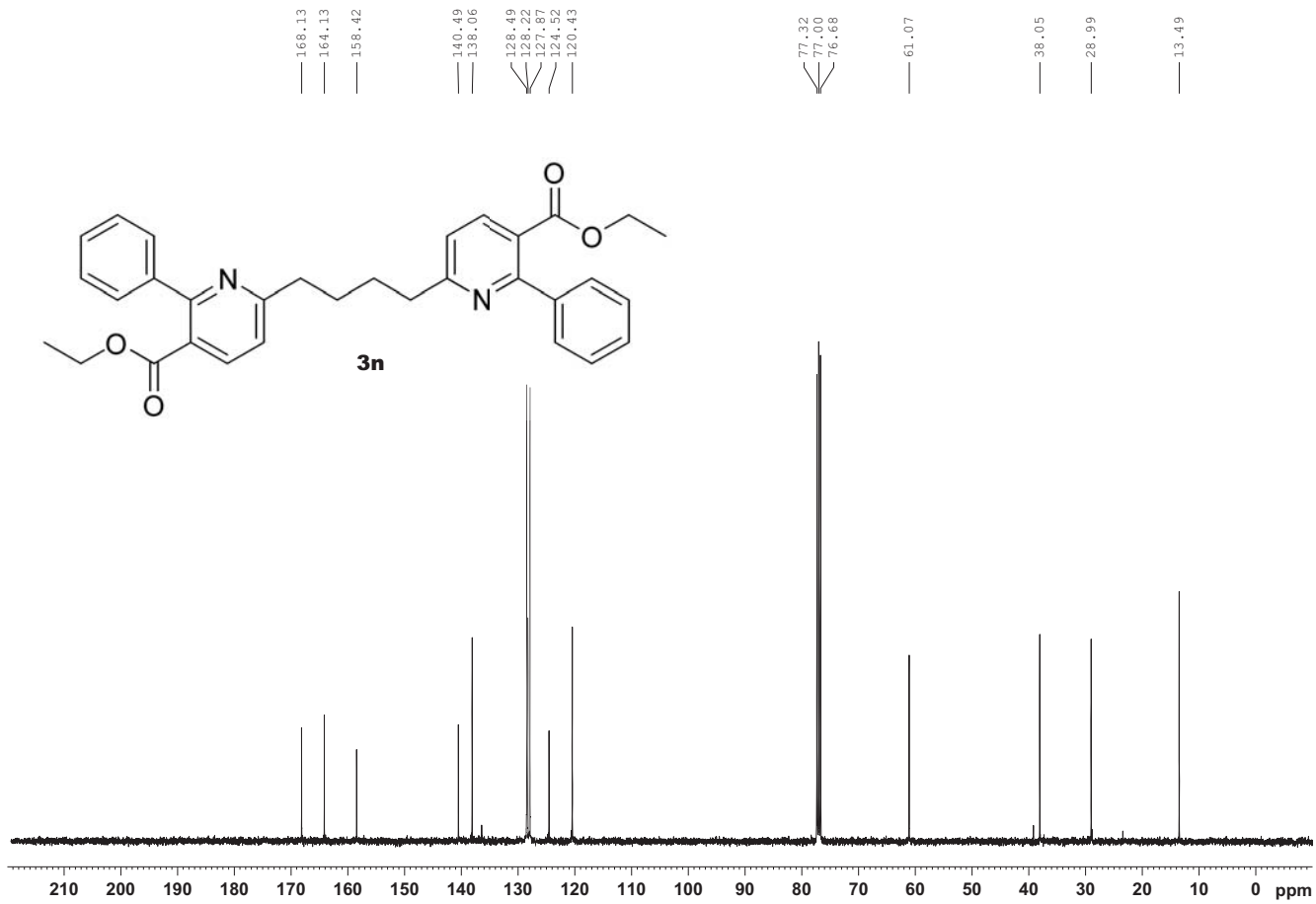
4.06
6.03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76.68
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3n
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200
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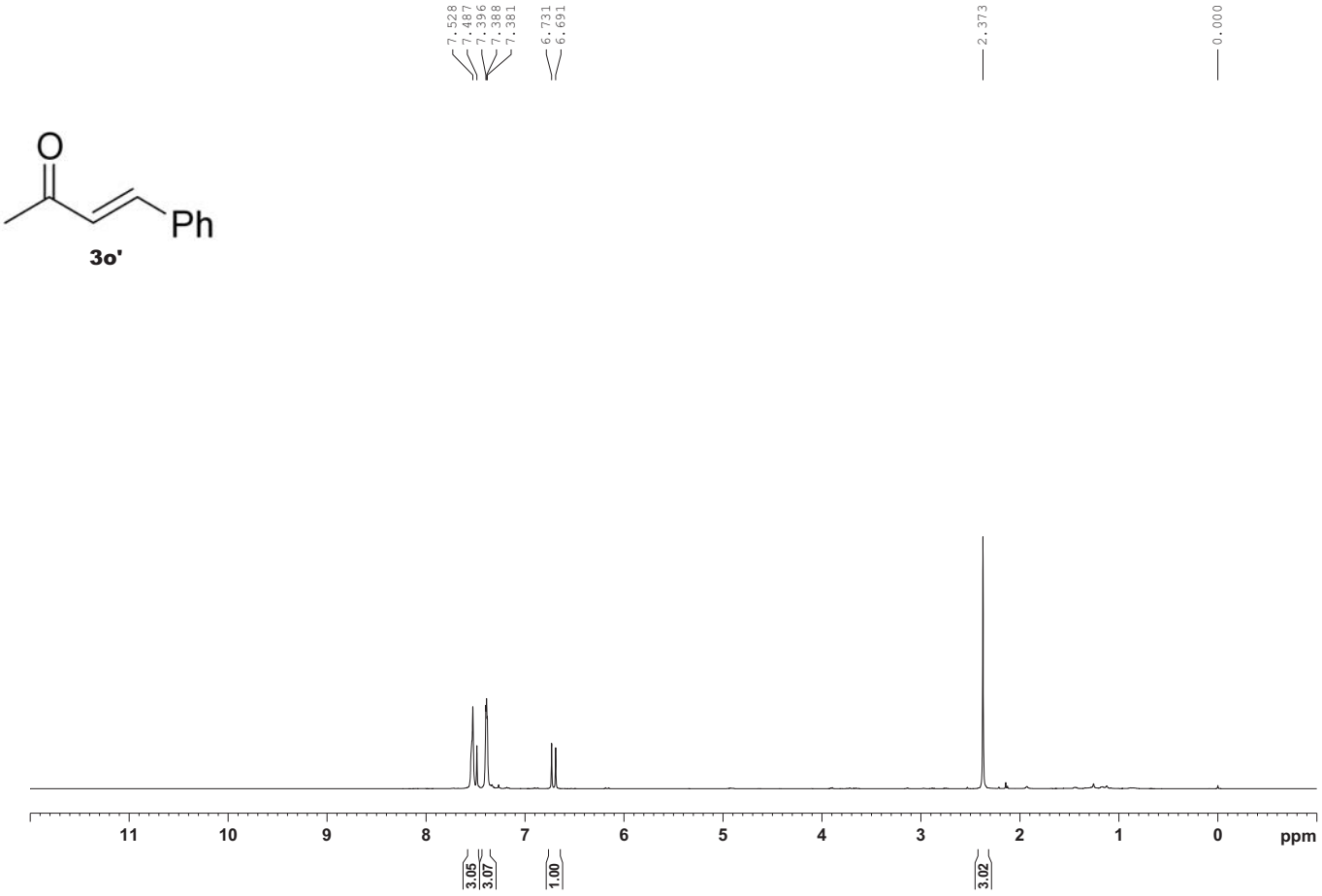
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Ph
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6
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4
3
2
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ppm
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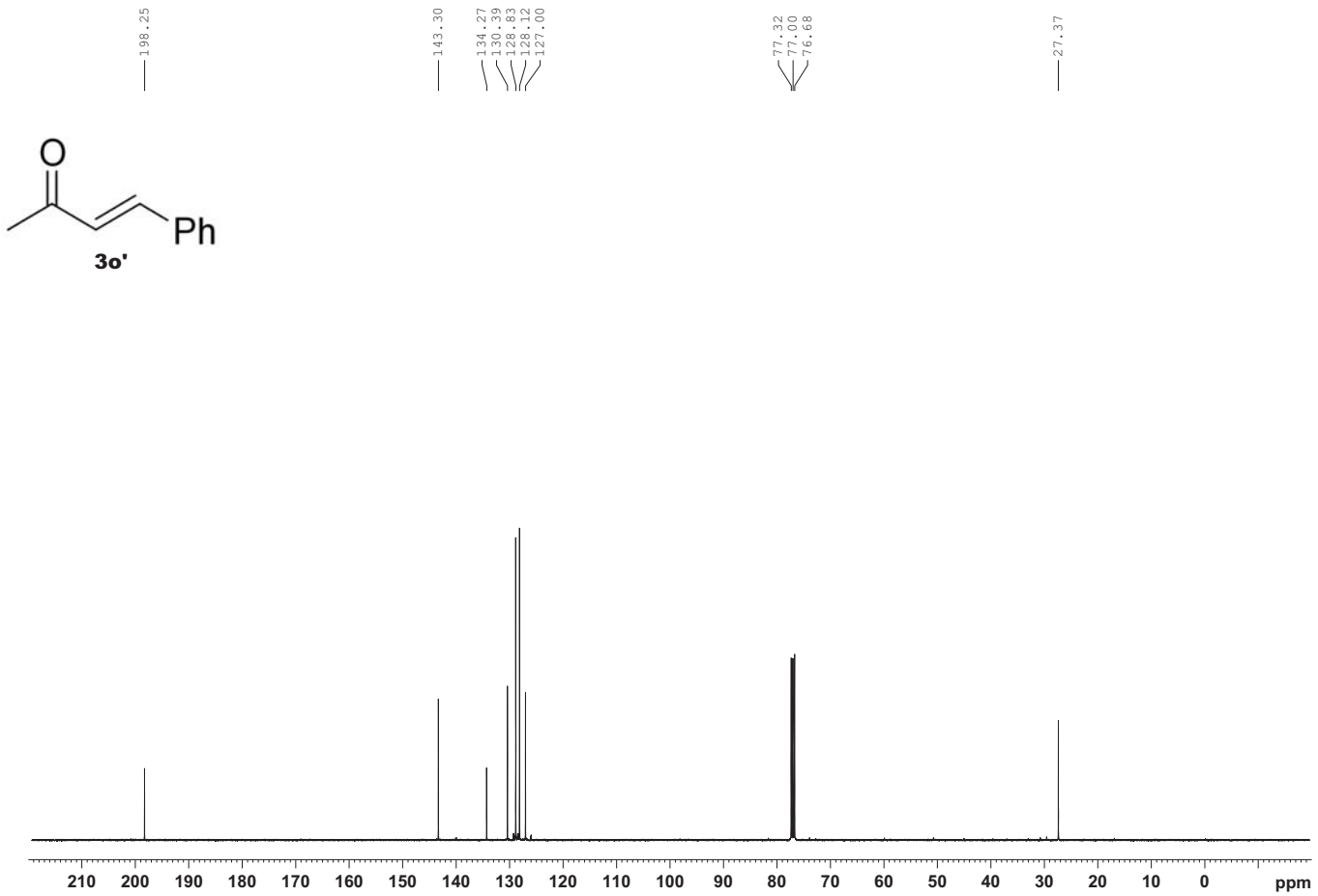
1.00
3.02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77.00
76.68
27.37
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200
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130
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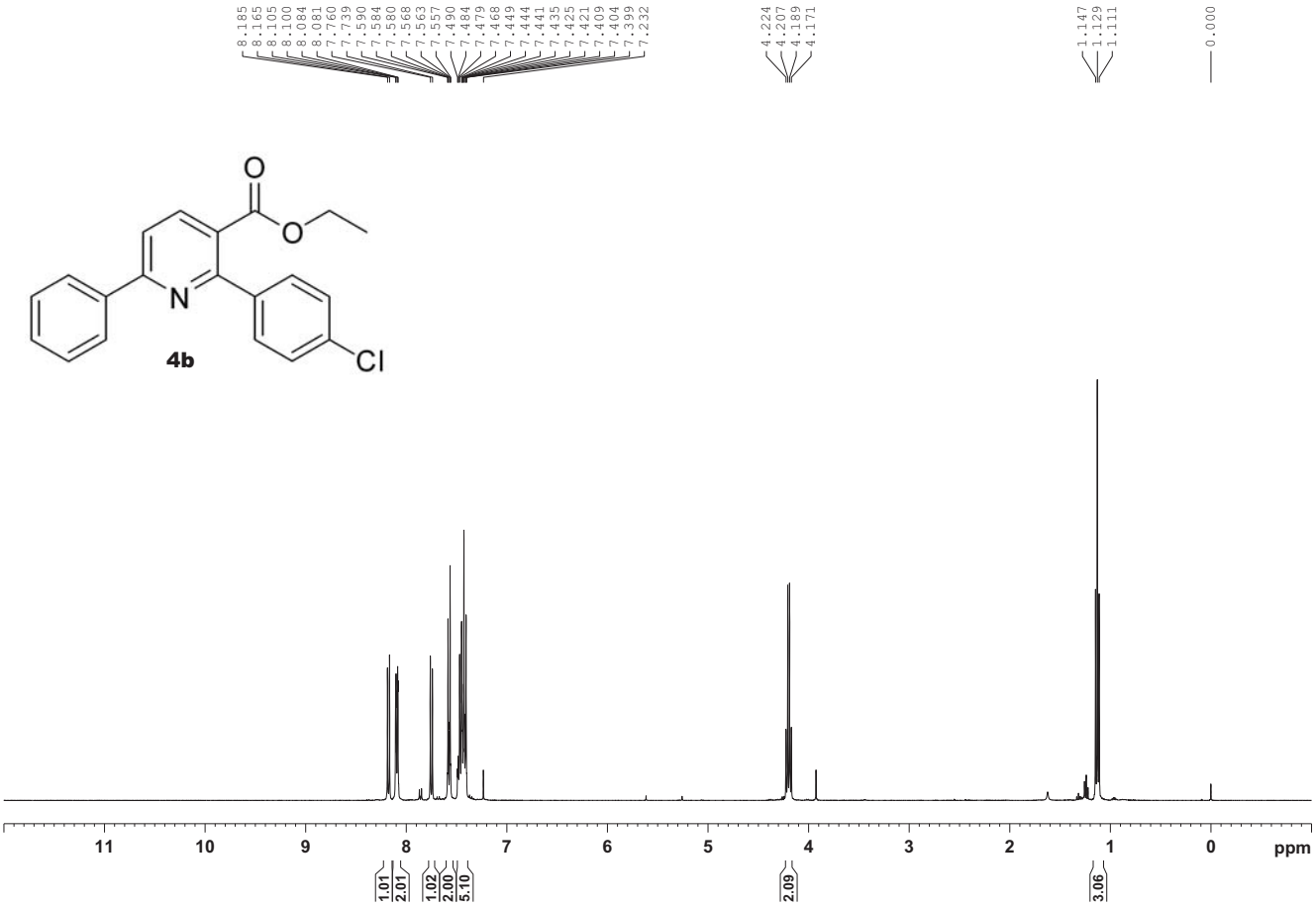
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7.435
7.425
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7.404
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7.232
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O
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4b
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1.02
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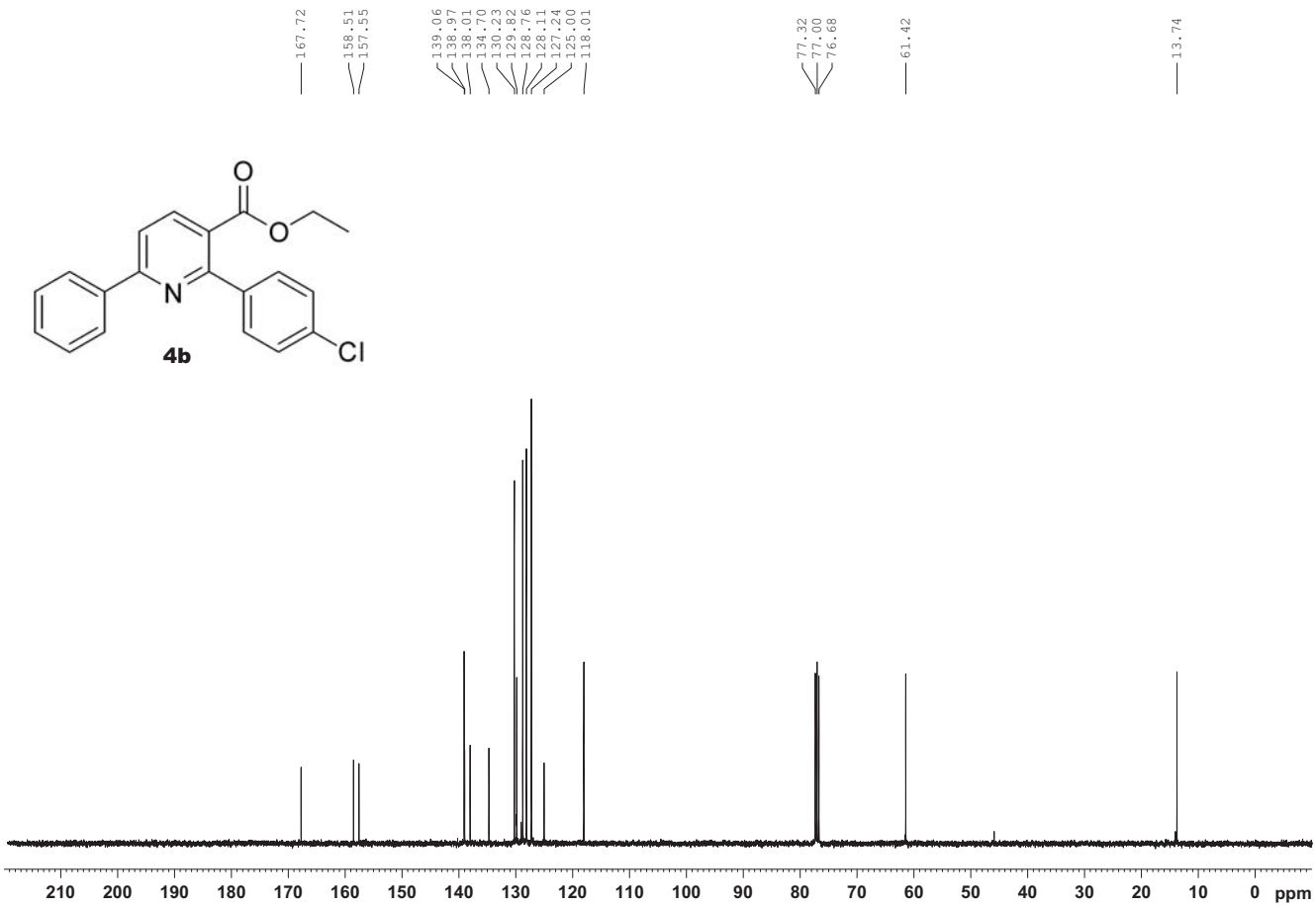
2.09
3.06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77.00
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O
N
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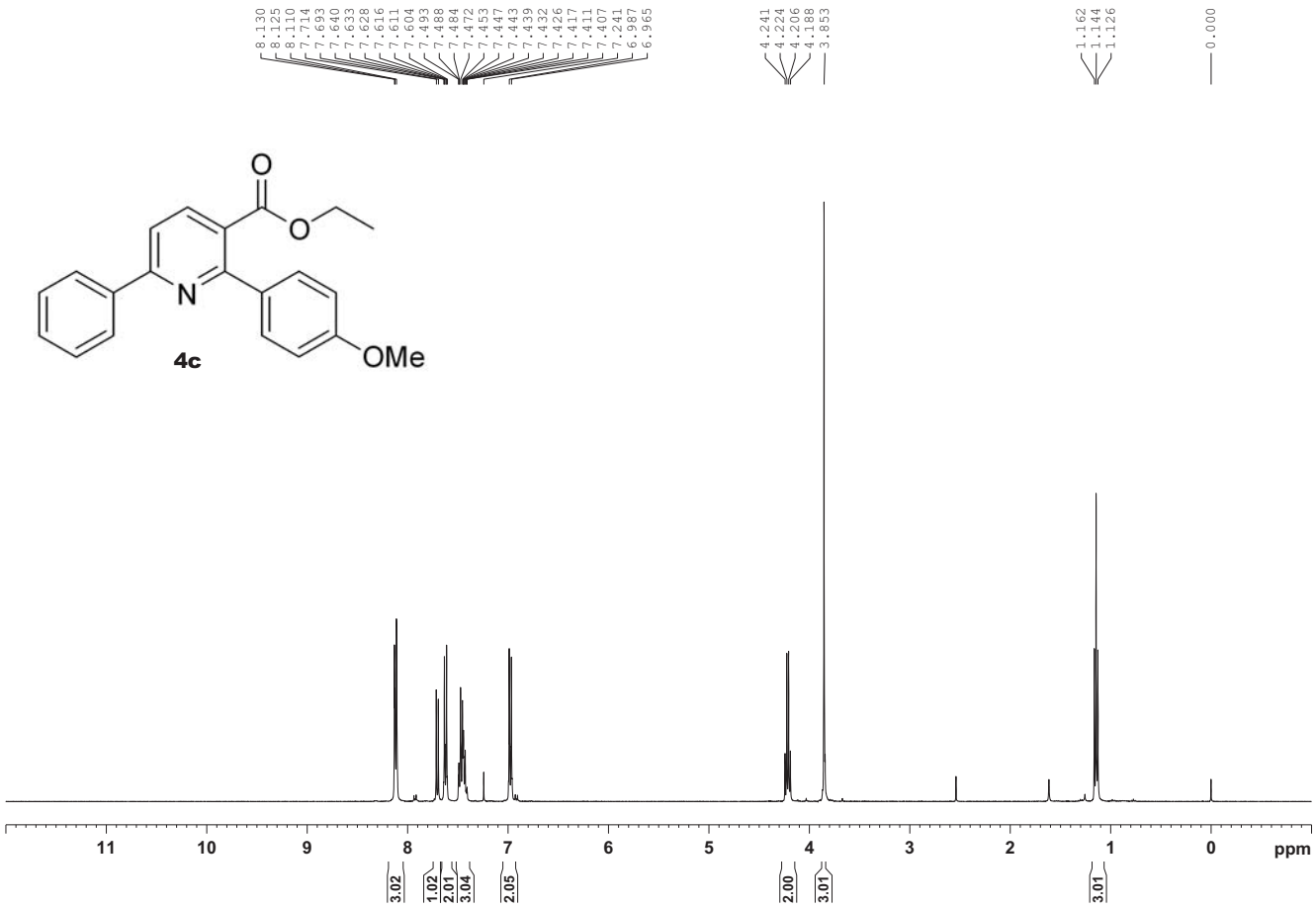
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7.443
7.439
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7.426
7.417
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7.407
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4.188
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O
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OMe
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3.04
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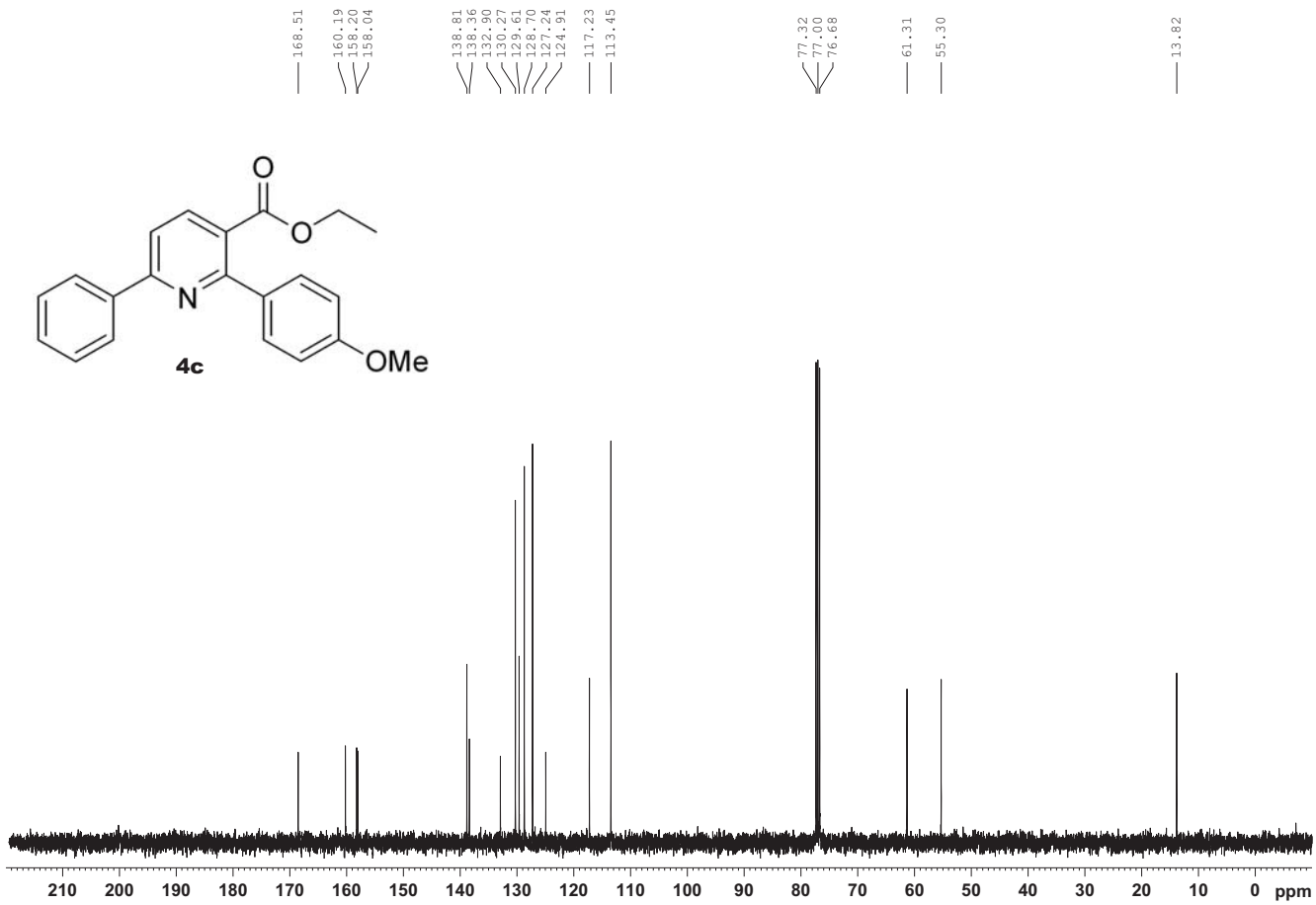
2.00
3.01
3.01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O
N
OMe
4c
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200
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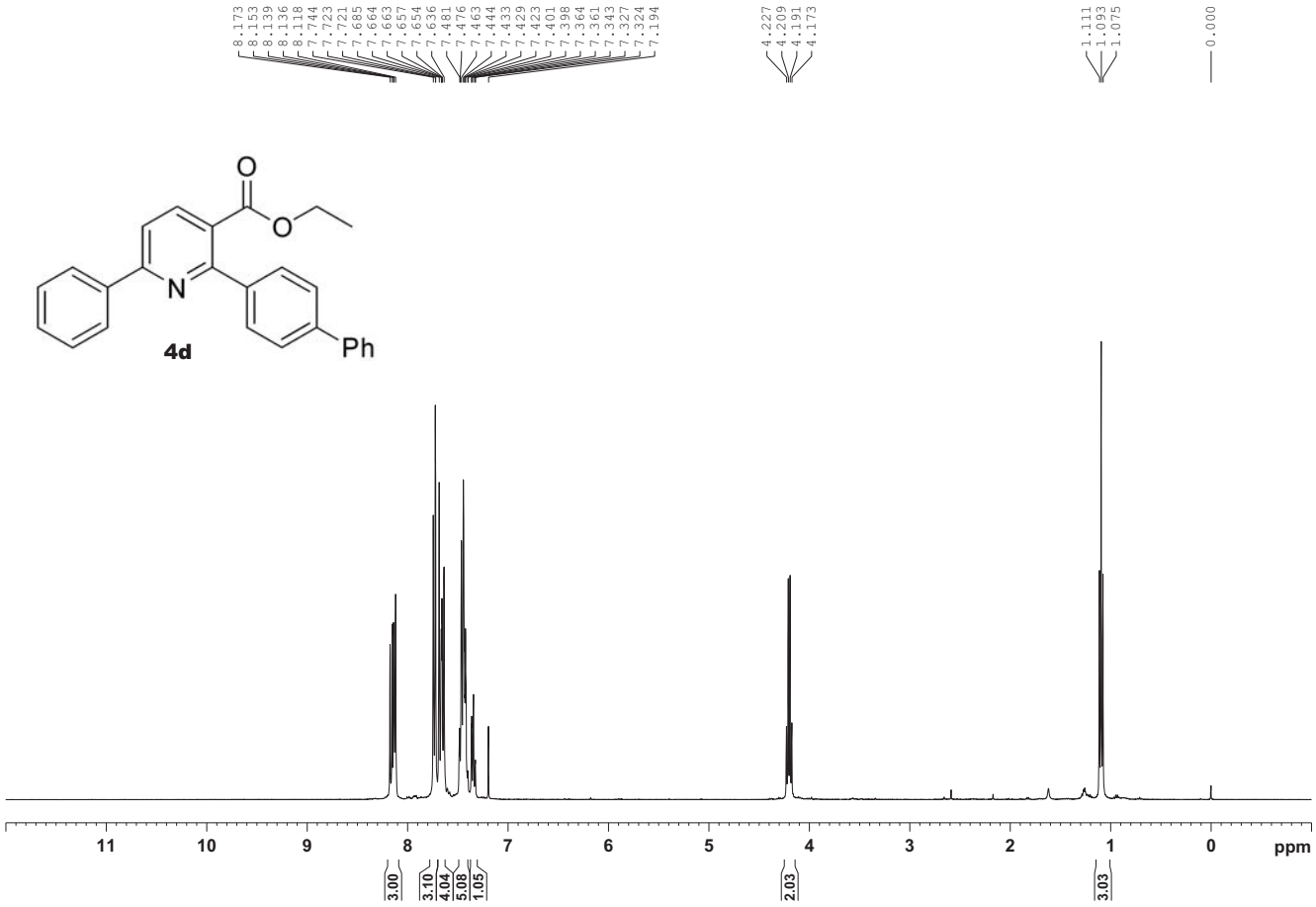
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7.429
7.423
7.401
7.398
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7.361
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7.327
7.324
7.194
4.227
4.209
4.191
4.173
1.111
1.093
1.075
0.000
O
O
N
Ph
4d
11
10
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8
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3.10
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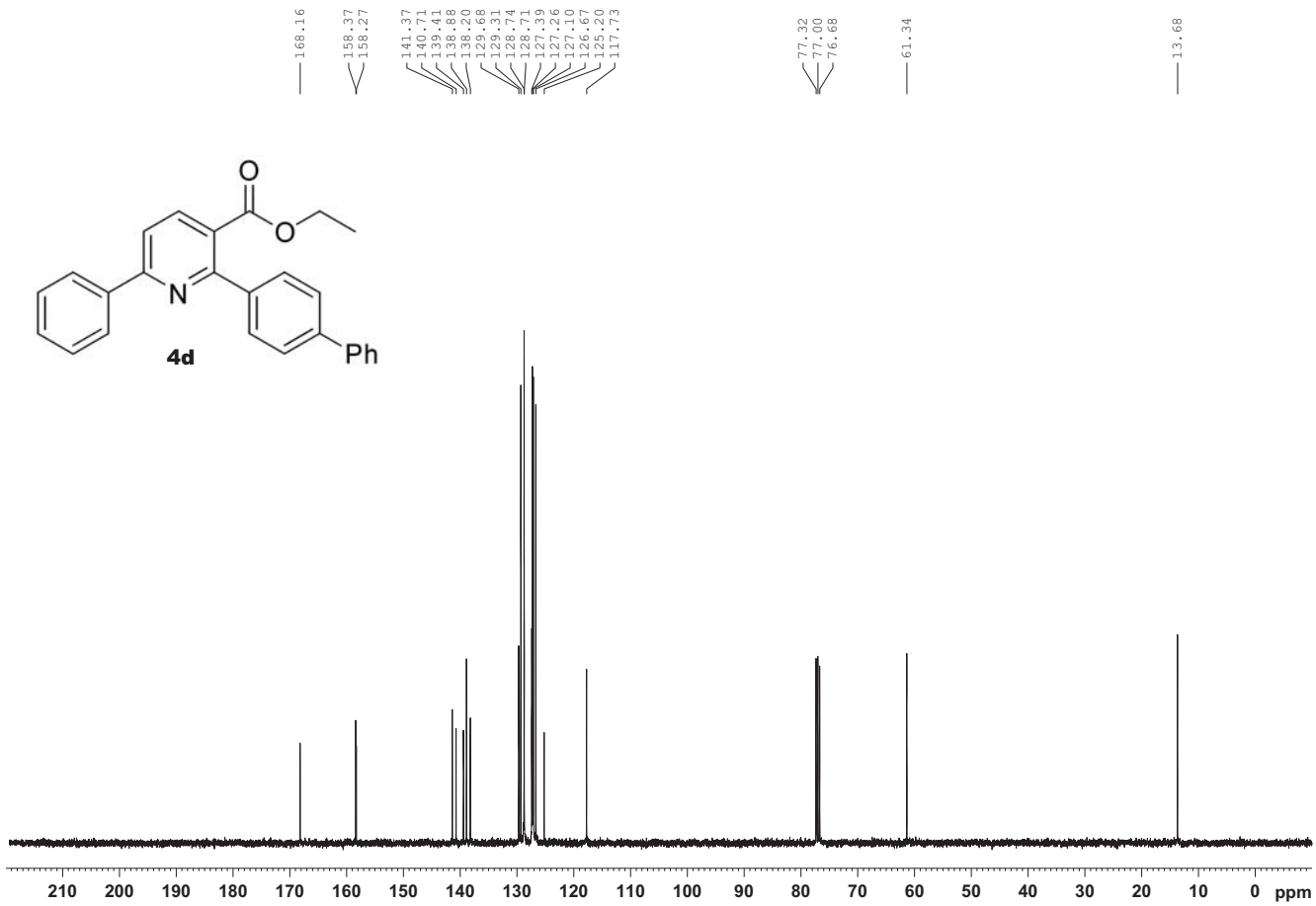
2.03
3.03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117.73
77.32
77.00
76.68
61.34
13.68
O
O
N
Ph
4d
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200
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180
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140
130
120
110
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90
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70
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50
40
30
20
10
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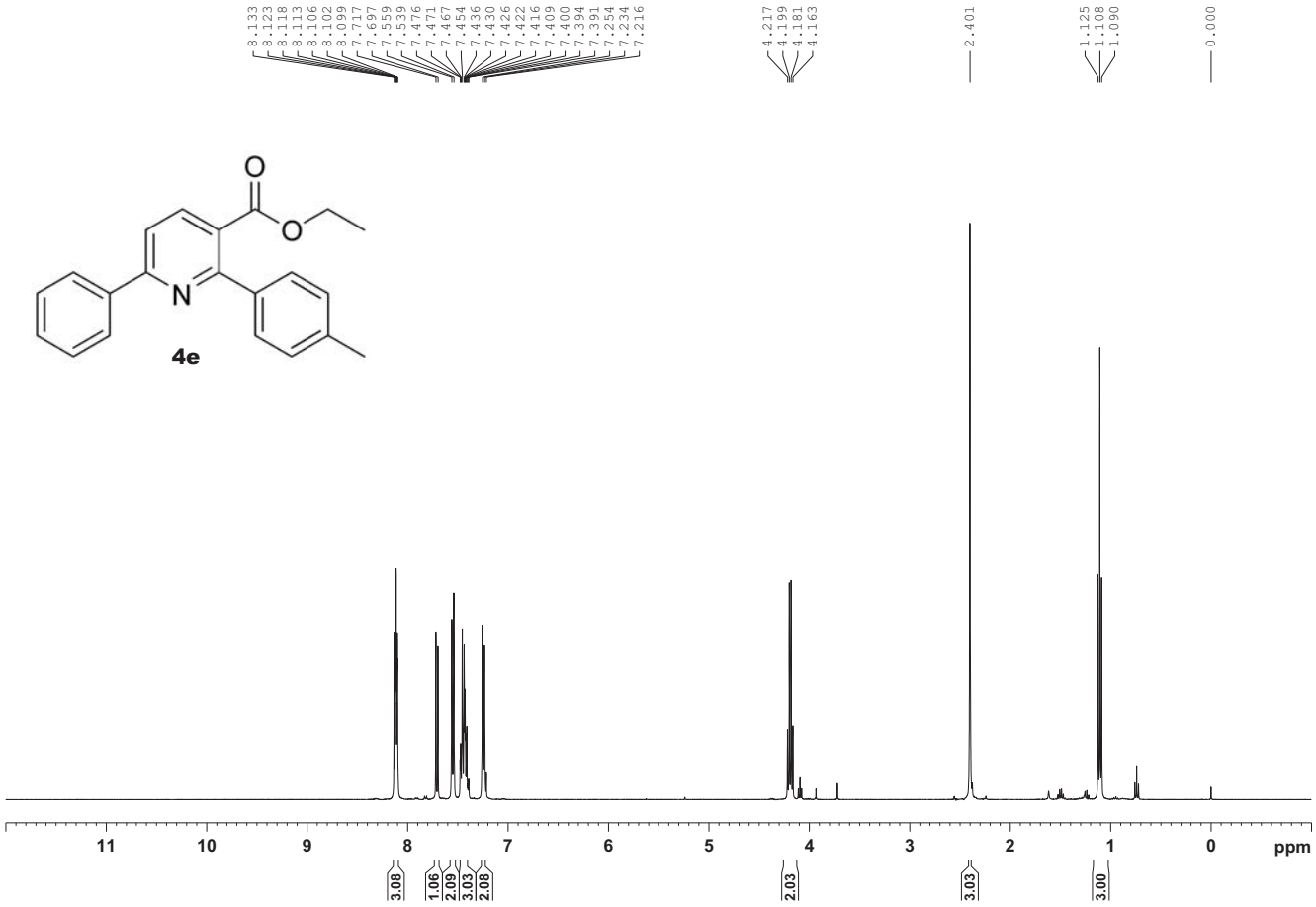
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7.436
7.430
7.426
7.422
7.416
7.409
7.400
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7.391
7.254
7.234
7.216
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4.163
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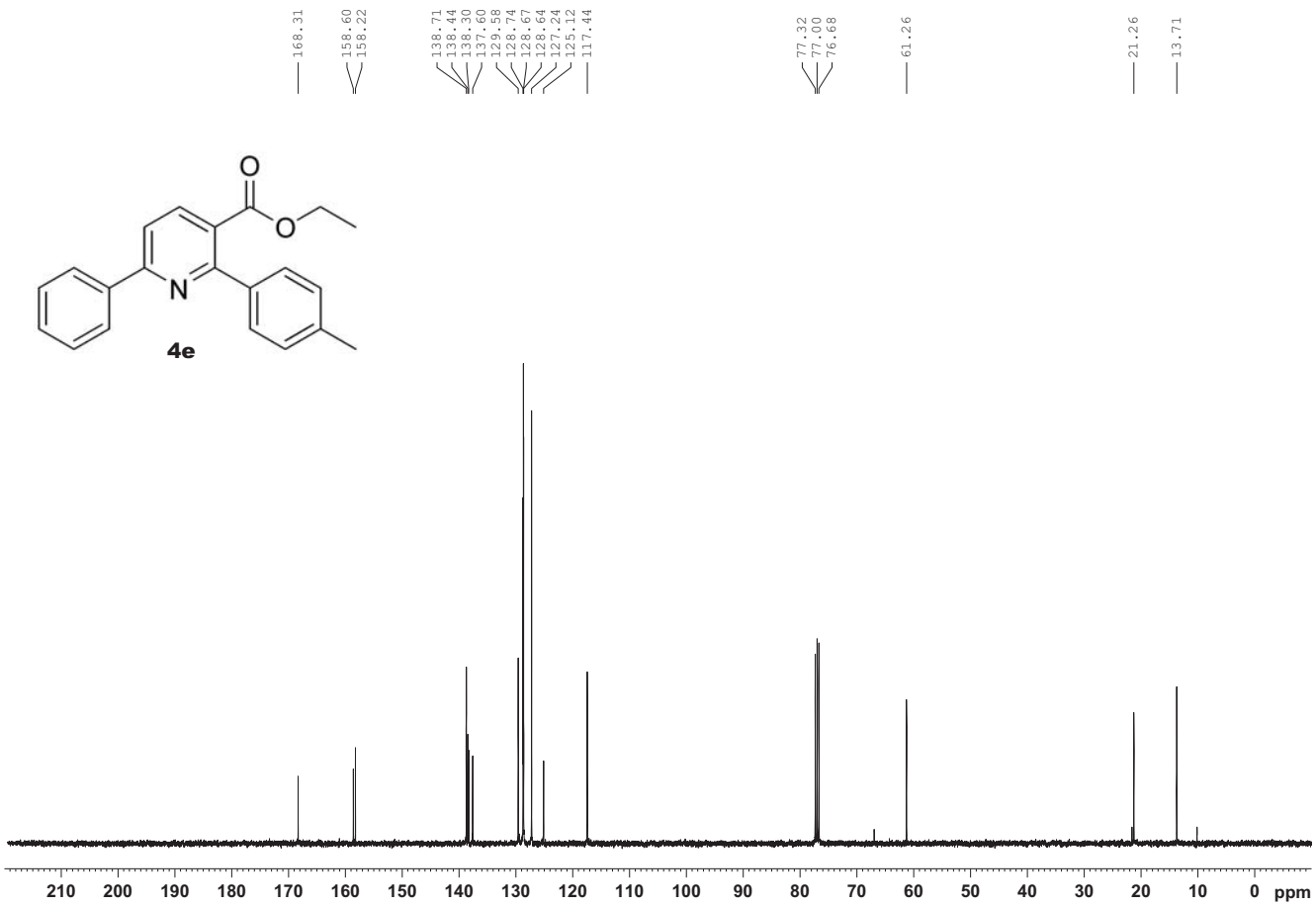
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O
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4e
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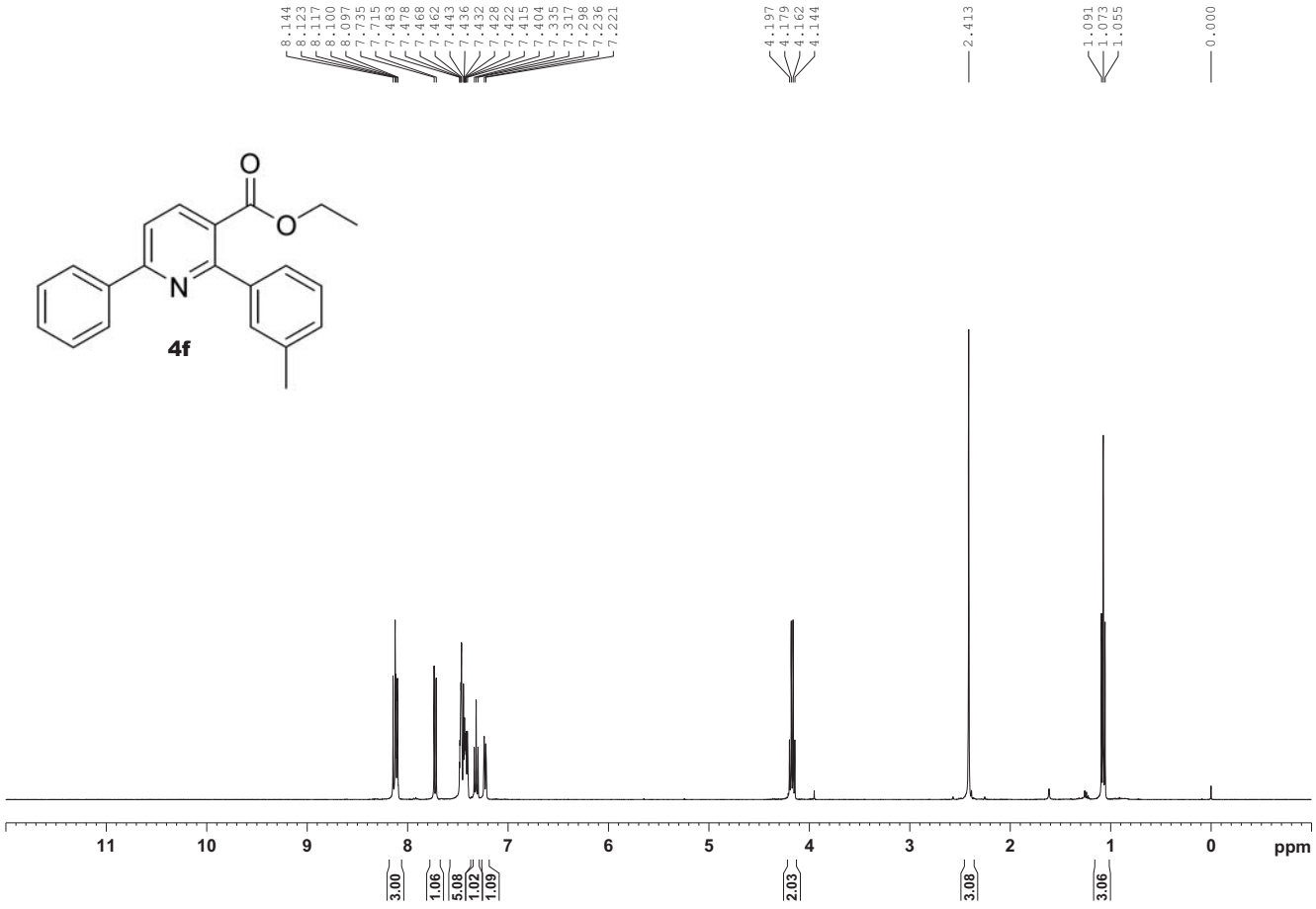
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7.428
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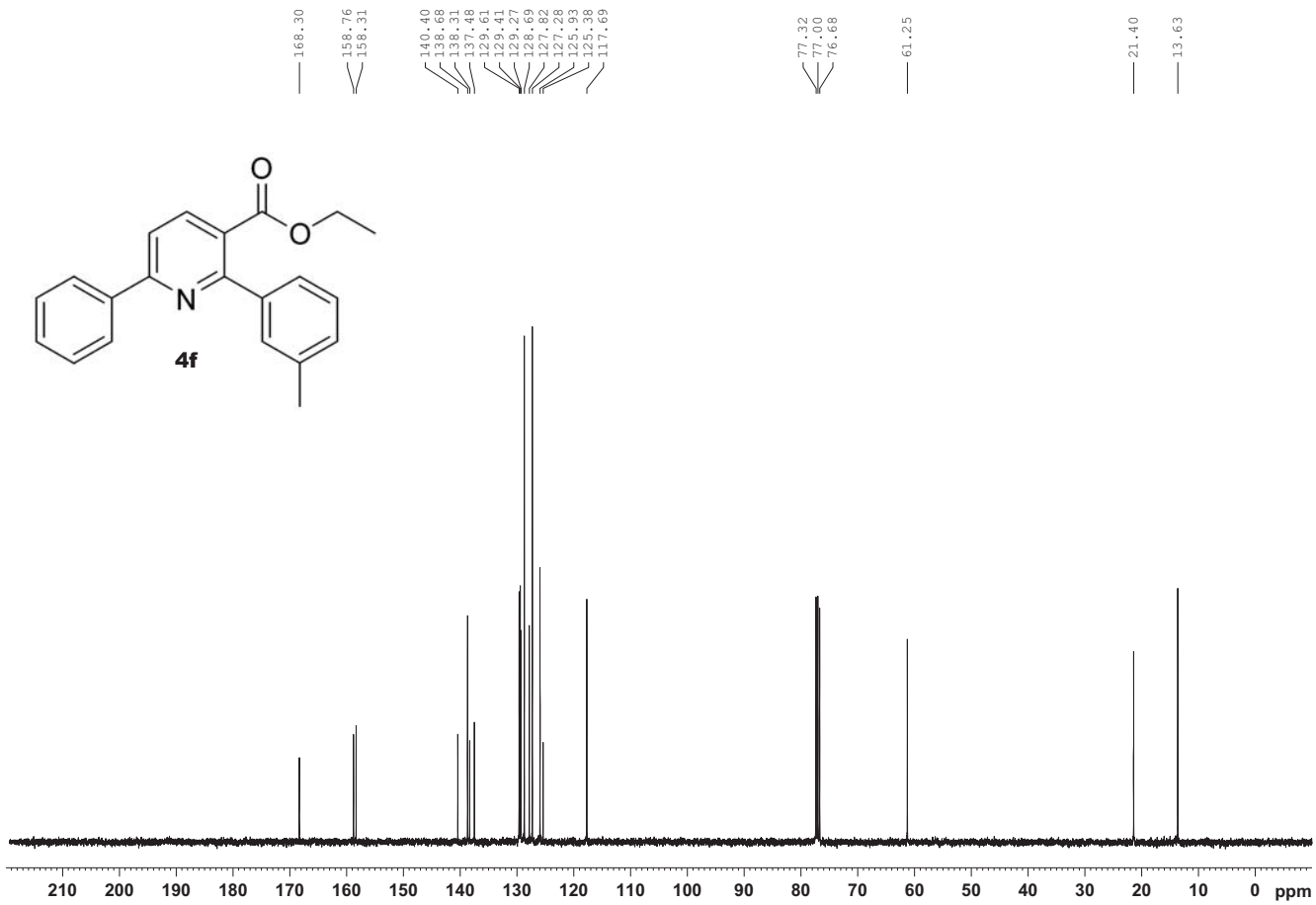
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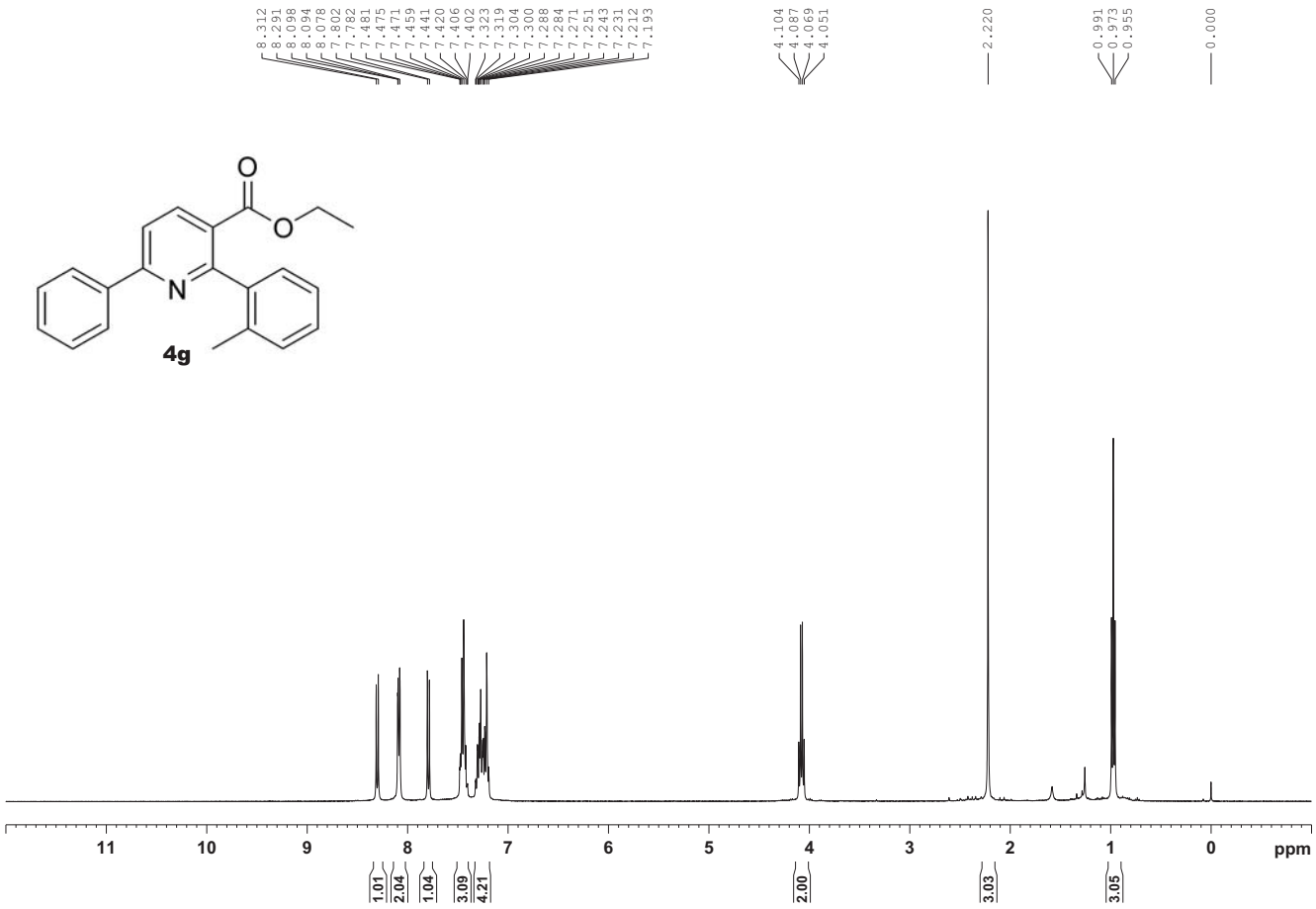
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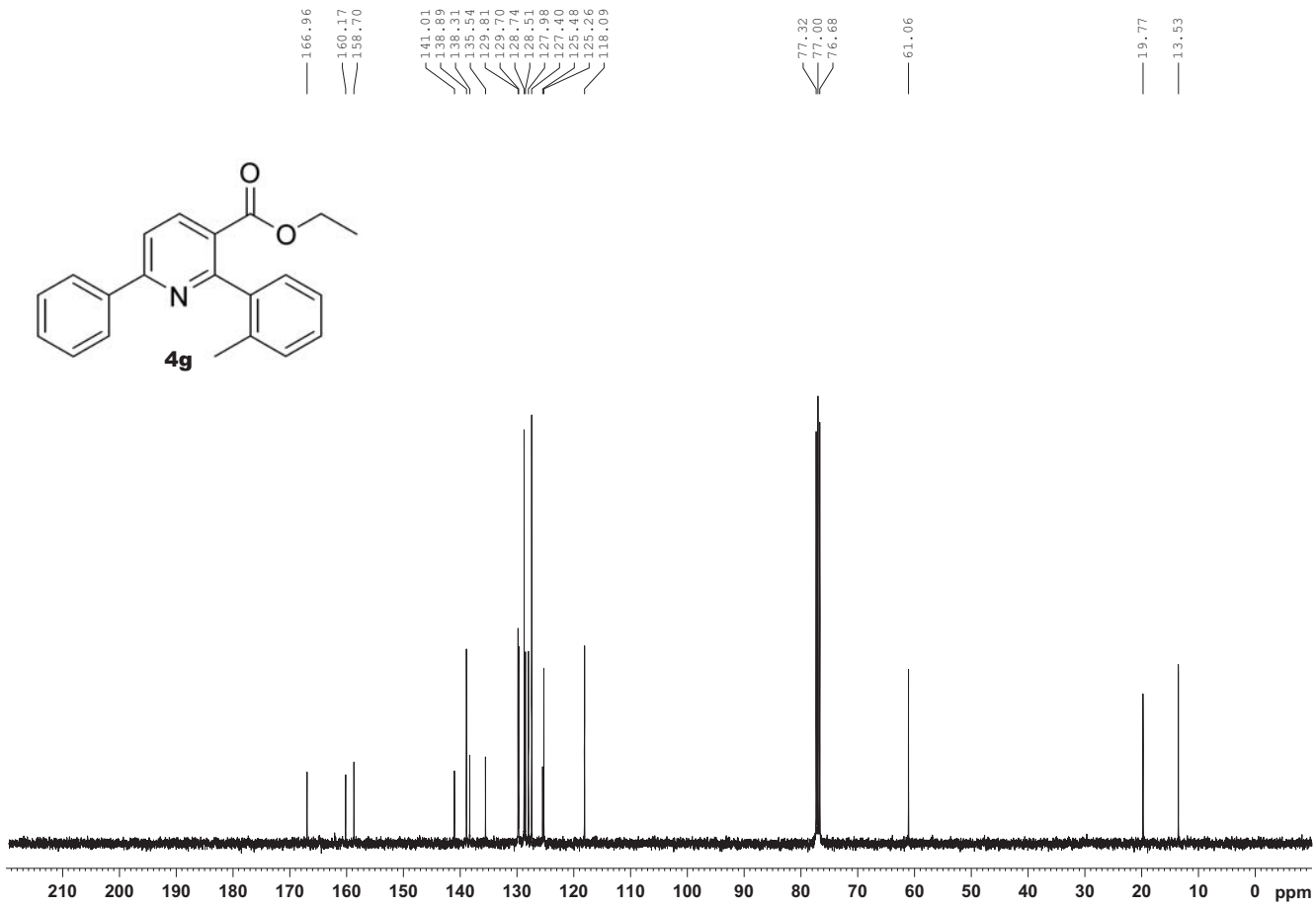
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4g
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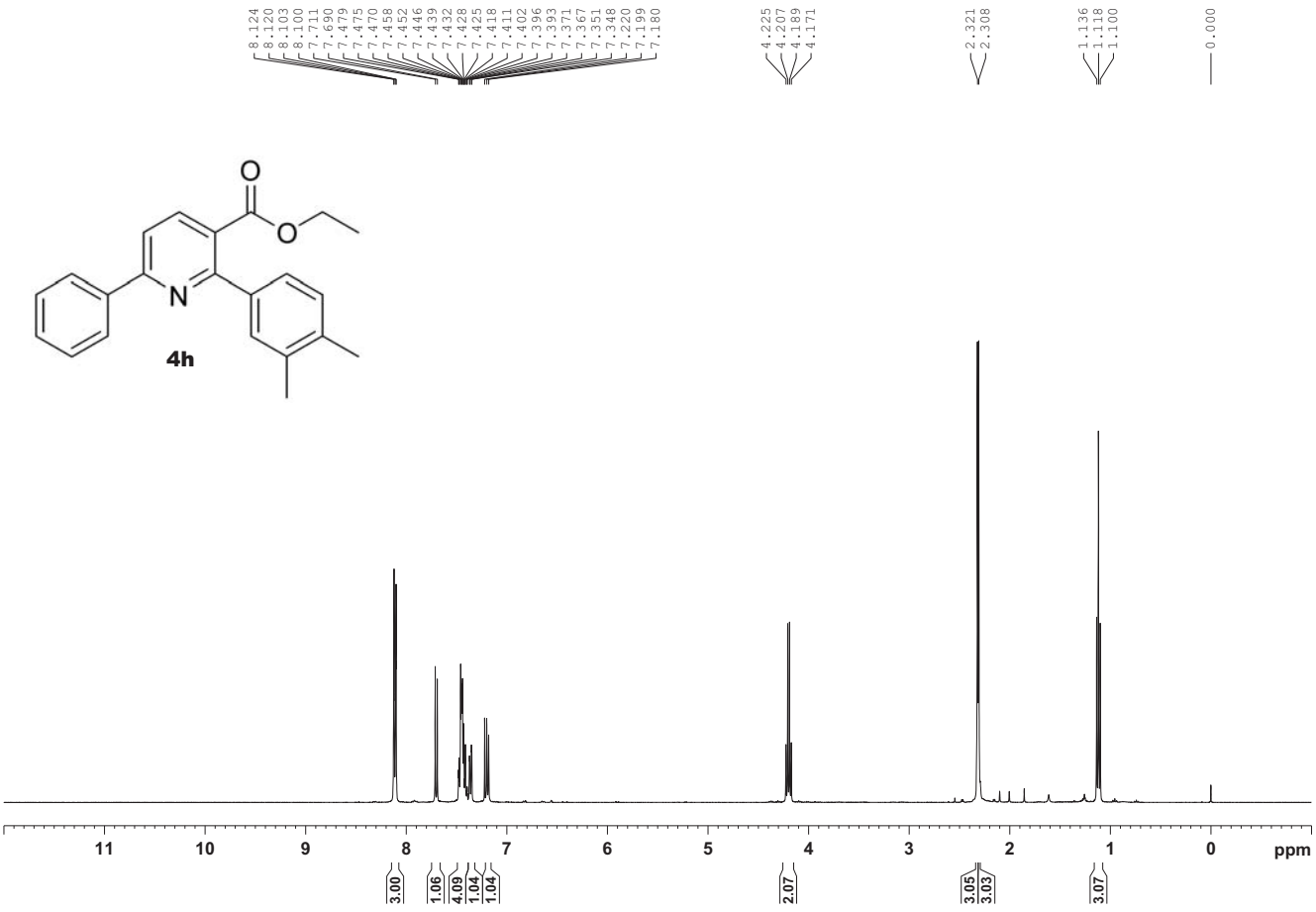
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7.428
7.425
7.418
7.411
7.402
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7.393
7.371
7.367
7.351
7.348
7.220
7.199
7.180
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4.207
4.189
4.171
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1.118
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4h
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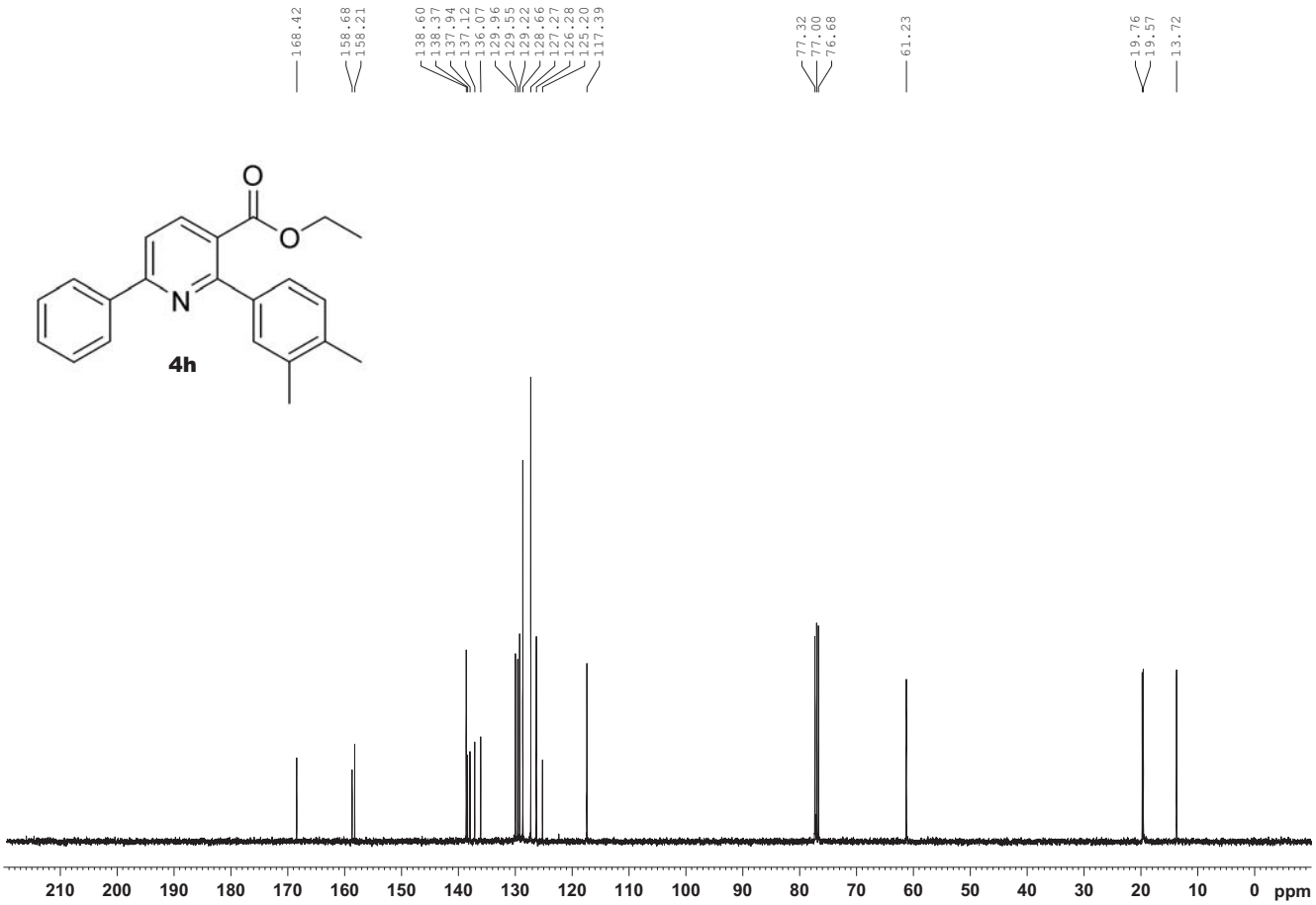
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77.32
77.00
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61.23
19.76
19.57
13.72
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O
N
4h
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200
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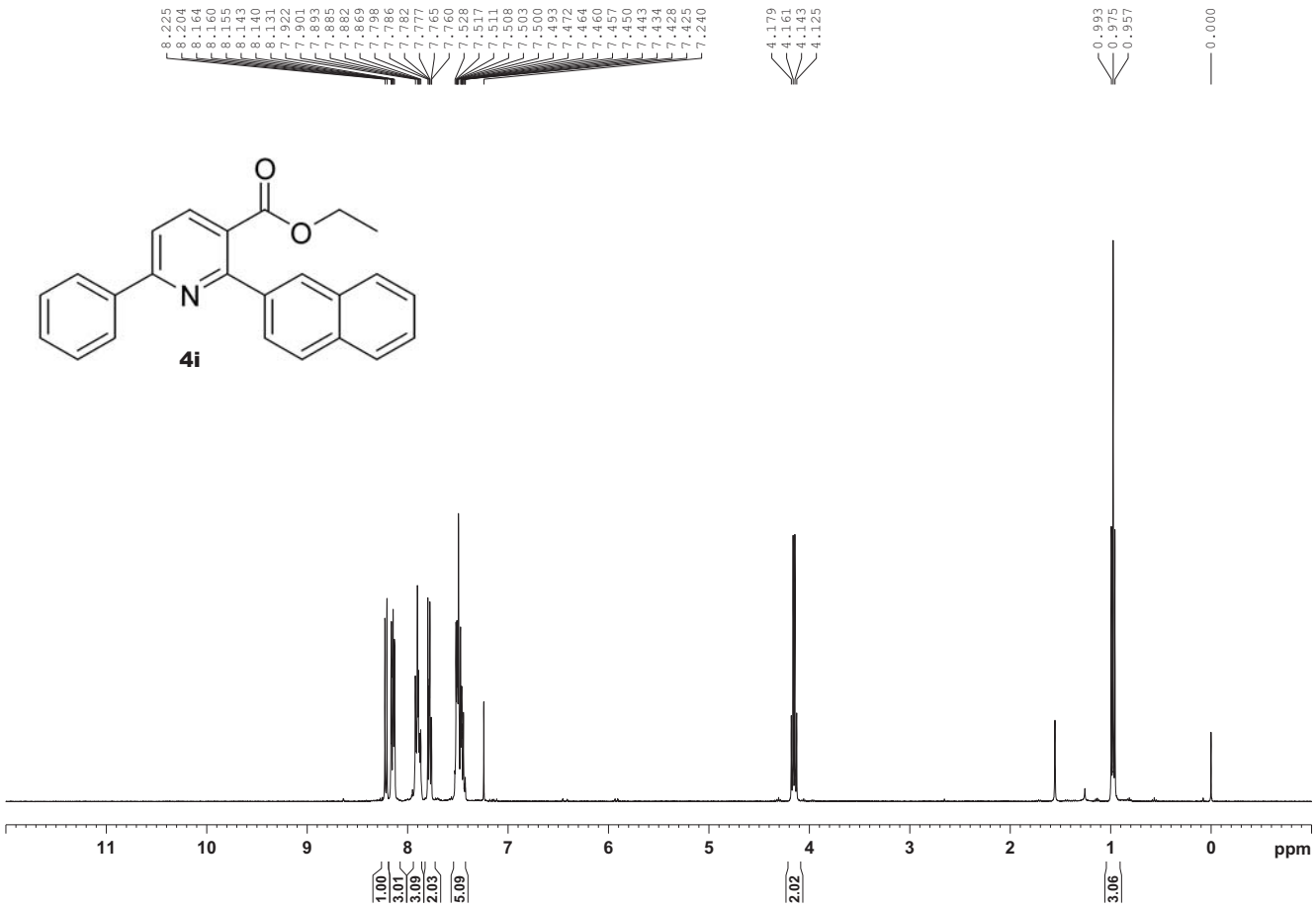
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7.760
7.528
7.517
7.511
7.508
7.503
7.500
7.493
7.472
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7.460
7.457
7.450
7.443
7.434
7.428
7.425
7.240
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4.161
4.143
4.125
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0.957
0.000
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O
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8
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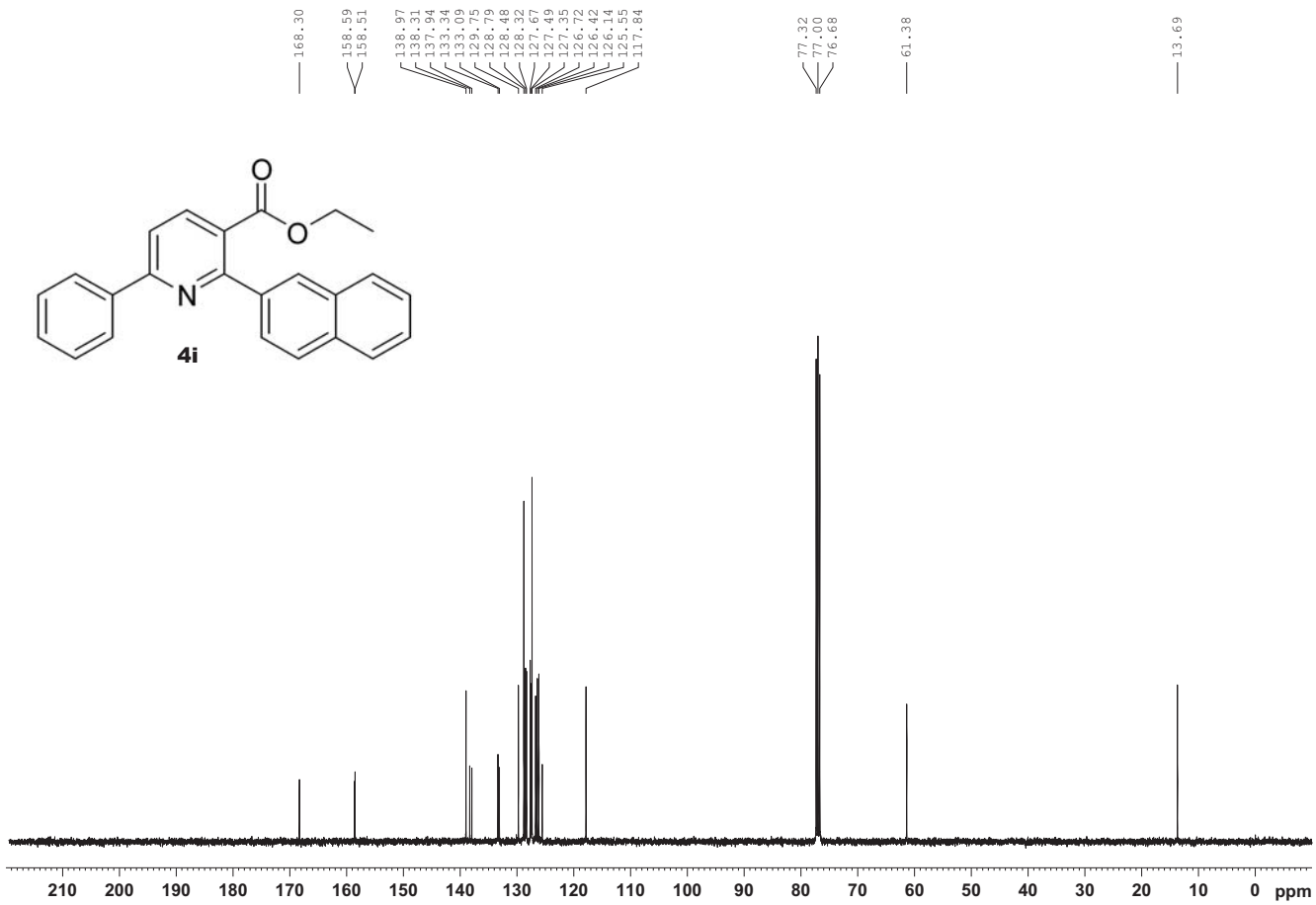
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126.72
126.42
126.14
125.55
117.84
77.32
77.00
76.68
61.38
13.69
O
O
N
4i
210
200
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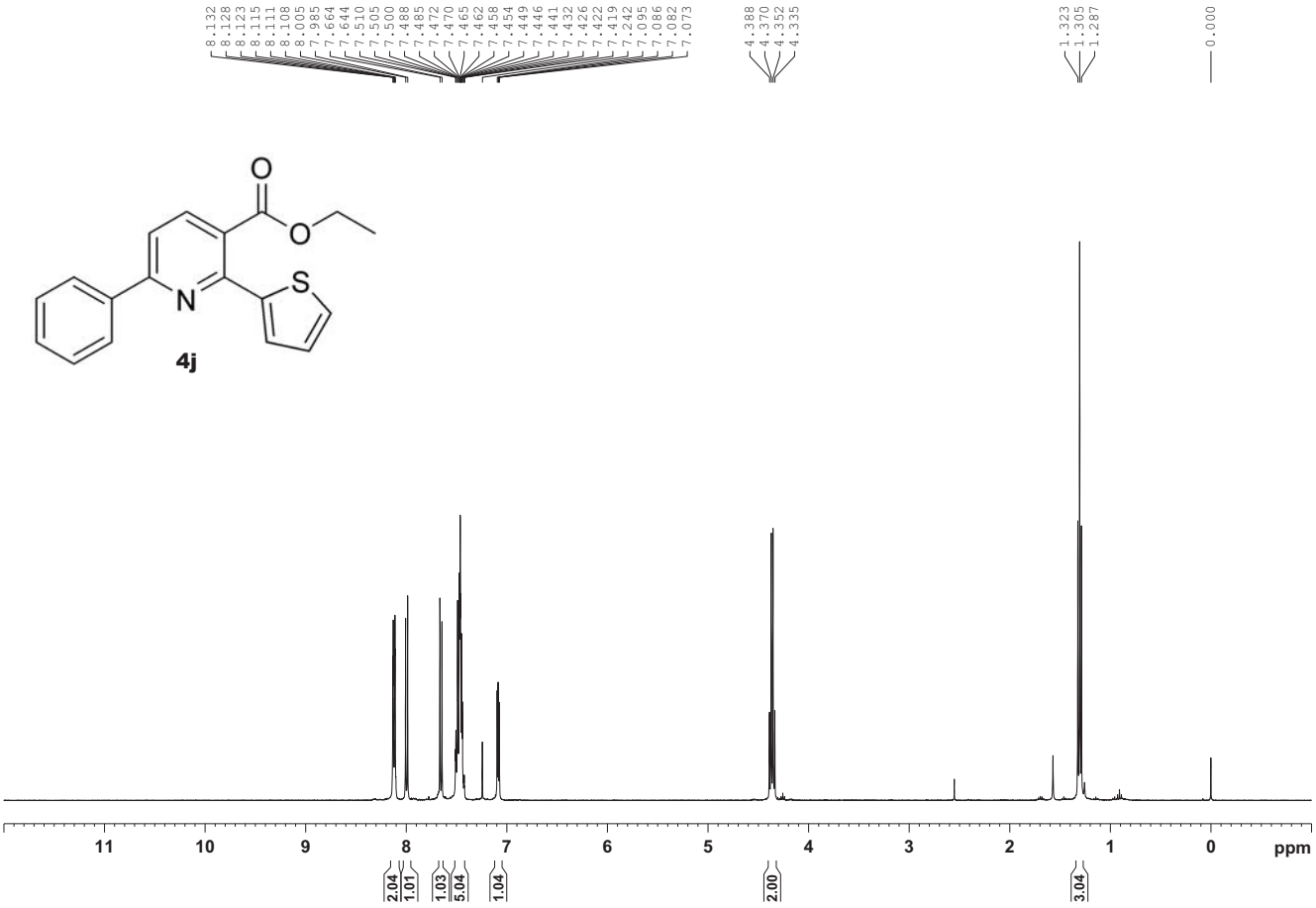
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7.485
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7.462
7.458
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7.449
7.446
7.441
7.432
7.426
7.422
7.419
7.242
7.095
7.086
7.082
7.073
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4.370
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O
O
N
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1.03
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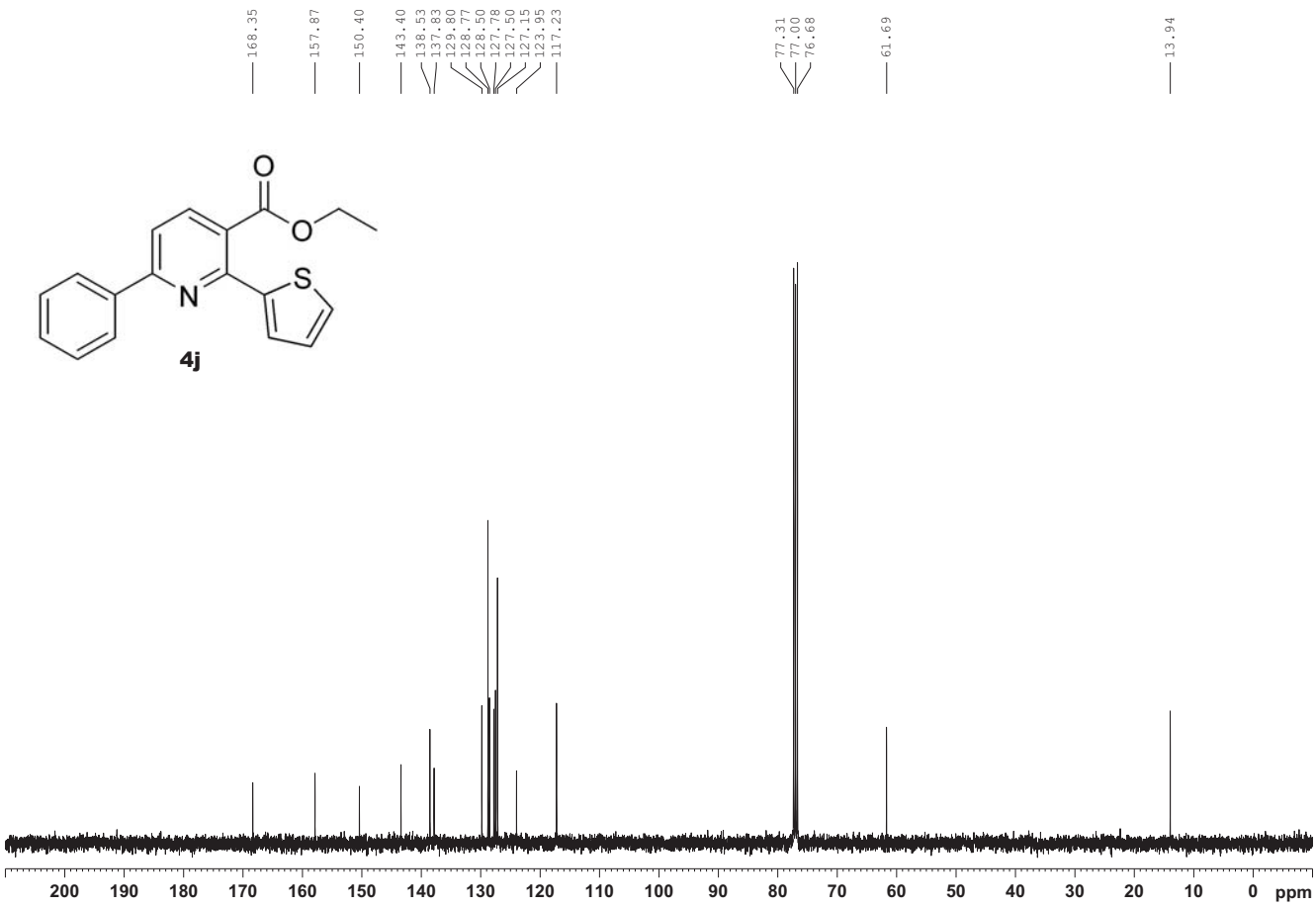
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77.00
76.68
61.69
13.94
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O
N
S
4j
200
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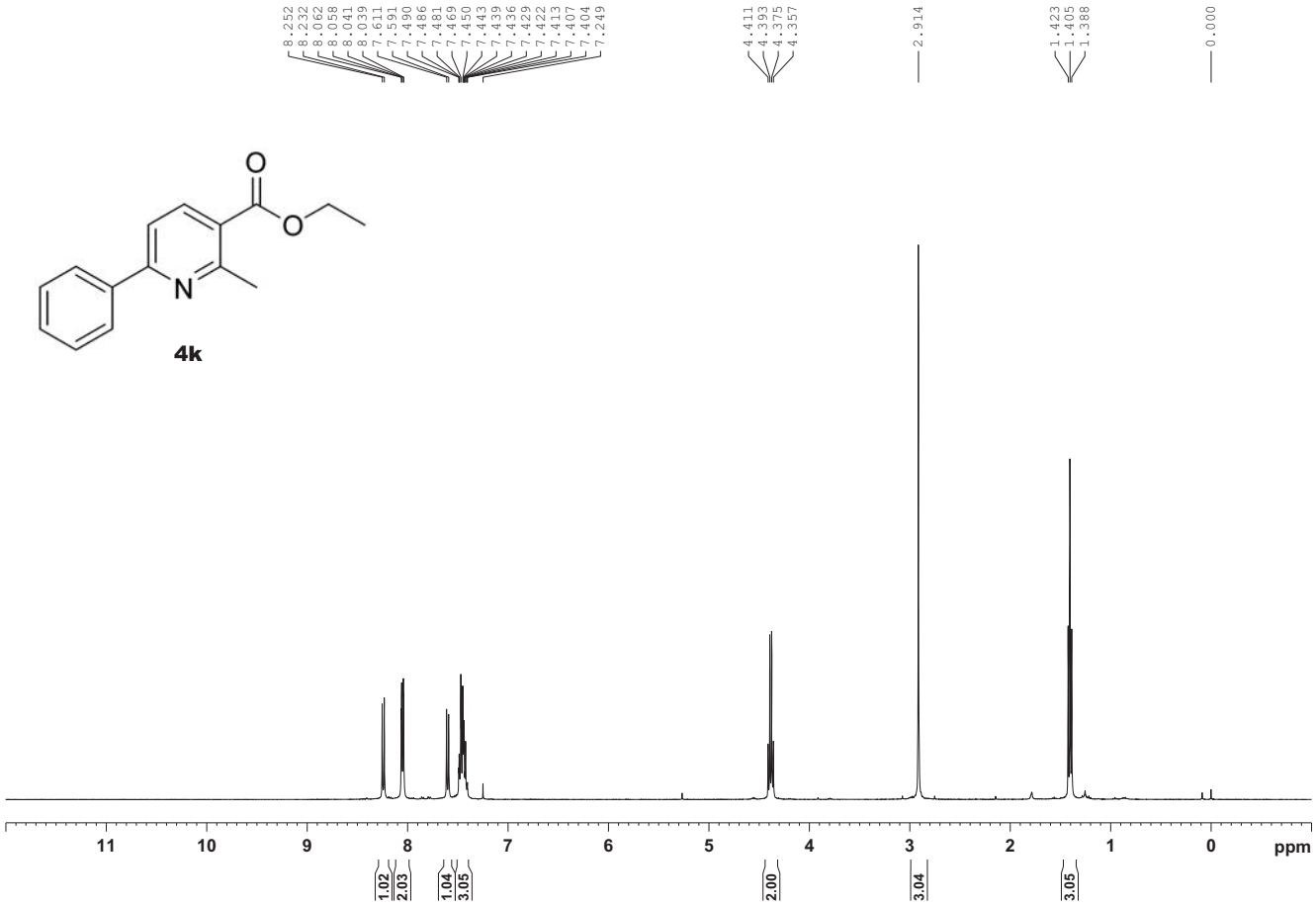
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7.439
7.436
7.429
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7.413
7.407
7.404
7.249
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4.393
4.375
4.357
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1.405
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1.04
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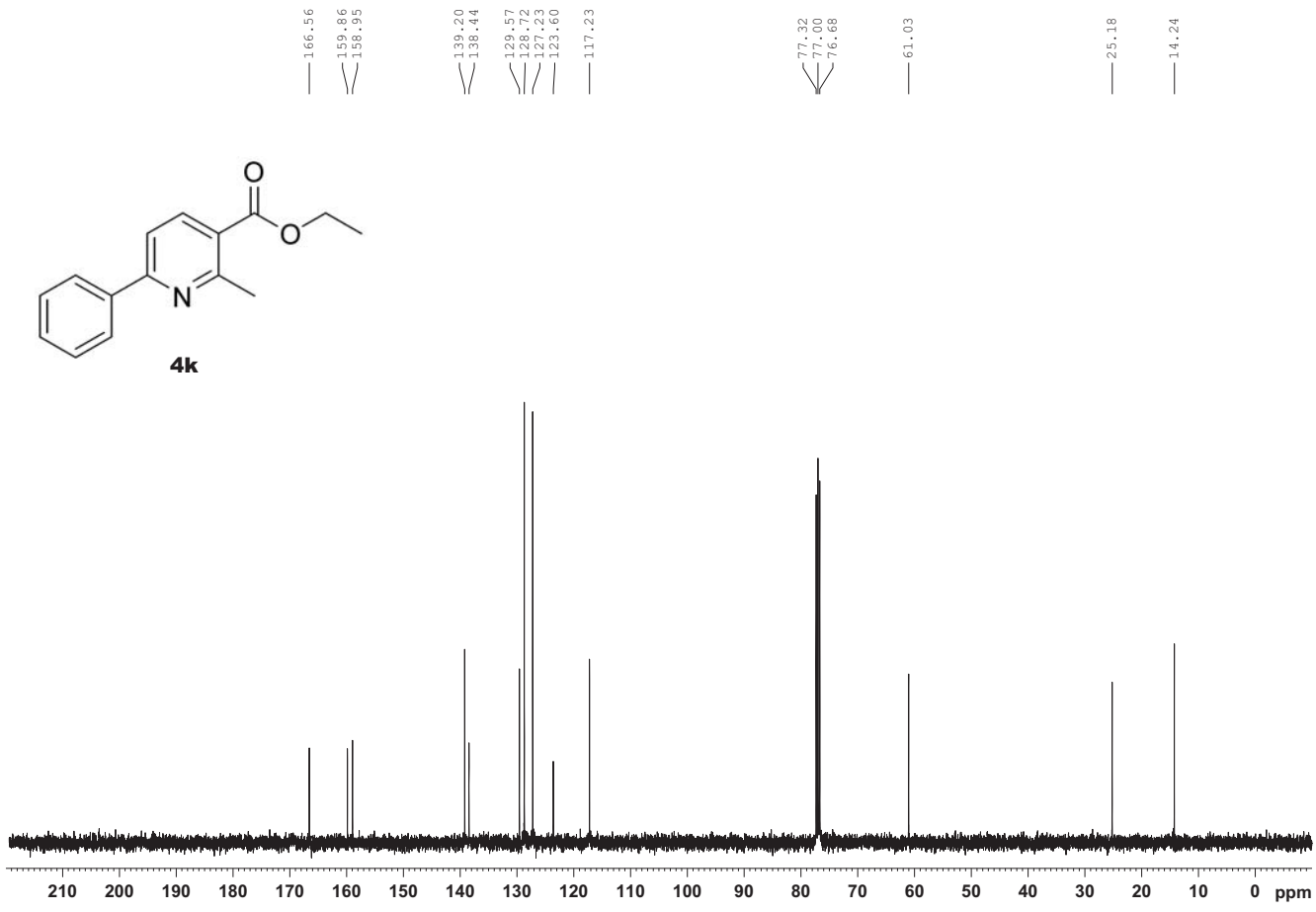
3.05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76.68
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14.24
4k
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200
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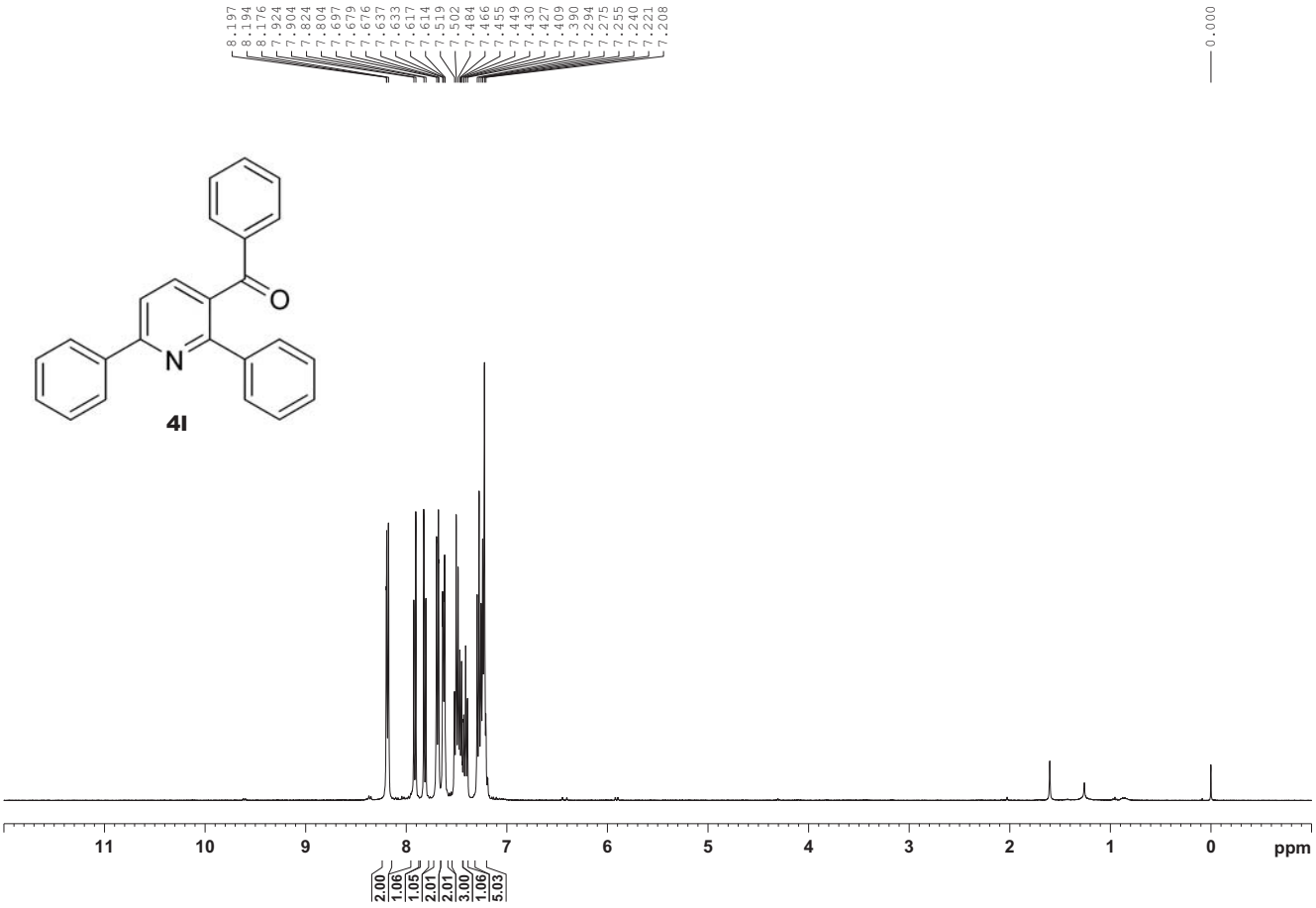
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7.614
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7.502
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7.449
7.430
7.427
7.409
7.390
7.294
7.275
7.255
7.240
7.221
7.208
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O
N
4l
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10
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8
7
6
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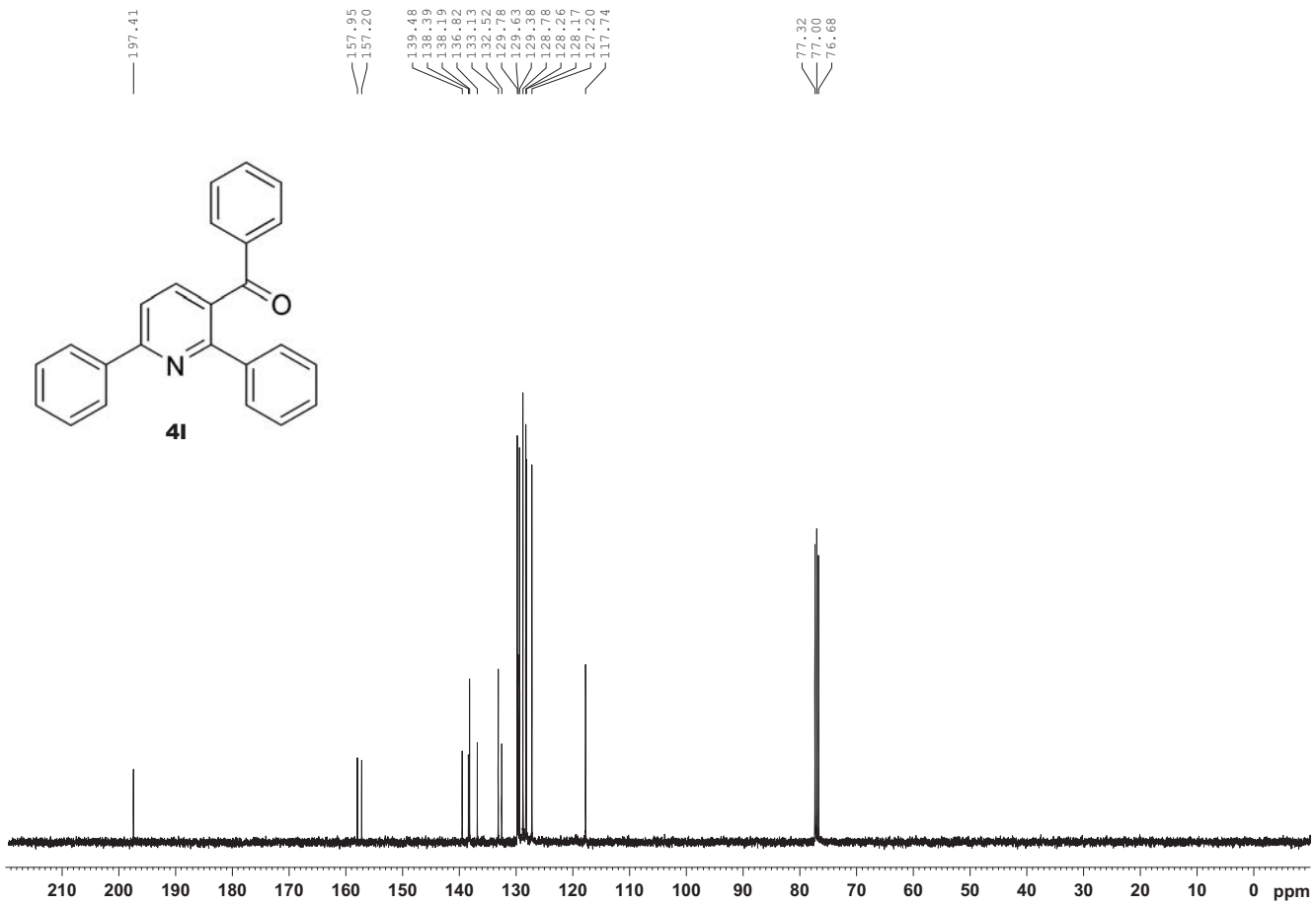
5.03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128.17
127.20
117.74
77.32
77.00
76.68
O
N
4l
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200
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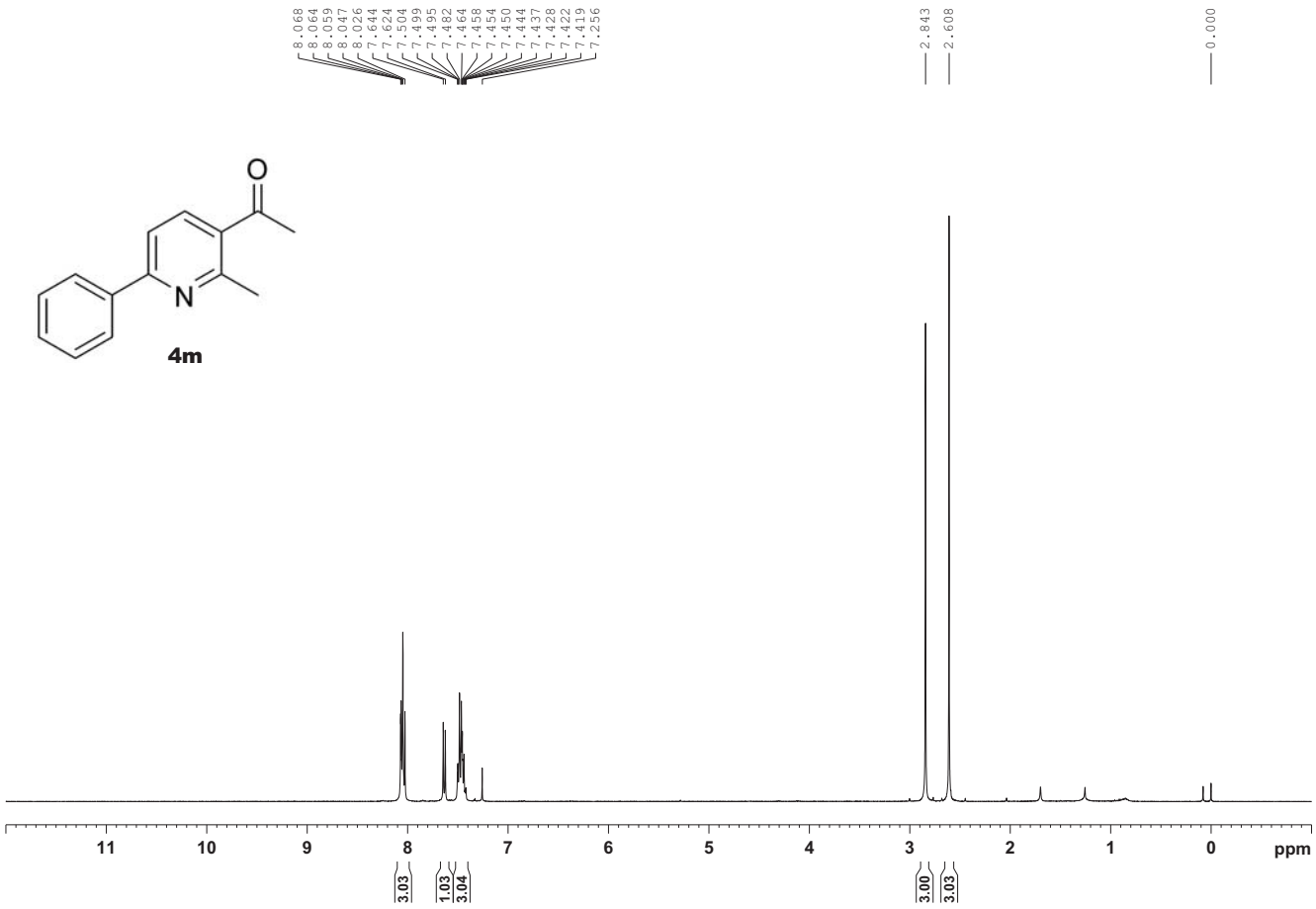
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7.450
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7.437
7.428
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7.419
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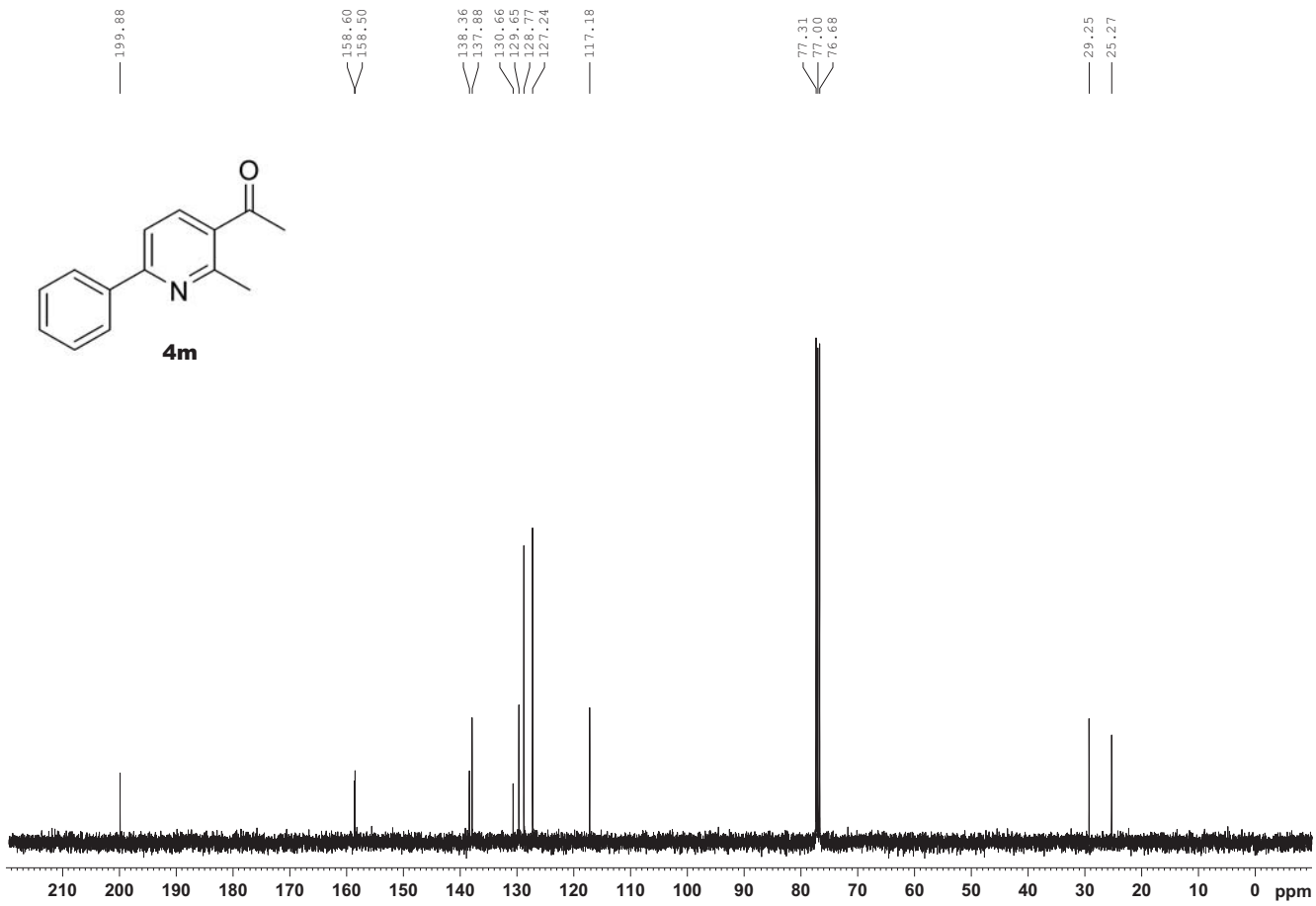
3.00
3.03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77.00
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29.25
25.27
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N
4m
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200
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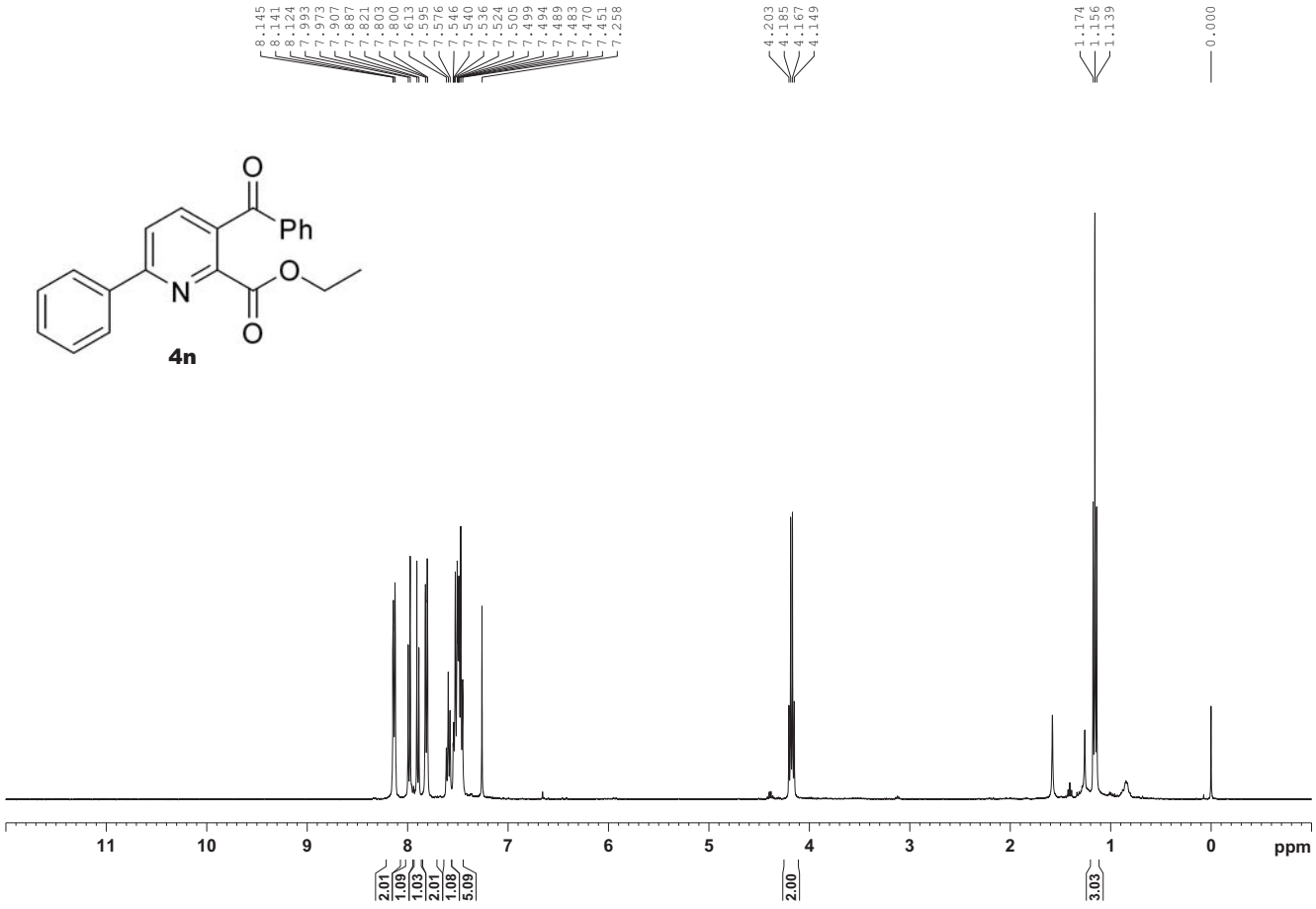
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7.536
7.524
7.505
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1.156
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2.01
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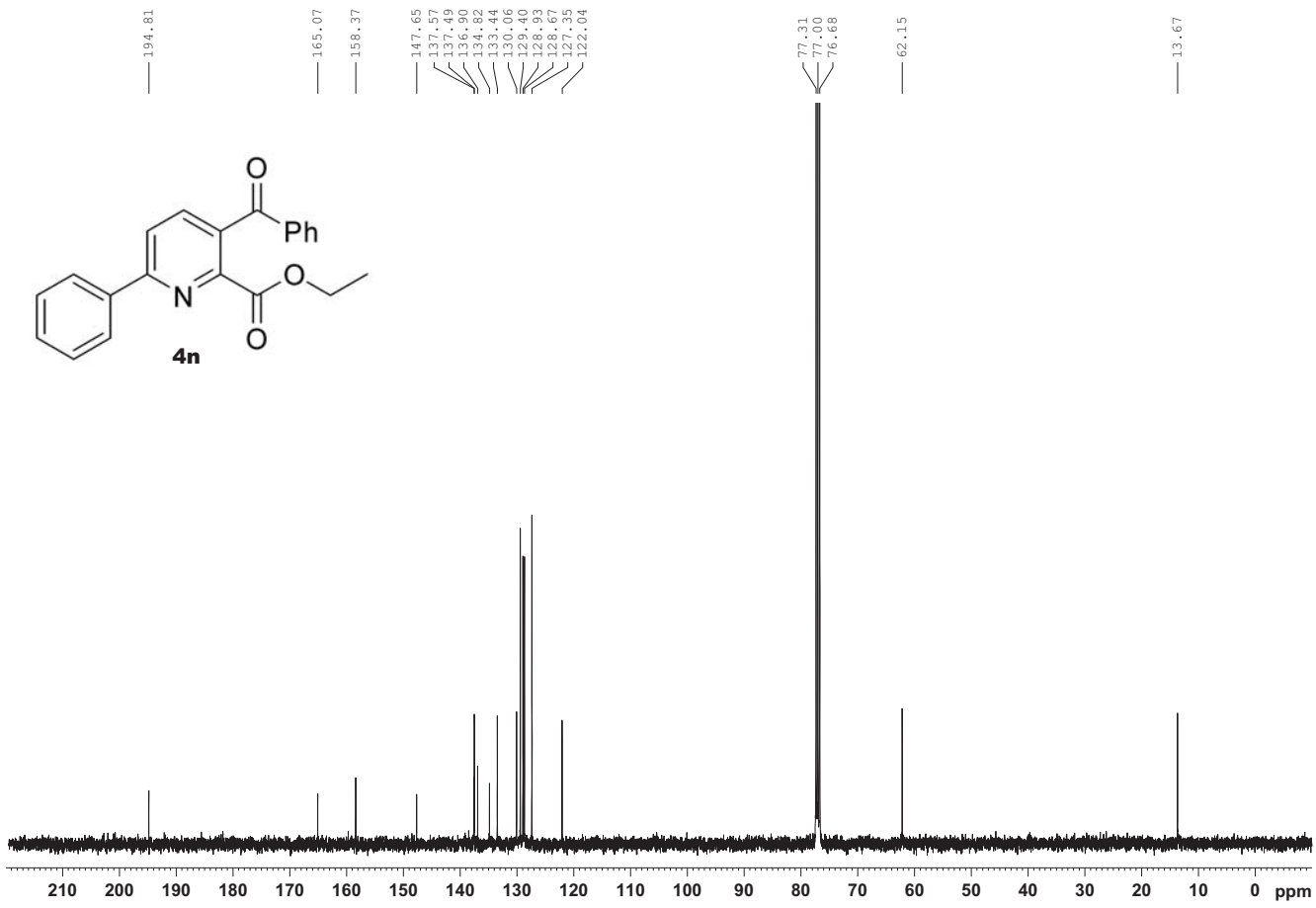
3.03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127.35
122.04
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77.00
76.68
62.15
13.67
O
Ph
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O
O
O
4n
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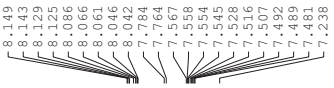
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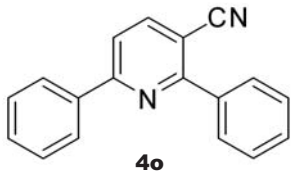
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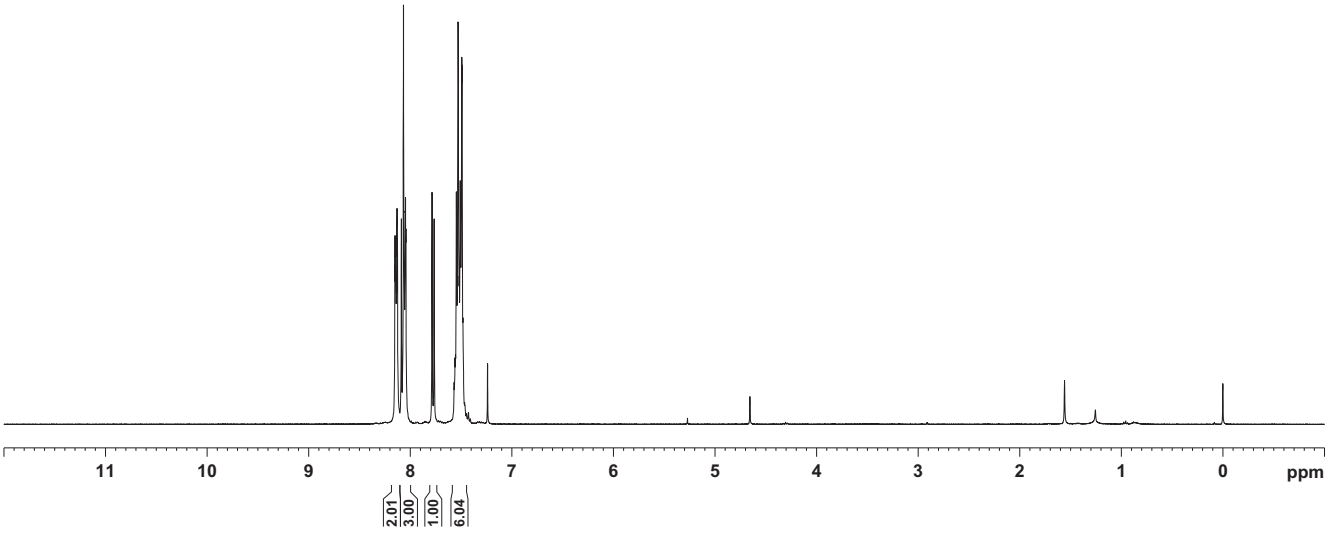
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ppm
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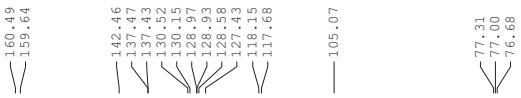
3.00
1.00
6.04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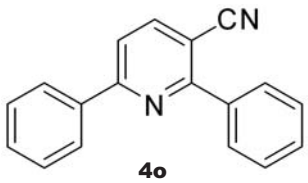
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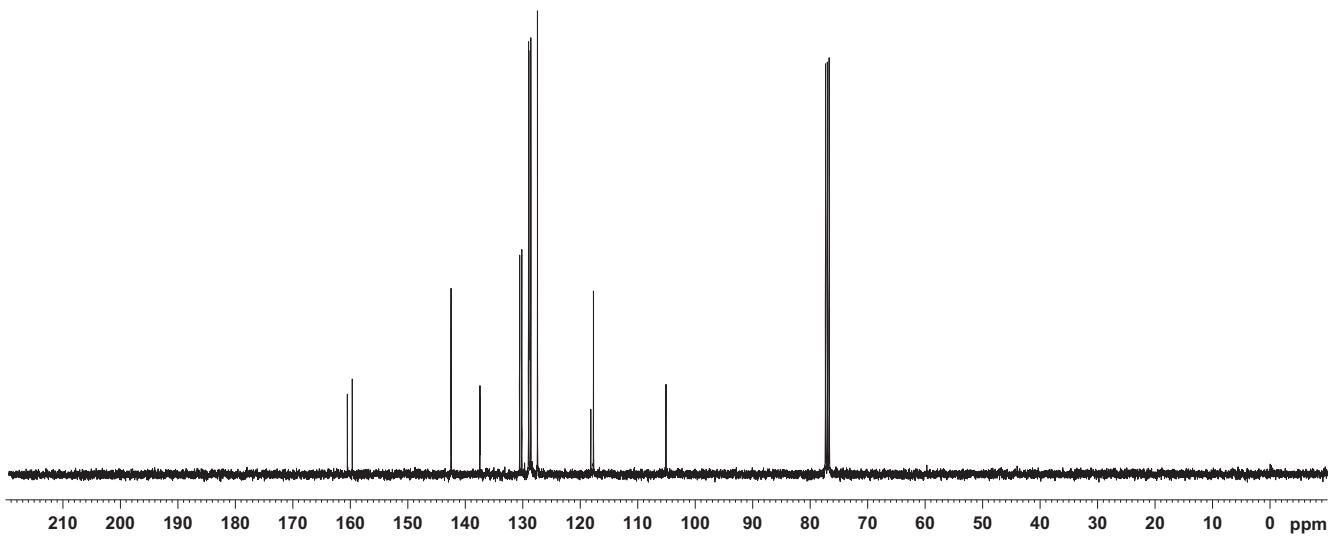
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60
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30
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10
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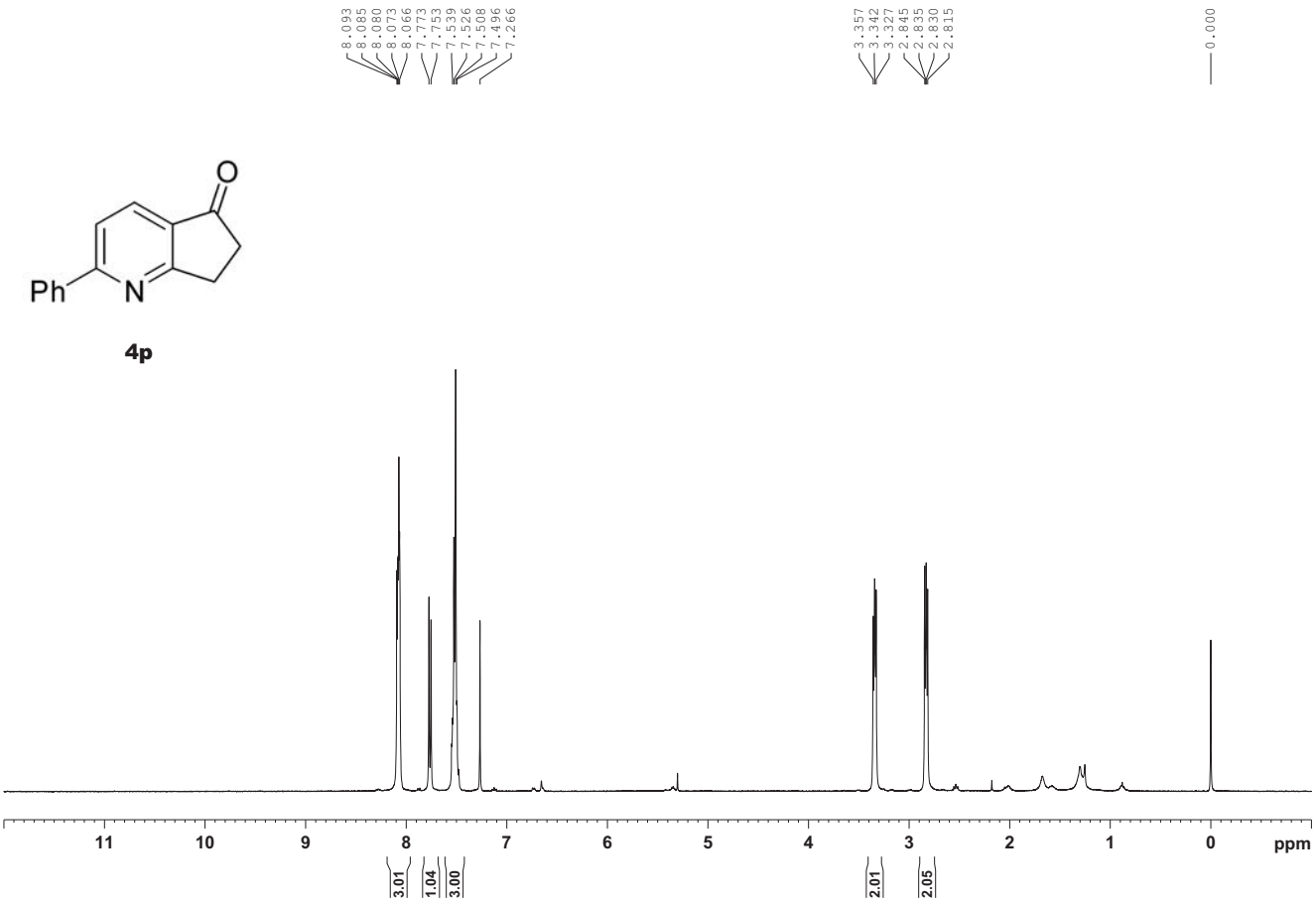
ppm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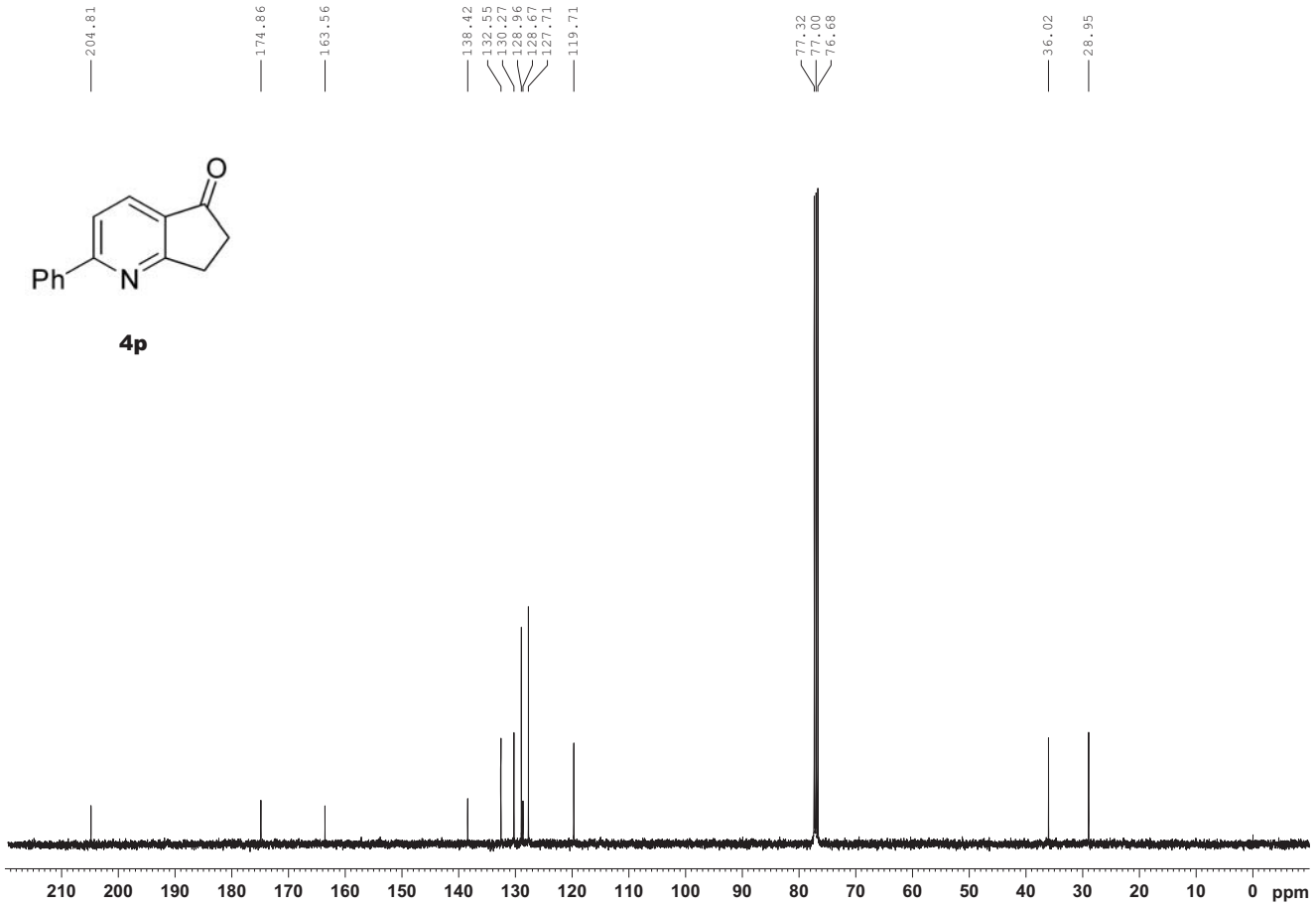
8.080
8.073
8.066
7.773
7.753
7.539
7.526
7.508
7.496
7.266
3.357
3.342
3.327
2.845
2.835
2.830
2.815
0.000
O
Ph
N
4p
11
10
9
8
7
6
5
4
3
2
1
0
ppm
3.01
1.04
3.00
2.01
2.05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163.56
138.42
132.55
130.27
128.96
128.67
127.71
119.71
77.32
77.00
76.68
36.02
28.95
O
Ph
N
4p
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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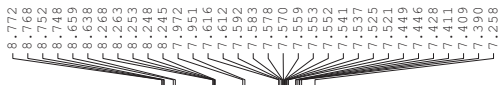
30
20
10
0
ppm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8.768
8.752
8.748
8.659
8.638
8.268
8.263
8.253
8.248
8.245
7.972
7.951
7.616
7.612
7.592
7.583
7.578
7.570
7.559
7.553
7.552
7.541
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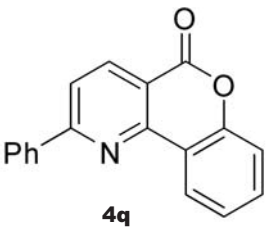
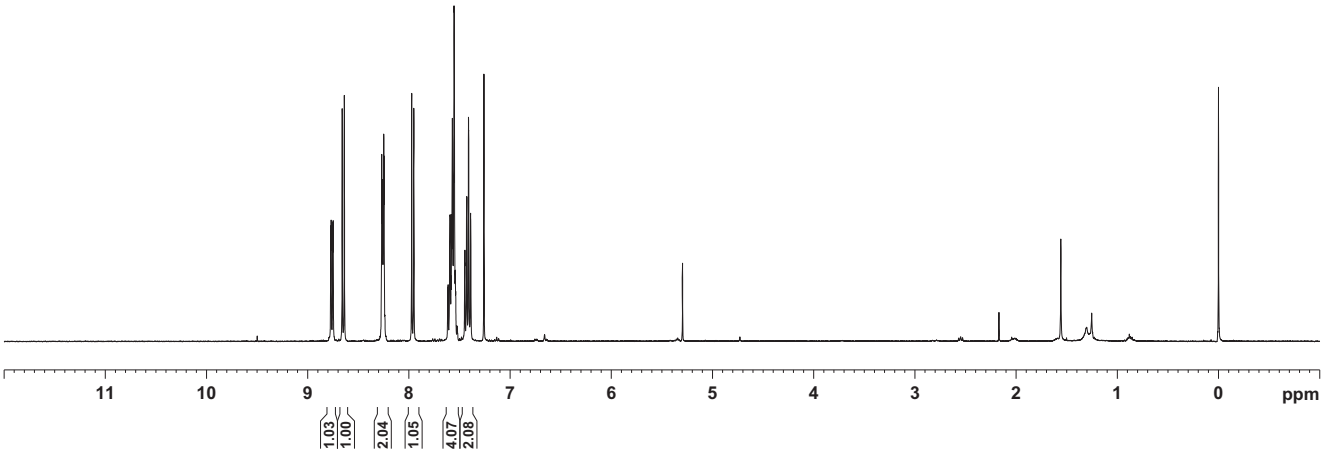
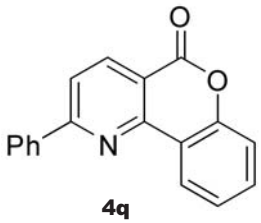
7.521
7.449
7.446
7.428
7.411
7.409
7.390
7.258
0.000


O
O
Ph
N

4q


11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.00
2.04
1.05
4.07
2.08


162.49
161.25
152.86
151.68
138.94
137.79
132.12
130.77
129.01
127.74
124.92
124.75
120.31
119.60
117.17
115.61
77.32
77.00
76.68


O
O
Ph
N

4q

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm