Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of 3-aryl-1-phosphinoimidazo[1,5-*a*]pyridine ligands for use in palladium-catalyzed cross-coupling reactions

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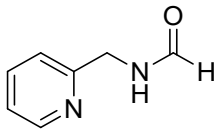
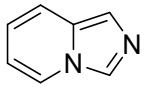
General Considerations

^{1}H, ^{13}C, and ^{31}P NMR spectra were obtained on a JEOL 500 MHz NMR at 500 MHz, 125 MHz, and 202 MHz, respectively, as solutions in $CDCl_3$ or in DMSO-d_6. Chemical shifts were reported in parts per million (ppm, δ). TLC analyses were performed on Whatman flexible aluminum backed TLC plates with a fluorescent indicator. Detection was conducted by UV absorption (254 nm). High-purity grade silica gel (Merck Grade 7734), pore size 60 Å, 70-230 mesh was used for all chromatographic separations. All chemicals used for synthetic procedures were reagent grade or better. Solutions were concentrated *in vacuo* with a rotary evaporator and the residue was purified by column chromatography using silica gel.



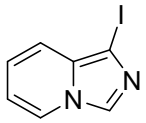
***N*-[(Pyridin-2-yl)methyl]formamide.** To a 500 mL round-bottom flask, formic acid (60 mL) was added dropwise to 2-aminomethylpyridine (12.0 g, 0.11 mmol) at 0 °C under argon. After the addition, the solution mixture was stirred at 100 °C for 5 h. The reaction mixture was quenched with 50% w/w NaOH solution until the pH of 10. The reaction mixture was extracted with dichloromethane (6 x 100 mL). The organic layers were combined, dried over Na_2SO_4 and condensed *in vacuo* to give a yellow oil (11.5 g, 77%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 – 8.48 (m, 1H), 8.29 (dd, J = 1.8, 0.9 Hz, 1H), 7.86 (m, 1H), 7.68 – 7.63 (m, 1H), 7.28 (dd, J = 7.8, 0.9

Hz, 1H), 7.21 – 7.17 (m, 1H), 4.57 (d, J = 5.6 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 208.5, 161.7, 149.0, 137.0, 122.6, 122.1, 43.1.



5

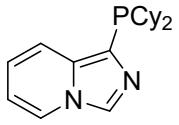
Imidazo[1,5-*a*]pyridine (5). To a 500 mL round-bottom flask was added *N*-[(pyridin-2-yl)methyl]formamide (2.1 g, 0.015 mol) in toluene (10 mL). $POCl_3$ (2 mL, 0.021 mol) was added dropwise to the solution while stirring. The reaction mixture was stirred and reflux for 2 h under argon. The reaction mixture was quenched with 50% w/w NaOH until the pH of 10. The solution mixture was extracted with dichloromethane (4 x 70 mL). The organic layers were combined, dried over Na_2SO_4 and condensed *in vacuo* to give a brown solid (1.36 g, 76%). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 8.10 (s, 1H), 7.91 (m, 1H), 7.45 – 7.38 (m, 2H), 6.71 – 6.66 (m, 1H), 6.53 (d, J = 7.0 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 130.4, 127.7, 122.2, 119.9, 119.1, 118.4, 112.8.



6

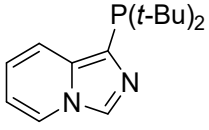
1-Iodoimidazo[1,5-*a*]pyridine (6). To a 500 mL round-bottom flask was added imidazo[1,5-*a*]pyridine (2.0 g, 17 mmol) in THF (121 mL) under argon. To the solution was added dropwise NIS (4.0 g, 17.7 mmol) dissolved in THF (80 mL). The reaction mixture was allowed to stir on ice overnight. The reaction mixture was quenched with $Na_2S_2O_3$ solution (80 mL) and extracted with dichloromethane (4 x 100 mL). The organic layers were combined, dried over Na_2SO_4 and condensed *in vacuo*. Column chromatography was performed using chloroform:acetone (9:1) eluent to give a brown solid (2.63 g, 63%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.89 (d, J

= 7.1 Hz, 1H), 7.12 (dd, *J* = 9.2, 1.1 Hz, 1H), 6.67 – 6.63 (m, 1H), 6.51 – 6.46 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 132.1, 129.5, 122.9, 120.7, 117.8, 113.5, 72.2.



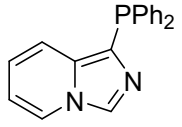
7a

1-Dicyclohexylphosphino-imidazo[1,5-*a*]pyridine (7a). To a 20 mL brown vial, 1-iodoimidazo[1,5-*a*]pyridine (600 mg, 1.86 mmol) was dissolved in 1,4-dioxane (6 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (721 mg, 2.2 mmol), DIPPF (8.37 mg, 0.037 mmol) and $Pd(OAc)_2$ (19.4 mg, 0.047 mmol). The solution was capped and stirred at room temperature for 2 h. Dicyclohexylphophine (1.86 mmol, 3.27 mL in 0.5 M hexane solution) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL). The mixture was further purified by column chromatography using a chloroform:acetone (97:3) eluent to give a yellow solid (191 mg, 33%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.89 (m, 1H), 7.67 (d, *J* = 9.3 Hz, 1H), 6.72 – 6.68 (m, 1H), 6.56 – 6.51 (m, 1H), 2.16 (td, *J* = 11.9, 2.9 Hz, 2H), 1.92 – 1.54 (m, 12H), 1.35 – 1.00 (m, 8H). ^{13}C NMR (126 MHz, $CDCL_3$) δ 138.1 137.7, 129.3, 122.4, 119.6, 118.9, 112.8, 32.8, 30.4, 29.2, 27.2, 27.0, 26.6. ^{31}P NMR (202 MHz, $CDCl_3$) δ -26.6.



7b

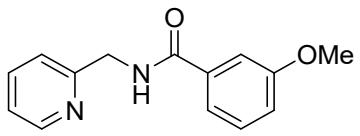
1-Di-(*t-butyl*)phosphino-imidazo[1,5-*a*]pyridine (7b). To a 20 mL brown vial, 1-iodoimidazo[1,5-*a*]pyridine (200 mg, 0.62 mmol) was dissolved in 1,4 dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (240 mg, 0.74 mmol), DIPPF (2.7 mg, 0.012 mmol) and $Pd(OAc)_2$ (6.7 mg, 0.016 mmol).The solution was capped and stirred at room temperature for 2 h. Di-(*t*-butyl*)*phosphine (0.62 mmol, 1.24 mL in 0.5 M hexane solution) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a chloroform:acetone (9:1) eluent to give a yellow solid (78 mg, 48%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (d, *J* = 2.6 Hz, 1H), 7.90 – 7.85 (m, 1H), 7.77 – 7.71 (m, 1H), 6.72 – 6.66 (m, 1H), 6.54 – 6.47 (m, 1H), 1.27 – 1.10 (m, 18H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.7, 129.1, 122.4, 120.5, 119.8, 119.3, 112.8, 33.1, 30.5. ^{31}P NMR (202 MHz, $CDCl_3$) δ 4.3.



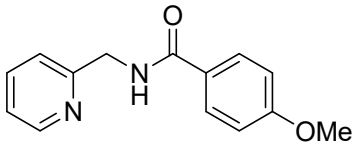
7c

1-Diphenylphosphino-imidazo[1,5-a]pyridine (7c). To a 20 mL brown vial, 1-iodoimidazo[1,5-*a*]pyridine (300 mg, 0.93 mmol) was dissolved in 1,4-dioxane (3 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (355 mg, 1.10 mmol), DIPPF (9.6 mg, 0.023 mmol) and $Pd(OAc)_2$ (4.3 mg, 0.019 mmol). The solution was capped and stirred at room temperature for 2 h. Diphenylphosphine (173 mg, 0.93 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a

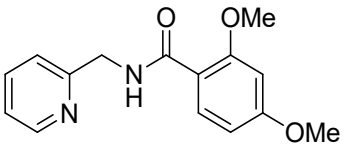
chloroform:acetone (9:1) eluent to give a brown solid (70 mg, 25%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (s, 1H), 7.88 (d, *J* = 7.4 Hz, 1H), 7.57 – 7.50 (m, 5H), 7.34 – 7.23 (m, 6H), 6.73 (t, *J* = 9.0 Hz, 1H), 6.55 (t, *J* = 6.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.1, 133.6, 133.4, 131.7, 130.5, 128.3, 125.6, 122.9, 120.8, 118.6, 113.2. ^{31}P NMR (202 MHz, $CDCl_3$) δ -33.0.



3-Methoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8c). To a 50 mL round-bottom flask was added 3-methoxybenzoic acid (1.2 g, 7.89 mmol) in dicholoromethane (40 mL) under argon. Oxalyl chloride (709 μL, 8.27 mmol) and DMF (6 drops) were slowly added to the reaction mixture over 30 min through a septum. The reaction mixture was allowed to stir at room temperature for 2 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (40 mL) and purged with argon. 2-Aminomethylpyridine (832 mg, 7.51 mmol) and triethylamine (1.3 mL, 9.02 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir on ice overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (1.82 g, 100%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 – 8.52 (m, 1H), 7.86 (t, *J* = 5.1 Hz, 1H), 7.65 (td, *J* = 7.7, 1.8 Hz, 1H), 7.45 (dd, *J* = 2.7, 1.6 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.33 – 7.28 (m, 2H), 7.21 – 7.17 (m, 1H), 7.03 – 7.00 (m, 1H), 4.73 (d, *J* = 5.0 Hz, 2H), 3.81 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.5, 159.6, 157.1, 148.8, 136.8, 135.6, 129.4, 122.3, 121.9, 119.2, 117.6, 112.4, 55.2, 45.0.

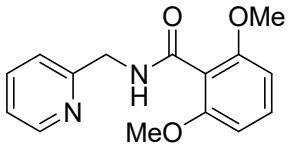


4-Methoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8d). To a 50 mL round-bottom flask was added 4-methoxybenzoic acid (1.6 g, 10.5 mmol) in dicholoromethane (50 mL) under argon. Oxalyl chloride (950 µL, 11.0 mmol) and DMF (6 drops) were slowly added to the reaction mixture over 30 minutes through a septum. The reaction mixture was allowed to stir at room temperature for 3 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (50 mL) and purged with argon. 2-Aminomethylpyridine (1.08 g, 10.0 mmol) and triethylamine (1.7 mL, 12.0 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir on ice overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (2.44 g, 100%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (ddd, J = 5.0, 1.8, 0.9 Hz, 1H), 7.85 – 7.77 (m, 2H), 7.66 (td, J = 7.7, 1.8 Hz, 1H), 7.54 (t, J = 5.1 Hz, 1H), 7.31 (dt, J = 7.8, 1.1 Hz, 1H), 7.21 – 7.17 (m, 1H), 6.93 – 6.88 (m, 2H), 4.73 (d, J = 4.9 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.0, 162.3, 156.6, 149.1, 136.9, 129.0, 126.8, 122.5, 122.3, 113.8, 55.5, 44.8.



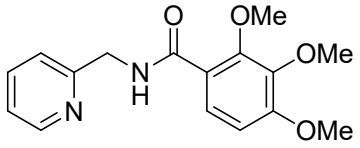
2,4-Dimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8e). To a 50 mL round-bottom flask was added 2,4-dimethoxybenzoic acid (1.6 g, 8.8 mmol) in dichloromethane (50 mL) under argon. Oxalyl chloride (800 µL, 9.2 mmol) and DMF (6 drops) were slowly added to the reaction mixture

over 30 minutes through a septum. The reaction mixture was allowed to stir at room temperature for 3 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (50 mL) and purged with argon. 2-Aminomethylpyridine (905 mg, 8.4 mmol) and triethylamine (970 µL, 10.1 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (2.13 g, 100%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.78 (t, *J* = 5.3 Hz, 1H), 8.52 (ddd, *J* = 5.0, 1.8, 1.0 Hz, 1H), 8.16 (d, *J* = 8.7 Hz, 1H), 7.60 (td, *J* = 7.7, 1.8 Hz, 1H), 7.29 (m, 1H), 7.13 (m, 1H), 6.54 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.44 (d, *J* = 2.3 Hz, 1H), 4.74 (d, *J* = 5.2 Hz, 2H), 3.91 (s, 3H), 3.79 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.3, 163.5, 159.2, 157.7, 149.2, 136.8, 133.9, 122.2, 122.1, 114.5, 105.3, 98.6, 56.0, 55.6, 45.3.



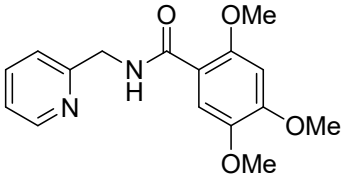
2,6-Dimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8g). To a 50 mL round-bottom flask was added 2,6-dimethoxybenzoic acid (1.6 g, 8.8 mmol) in dichloromethane (50 mL) under argon. Oxalyl chloride (800 µL, 9.2 mmol) and DMF (6 drops) were slowly added to the reaction mixture over 30 minutes through a septum. The reaction mixture was allowed to stir at room temperature for 3 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (50 mL) and purged with argon. 2-Aminomethylpyridine (905 mg, 8.4 mmol) and triethylamine (970 µL, 10.1 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir

overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (2.25 g, 98%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (m, 1H), 7.66 (td, *J* = 7.7, 1.8 Hz, 1H), 7.43 (dt, *J* = 7.9, 1.0 Hz, 1H), 7.29 – 7.23 (m, 1H), 7.18 – 7.13 (m, 1H), 6.86 (d, *J* = 6.1 Hz, 1H), 6.55 (d, *J* = 8.4 Hz, 2H), 4.78 (d, *J* = 5.4 Hz, 2H), 3.79 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.1, 157.6, 157.1, 149.0, 136.8, 130.8, 122.3, 122.0, 115.8, 104.1, 56.0, 45.0.

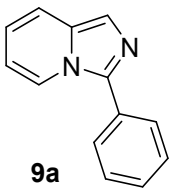


2,3,4-Trimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8h). To a 50 mL round-bottom flask was added 2,3,4-trimethoxybenzoic acid (1.6 g, 7.6 mmol) in dichloromethane (50 mL) under argon. Oxalyl chloride (680 µL, 7.9 mmol) and DMF (4 drops) were slowly added to the reaction mixture over 30 minutes through a septum. The reaction mixture was allowed to stir at room temperature for 3 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (50 mL) and purged with argon. 2-Aminomethylpyridine (765 mg, 7.2 mmol) and triethylamine (1.2 mL, 8.7 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (2.2 g, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.10 (t, *J* = 5.1 Hz, 1H), 8.59 (dd, *J* = 4.9, 0.9 Hz, 1H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.67 (td, *J* = 7.6, 1.8 Hz, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.22 – 7.16 (m, 1H), 6.79 (d, *J* = 9.0 Hz, 1H), 4.80 (d, *J* = 5.1 Hz, 2H),

4.02 (s, 3H), 3.91 (s, 3H), 3.88 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 157.3, 156.5, 152.9, 149.2, 141.9, 136.7, 126.8, 122.3, 122.0, 122.0, 118.9, 107.5, 61.8, 61.0, 56.1, 45.1.

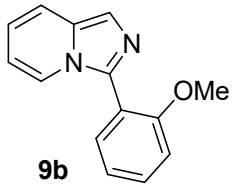


2,4,5-Trimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (8i). To a 50 mL round-bottom flask was added 2,4,5-trimethoxybenzoic acid (1.2 g, 5.7 mmol) in dichloromethane (50 mL) under argon. Oxalyl chloride (520 μL, 5.9 mmol) and DMF (6 drops) were slowly added to the reaction mixture over 30 minutes through a septum. The reaction mixture was allowed to stir at room temperature for 3 h. The solvent was removed *in vacuo* and the crude material was collected and used in the next step. The crude product was re-dissolved in dichloromethane (50 mL) and purged with argon. 2-Aminomethylpyridine (624 mg, 5.4 mmol) and triethylamine (900 μL, 6.5 mmol) were slowly injected to the reaction mixture through a septum. The reaction mixture was allowed to stir overnight. The reaction mixture was quenched with $NaHCO_3$ (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a white solid (1.4 g, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.98 (t, J = 5.2 Hz, 1H), 8.60 – 8.54 (m, 1H), 7.79 (s, 1H), 7.65 (td, J = 7.7, 1.8 Hz, 1H), 7.35 (dt, J = 7.9, 1.0 Hz, 1H), 7.19 – 7.16 (m, 1H), 6.54 (s, 1H), 4.79 (d, J = 5.2 Hz, 2H), 3.98 (s, 3H), 3.93 (s, 3H), 3.90 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 165.2, 157.5, 153.0, 152.4, 149.1, 143.1, 136.7, 122.2, 121.9, 114.0, 112.9, 96.6, 56.7, 56.2, 56.1, 45.3.



9a

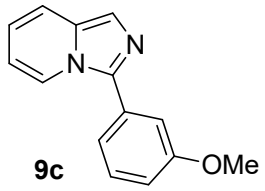
3-Phenylimidazo[1,5-*a*]pyridine (9a). 2-Aminomethylpyridine (1.00 g, 9.24 mmol) was combined with benzaldehyde (1.96 g, 18.5 mmol) and iodine (235 mg, 0.925 mmol) in DMF (35 mL) under argon. After stirring for 1 h, TBHP (70%, 1.89 mL, 13.9 mmol) was added through a septum, and the resulting solution was stirred overnight at 80 ºC. The crude mixture was quenched with water (300 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layers were rinsed with LiCl (3 x 100 mL). The remaining organic solution was dried over Na_2SO_4, condensed *in vacuo*, and purified via chromatography using a hexanes:ethyl acetate (1:1) eluent to give a solid (1.26 g, 70%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.55 (d, *J* = 0.9 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.48 (d, *J* = 9.1 Hz, 1H), 7.45 – 7.41 (m, 1H), 6.72 (ddd, *J* = 9.1, 6.3, 0.9 Hz, 1H), 6.57 – 6.53 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.4, 131.7, 130.5, 129.1, 128.7, 128.0, 121.5, 120.7, 118.9, 118.8, 113.1.



9b

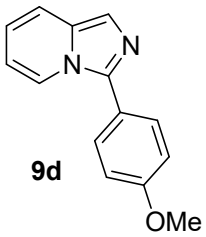
3-(2-Methoxyphenyl)imidazo[1,5-*a*]pyridine (9b). 2-Aminomethylpyridine (1.00 g, 9.24 mmol) was combined with 2-methoxybenzaldehyde (2.52 g, 18.5 mmol) and iodine (235 mg, 0.925 mmol) in DMF (35 mL) under argon. After stirring for 1 h, TBHP (70%, 1.89 mL, 13.9 mmol) was added through a septum, and the resulting solution was stirred overnight at 80 ºC. The crude mixture was quenched with water (300 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layers were rinsed with LiCl (3 x 100 mL). The remaining organic solution was dried over Na_2SO_4, condensed *in vacuo*, and purified via chromatography using a hexanes:ethyl acetate (1:1) eluent to give a solid (1.19 g, 36%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.57 (m, 2H), 7.56 (s, 1H), 7.47 – 7.41 (m, 2H), 7.09 (td, *J* = 7.5, 0.9 Hz, 1H), 7.02 (d, *J* =

8.0 Hz, 1H), 6.70 (dd, *J* = 9.2, 6.3 Hz, 1H), 6.51 – 6.46 (m, 1H), 3.78 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 136.3, 132.6, 131.3, 130.6, 123.3, 121.4, 120.3, 119.5, 118.5, 118.2, 111.9, 111.4, 111.1, 55.7.



9c

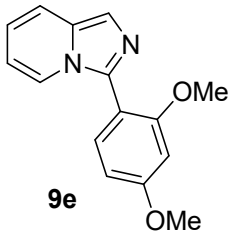
3-(3-Methoxyphenyl)imidazo[1,5-*a*]pyridine (9c). To a 50 mL round-bottom flask was dropwise added $POCl_3$ (30.5 mL) to 3-methoxy-*N*-[(pyridin-2-yl)methyl]benzamide (1.85 g, 7.64 mmol). A condenser was applied and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50% w/w NaOH to the pH of 10 and extracted with dichloromethane (4 x 100 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (1.69 g, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.51 (d, *J* = 1.0 Hz, 1H), 7.36 (d, *J* = 9.2 Hz, 1H), 7.34 – 7.29 (m, 3H), 6.91 – 6.88 (m, 1H), 6.58 (ddd, *J* = 9.1, 6.3, 1.0 Hz, 1H), 6.43 – 6.39 (m, 1H), 3.78 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 138.0, 131.7, 131.7, 129.9, 121.4, 120.6, 119.7, 118.8, 118.6, 114.5, 113.3, 113.0, 55.3.



9d

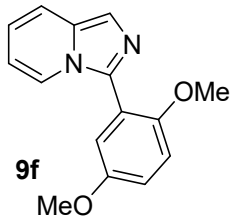
3-(4-Methoxyphenyl)imidazo[1,5-*a*]pyridine (9d). To a 50 mL round-bottom flask was dropwise added $POCl_3$ (40.4 mL) to 4-methoxy-*N*-[(pyridin-2-yl)methyl]benzamide (2.44 g, 10.1 mmol). A condenser was applied and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50% w/w NaOH

to the pH of 10 and extracted with dichloromethane (4 x 100 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (2.20 g, 98%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.72 – 7.68 (m, 2H), 7.51 (d, *J* = 0.9 Hz, 1H), 7.44 (dt, *J* = 9.1, 1.3 Hz, 1H), 7.06 – 7.00 (m, 2H), 6.67 (ddd, *J* = 9.1, 6.4, 1.0 Hz, 1H), 6.51 (m, 1H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 138.4, 131.4, 129.5, 123.0, 121.5, 120.3, 118.9, 118.5, 114.5, 112.9, 55.5.



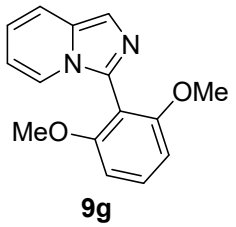
9e

3-(2,4-Dimethoxyphenyl)imidazo[1,5-*a*]pyridine (9e). To a 50 mL round-bottom flask was dropwise added $POCl_3$ (31.3 mL) to 2,4-dimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (2.13 g, 7.8 mmol). A condenser was applied and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50% w/w NaOH to the pH of 10 and extracted with dichloromethane (4 x 100 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (1.7 g, 85%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 – 7.82 (m, 1H), 7.79 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.67 (d, *J* = 9.4 Hz, 1H), 7.63 (d, *J* = 8.6 Hz, 1H), 7.13 (ddd, *J* = 9.3, 6.6, 0.9 Hz, 1H), 6.97 – 6.93 (m, 1H), 6.71 (dd, *J* = 8.6, 2.3 Hz, 1H), 6.60 (d, *J* = 2.3 Hz, 1H), 3.87 (s, 3H), 3.83 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 164.8, 158.9, 133.6, 133.0, 129.8, 123.6, 123.5, 119.2, 116.9, 111.0, 106.5, 103.2, 99.4, 56.1, 55.9.



9f

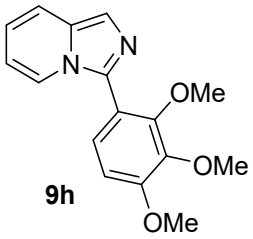
3-(2,5-Dimethoxyphenyl)imidazo[1,5-*a*]pyridine (9f). 2-Aminomethylpyridine (1.00 g, 9.24 mmol) was combined with 2,5-dimethoxybenzaldehyde (3.07 g, 18.5 mmol) and iodine (235 mg, 0.925 mmol) in DMF (35 mL) under argon. After stirring for 1 h, TBHP (70%, 1.89 mL, 13.86 mmol) was added through a septum, and the resulting solution was stirred overnight at 80 ºC. The crude mixture was quenched with water (300 mL) and extracted with ethyl acetate (3 x 50 mL). The combined organic layers were rinsed with LiCl (3 x 100 mL). The remaining organic solution was dried over Na_2SO_4, condensed *in vacuo*, and purified via chromatography using a hexanes:ethyl acetate (1:1) eluent to give a solid (1.23 g, 54%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.62 (m, 1H), 7.56 (s, 1H), 7.47 (d, *J* = 9.1 Hz, 1H), 7.17 (d, *J* = 2.9 Hz, 1H), 6.99 – 6.92 (m, 2H), 6.73 (dd, *J* = 9.2, 6.3 Hz, 1H), 6.53 – 6.49 (m, 1H), 3.81 (s, 3H), 3.73 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.0, 151.6, 136.2, 131.5, 123.4, 120.3, 120.1, 118.7, 118.2, 116.8, 116.8, 112.9, 111.9, 56.3, 56.0.



9g

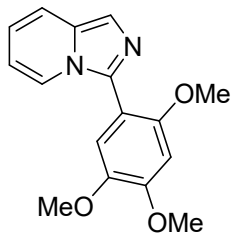
3-(2,6-Dimethoxyphenyl)imidazo[1,5-*a*]pyridine (9g). To a 50 mL round-bottom flask was dropwise added $POCl_3$ (32.0 mL) to 2,6-dimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (2.25 g, 8.3 mmol). A condenser was applied and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50%

w/w NaOH to the pH of 10 and extracted with dichloromethane (4 x 100 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (1.85 g, 88%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 1.0 Hz, 1H), 7.47 – 7.35 (m, 3H), 6.70 – 6.62 (m, 3H), 6.46 – 6.39 (m, 1H), 3.71 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 132.2, 131.5, 130.7, 122.5, 119.9, 118.4, 111.7, 107.4, 104.1, 56.0.



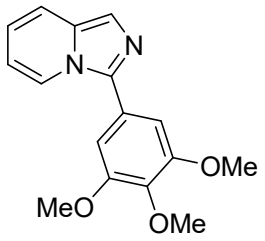
9h

3-(2,3,4-Trimethoxyphenyl)imidazo[1,5-*a*]pyridine (9h). To a 250 mL round-bottom flask was dropwise added $POCl_3$ (30 mL) to 2,3,4-trimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (2.2 g, 7.2 mmol). A condenser was applied, and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50% w/w NaOH to the pH of 10 and extracted with dichloromethane (4 x 50 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (2.1 g, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 7.3, 1.1 Hz, 1H), 7.54 (d, *J* = 1.0 Hz, 1H), 7.45 (d, *J* = 9.1 Hz, 1H), 7.30 (d, *J* = 8.7 Hz, 1H), 6.82 (d, *J* = 8.7 Hz, 1H), 6.70 (ddd, *J* = 9.2, 6.3, 1.0 Hz, 1H), 6.51 – 6.47 (m, 1H), 3.96 (s, 3H), 3.91 (s, 3H), 3.54 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.5, 152.1, 142.2, 135.7, 131.1, 126.6, 122.9, 120.0, 118.6, 117.9, 117.1, 111.9, 108.0, 61.0, 55.9, 53.9.



9i

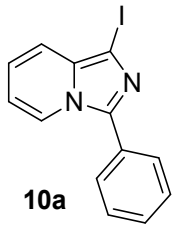
3-(2,4,5-Trimethoxyphenyl)imidazo[1,5-*a*]pyridine (9i). To a 50 mL round-bottom flask was dropwise added $POCl_3$ (18.5 mL) to 2,4,5-trimethoxy-*N*-[(pyridin-2-yl)methyl]benzamide (1.38 g, 4.6 mmol). A condenser was applied and the reaction mixture was stirred at reflux for 3 h. The reaction mixture was allowed to cool down to room temperature, then was quenched with 50% w/w NaOH to the pH of 10 and extracted with dichloromethane (4 x 50 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a brown solid (940 mg, 70%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.2 Hz, 1H), 7.46 (s, 1H), 7.35 (t, *J* = 9.7 Hz, 1H), 7.06 (s, 1H), 6.61 (dd, *J* = 9.1 Hz, 1H), 6.56 (s, 1H), 6.41 (t, *J* = 6.7 Hz, 1H), 3.87 (s, 3H), 3.80 (s, 3H), 3.65 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.8, 150.8, 143.5, 136.2, 131.2, 123.3, 119.9, 118.5, 118.1, 115.1, 111.7, 110.8, 97.8, 56.5, 56.5, 56.2.



9j

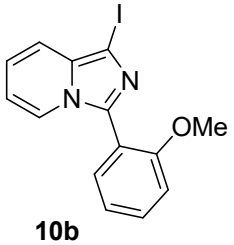
3-(3,4,5-Trimethoxyphenyl)imidazo[1,5-*a*]pyridine (9j). To a 25 mL reaction vial was added 3,4,5-trimethoxybenzaldehyde (1.8 g, 9.2 mmol) to DMF (15 mL). The reaction mixture was purged with argon. 2-Aminomethylpyridine (495 mg, 4.6 mmol), I_2 (117 mg, 0.46 mmol) and 70% w/w TBHP (667 µL, 6.9 mmol) were added. The reaction mixture was capped and stirred at 80 °C overnight. The reaction mixture was extracted with ethyl acetate (3 x 30 mL) and the combined organic layers were washed with 5% w/v LiCl solution (3 x 50 mL). The organic layer was dried over sodium sulfate and condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (1:1) eluent to give a brown solid (535 mg, 41%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.50 (s, 1H), 7.43 (dt, *J* = 9.2, 1.3 Hz, 1H), 6.99 (s, 2H),

6.69 – 6.63 (m, 1H), 6.54 – 6.51 (m, 1H), 3.91 (s, 3H), 3.88 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.5, 138.4, 137.9, 131.5, 125.7, 121.2, 120.2, 118.6, 113.1, 105.1, 60.7, 56.1, 55.9.



10a

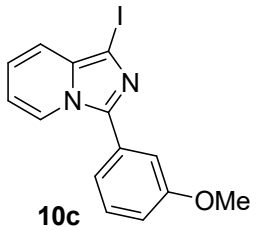
1-Iodo-3-phenylimidazo[1,5-a]pyridine (10a). To a 50 mL round-bottom flask was dissolved 3-phenylimidazo[1,5-*a*]pyridine (600 mg, 3.08 mmol) in acetonitrile (15 mL). The reaction mixture was purged with argon. NIS (904 mg, 4.02 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (951 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (dt, *J* = 7.3, 1.1 Hz, 1H), 7.72 – 7.65 (m, 2H), 7.47 – 7.41 (m, 2H), 7.40 – 7.34 (m, 1H), 7.27 (dt, *J* = 9.2, 1.2 Hz, 1H), 6.71 (ddd, *J* = 9.2, 6.4, 1.0 Hz, 1H), 6.54 – 6.50 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.5, 133.5, 129.4, 129.2, 129.1, 128.0, 121.9, 120.4, 119.0, 114.1, 74.2.



10b

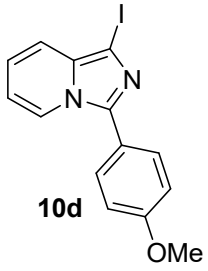
1-Iodo-3-(2-methoxyphenyl)imidazo[1,5-a]pyridine (10a). To a 50 mL round-bottom flask was dissolved 3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridine (600 mg, 2.67 mmol) in acetonitrile (15 mL). The reaction mixture was purged with argon. NIS (743 mg, 3.48 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was

quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (926 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.35 (d, *J* = 9.2 Hz, 1H), 7.09 (t, *J* = 7.3 Hz, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 6.81 (dd, *J* = 9.1, 6.1 Hz, 1H), 6.56 (t, *J* = 6.3 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.2, 157.2, 138.6, 133.3, 132.9, 131.3, 123.9, 121.5, 120.2, 118.6, 112.8, 111.6, 73.2, 55.5.



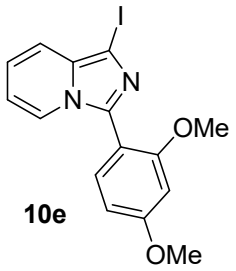
10c

1-Iodo- 3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (10c). To a 50 mL round-bottom flask was dissolved 3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (762 mg, 3.39 mmol) in acetonitrile (20 mL). The reaction mixture was purged with argon. NIS (1.03 g, 4.06 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (968 mg, 82%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (dt, *J* = 7.3, 1.0 Hz, 1H), 7.40 – 7.35 (m, 1H), 7.32 – 7.28 (m, 3H), 6.95 (ddd, *J* = 8.3, 2.4, 1.2 Hz, 1H), 6.77 – 6.72 (m, 1H), 6.59 – 6.53 (m, 1H), 3.84 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 140.4, 133.5, 130.6, 130.1, 122.1, 120.4, 120.0, 119.0, 115.2, 114.1, 113.5, 74.2, 55.6.



10d

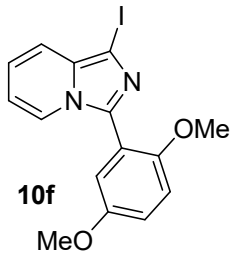
1-Iodo-3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (10d). To a 50 mL round-bottom flask was dissolved 3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (730 mg, 3.26 mmol) in acetonitrile (20 mL). The reaction mixture was purged with argon. NIS (953 g, 4.24 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (826 mg, 72%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.07 (dt, J = 7.2, 1.1 Hz, 1H), 7.70 – 7.51 (m, 2H), 7.25 (dt, J = 9.2, 1.2 Hz, 1H), 6.99 – 6.92 (m, 2H), 6.77 – 6.64 (m, 1H), 6.51 (ddd, J = 7.4, 6.4, 1.2 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 138.3, 131.3, 129.4, 123.0, 121.4, 120.3, 118.8, 118.5, 114.4, 112.9, 55.4.



10e

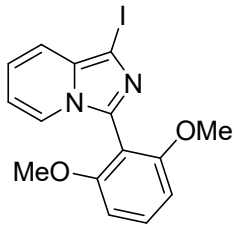
3-(2,4-Dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10e). To a 50 mL round-bottom flask was dissolved 3-(2,4-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (480 mg, 1.9 mmol) in acetonitrile (15 mL). The reaction mixture was purged with argon. NIS (553 mg, 2.5 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane

(4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green-brown oil (712 mg, 99%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.0 Hz, 1H), 7.44 (d, *J* = 7.0 Hz, 1H), 7.25 (d, *J* = 7.0 Hz, 1H), 6.73 – 6.71 (m, 1H), 6.57 (dd, *J* = 8.5 Hz, 1H), 6.52 (d, *J* = 2.3 Hz, 1H), 6.47 (dd, *J* = 10.0 Hz, 1H), 3.80 (s, 3H), 3.70 (s, 3H). ^{13}C NMR (125 MHz $CDCl_3$) δ 162.4, 158.4, 138.6, 133.5 133.1, 123.7, 120.0, 118.3, 112.6, 111.1, 105.4, 98.7, 72.8, 55.7, 55.6.



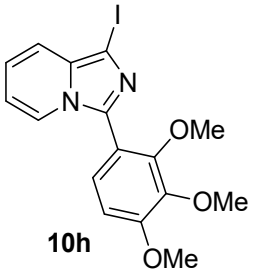
10f

3-(2,5-Dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10f). To a 50 mL round-bottom flask was dissolved 3-(2,5-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (897 mg, 3.53 mmol) in acetonitrile (20 mL). The reaction mixture was purged with argon. NIS (1.03 mg, 4.59 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo,* and purified with chromatography using a hexanes:ethyl acetate (3:1) eluent to give a yellow crystals (667 mg, 50%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.0 Hz, 1H), 7.33 (dd, *J* = 9.2, 1.0 Hz, 1H), 7.14 (d, *J* = 3.0 Hz, 1H), 6.99 (dd, *J* = 9.1, 3.0 Hz, 1H), 6.94 (d, *J* = 9.0 Hz, 1H), 6.79 (ddd, *J* = 9.2, 6.3, 0.8 Hz, 1H), 6.58 – 6.52 (m, 1H), 3.79 (s, 3H), 3.71 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.9, 151.4, 138.4, 133.4, 124.0, 120.2, 118.9, 118.4, 117.3, 117.0, 112.8, 73.2, 56.3, 56.0.



10g

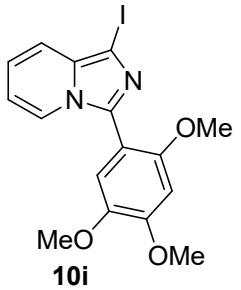
3-(2,6-Dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10g). To a 50 mL round-bottom flask was dissolved 3-(2,6-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (600 mg, 2.4 mmol) in acetonitrile (15 mL). The reaction mixture was purged with argon. NIS (640 mg, 2.8 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with dichloromethane (4 x 20 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (840 mg, 94%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.24 (m, 2H), 7.17 (d, J = 9.2 Hz, 1H), 6.60 (dt, J = 10.0 Hz, 1H), 6.51 (d, J = 8.5 Hz, 2H), 6.35 (t, J = 6.6 Hz, 1H), 3.54 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.7, 134.3, 132.7, 132.1, 122.8, 120.0, 118.2, 112.7, 106.1, 104.0, 72.4, 56.0.



10h

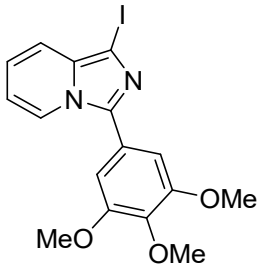
3-(2,3,4-Trimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10h). To a 250 mL round-bottom flask was dissolved 3-(2,3,4-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (606 mg, 2.13 mmol) in acetonitrile (10 mL). The reaction mixture was purged with argon. NIS (650 mg, 2.56 mmol) was added. The reaction mixture was capped and stirred at room temperature for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (20 mL) and extracted with

dichloromethane (3 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo* to give a green solid (831 mg, 95%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, J = 7.1 Hz, 1H), 7.35 – 7.27 (m, 2H), 6.81 (dd, J = 9.1, 5.7 Hz, 2H), 6.57 (t, J = 6.7 Hz, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.57 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.0, 151.8, 141.9, 138.0, 133.0, 126.9, 123.6, 120.2, 118.1, 115.9, 112.8, 107.9, 72.8, 61.4, 61.2, 56.1.



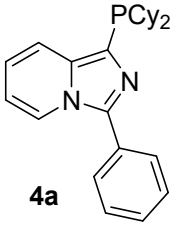
10i

3-(2,4,5-Trimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10i). To a 50 mL round-bottom flask was dissolved 3-(2,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (780 mg, 3.0 mmol) in THF (25 mL). The reaction mixture was purged with argon. Iodine (2.3 g, 9.0 mmol) was added. The reaction mixture was capped and stirred over reflux for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo*. Column chromatography was performed using dichloromethane:acetone (96:4) eluent to give a yellow oil (790 mg, 64%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, J = 6.9 Hz, 1H), 7.28 (d, J = 9.0 Hz, 1H), 7.08 (s, 1H), 6.75 (t, J = 6.5 Hz , 1H), 6.58 (s, 1H), 6.51 (t, J = 6.5 Hz, 1H), 3.92 (s, 3H), 3.83 (s, 3H), 3.69 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.7, 151.2, 143.5, 138.5, 133.1, 123.7, 120.7, 118.7, 115.7, 114.6, 113.24, 112.1, 109.6, 97.9, 72.8, 56.4, 56.3, 56.2.



10j

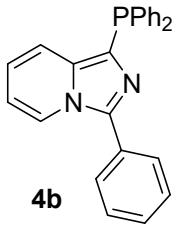
3-(3,4,5-Trimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (10j). To a 50 mL round-bottom flask was dissolved 3-(3,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (1.45 g, 4.9 mmol) in THF (25 mL). The reaction mixture was purged with argon. Iodine (3.8 g, 14.8 mmol) was added. The reaction mixture was capped and stirred over reflux for 3 h. The reaction mixture was quenched with saturated sodium thiosulfate solution (30 mL) and extracted with dichloromethane (4 x 30 mL). The organic layers were combined, dried over sodium sulfate and condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (1:1) eluent to give a green solid (1.05 g, 50%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, J = 7.1 Hz, 1H), 7.11 (d, J = 9.1 Hz, 1H), 6.78 (s, 2H), 6.59 (td, J = 6.7 Hz, 1H), 6.43 (t, J = 6.7 Hz, 1H), 3.74 (s, 9H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.6, 140.2, 138.8, 133.3, 124.7, 121.9, 120.3, 118.8, 114.1, 105.4, 73.9, 60.9, 56.4.



4a

1-(Dicyclohexylphosphino)-3-phenylimidazo[1,5-*a*]pyridine (4a). To a 20 mL brown vial, 1-iodo-3-phenylimidazo[1,5-*a*]pyridine (300 mg, 0.937 mmol) was dissolved in 1,4-dioxane (5 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (363 mg, 1.12 mmol),

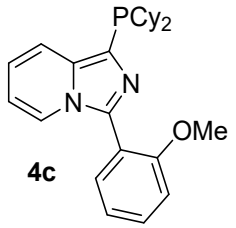
DIPPF (10.0 mg, 0.023 mmol) and $Pd(OAc)_2$ (5.00 mg, 0.019 mmol). The solution was capped and stirred at room temperature for 2 h. Dicyclohexylphosphine (205 mg, 185 μL, 0.937 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (5:1) eluent to give a solid (250 mg, 68%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (dd, J = 7.2, 1.1 Hz, 1H), 7.78 – 7.72 (m, 4H), 7.52 (t, J = 7.6 Hz, 2H), 7.45 – 7.40 (m, 1H), 6.75 – 6.71 (m, 1H), 6.57 – 6.52 (m, 1H), 2.29 – 2.22 (m, 2H), 1.96 – 1.59 (m, 12H), 1.38 – 1.08 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.0, 139.3, 139.0, 130.6, 129.1, 128.7, 126.3, 121.7, 119.5, 119.3, 113.1, 33.0, 30.8, 29.6, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.8.



4b

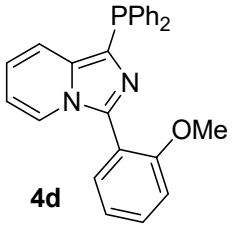
1-(Diphenyllphosphino)-3-phenylimidazo[1,5-*a*]pyridine (4b). To a 20 mL brown vial, 1-iodo-3-phenylimidazo[1,5-*a*]pyridine (220 mg, 0.687 mmol) was dissolved in 1,4-dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (226 mg, 0.825 mmol), DIPPF (7.00 mg, 0.017 mmol) and $Pd(OAc)_2$ (3.00 mg, 0.014 mmol). The solution was capped and stirred at room temperature for 2 h. Diphenylphosphine (128 mg, 119μL, 0.687 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (2:1) eluent to give a solid (100 mg, 38%). ^{1}H NMR (500 MHz,

$CDCl_3$) δ 8.26 (dd, *J* = 7.4, 0.9 Hz, 1H), 7.78 (dt, *J* = 3.1, 1.9 Hz, 2H), 7.61 – 7.57 (m, 4H), 7.52 – 7.41 (m, 5H), 7.31 – 7.28 (m, 5H), 6.75 – 6.70 (m, 1H), 6.60 – 6.56 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.8, 140.7, 138.2, 138.1, 138.0, 138.0, 133.7, 133.6, 133.5, 133.4, 130.1, 129.1, 128.9, 128.6, 128.5, 128.2, 128.2, 126.2, 122.3, 122.0, 120.5, 120.38, 119.3, 119.2, 119.1, 119.0, 113.4. ^{31}P NMR (202 MHz, $CDCl_3$) δ -31.3.



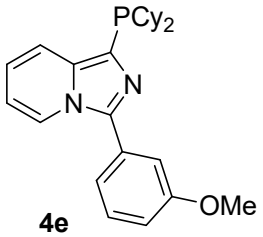
4c

1-(Dicyclohexylphosphino)-3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridine (4c). To a 20 mL brown vial, 1-iodo-3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridine (200 mg, 0.571 mmol) was dissolved in 1,4-dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (221 mg, 0.685 mmol), DIPPF (6.0 mg, 0.014 mmol) and $Pd(OAc)_2$ (2.5 mg, 0.011 mmol).The solution was capped and stirred at room temperature for 2 h. Dicyclohexylphosphine (113 mg, 0.571 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (8:1) eluent to give a yellow solid (170 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 9.1 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.46 – 7.39 (m, 1H), 7.08 (td, *J* = 7.5, 0.7 Hz, 1H), 7.02 (d, *J* = 8.5 Hz, 1H), 6.72 (dd, *J* = 8.9, 6.5 Hz, 1H), 6.48 (t, *J* = 6.7 Hz, 1H), 3.78 (d, *J* = 8.6 Hz, 3H), 2.26 (t, *J* = 10.0 Hz, 2H), 1.73 (d, *J* = 12.9 Hz, 2H), 1.63 (dd, *J* = 22.5, 11.1 Hz, 6H), 1.38 – 1.06 (m, 12H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.6, 139.1, 138.8, 138.1, 133.0, 130.8, 123.3, 121.3, 119.7, 119.0, 118.9, 111.9, 111.6, 55.7, 33.0, 30.8, 29.6, 27.3, 27.0, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.9.



4d

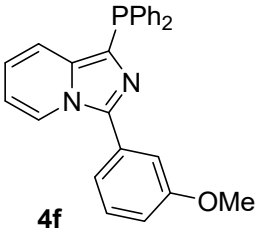
1-(Diphenylphosphino)-3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridine (4d). To a 20 mL brown vial, 1-iodo-3-(2-methoxyphenyl)imidazo[1,5-*a*]pyridine (200 mg, 0.571 mmol) was dissolved in 1,4-dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (221.1 mg, 0.685 mmol), DIPPF (6.00 mg, 0.014 mmol) and $Pd(OAc)_2$ (2.5 mg, 0.011 mmol).The solution was capped and stirred at room temperature for 2 h. Diphenylphosphine (106 mg, 0.571 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (2:1) eluent to give a yellow solid (140 mg, 62%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.62 – 7.57 (m, 4H), 7.49 – 7.41 (m, 3H), 7.32 – 7.24 (m, 6H), 7.10 – 7.06 (m, 1H), 7.02 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.77 – 6.73 (m, 1H), 6.56 – 6.52 (m, 1H), 3.80 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.4, 139.1, 138.4, 138.2, 137.9, 133.7, 133.5, 133.2, 131.9, 131.0, 128.2, 123.9, 121.3, 120.2, 119.3, 118.6, 112.1, 111.3, 55.6. ^{31}P NMR (202 MHz, $CDCl_3$) δ -31.3.



4e

1-(Dicyclohexylphosphino)-3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (4e). To a 25 mL reaction vial was added 1-iodo-3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (380 mg, 1.09 mmol),

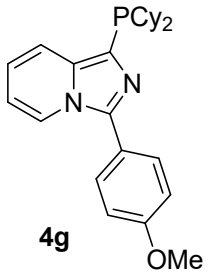
Cs_2CO_3 (421 mg, 1.302 mmol), DIPPF (11.3 mg, 0.027 mmol), and $Pd(OAc)_2$ (4.9 mg, 0.0217 mmol) in 1,4-dioxane (5 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added dicyclohexylphosphine (220 µL, 1.085 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (4:1) eluent to give a yellow solid (263 mg, 58%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (dd, *J* = 7.2, 1.3 Hz, 1H), 7.76 (dd, *J* = 9.2, 1.4 Hz, 1H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.34 (dt, *J* = 7.6, 1.3 Hz, 1H), 7.30 (s, 1H), 6.99 – 6.95 (m, 1H), 6.73 (dd, *J* = 9.2, 6.3 Hz, 1H), 6.56 – 6.51 (m, 1H), 3.85 (s, 3H), 2.31 – 2.23 (m, 2H), 1.96 – 1.58 (m, 12H), 1.38 – 1.07 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 139.8, 139.3, 131.9, 130.1, 126.3, 121.8, 120.8, 119.4, 119.3, 114.5, 114.3, 113.1, 55.5, 33.0, 30.8, 29.6, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.8.



4f

1-(Diphenylphosphino)-3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (4f). To a 25 mL reaction vial was added 1-iodo-3-(3-methoxyphenyl)imidazo[1,5-*a*]pyridine (380 mg, 1.09 mmol), Cs_2CO_3 (421 mg, 1.302 mmol), DIPPF (11.3 mg, 0.027 mmol), and $Pd(OAc)_2$ (4.9 mg, 0.022 mmol) in 1,4-dioxane (5 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added dicyclohexylphosphine (189 µL, 1.085 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate

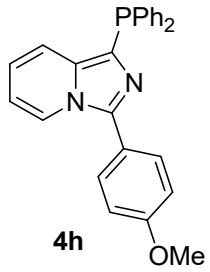
(4:1) eluent to give a yellow solid (150 mg, 33%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.61 – 7.55 (m, 4H), 7.45 – 7.42 (m, 1H), 7.41 – 7.39 (m, 1H), 7.36 (m, 1H), 7.33 (dt, *J* = 2.5, 1.3 Hz, 1H), 7.32 – 7.28 (m, 6H), 6.99 – 6.96 (m, 1H), 6.74 – 6.70 (m, 1H), 6.61 – 6.55 (m, 1H), 3.86 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.1, 140.6, 140.5, 138.2, 138.0, 138.0, 137.9, 133.6, 133.5, 131.4, 130.0, 128.3, 128.3, 126.2, 122.3, 120.6, 120.5, 119.1, 119.1, 114.8, 114.2, 113.4, 55.5. ^{31}P NMR (202 MHz, $CDCl_3$) δ -30.9.



4g

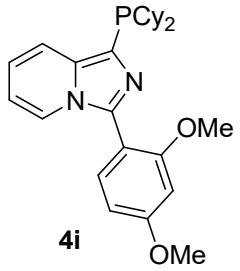
1-(Dicyclohexylphosphino)-3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (4g). To a 25 mL reaction vial was added 1-iodo-3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (241 mg, 0.691 mmol), Cs_2CO_3 (268 mg, 0.829 mmol), DIPPF (7.2 mg, 0.017 mmol), and $Pd(OAc)_2$ (3.1 mg, 0.014 mmol) in 1,4-dioxane (4 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added dicyclohexylphosphine 0.5M (1.52 mL, 0.8 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (4:1) eluent to give a yellow solid (128 mg, 44%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.71 (dd, *J* = 9.2, 1.3 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.69 – 6.66 (m, 1H), 6.50 – 6.47 (m, 1H), 3.84 (s, 3H), 2.27 – 2.20 (m, 2H), 1.96 – 1.54 (m, 12H), 1.36 – 1.05 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 139.9, 139.1, 130.1, 125.7, 123.1,

121.7, 119.4, 119.0, 114.5, 112.8, 55.5, 33.0, 30.8, 29.6, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.9.



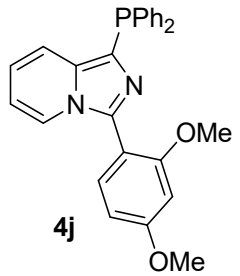
4h

1-(Diphenylphosphino)-3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (4h). To a 25 mL reaction vial was added 1-iodo-3-(4-methoxyphenyl)imidazo[1,5-*a*]pyridine (280 mg, 0.8 mmol), Cs_2CO_3 (311 mg, 0.96 mmol), DIPPF (8.4 mg, 0.02 mmol), and $Pd(OAc)_2$ (10 mg, 0.02 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added diphenylphosphine (140 µL, 0.8 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (7:3) eluent to give a yellow solid (211 mg, 65%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 2H), 7.58 (td, *J* = 7.9, 1.6 Hz, 4H), 7.40 (dd, *J* = 9.2, 1.1 Hz, 1H), 7.31 – 7.22 (m, 6H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.63 (ddd, *J* = 9.2, 6.4, 1.0 Hz, 1H), 6.49 – 6.45 (m, 1H), 3.79 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 160.0, 140.6, 138.1, 137.9, 133.4, 133.3, 129.8, 128.1, 125.5, 122.5, 122.0, 120.1, 118.8, 114.2, 113.1, 55.3. ^{31}P NMR (202 MHz, $CDCl_3$) δ -31.3.



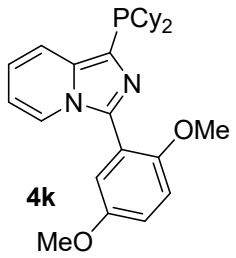
4i

1-(Dicyclohexylphosphino)-3-(2,4-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4i). To a 25 mL reaction vial was added 3-(2,4-dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (220 mg, 0.63 mmol), Cs_2CO_3 (244 mg, 0.75 mmol), DIPPF (6.6 mg, 0.018 mmol), and $Pd(OAc)_2$ (3.0 mg, 0.013 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added 0.5 M dicyclohexylphosphine (1.3 mL, 0.63 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (2:1) eluent to give a brown oil (110 mg, 41%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.72 (dd, *J* = 9.2, 1.1 Hz, 1H), 7.54 (dd, *J* = 7.2, 1.1 Hz, 1H), 7.43 (d, *J* = 8.2 Hz, 1H), 6.74 – 6.68 (m, 1H), 6.64 – 6.60 (m, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 6.47 (t, *J* = 6.5 Hz, 1H), 3.86 (s, 3H), 3.76 (s, 3H), 2.24 (dt, *J* = 9.0, 3.0 Hz, 2H), 1.94 – 1.57 (m, 12H), 1.36 – 1.06 (m, 8H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 158.8, 139.0, 138.6, 138.0, 133.7, 123.2, 118.9, 118.9, 112.4, 111.8, 105.4, 99.1, 55.7, 55.6, 33.0, 30.8, 29.6, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -26.0.



4j

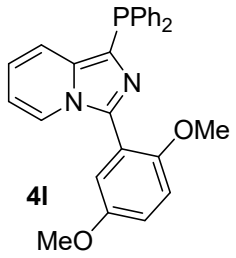
1-(Diphenylphosphino)-3-(2,4-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4j). To a 25 mL reaction vial was added 3-(2,4-dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (220 mg, 0.63 mmol), Cs_2CO_3 (244 mg, 0.75 mmol), DIPPF (6.6 mg, 0.018 mmol), and $Pd(OAc)_2$ (3.0 mg, zz0.013 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added diphenylphosphine (110 µL, 0.63 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (3:2) eluent to give a yellow oil (166 mg, 65%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 1.4 Hz, 1H), 7.64 – 7.60 (m, 4H), 7.54 – 7.51 (m, 1H), 7.47 (d, *J* = 9.1 Hz, 1H), 7.33 – 7.25 (m, 6H), 6.71 (dd, *J* = 9.1 Hz, 1H), 6.63 – 6.61 (m, 1H), 6.58 (d, *J* = 2.2 Hz, 1H), 6.50 (dd, *J* = 10.1 Hz, 1H), 3.84 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.3, 158.6, 139.2, 139.1, 138.5, 133.6, 128.7, 127.9, 125.0, 123.8, 120.8, 118.3, 112.0, 104.8, 99.4, 98.3, 55.6, 55.40. ^{31}P NMR (202 MHz, $CDCl_3$) δ -31.2.



4k

1-(Dicyclohexylphosphino)-3-(2,5-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4k). To a 20 mL brown vial, 1-iodo-3-(2,5-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (200 mg, 0.53 mmol) was dissolved in 1,4-dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (204 mg, 0.63 mmol), DIPPF (6.00 mg, 0.013 mmol) and $Pd(OAc)_2$ (3 mg, 0.011 mmol).The solution was capped and stirred at room temperature for 2 h. Dicyclohexylphosphine (104 mg, 133µL, 0.53 mmol) was added to the solution; the solution was again purged with argon

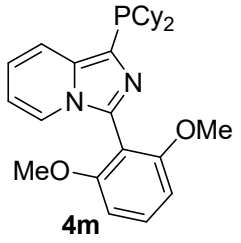
and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (3:1) eluent to give a white solid (241 mg, 90%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (dt, *J* = 9.1, 1.2 Hz, 1H), 7.59 (dt, *J* = 7.2, 1.1 Hz, 1H), 7.08 (dd, *J* = 2.6, 0.9 Hz, 1H), 6.97 (d, *J* = 2.7 Hz, 1H), 6.96 (d, *J* = 0.8 Hz, 1H), 6.76 – 6.71 (m, 1H), 6.52 – 6.47 (m, 1H), 2.31 – 2.21 (m, 2H), 2.00 – 1.85 (m, 2H), 1.77 – 1.69 (m, 2H), 1.69 – 1.54 (m, 8H), 1.38 – 1.05 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.0, 151.9, 139.1, 137.9, 125.5, 123.4, 120.5, 119.2, 118.8, 118.0, 116.1, 113.3, 112.0, 56.6, 55.9, 33.0, 30.8, 29.6, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.8.



4l

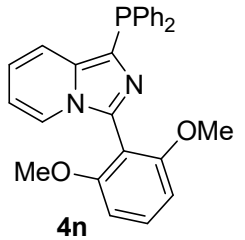
1-(Diphenylphosphino)-3-(2,5-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4l). To a 20 mL brown vial, 1-iodo-3-(2,5-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (200 mg, 0.53 mmol) was dissolved in 1,4-dioxane (4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (204 mg, 0.63 mmol), DIPPF (6.00 mg, 0.013 mmol) and $Pd(OAc)_2$ (3 mg, 0.011 mmol).The solution was capped and stirred at room temperature for 2 h. Diphenylphosphine (99.0 mg, 92.5µL, 0.53 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (5:1) eluent to give a yellow solid (147 mg, 63%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.0, 0.8 Hz, 1H), 7.58

(td, J = 7.8, 1.6 Hz, 4H), 7.43 (d, J = 9.0 Hz, 1H), 7.33 – 7.26 (m, 6H), 7.16 (d, J = 3.0 Hz, 1H), 7.01 – 6.94 (m, 2H), 6.77 – 6.72 (m, 1H), 6.55 (dd, J = 10.1, 3.8 Hz, 1H), 3.79 (s, 3H), 3.73 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.9, 151.7, 138.8, 138.8, 138.2, 138.2, 138.0, 137.7, 133.6, 133.5, 128.3, 128.3, 124.1, 120.4, 118.5, 118.5, 117.8, 116.7, 112.9, 112.3, 56.4, 56.0. ^{31}P NMR (202 MHz, $CDCl_3$) δ -30.8.



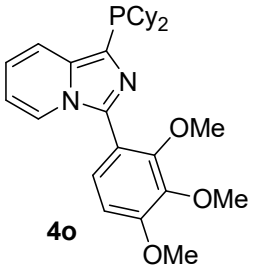
4m

1-(Dicyclohexylphosphino)-3-(2,6-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4m). To a 25 mL reaction vial was added 3-(2,6-dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (250 mg, 0.66 mmol), Cs_2CO_3 (255 mg, 0.79 mmol), DIPPF (6.9 mg, 0.017 mmol), and $Pd(OAc)_2$ (3.0 mg, 0.013 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added 0.5 M dicyclohexylphosphine (1.32 mL, 0.66 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (3:2) eluent to give a yellow oil (151 mg, 51%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 – 7.72 (m, 1H), 7.41 – 7.33 (m, 2H), 6.72 – 6.67 (m, 1H), 6.64 (dd, J = 8.5, 1.5 Hz, 2H), 6.46 – 6.40 (m, 1H), 3.68 (s, 6H), 2.32 – 2.21 (m, 2H), 1.95 – 1.56 (m, 12H), 1.36 – 1.06 (m, 8H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.1, 138.5, 133.9, 131.5, 124.6, 122.7, 118.9, 118.8, 111.7, 108.0, 104.6. 56.1, 33.0, 30.9, 29.4, 27.3, 27.1, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -26.5.



4n

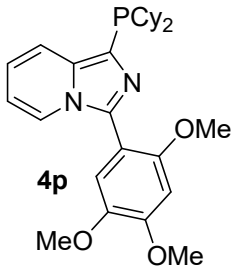
1-(Diphenylphosphino)-3-(2,6-dimethoxyphenyl)imidazo[1,5-*a*]pyridine (4n). To a 25 mL reaction vial was added 3-(2,6-dimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (220 mg, 0.63 mmol), Cs_2CO_3 (244 mg, 0.75 mmol), DIPPF (6.6 mg, 0.018 mmol), and $Pd(OAc)_2$ (3.0 mg, 0.013 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added diphenylphosphine (115 μL, 0.63 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (3:2) eluent to give a yellow oil (155 mg, 54%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 – 7.64 (m, 4H), 7.52 – 7.47 (m, 2H), 7.42 – 7.36 (m, 1H), 7.33 – 7.24 (m, 6H), 6.73 – 6.69 (m, 1H), 6.65 (d, *J* = 8.4 Hz, 2H), 6.49 – 6.45 (m, 1H), 3.68 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.0, 138.7, 137.9, 137.6, 135.0, 133.7, 133.5, 128.2, 124.5, 123.1, 120.2, 118.5, 112.2, 107.5, 104.5, 56.1; ^{31}P NMR (202 MHz, $CDCl_3$) δ -31.9.



4o

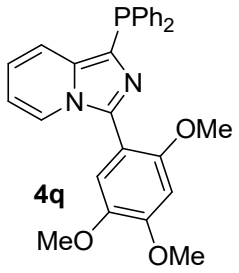
1-(Dicyclohexylphosphino)-3-(2,3,4-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (4o). To a 20 mL brown vial, 1-iodoimidazo[1,5-*a*]pyridine (220 mg, 0.54 mmol) was dissolved in 1,4-dioxane

(4 mL). The reaction was purged with argon. To the solution was added Cs_2CO_3 (209 mg, 0.65 mmol), DIPPF (5.6 mg, 0.014 mmol) and $Pd(OAc)_2$ (2.4 mg, 0.011 mmol).The solution was capped and stirred at room temperature for 2 h. Dicyclohexylphosphine 0.5M (1.08 mL, 0.54 mmol) was added to the solution; the solution was again purged with argon and then capped. The solution was allowed to stir overnight at 80 °C for 12 h. The crude reaction mixture was filtered over Celite and rinsed with ethyl acetate (3 x 10 mL portions). The mixture was further purified by column chromatography using a hexanes:ethyl acetate (2:1) eluent to give a brown oil (104 mg, 40%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 9.2, 1.3 Hz, 1H), 7.72 (s, 0H), 7.65 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.24 (d, *J* = 8.6 Hz, 1H), 6.82 (d, *J* = 8.6 Hz, 1H), 6.75 (ddd, *J* = 9.2, 6.3, 1.0 Hz, 1H), 6.52 (ddd, *J* = 7.4, 6.3, 1.2 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.54 (s, 3H), 2.27 (ddt, *J* = 11.6, 8.2, 3.1 Hz, 2H), 1.98 – 1.56 (m, 12H), 1.38 – 1.06 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 154.9, 152.5, 142.4, 138.7, 137.4, 127.0, 125.0, 122.9, 119.3, 118.7, 117.3, 112.2, 108.1, 77.1, 61.3, 56.2, 33.0, 30.8, 29.5, 27.2, 27.0, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -26.5.



1-(Dicyclohexylphosphino)-3-(2,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (4p). To a 25 mL reaction vial was added 3-(2,4,5-trimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (200 mg, 0.5 mmol), Cs_2CO_3 (190 mg, 0.6 mmol), DIPPF (5.1 mg, 0.013 mmol), and $Pd(OAc)_2$ (2.2 mg, 0.01 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added 0.5 M dicyclohexylphosphine (0.98 mL, 0.5 mmol) and capped. The reaction was stirred overnight at 80

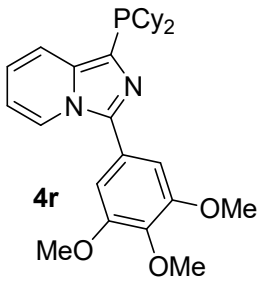
°C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (2:1) eluent to give an orange solid (122 mg, 52%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, *J* = 9.2 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.05 (s, 1H), 6.74 (d, *J* = 8.1 Hz, 1H), 6.66 (d, *J* = 2.2 Hz, 1H), 6.50 (d, *J* = 6.9 Hz, 1H), 3.96 (s, 3H), 3.88 (s, 3H), 3.72 (s, 3H), 2.35 – 2.22 (m, 2H), 1.98 – 1.60 (m, 12H), 1.37 – 1.10 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.4, 151.0, 143.7, 138.6, 123.3, 119.1, 118.8, 118.8, 115.7, 111.9, 111.2, 100.0, 98.4, 57.0, 56.5, 56.3, 33.1, 30.8, 29.6, 27.3, 27.0, 26.7. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.9.



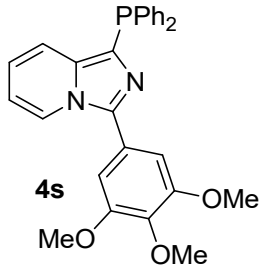
4q

1-(Diphenylphosphino)-3-(2,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (4q). To a 25 mL reaction vial was added 3-(2,4,5-trimethoxyphenyl)-1-iodoimidazo[1,5-*a*]pyridine (200 mg, 0.5 mmol), Cs_2CO_3 (190 mg, 0.6 mmol), DIPPF (5.1 mg, 0.013 mmol), and $Pd(OAc)_2$ (2.2 mg, 0.01 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added diphenylphosphine (89 µL, 0.5 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (2:1) eluent to give an orange solid (128 mg, 56%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.0 Hz, 1H), 7.56 (td, *J* = 7.7 Hz, 4H), 7.34 (d, *J* = 9.2 Hz, 1H), 7.30 – 7.24 (m, 6H), 7.11 (s, 1H), 6.69 (dd, *J* = 8.8 Hz, 1H), 6.61 (d, *J* = 5.1 Hz, 1H), 6.52 (t, *J* = 6.8 Hz, 1H), 3.92 (s, 3H), 3.84 (s, 3H),

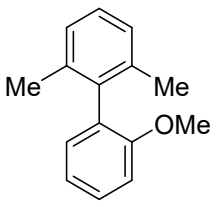
3.70 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 152.0, 151.0, 143.5, 138.2, 137.6, 137.4, 133.5, 133.3, 128.2, 128.1, 123.9, 120.1, 118.4, 115.6, 112.0, 99.9, 97.6, 56.6, 56.5, 56.2. δ ^{31}P NMR (202 MHz, $CDCl_3$) δ -30.1.



3-(3,4,5-Trimethoxyphenyl)-1-(dicyclohexylphosphino)imidazo[1,5-*a*]pyridine (4r). To a 25 mL reaction vial was added 1-iodo-3-(3,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (300 mg, 0.731 mmol), Cs_2CO_3 (284 mg, 0.877 mmol), DIPPF (7.7 mg, 0.0183 mmol), and $Pd(OAc)_2$ (3.0 mg, 0.0146 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added dicyclohexylphosphine (1.46 mL, 0.731 mmol, 0.5 M in hexanes) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (4:1) eluent to give a yellow solid (169 mg, 48%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (dd, J = 7.2, 1.2 Hz, 1H), 7.72 (dd, J = 9.1, 1.2 Hz, 1H), 6.91 (s, 2H), 6.71 (ddd, J = 9.1, 6.3, 1.0 Hz, 1H), 6.55 – 6.51 (m, 1H), 3.90 (s, 6H), 3.88 (s, 3H), 2.29 – 2.19 (m, 2H), 1.95 – 1.58 (m, 12H), 1.38 – 1.03 (m, 8H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.8, 139.8, 139.1, 138.9, 126.2, 126.0, 121.7, 119.5, 119.2, 113.1, 106.2, 61.0, 56.4, 33.0, 30.8, 29.6, 27.3, 27.0, 26.6. ^{31}P NMR (202 MHz, $CDCl_3$) δ -25.5.



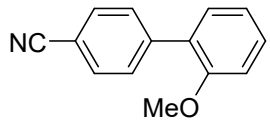
3-(3,4,5-Trimethoxyphenyl)-1-(diphenyllphosphino)imidazo[1,5-*a*]pyridine (4s). To a 25 mL reaction vial was added 1-iodo-3-(3,4,5-trimethoxyphenyl)imidazo[1,5-*a*]pyridine (300 mg, 0.731 mmol), Cs_2CO_3 (284 mg, 0.877 mmol), DIPPF (7.7 mg, 0.0183 mmol), and $Pd(OAc)_2$ (3.0 mg, 0.0146 mmol) in 1,4-dioxane (3 mL) was purged with argon. The reaction vial was capped and stirred at room temperature for 2 h. The reaction was purged with argon for 5 minutes then added dicyclohexylphosphine (127 μL, 0.731 mmol) and capped. The reaction was stirred overnight at 80 °C. The reaction mixture was filtered over Celite and transferred using ethyl acetate. The filtrate was condensed *in vacuo*. Column chromatography was performed using hexanes:ethyl acetate (4:1) eluent to give a yellow solid (167 mg, 49%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (dd, J = 7.2, 1.1 Hz, 1H), 7.59 – 7.54 (m, 4H), 7.35 (dd, J = 9.2, 1.1 Hz, 1H), 7.32 – 7.24 (m, 6H), 6.98 (s, 2H), 6.70 (ddd, J = 9.2, 6.4, 1.0 Hz, 1H), 6.61 – 6.56 (m, 1H), 3.91 (s, 3H), 3.89 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.8, 140.7, 139.0, 138.0, 137.7, 133.6, 133.4, 128.3, 126.2, 125.6, 122.3, 120.5, 119.2, 113.5, 106.2, 61.1, 56.5. ^{31}P NMR (202 MHz, $CDCl_3$) δ -30.0.



13

2,6-Dimethyl-(2'-methoxy)biphenyl (13):[1] In a 25 mL brown vial, 2-bromo-*m*-xylene (200 mg, 1.10 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 2-methoxyphenyl boronic acid (243 mg, 1.60 mmol), Cs_2CO_3 (888 mg, 2.75 mmol), $Pd(OAc)_2$ (6.2 mg, 0.0275 mmol), and ligand **4m** (25 mg, 0.055 mmol). The vial was purged with nitrogen for 10 min. The reaction was stirred overnight at 80 °C and the crude mixture was filtered over Celite washing with ethyl acetate. The mixture was purified utilizing column chromatography using 9:1 hexanes:ethyl acetate (9:1) eluent to give a yellow oil (225 mg, 96%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (ddd, J = 9.1, 6.9, 2.3 Hz, 1H), 7.13 (dd, J = 8.5, 6.3 Hz, 1H), 7.07 (s, 2H), 7.02 – 6.96 (m, 2H), 6.93 (d, J = 8.2 Hz, 1H), 3.67 (s, 3H), 2.00 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 138.5, 136.8, 130.9, 129.8, 128.7, 127.4, 127.3, 121.0, 111.2, 55.6, 20.8.

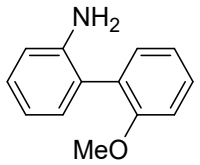
Large Scale Reaction of 2,6-Dimethyl-(2'-methoxy)biphenyl (13):[1] In a 250 mL sealed flask, 2-bromo-*m*-xylene (3.0 g, 16.2 mmol) was dissolved in 1,4-dioxane (50 mL). To the sealed flask was added 2-methoxyphenyl boronic acid (3.70 g, 24.3 mmol), Cs_2CO_3 (13.2 g, 40.5 mmol), $Pd(OAc)_2$ (9.1 mg, 0.040 mmol), and ligand **4m** (36 mg, 0.080 mmol). The vial was purged with nitrogen for 10 min. The reaction was stirred overnight at 80 °C and the crude mixture was filtered over Celite washing with ethyl acetate. The mixture was purified utilizing column chromatography using 9:1 hexanes:ethyl acetate (9:1) eluent to give a colorless oil (3.03 g, 88%). ^{1}H NMR was consistent with the above and the literature reference.



14

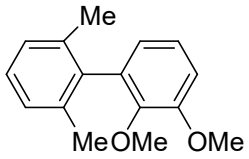
4-(2-Methoxyphenyl)benzonitrile (14).[2] In a 25 mL brown vial, 4-chlorobenzonitrile (200 mg, 1.45 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 2-methoxyphenyl boronic

acid (330 mg, 2.17 mmol), Cs_2CO_3 (937 mg, 2.90 mmol), $Pd(OAc)_2$ (8.2 mg, 0.036 mmol), and ligand **4m** (33 mg, 0.073 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with a 3:1 hexanes:ethyl acetate eluent to give a clear crystalline solid (280 mg, 92%). ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.82 – 7.78 (m, 2H), 7.65 – 7.61 (m, 2H), 7.37 (ddd, J = 8.3, 7.4, 1.7 Hz, 1H), 7.28 (dd, J = 7.6, 1.7 Hz, 1H), 7.10 (dd, J = 8.3, 1.0 Hz, 1H), 7.02 (td, J = 7.5, 1.1 Hz, 1H), 3.73 (s, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 156.6, 143.6, 132.4, 130.9, 130.7, 130.6, 128.4, 121.5, 119.5, 112.4, 110.0, 56.1.



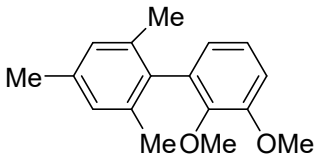
15

***2*-(2-Methoxyphenyl)aniline (15).**[3] In a 25 mL brown vial, 2-bromoaniline (200 mg, 1.16 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 2-methoxyphenyl boronic acid (266 mg, 1.74 mmol), Cs_2CO_3 (937 mg, 2.90 mmol), $Pd(OAc)_2$ (6.5 mg, 0.029 mmol), and ligand **4m** (27 mg, 0.058 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with a 3:1 hexanes:ethyl acetate eluent to give a brown crystalline solid (126 mg, 88%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.27 (ddd, J = 8.4, 7.4, 1.8 Hz, 1H), 7.20 (dd, J = 7.5, 1.8 Hz, 1H), 7.09 (td, J = 7.6, 1.7 Hz, 1H), 7.06 (dd, J = 7.6, 1.7 Hz, 1H), 6.97 (td, J = 7.4, 1.1 Hz, 1H), 6.91 (dd, J = 8.3, 1.1 Hz, 1H), 6.76 (td, J = 7.4, 1.2 Hz, 1H), 6.65 (dd, J = 7.9, 1.3 Hz, 1H), 3.67 (s, 3H), 3.57 (bs, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.6, 144.4, 131.7, 131.0, 128.9, 128.4, 128.2, 124.8, 121.0, 118.2, 115.5, 111.2, 55.5.



16

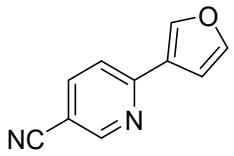
2,6-Dimethyl-(2',3'-dimethoxy)biphenyl (16). In a 25 mL brown vial, 2-bromo-*m*-xylene (200 mg, 1.1 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 2,3-dimethoxyphenyl boronic acid (292 mg, 1.6 mmol), Cs_2CO_3 (888 mg, 2.75 mmol), $Pd(OAc)_2$ (6.2 mg, 0.0275 mmol), and ligand **4m** (25 mg, 0.055 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with a 9:1 hexanes:ethyl acetate eluent to give a yellow crystalline solid (161 mg, 62%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.24 (dd, *J* = 8.4, 6.5 Hz, 1H), 7.20 – 7.15 (m, 3H), 6.99 (dd, *J* = 8.2, 1.5 Hz, 1H), 6.74 (dd, *J* = 7.6, 1.6 Hz, 1H), 3.96 (s, 3H), 3.61 (s, 3H), 2.17 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 148.4, 141.7, 133.3, 131.7, 130.3, 122.5, 119.4, 118.0, 106.5, 55.5, 51.1, 16.0.



17

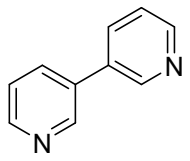
2,4,6-Trimethyl-(2',3'-dimethoxy)biphenyl (17). In a 25 mL brown vial, 2,4,6-trimethylbromobenzene (200 mg, 1.01 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 2,3-dimethoxyphenyl boronic acid (275 mg, 1.51 mmol), Cs_2CO_3 (653 mg, 2.02 mmol), $Pd(OAc)_2$ (5.7 mg, 0.025 mmol), and ligand **4m** (23 mg, 0.051 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with

a 9:1 hexanes:ethyl acetate eluent to give a clear solid (253 mg, 98%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (t, *J* = 7.9 Hz, 1H), 6.98 (s, 2H), 6.95 (dd, *J* = 8.0, 0.7 Hz, 1H), 6.70 – 6.67 (m, 1H), 3.94 (s, 3H), 3.57 (s, 3H), 2.37 (s, 3H), 2.09 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.0, 146.5, 136.6, 136.3, 135.1, 135.0, 128.0, 124.0, 123.0, 111.1, 60.2, 55.8, 21.2, 20.6.



18

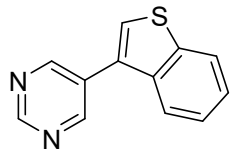
6-(Furan-3-yl)nicotinonitrile (18).[4] In a 25 mL brown vial, 2-chloronicotinonitrile (200 mg, 1..44 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 3-furanylboronic acid (242 mg, 2.16 mmol), Cs_2CO_3 (938 mg, 2.88 mmol), $Pd(OAc)_2$ (8 mg, 0.0356 mmol), and ligand **4m** (32 mg, 0.072 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with 30% ethyl acetate/hexanes eluent to give an off-white crystalline solid (191 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.11 (s, 1H), 7.89 (d, *J* = 8.3 Hz 1H), 7.52 (s, 1H), 7.51 (s, 1H), 6.88 (s, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 155.3, 152.7, 144.68, 143.4, 139.8, 126.2, 119.6, 117.1, 108.5, 107.2.



19

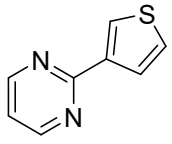
3,3'-Bipyridyl (19).[5] In a 25 mL brown vial, 3-bromopyridine (200 mg, 1.27 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added pyridine-3-boronic acid (234 mg, 1.90 mmol), Cs_2CO_3 (820 mg, 2.54 mmol), $Pd(OAc)_2$ (7.1 mg, 0.032 mmol), and ligand **4m** (29 mg, 0.064

mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with a 9:1 hexanes:ethyl acetate eluent to give a white crystalline solid (161 mg, 81%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.88 (s, 2H), 8.67 (s, 2H), 7.89 (s, 2H), 7.42 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.1, 147.9, 134.1, 133.1, 123.6.



20

5-(Benzo[*b*]thien-3-yl)pyrimidine (20).[6] In a 25 mL brown vial, 5-bromopyrimidine (200 mg, 1.26 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added benzo[*b*]thien-3-ylboronic acid (336 mg, 1.89 mmol), Cs_2CO_3 (820 mg, 2.52 mmol), $Pd(OAc)_2$ (7.9 mg, 0.0315 mmol), and ligand **4m** (29 mg, 0.063 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with 30% ethyl acetate /hexane eluent to give a yellow oil (231 mg, 86%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.13 (s, 1H), 8.97 (s, 2H), 7.78–7.81 (m, 2H), 7.57 (s, 1H), 7.33–7.36 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.8, 154.0, 140.2, 140.0, 136.2, 128.7, 125.6, 125.2, 124.2, 122.5, 122.0.



21

2-(Thiophen-3-yl)pyrimidine (21).[7] In a 25 mL brown vial, 2-bromopyrimidine (200 mg, 1.26 mmol) was dissolved in 1,4-dioxane (5 mL). To the vial was added 3-thienylboronic acid (240 mg,

1.89 mmol), Cs_2CO_3 (820 mg, 2.52 mmol), $Pd(OAc)_2$ (7.9 mg, 0.0315 mmol), and ligand **4m** (29 mg, 0.063 mmol). The vial was purged with nitrogen. The reaction stirred overnight at 80 °C. The crude mixture was filtered over Celite and rinsed with ethyl acetate. The mixture was further purified utilizing column chromatography with a 30% ethyl acetate in hexane eluent to give a colorless crystalline solid (162 mg, 79%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 4.9 Hz, 2H), 8.27 (d, *J* = 4.9 Hz, 1H), 7.87 (d, *J* = 4.3 Hz, 1H), 7.34 (m, 1H), 7.05 (t, *J* = 9.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 162.0, 157.3, 141.7, 128.1, 127.5, 126.2, 118.7**.**

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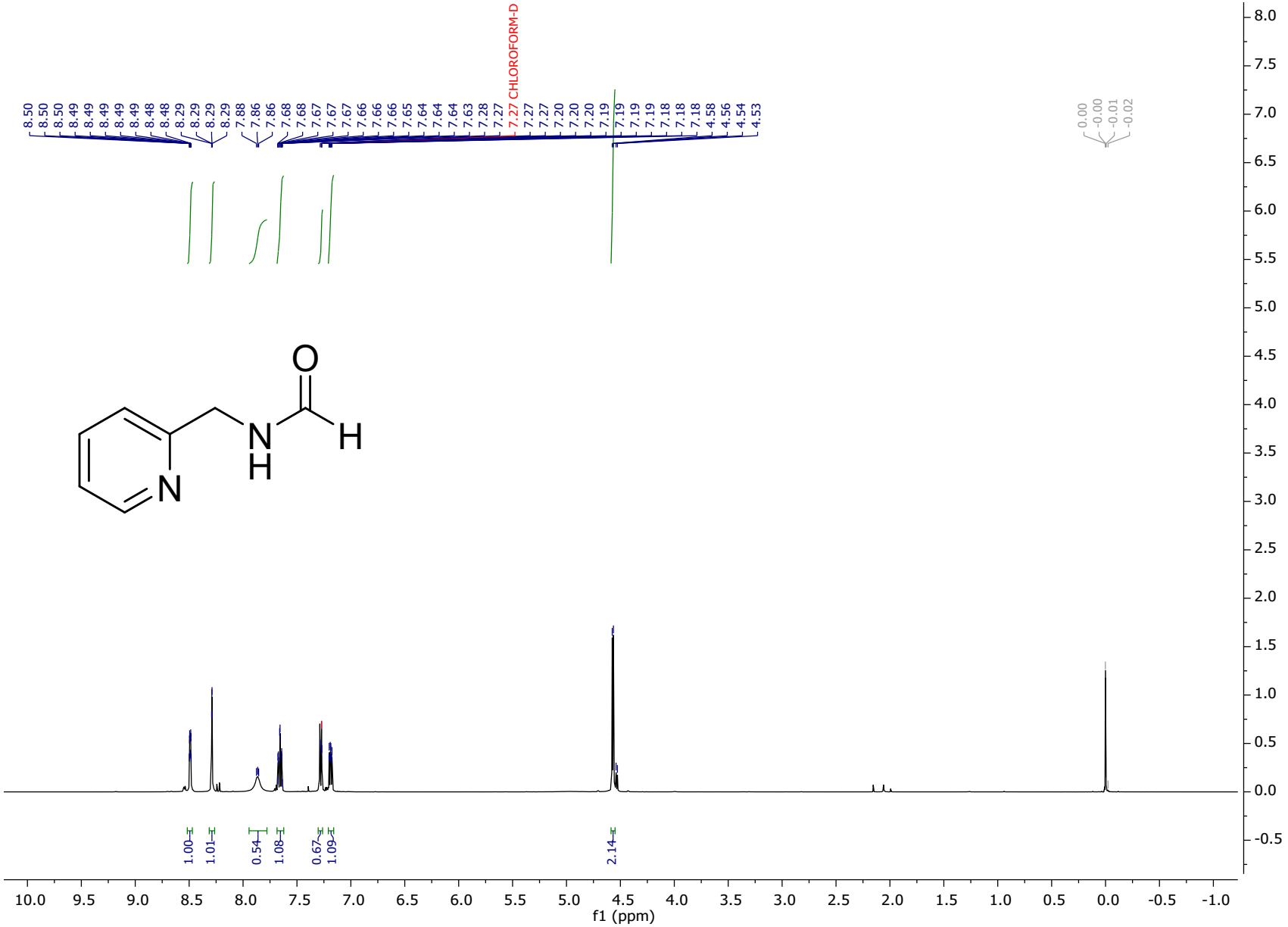
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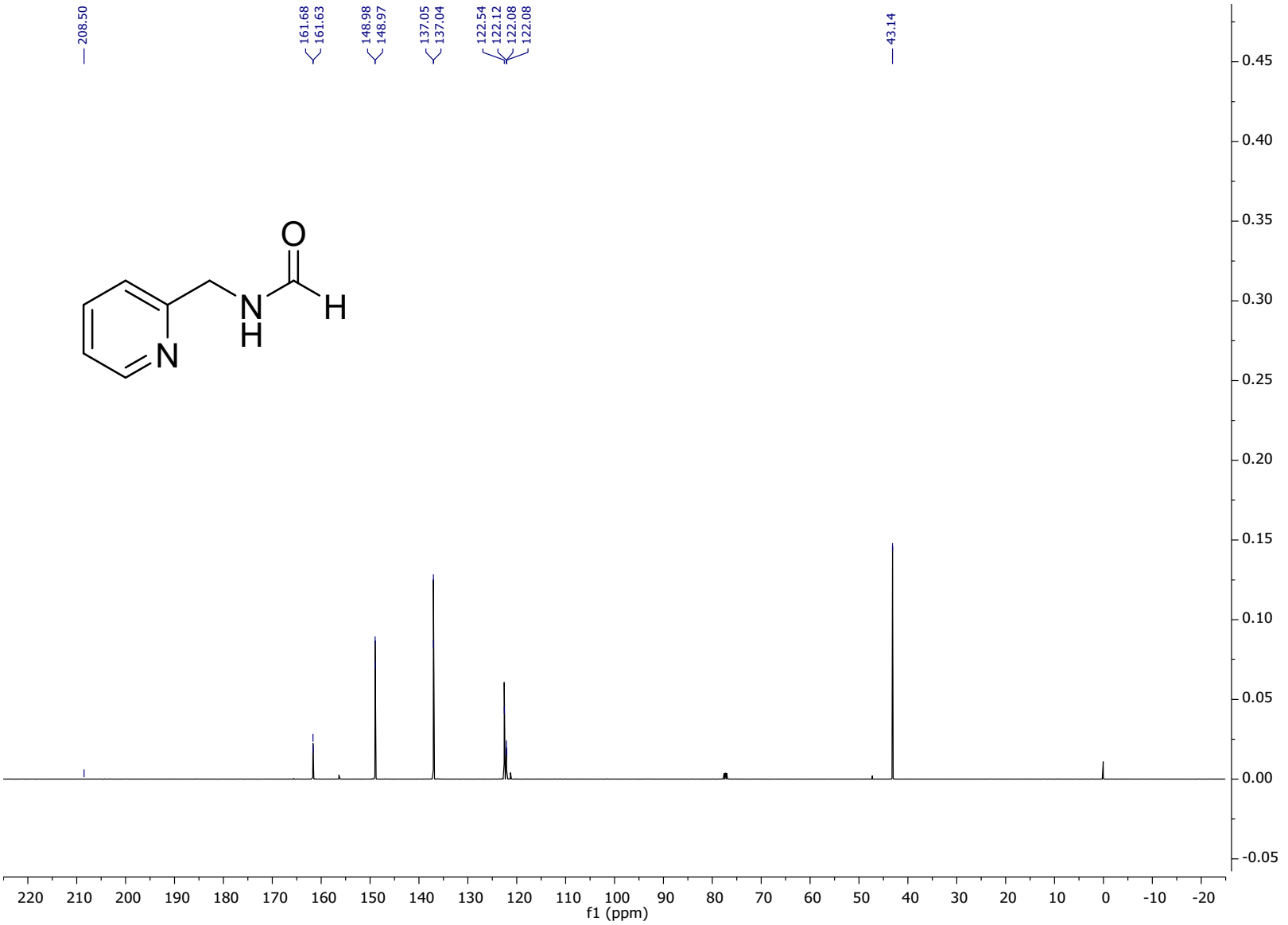
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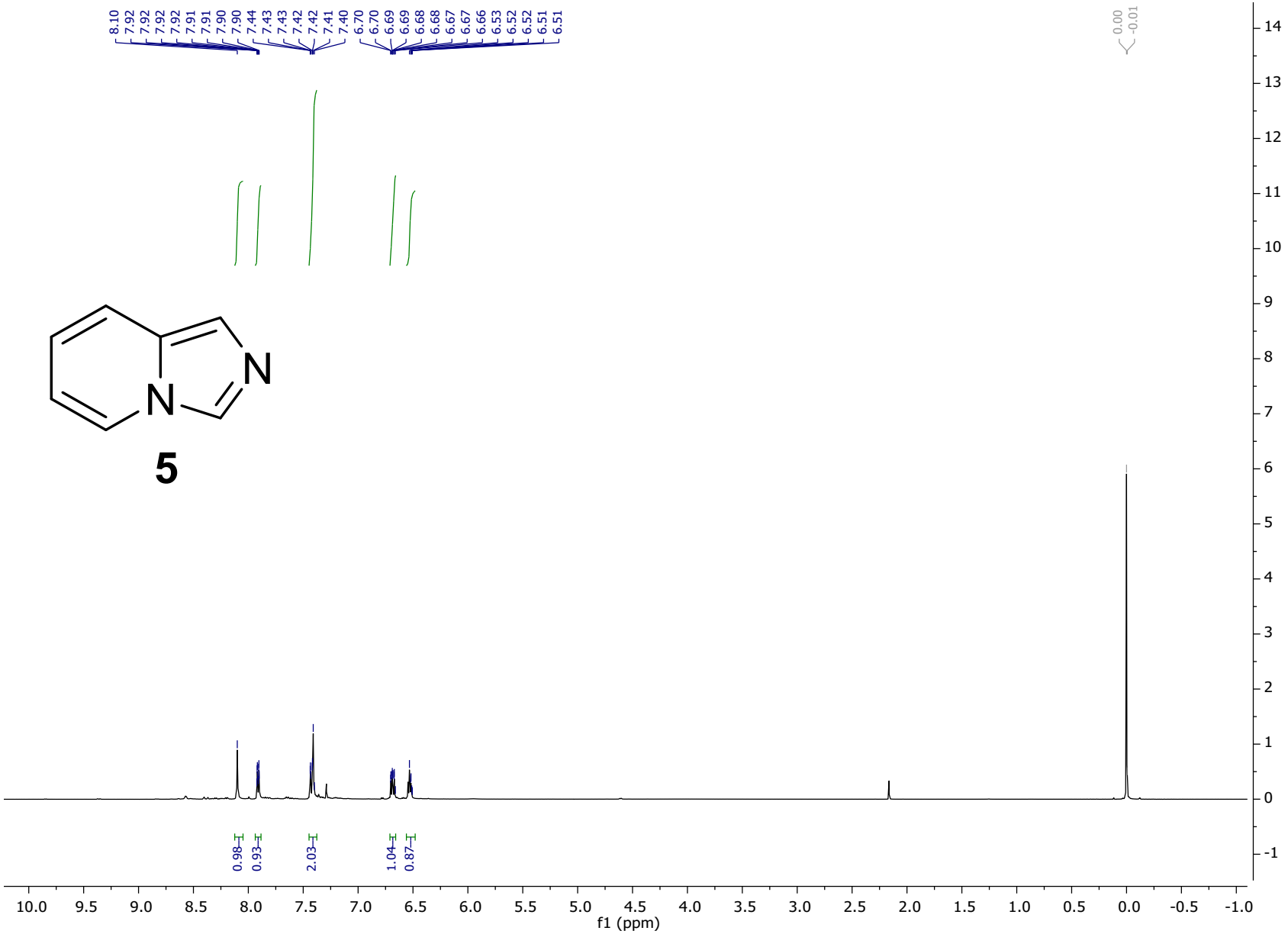
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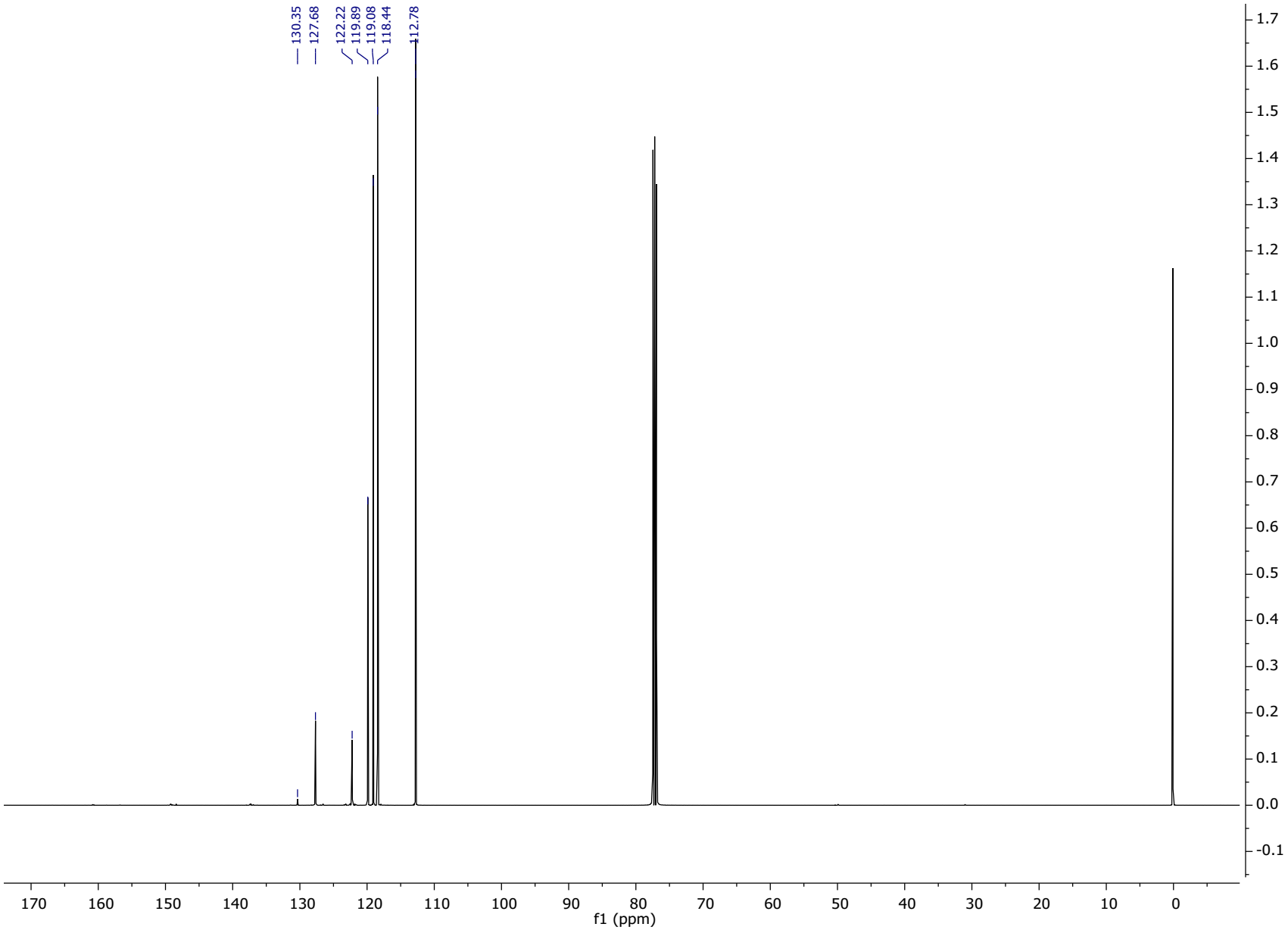
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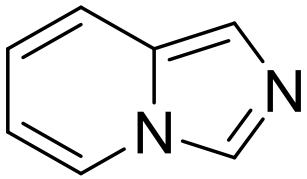
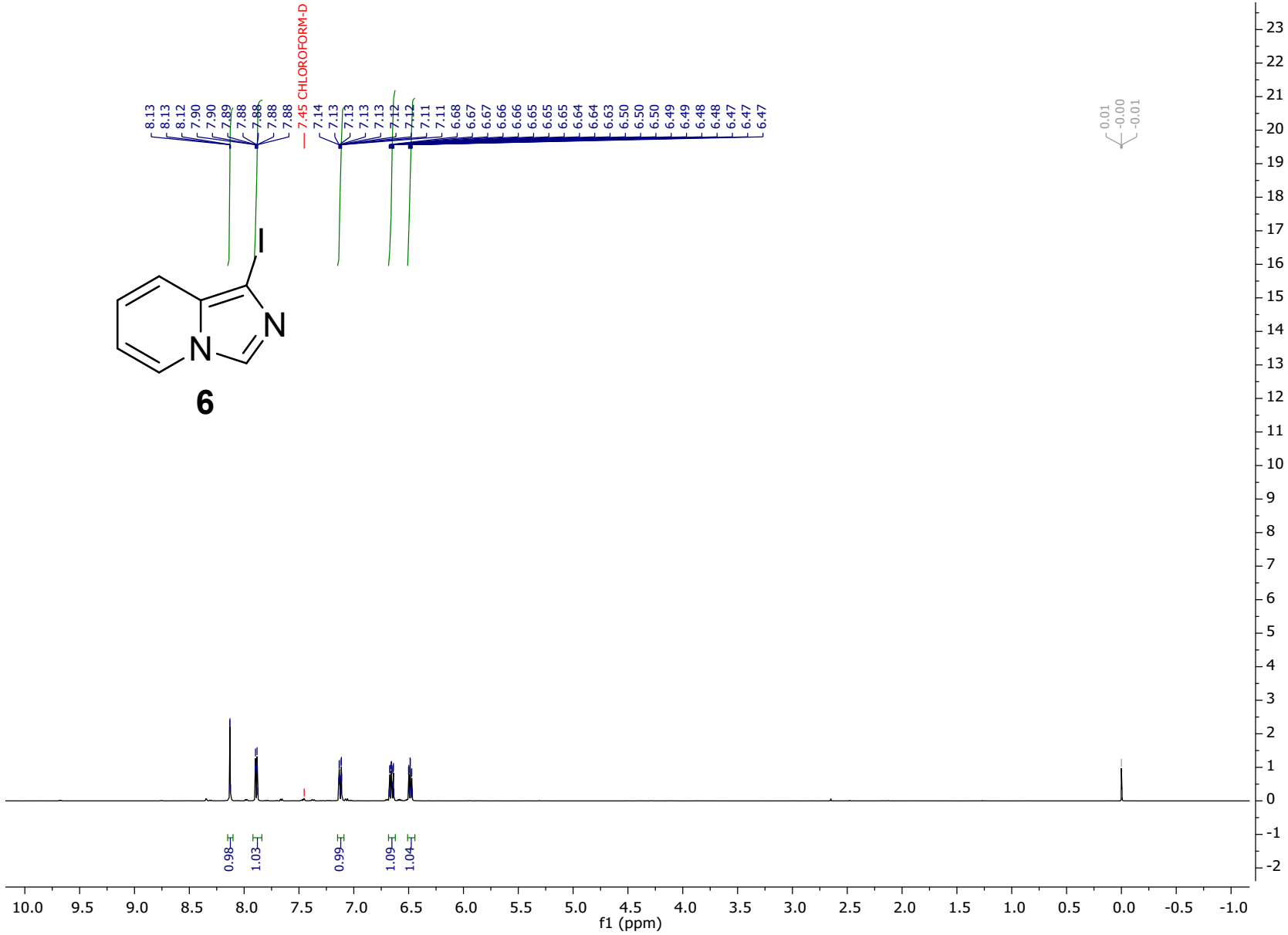


5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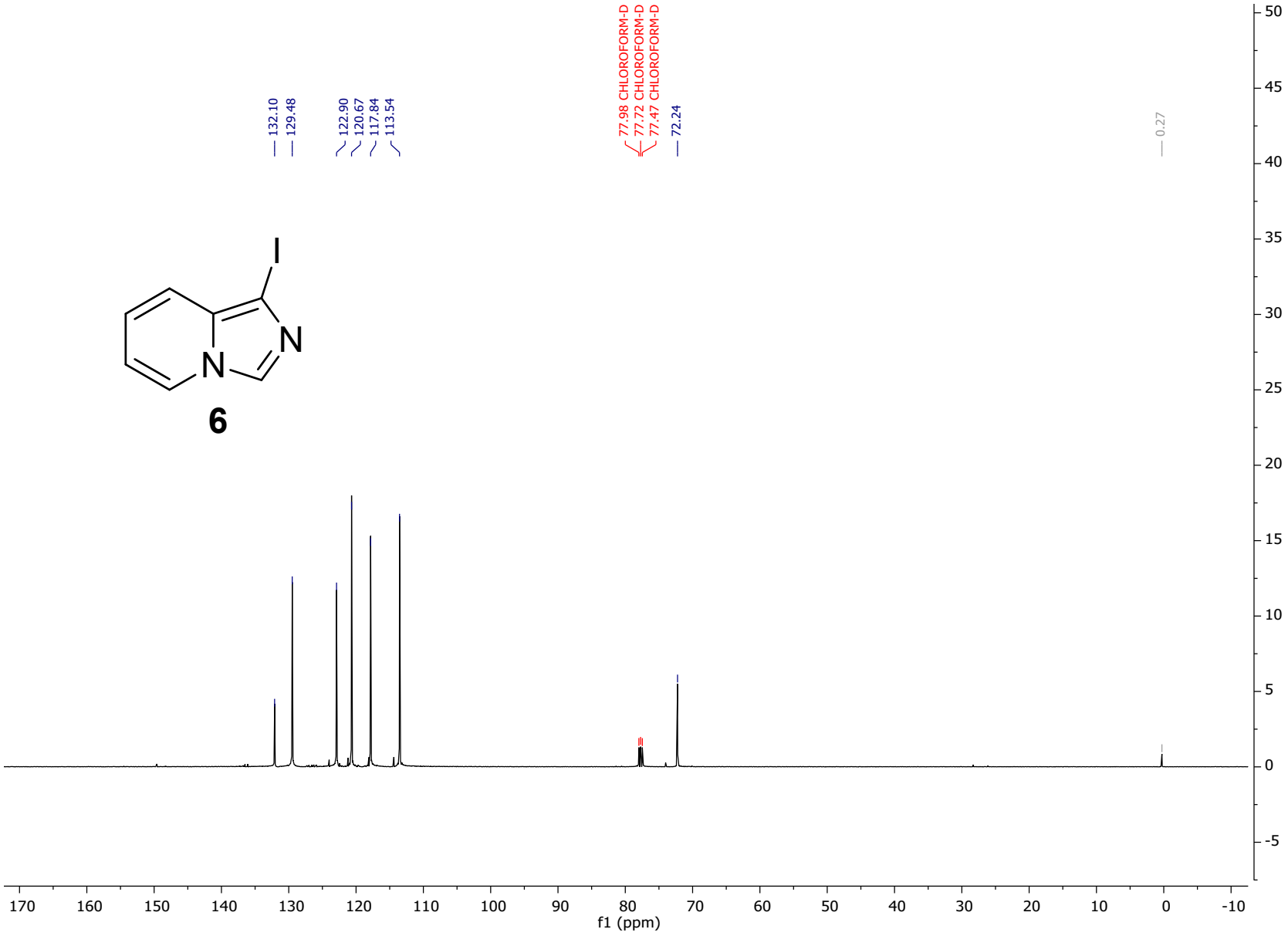
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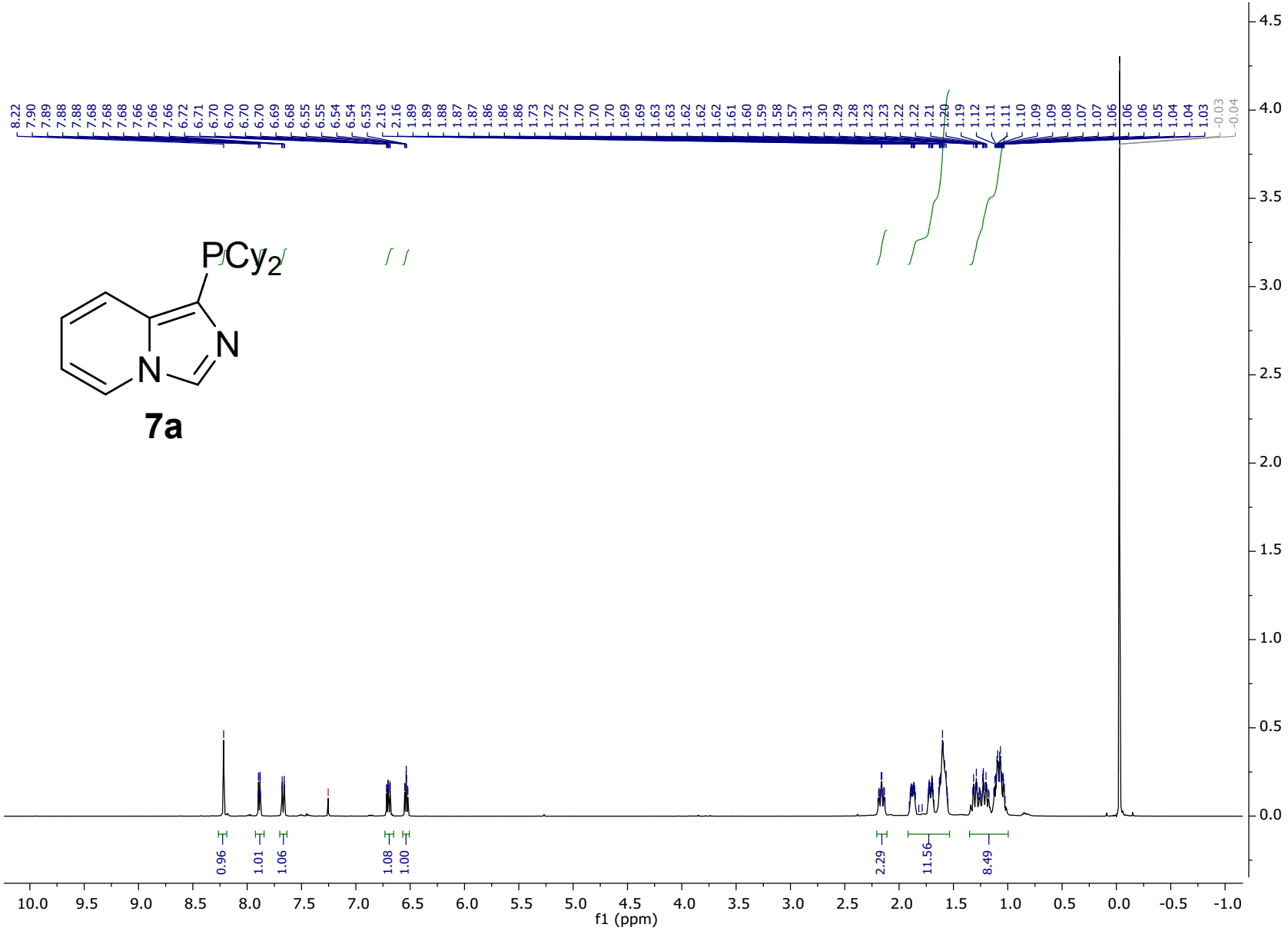
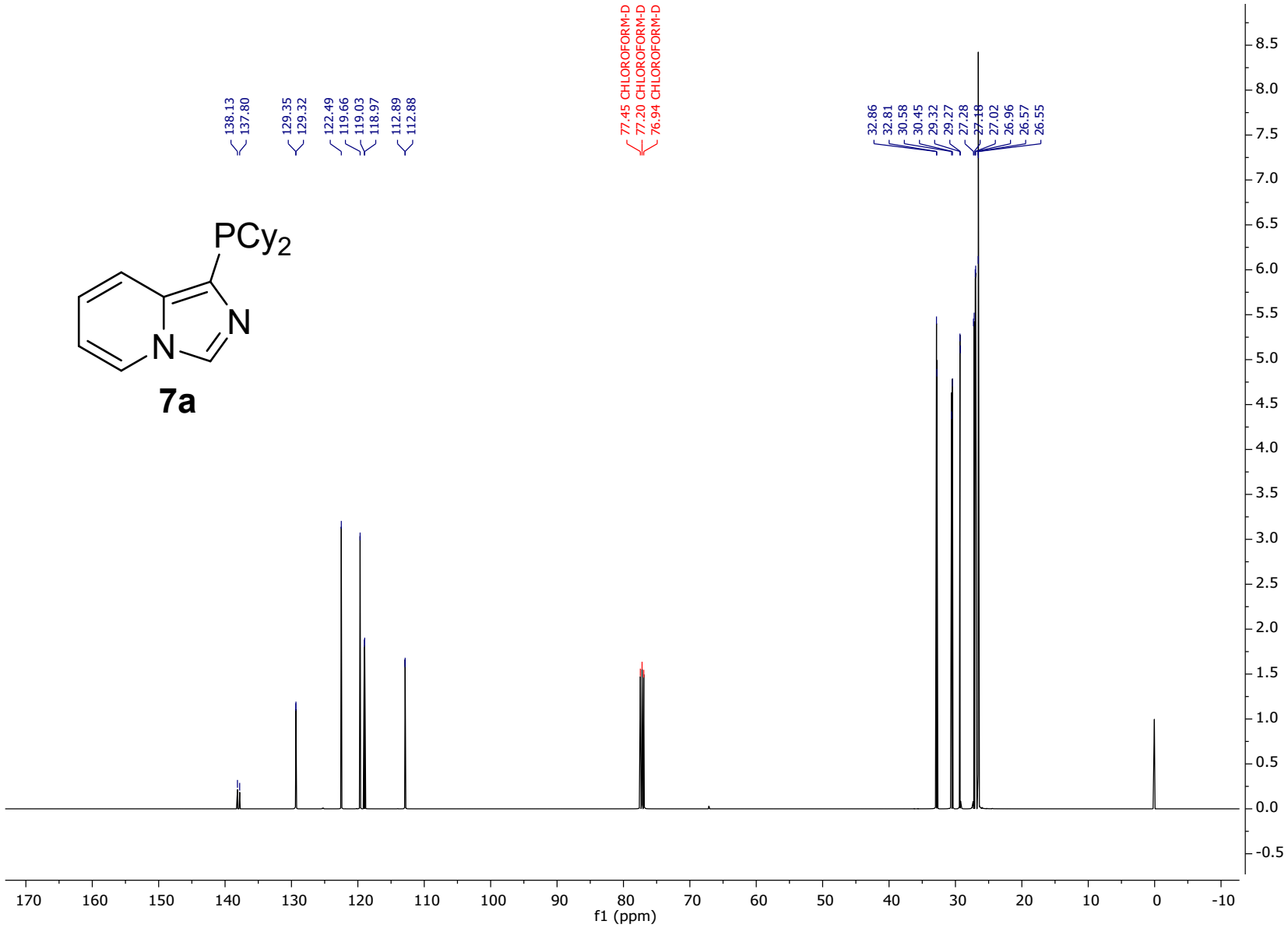
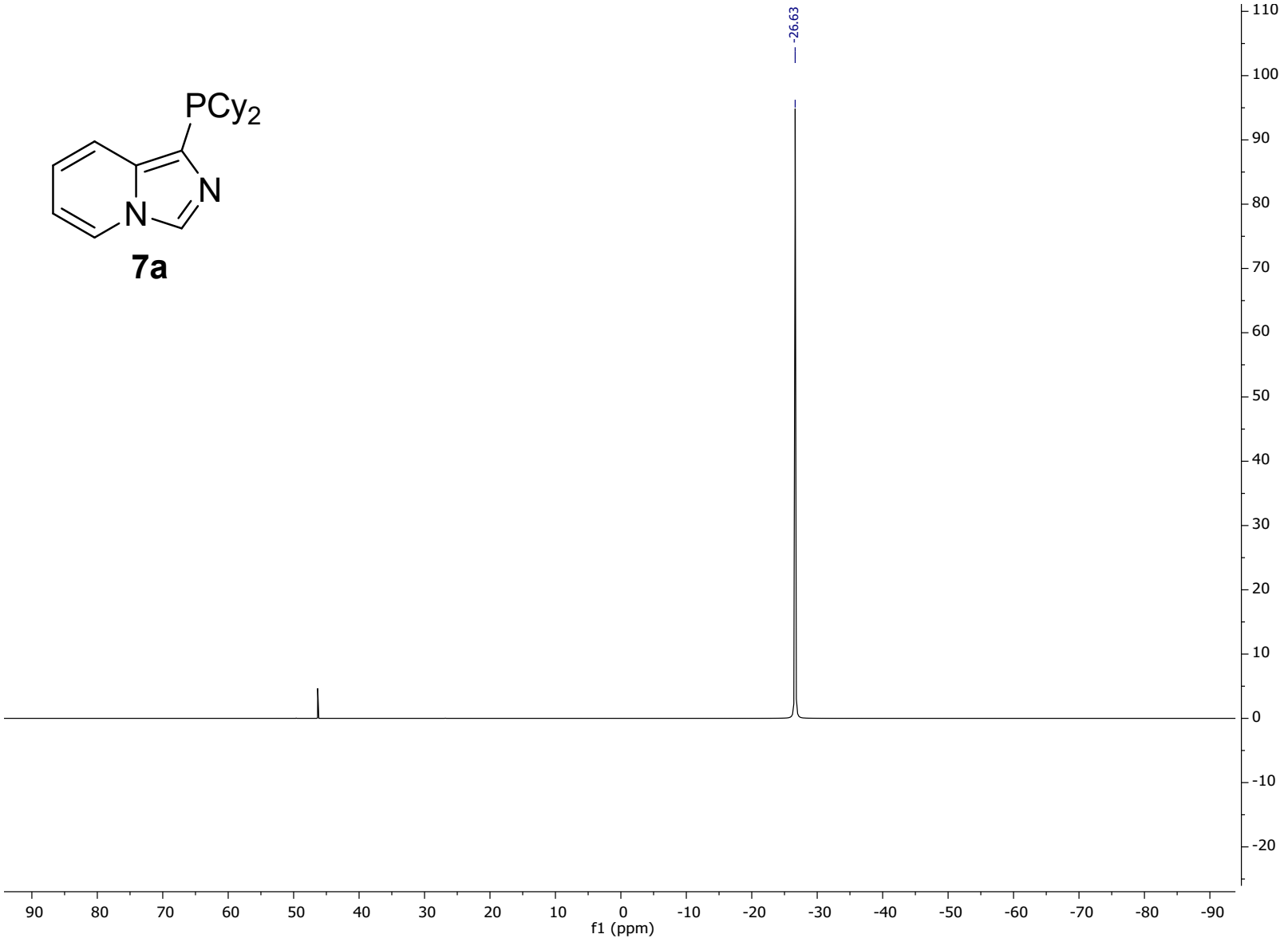
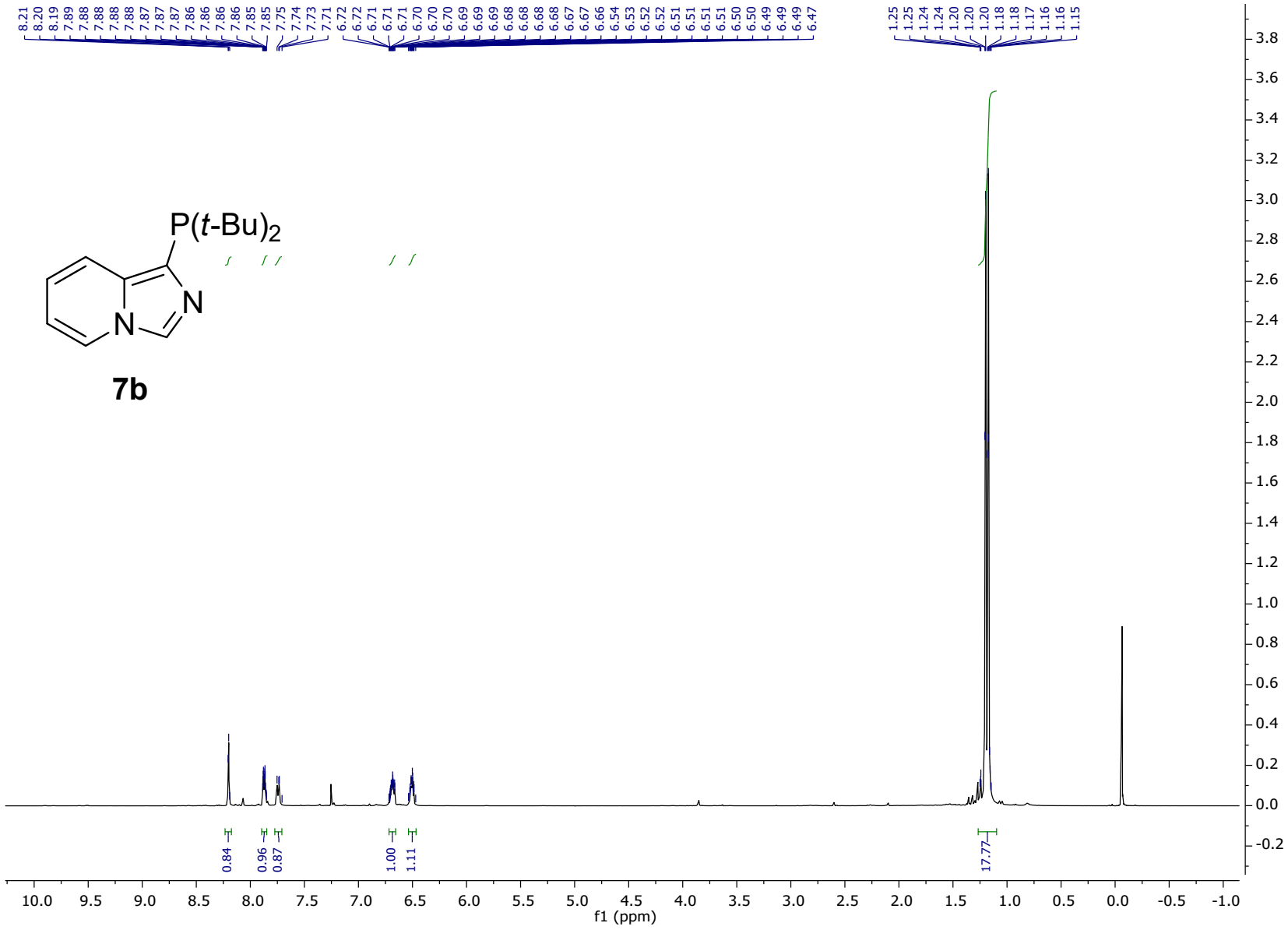
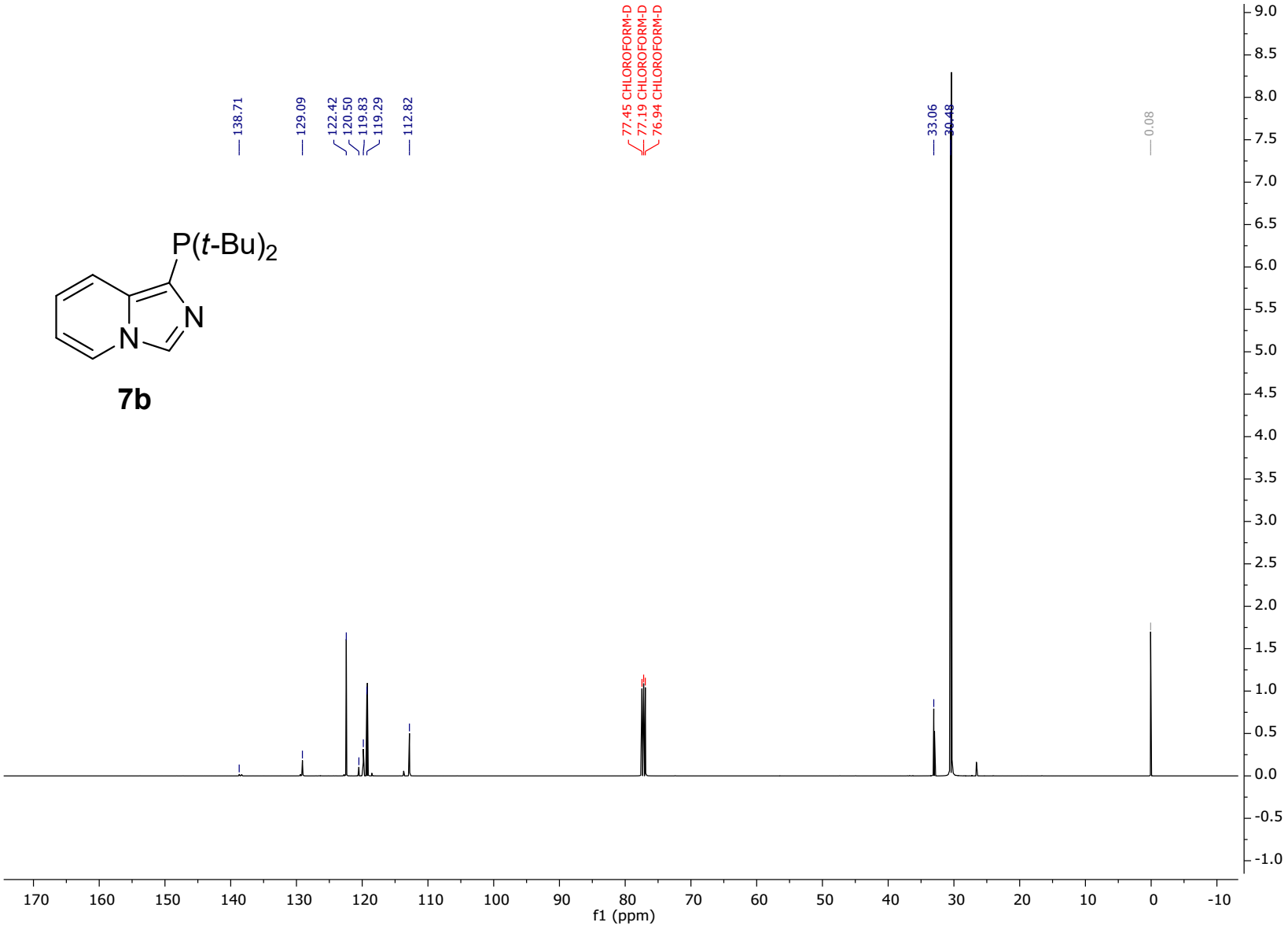
72.24
0.27
I
N
N
6
f1 (ppm)

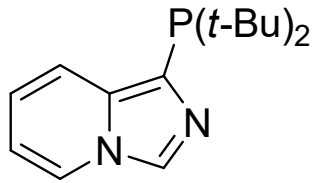

PCy2
N
N
7a
f1 (ppm)


138.13
137.80
129.35
129.32
122.49
119.66
119.03
118.97
112.89
112.88
77.45 CHLOROFORM-D
77.20 CHLOROFORM-D
76.94 CHLOROFORM-D
32.86
32.81
30.58
30.45
29.32
29.27
27.28
27.18
27.02
26.96
26.57
26.55
PCy2
N
N
7a
f1 (ppm)


PCy2
N
N
7a
-26.63
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

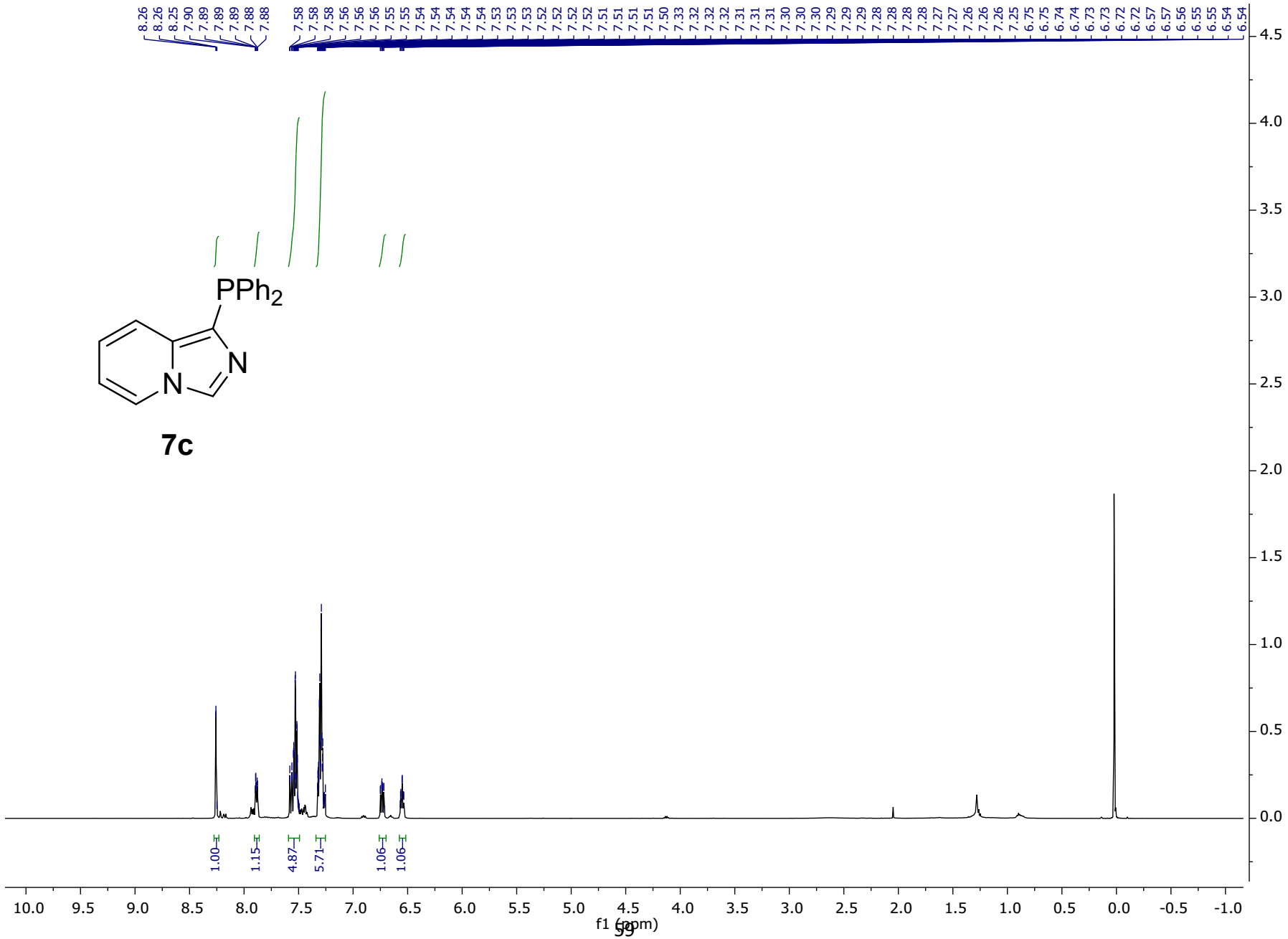

P(t-Bu)2
N
N
7b
f1 (ppm)

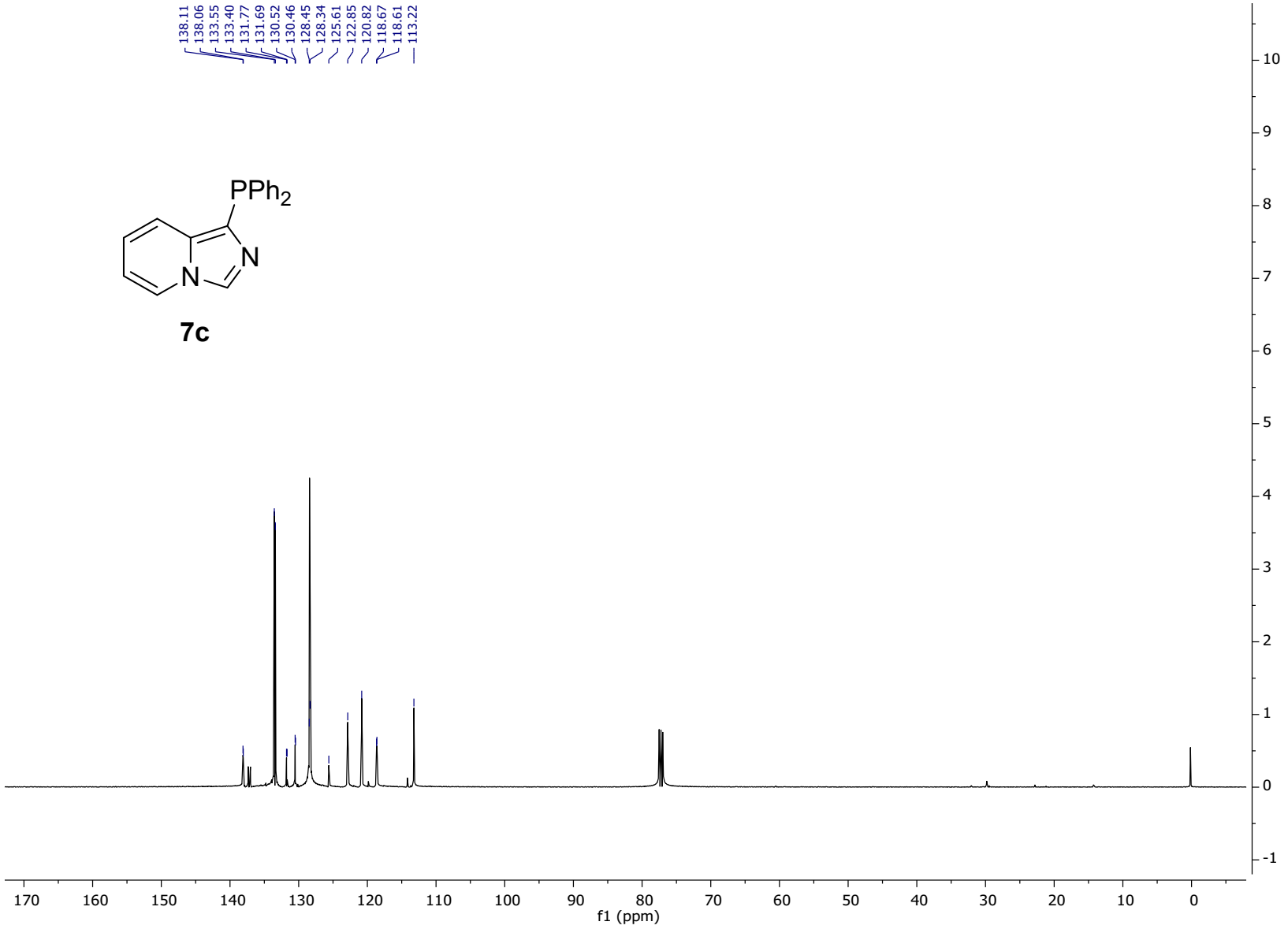

P(t-Bu)2
N
N
7b
138.71
129.09
122.42
120.50
119.83
119.29
112.82
77.45 CHLOROFORM-D
77.19 CHLOROFORM-D
76.94 CHLOROFORM-D
33.06
30.48
0.08
f1 (ppm)

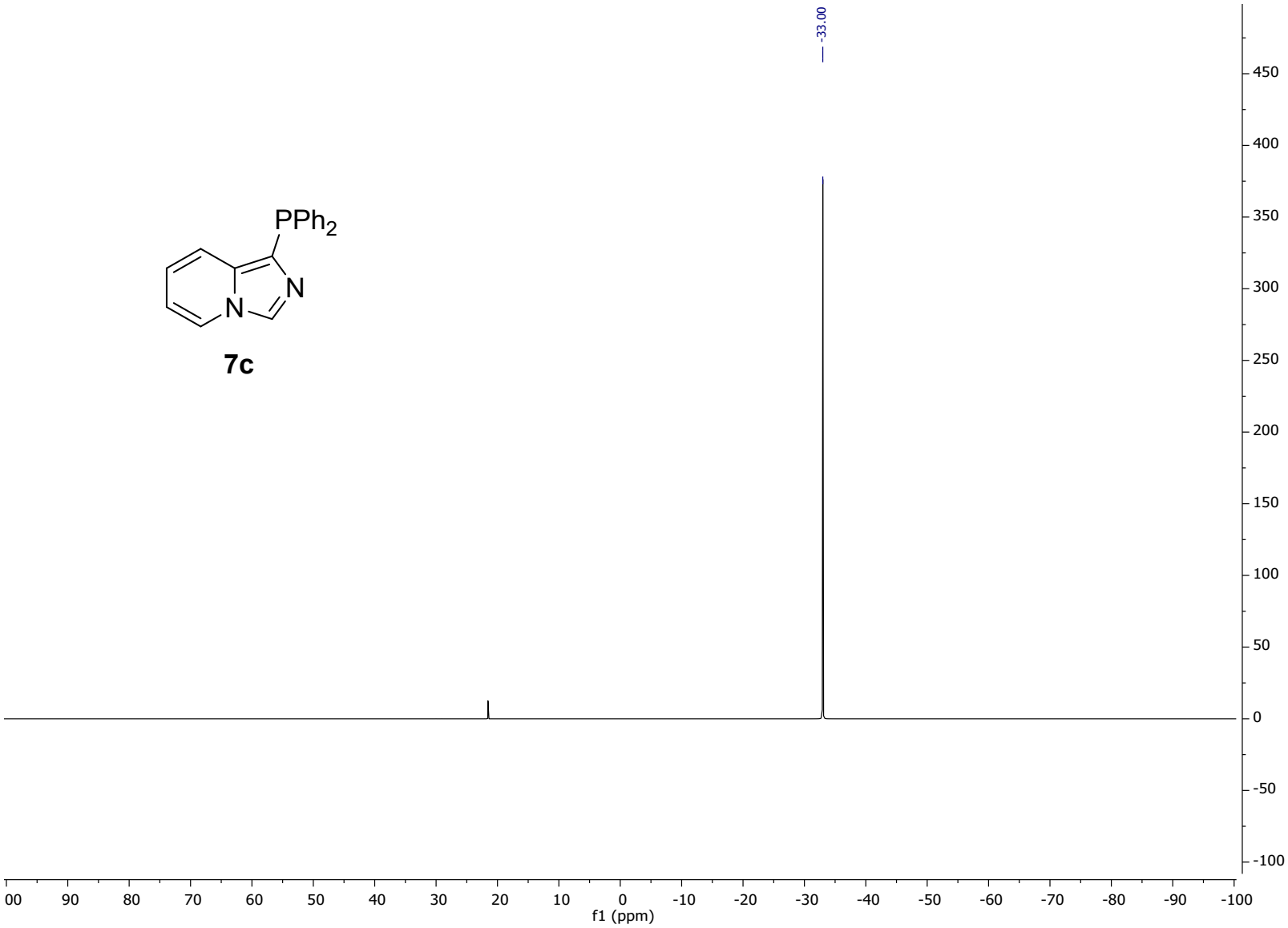

P(t-Bu)2
N
N

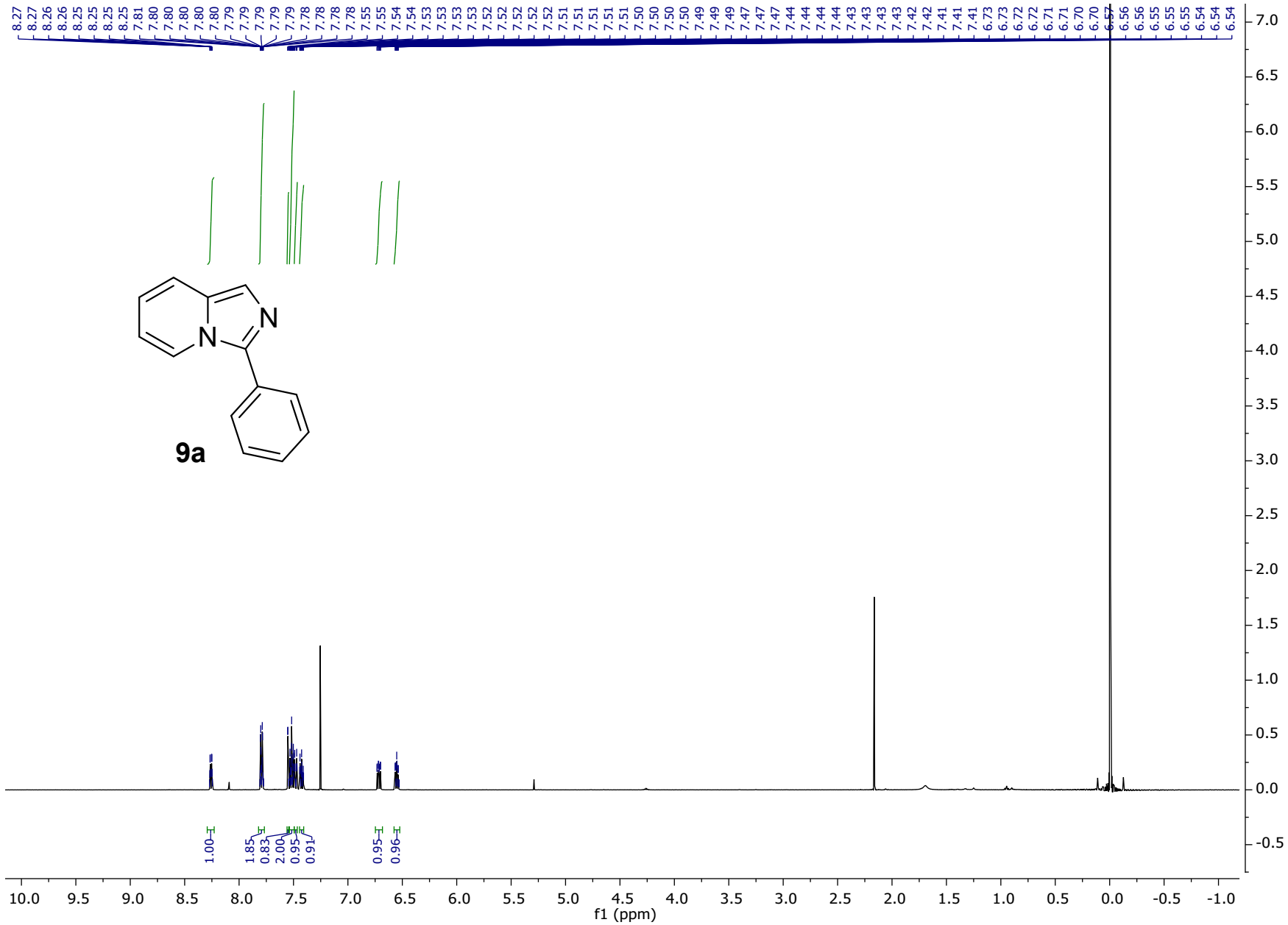
7b

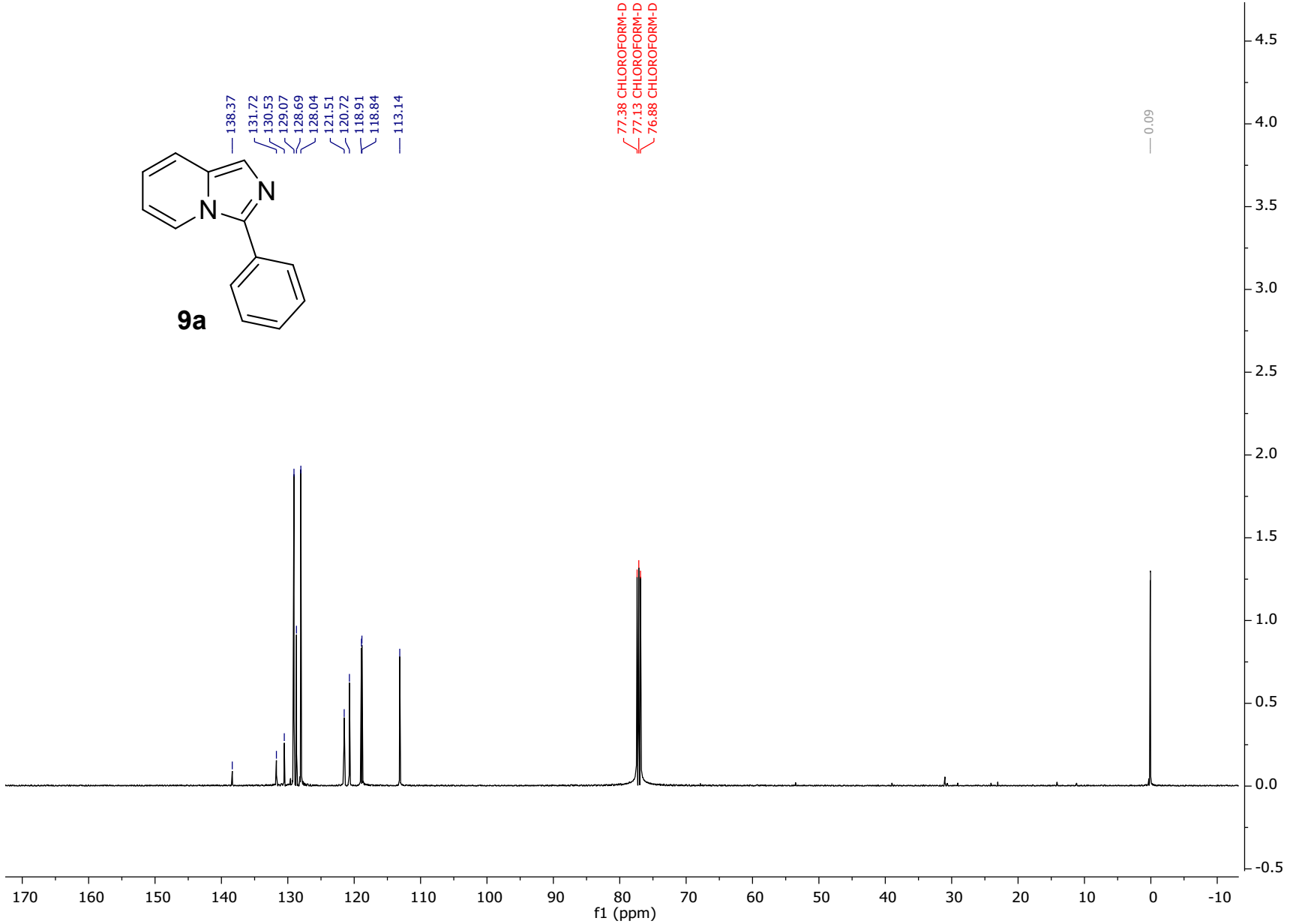
4.29
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

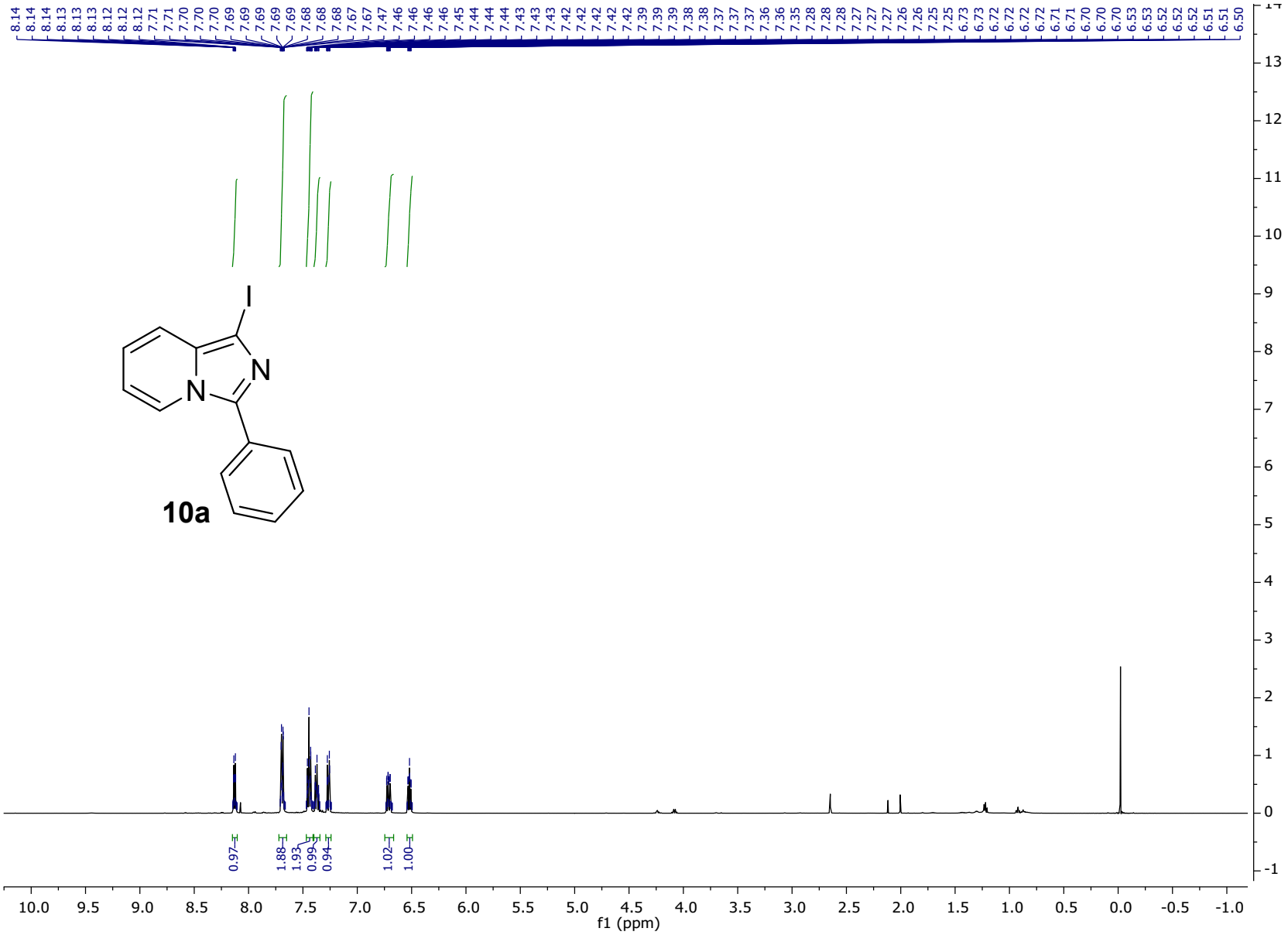

8.26 8.26 8.25 7.90 7.89 7.89 7.89 7.88 7.88
7.58 7.58 7.58 7.56 7.56 7.56 7.55 7.55 7.54 7.54 7.54 7.54 7.53 7.53 7.53 7.52 7.52 7.52 7.52 7.51 7.51 7.51 7.51 7.50 7.33 7.32 7.32 7.31 7.31 7.31 7.30 7.30 7.30 7.29 7.29 7.29 7.28 7.28 7.28 7.28 7.27 7.27 7.26 7.26 7.26 7.25 6.75 6.75 6.74 6.74 6.73 6.73 6.72 6.72 6.57 6.57 6.56 6.55 6.55 6.54 6.54
PPh2
N
N
7c
1.00
1.15
4.87
5.71
1.06
1.06
f1 (ppm)

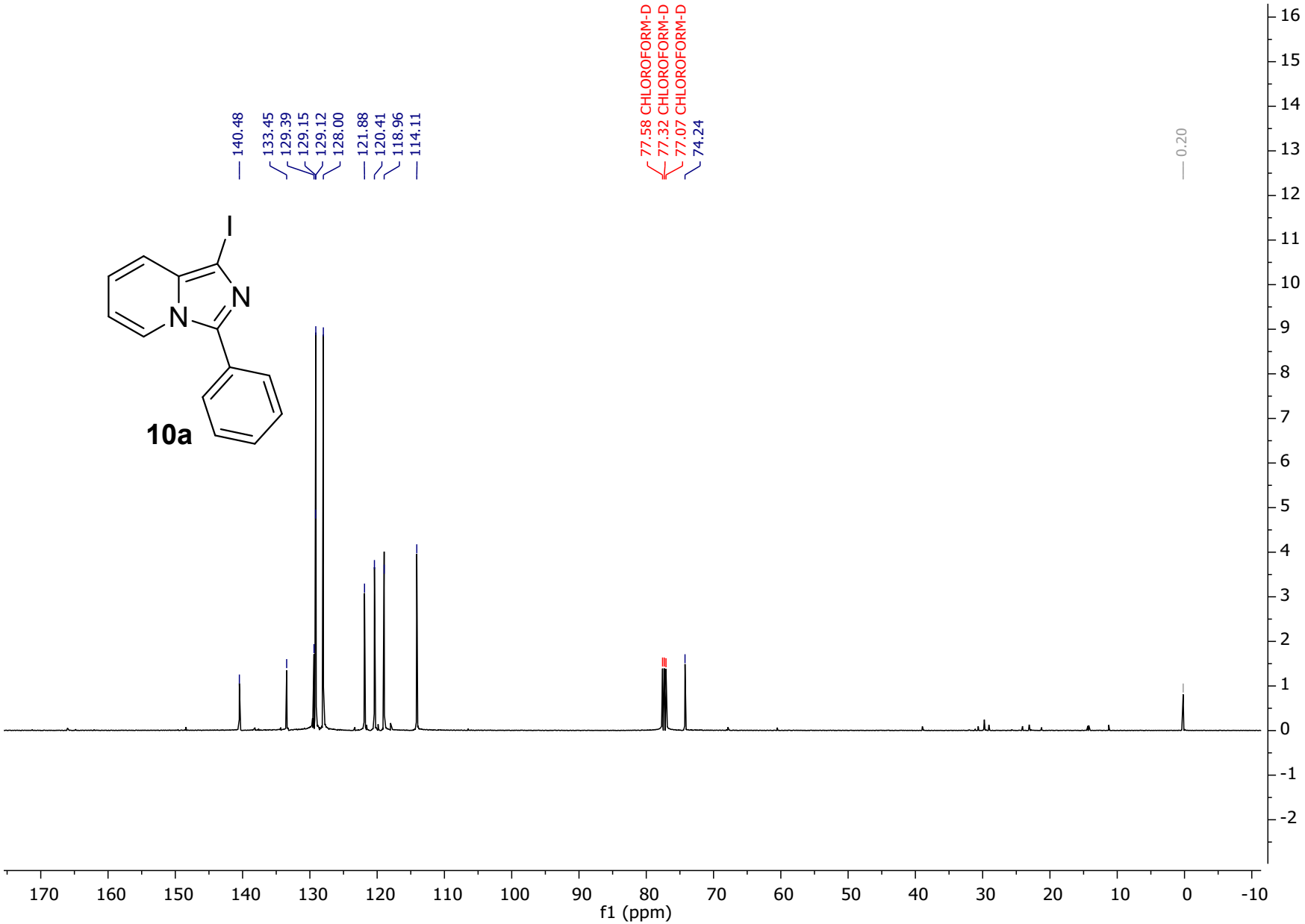

138.11
138.06
133.55
133.40
131.77
131.69
130.52
130.46
128.45
128.34
125.61
122.85
120.82
118.67
118.61
113.22
PPh2
N
N
7c
f1 (ppm)

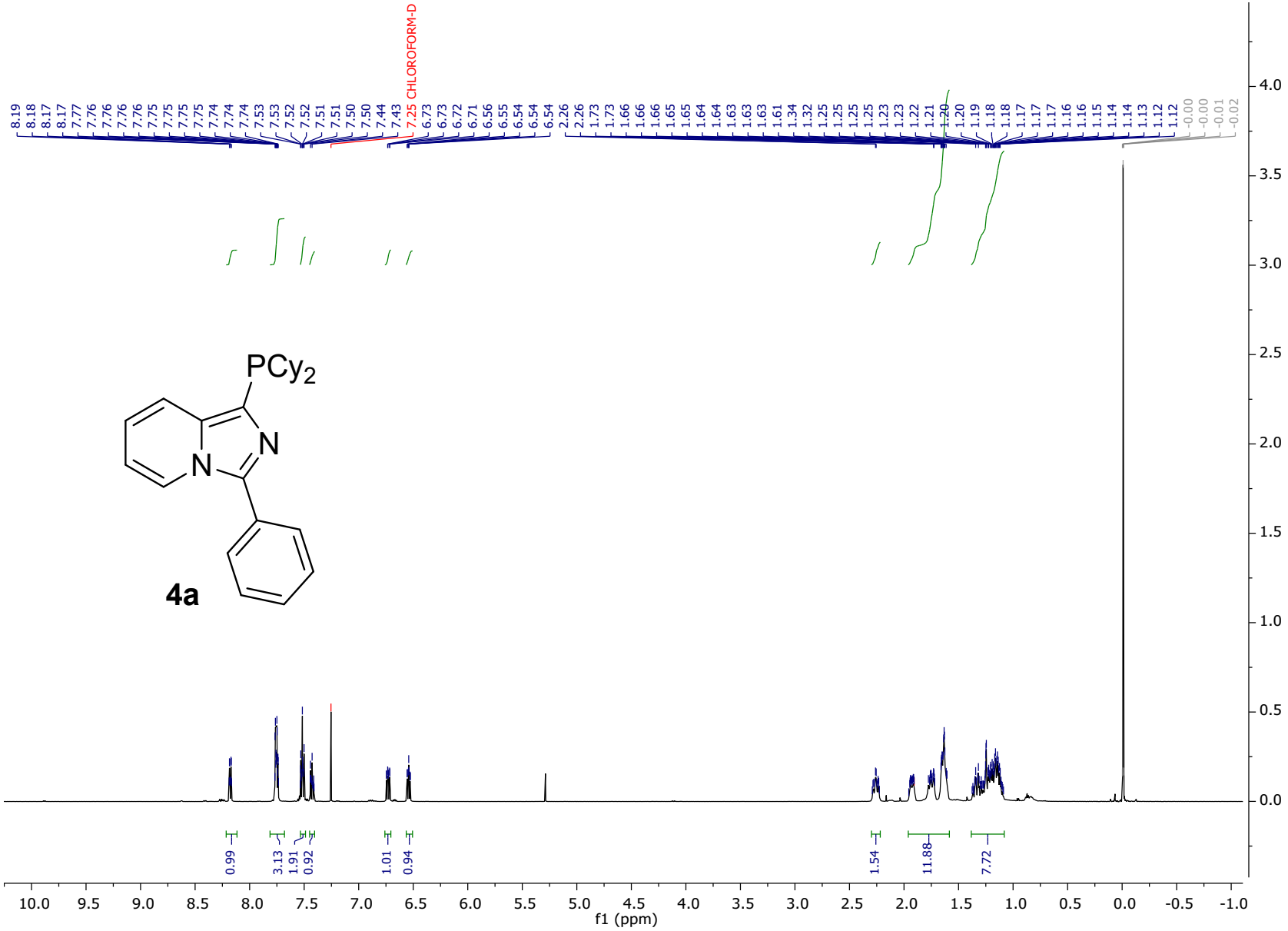

PPh2
N
N
7c
-33.00
450
400
350
300
250
200
150
100
50
0
-50
-100
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

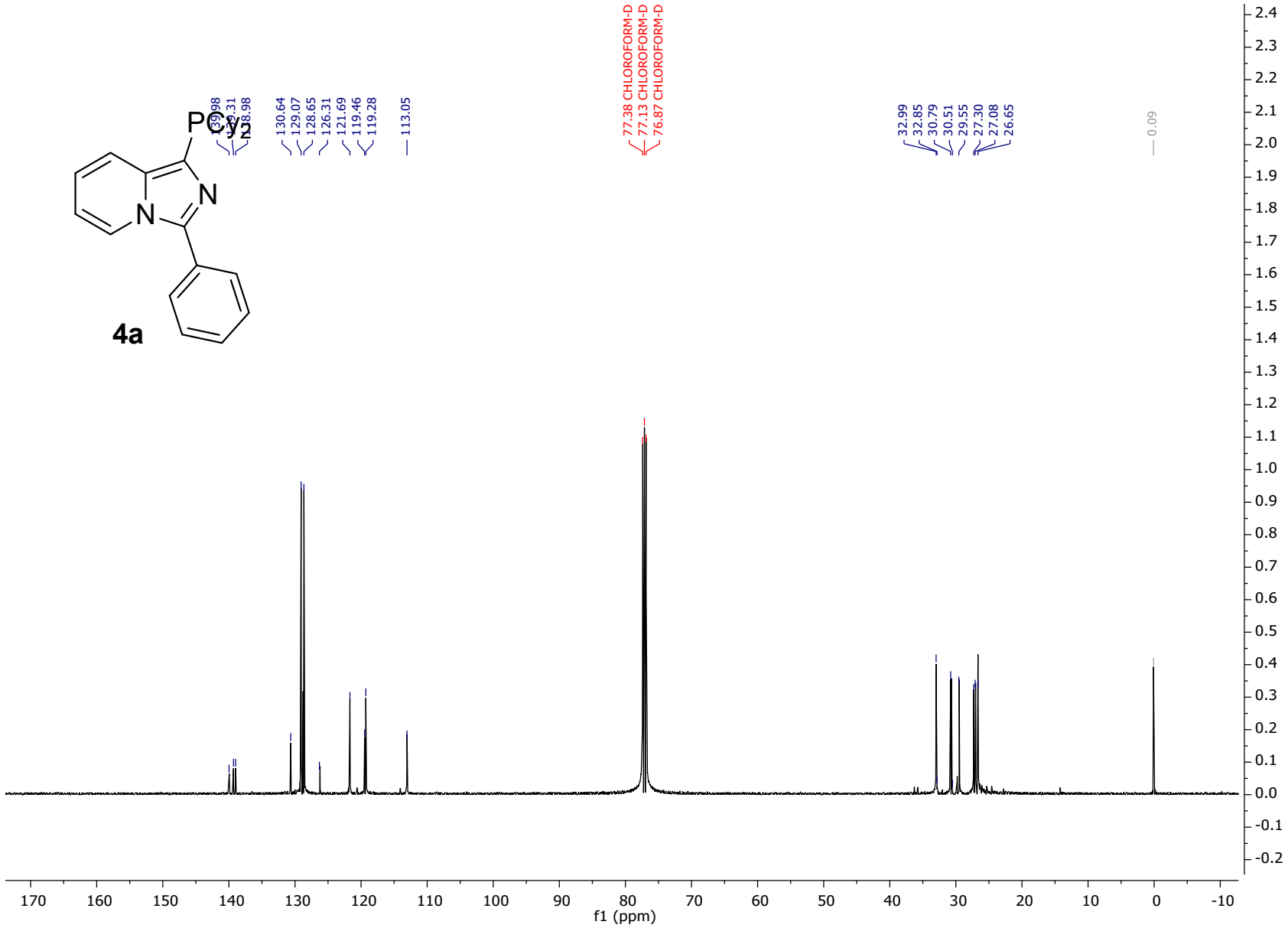

8.27 8.27 8.26 8.26 8.25 8.25 8.25 8.25 7.81 7.80 7.80 7.80 7.80 7.79 7.79 7.79 7.79 7.79 7.78 7.78 7.78 7.78 7.55 7.55 7.54 7.54 7.53 7.53 7.53 7.52 7.52 7.52 7.52 7.52 7.51 7.51 7.51 7.51 7.51 7.50 7.50 7.50 7.50 7.49 7.49 7.49 7.47 7.47 7.47 7.44 7.44 7.44 7.44 7.43 7.43 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.41 6.73 6.73 6.72 6.72 6.71 6.71 6.70 6.70 6.57 6.56 6.56 6.55 6.55 6.55 6.54 6.54 6.54
N
N
9a
1.00
1.85
0.83
2.00
0.95
0.91
0.95
0.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

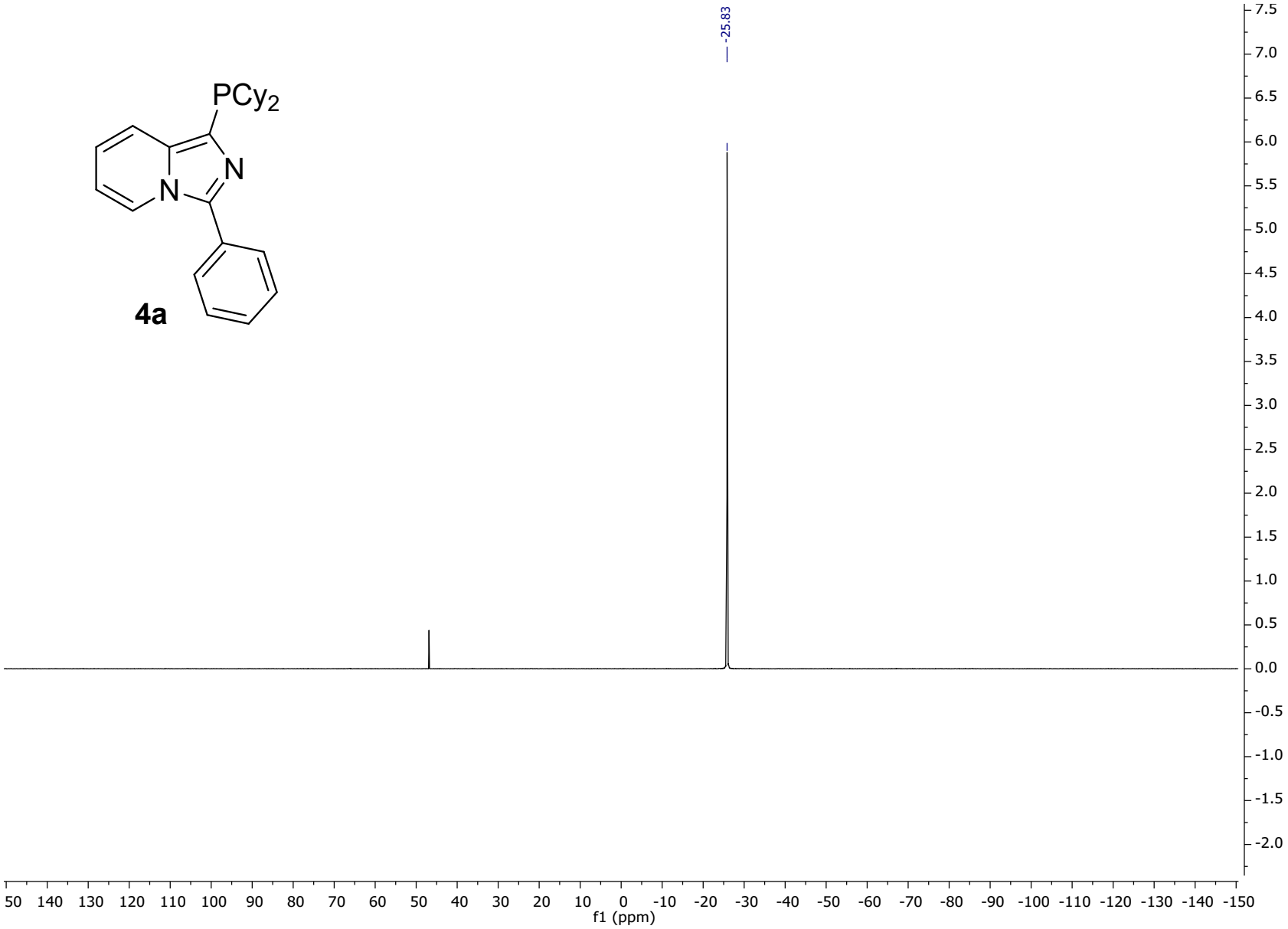

138.37
131.72
130.53
129.07
128.69
128.04
121.51
120.72
118.91
118.84
113.14
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
0.09
N
N
9a
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

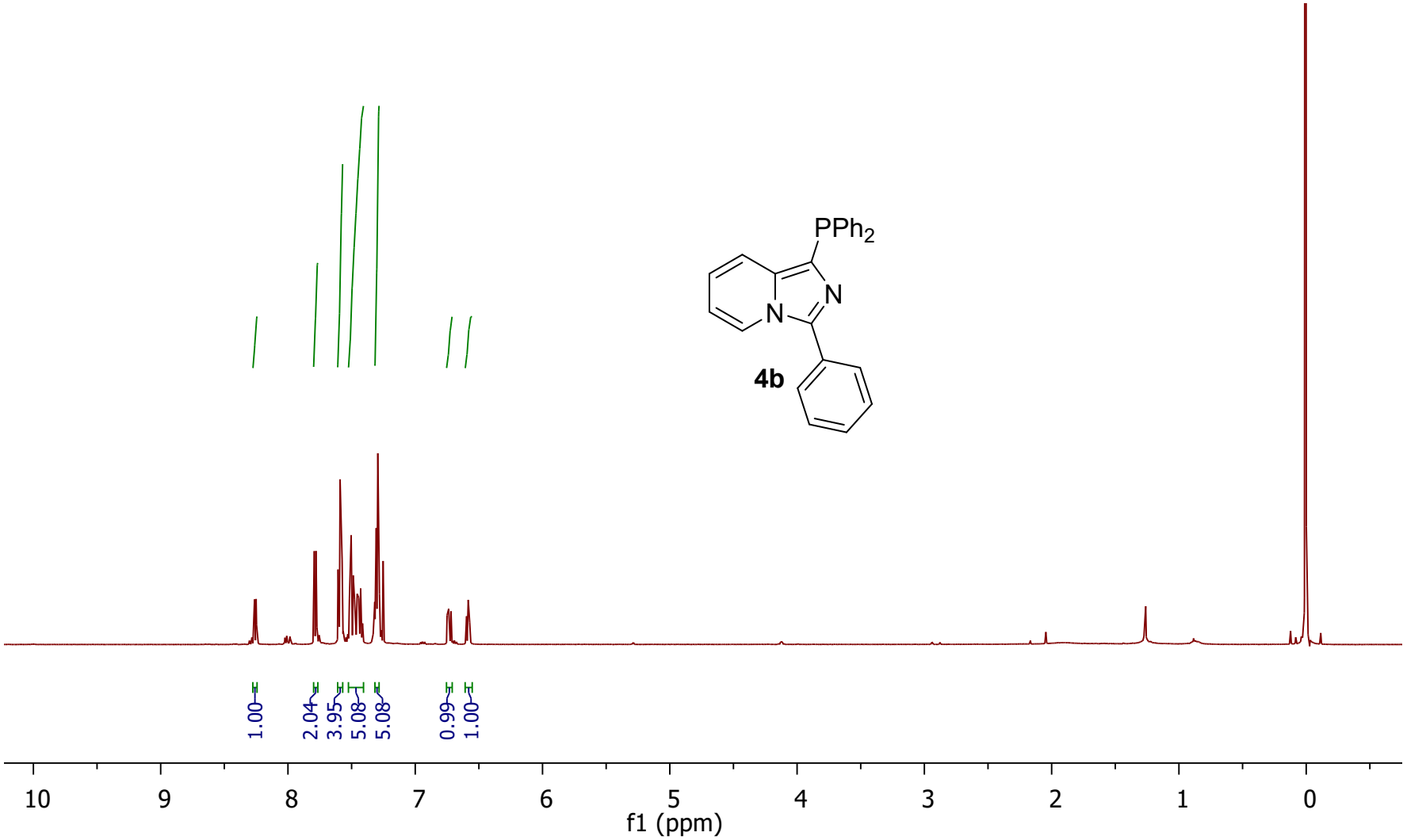

I
N
N
10a
f1 (ppm)

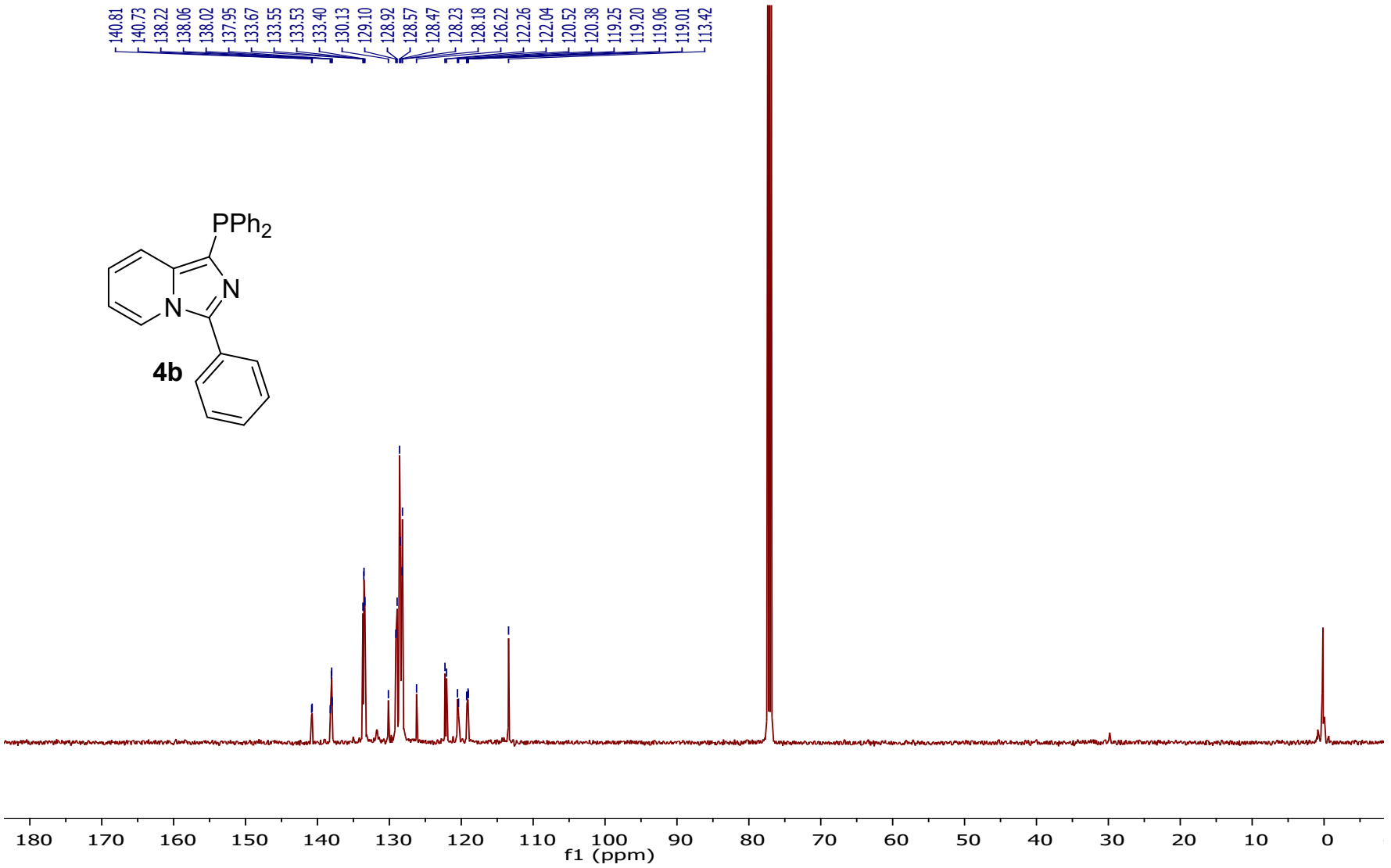

140.48
133.45
129.39
129.15
129.12
128.00
121.88
120.41
118.96
114.11
77.58 CHLOROFORM-D
77.32 CHLOROFORM-D
77.07 CHLOROFORM-D
74.24
0.20
I
N
N
10a
f1 (ppm)

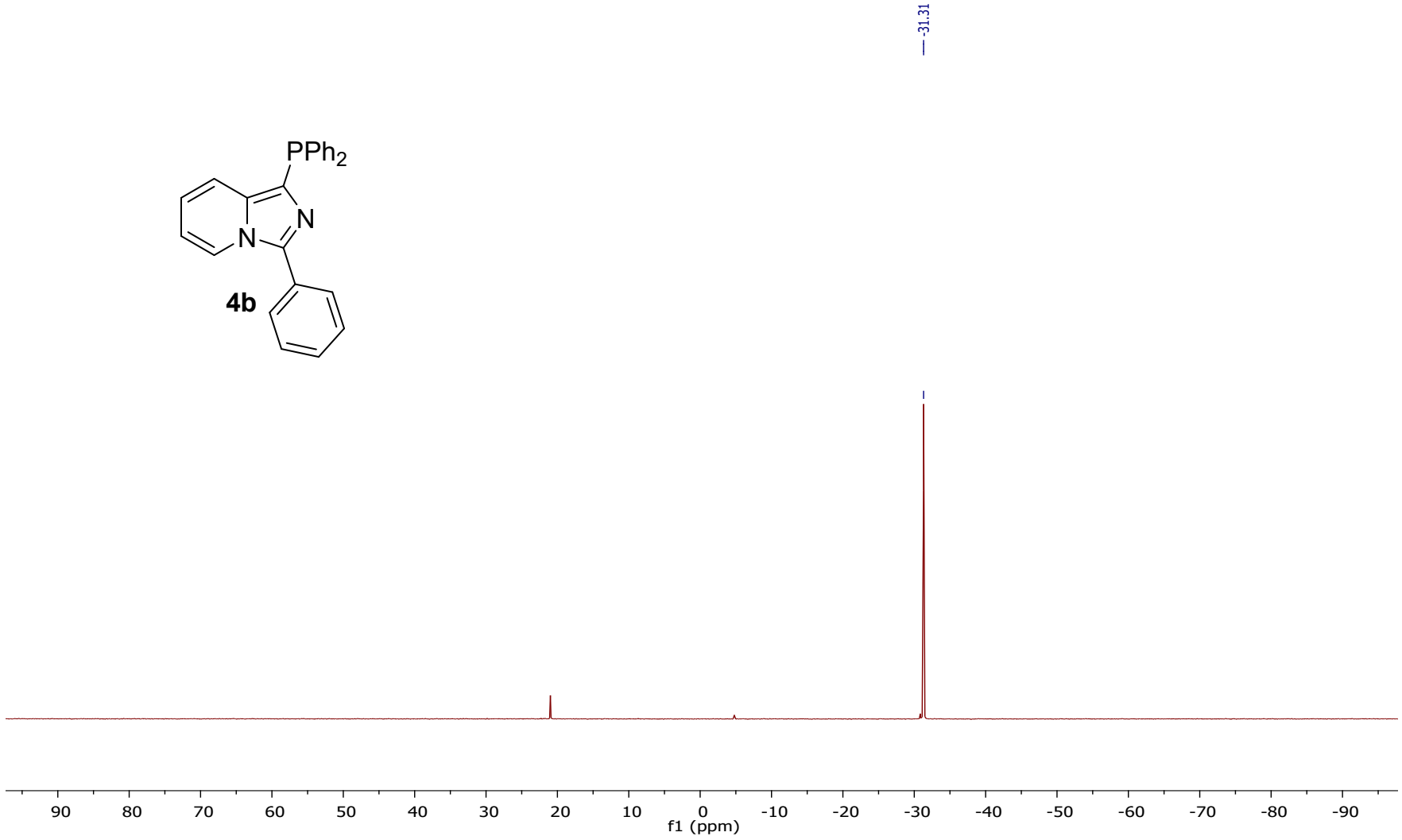

CHLOROFORM-D
PCy2
N
N
4a
0.99
3.13
1.91
0.92
1.01
0.94
1.54
11.88
7.72
f1 (ppm)

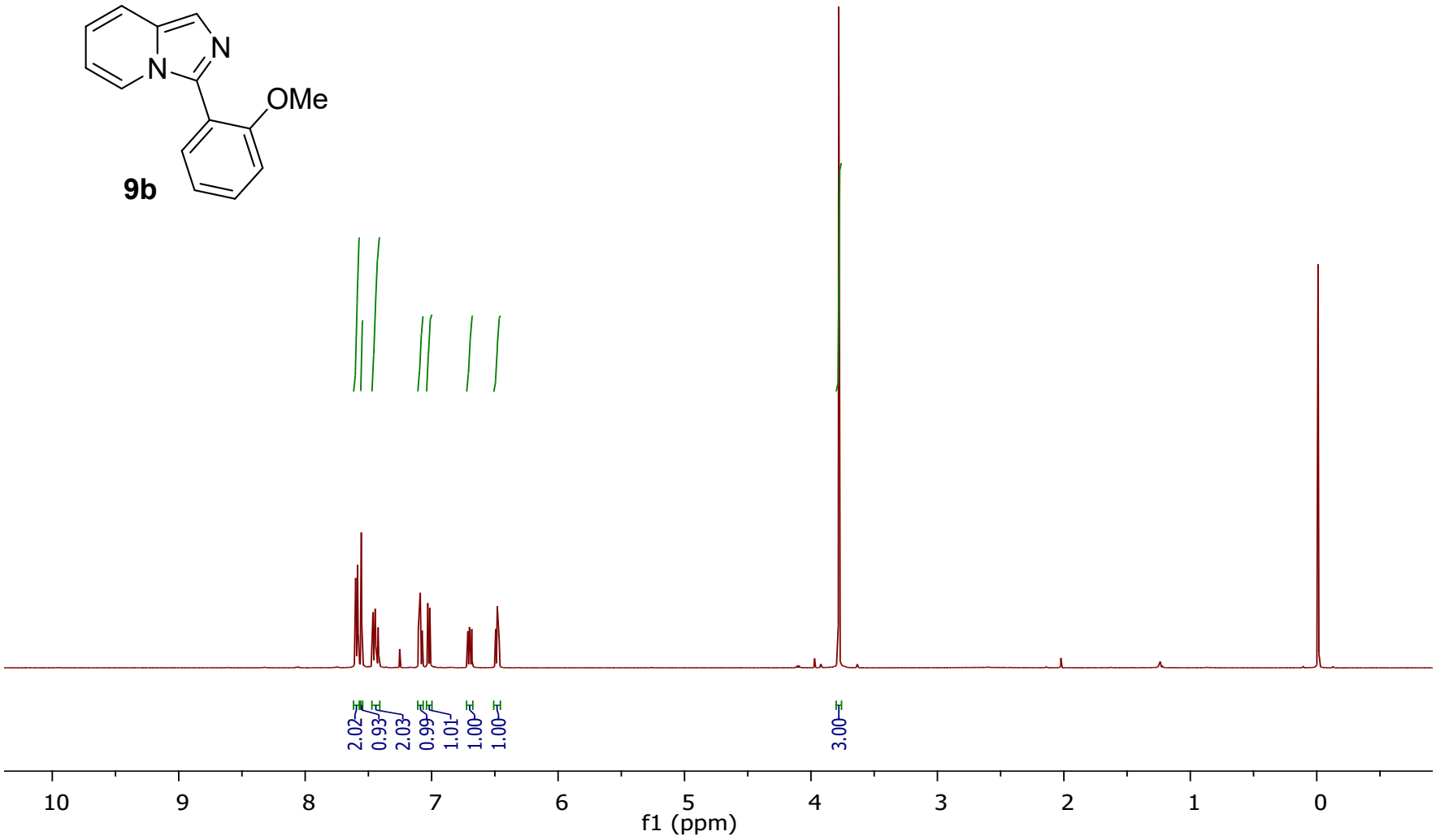

PCy2
N
N
4a
139.98
131.31
128.98
130.64
129.07
128.65
126.31
121.69
119.46
119.28
113.05
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
32.99
32.85
30.79
30.51
29.55
27.30
27.08
26.65
0.09
f1 (ppm)

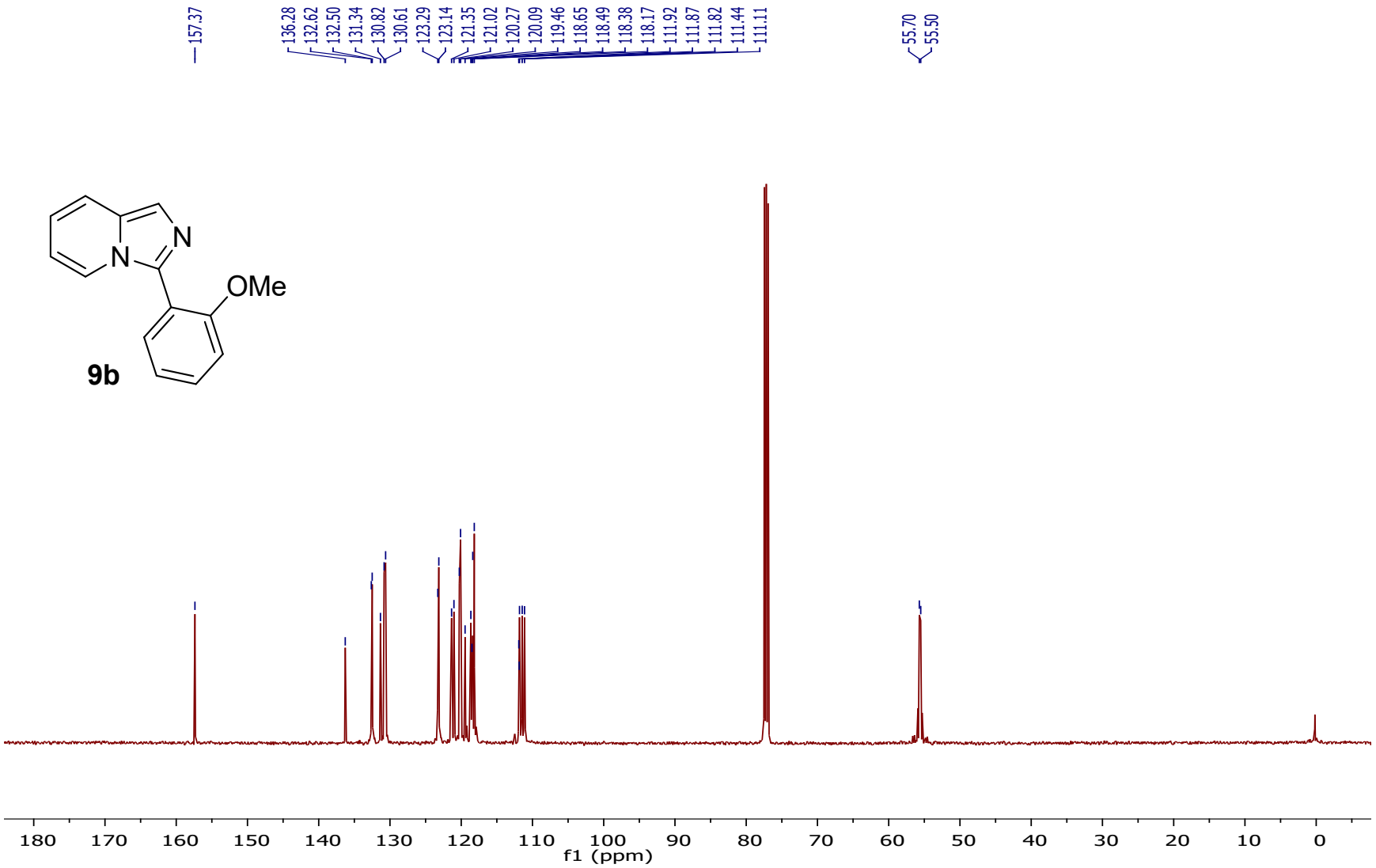

PCy2
N
N
4a
-25.83
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
50 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

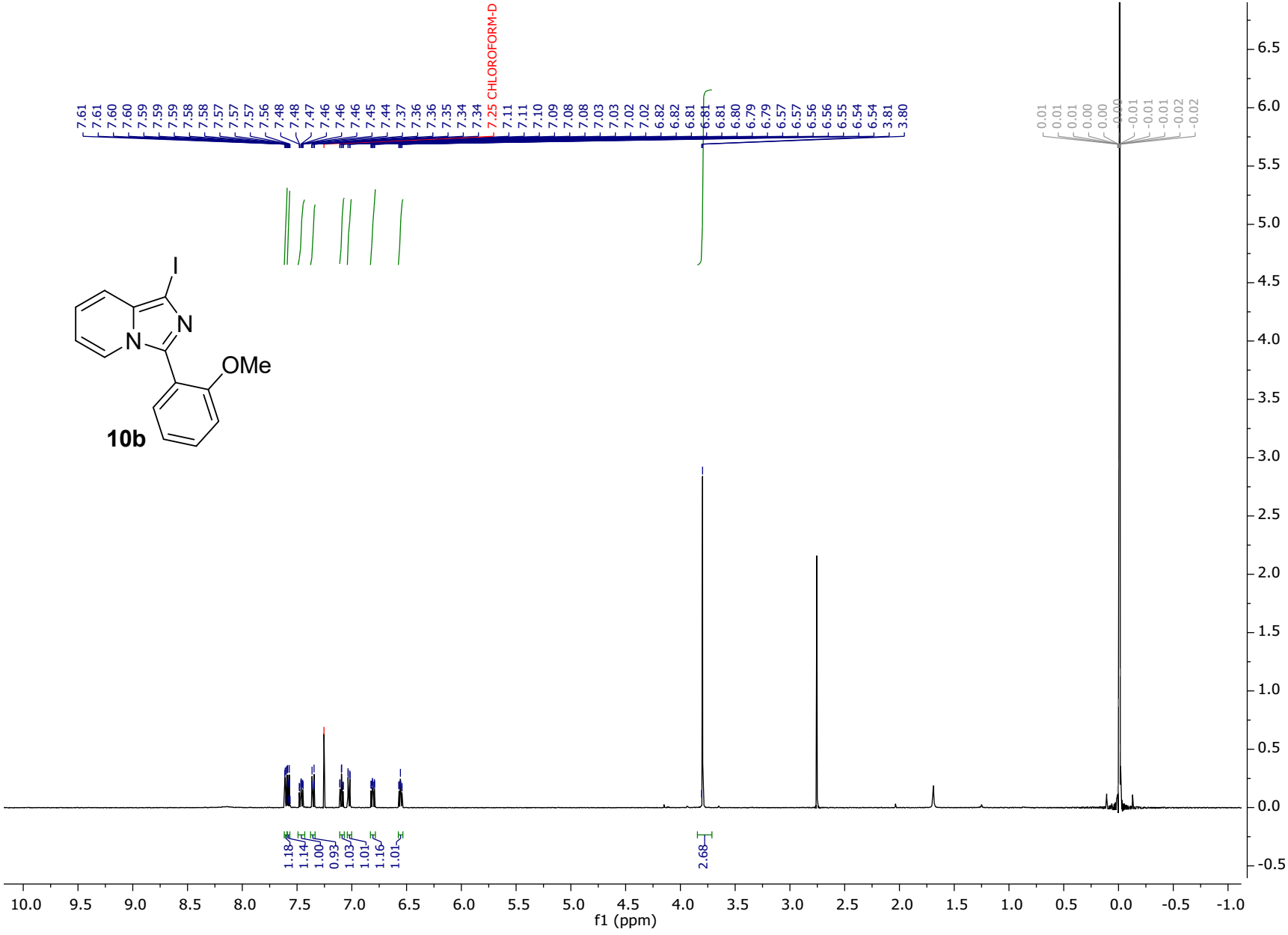

PPh2
N
N
4b
1.00
2.04
3.95
5.08
5.08
0.99
1.00
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

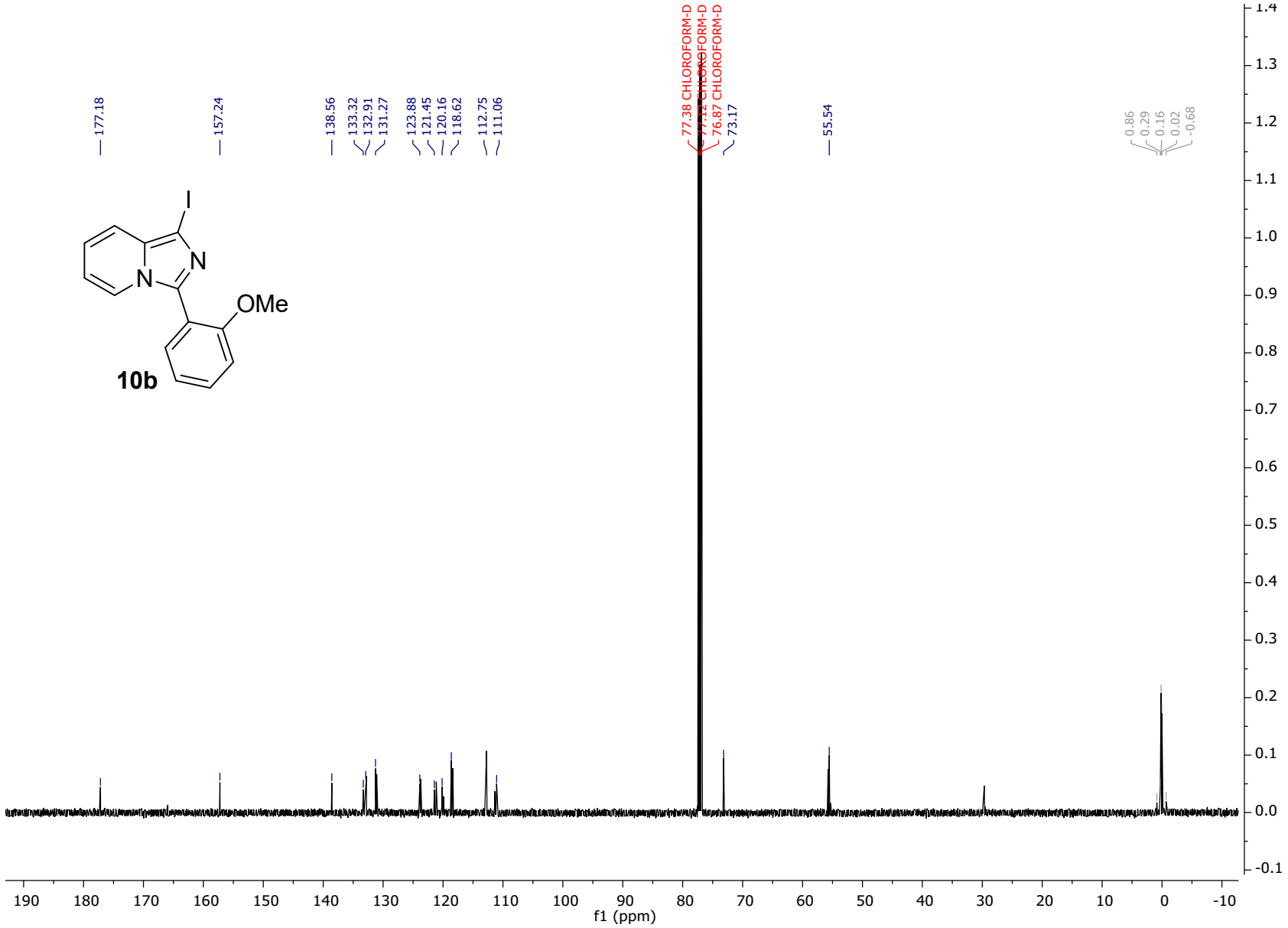

140.81
140.73
138.22
138.06
138.02
137.95
133.67
133.55
133.53
133.40
130.13
129.10
128.92
128.57
128.47
128.23
128.18
126.22
122.26
122.04
120.52
120.38
119.25
119.20
119.06
119.01
113.42
PPh2
N
N
4b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

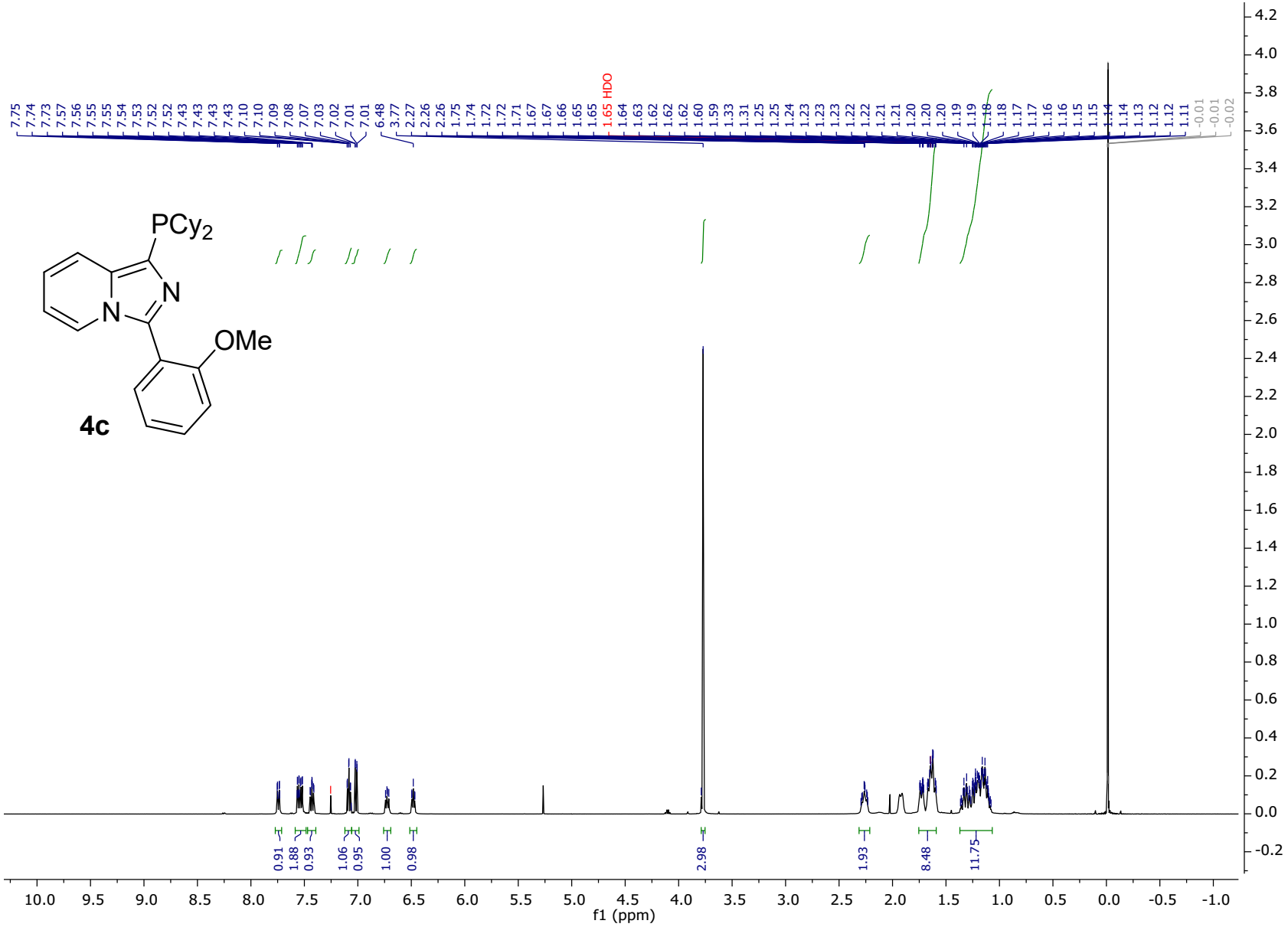

-31.31
PPh2
N
N
4b
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

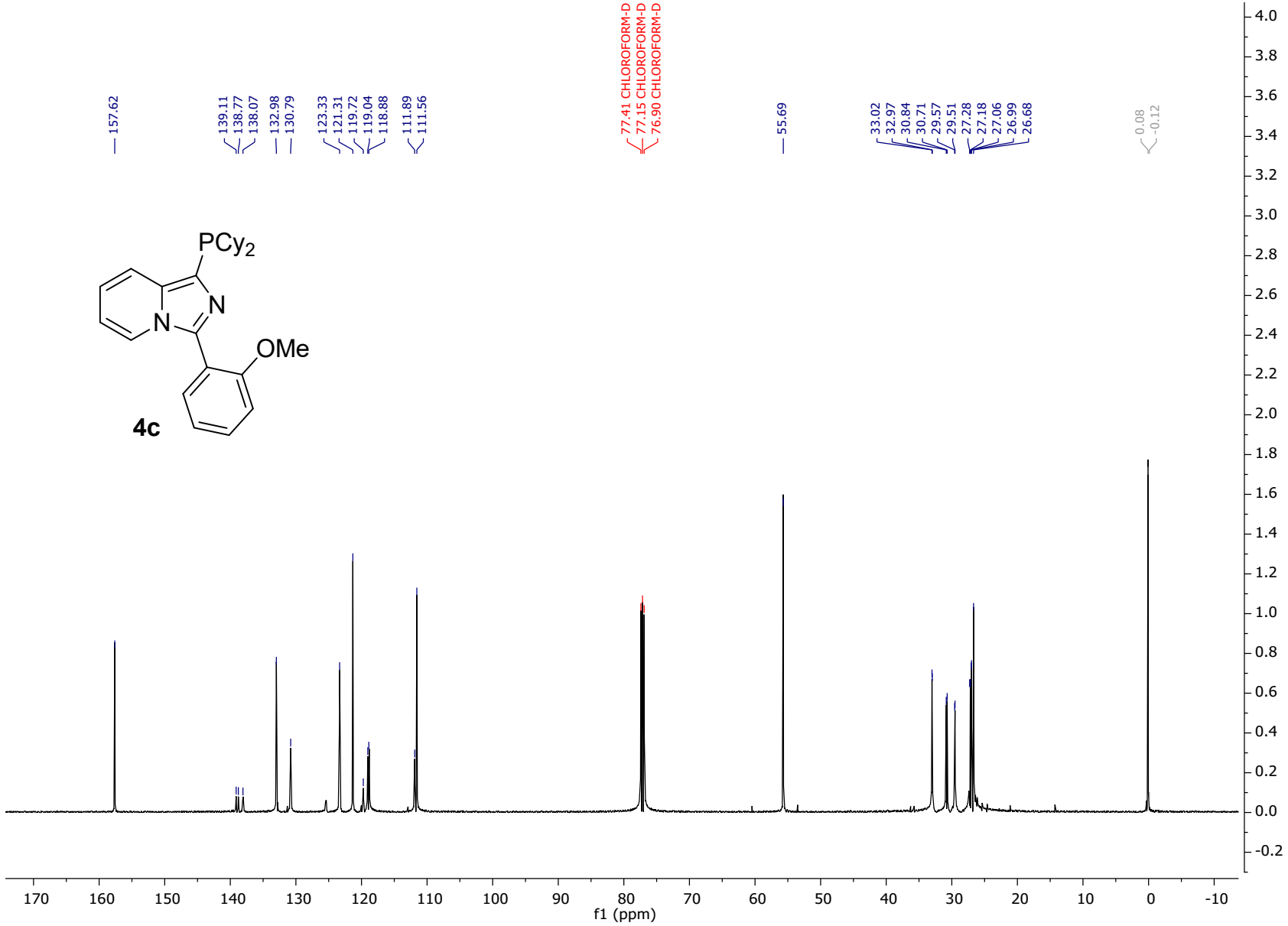

N
N
OMe
9b
2.02
0.93
2.03
0.99
1.01
1.00
1.00
3.00
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

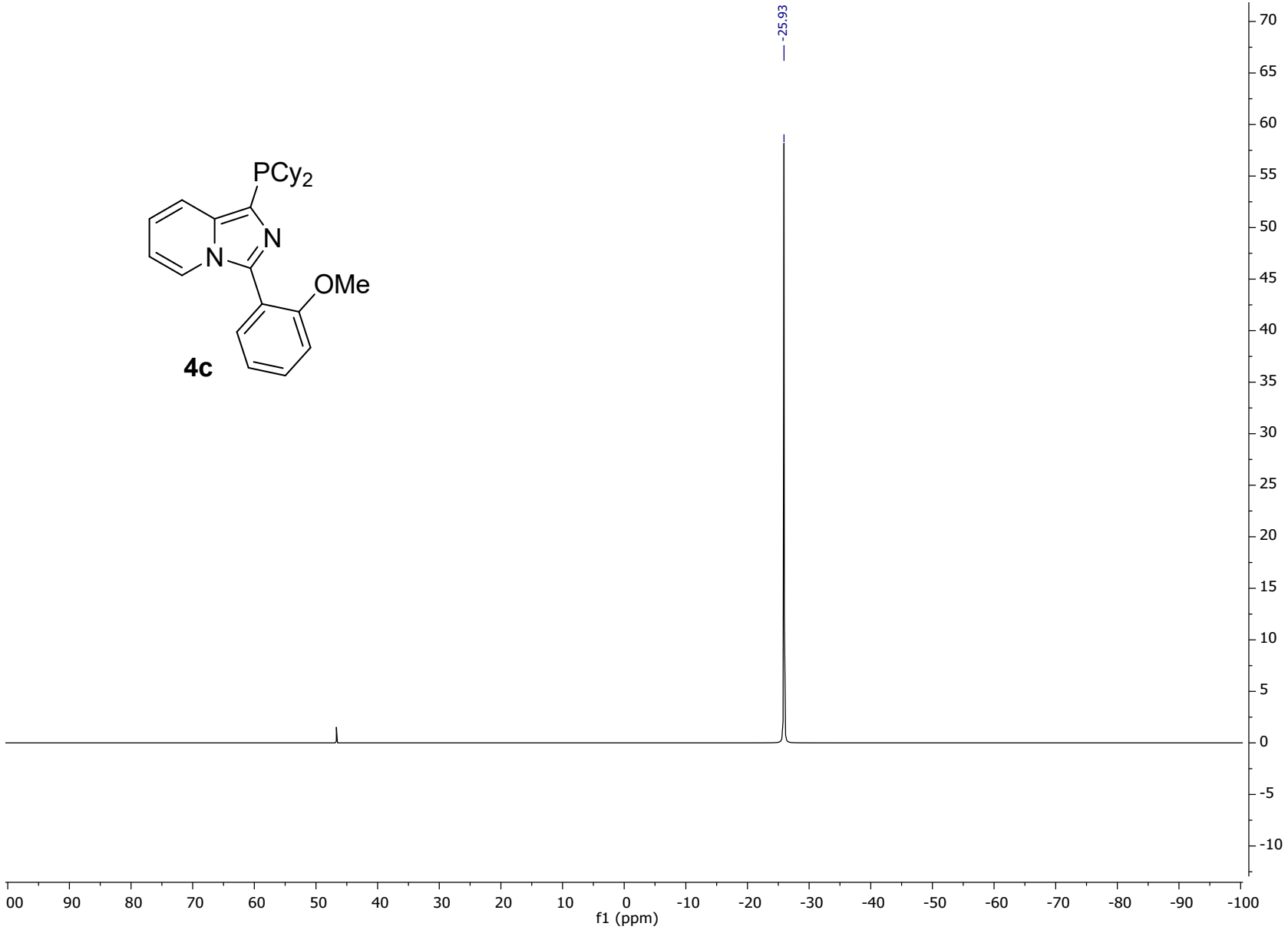

157.37
136.28
132.62
132.50
131.34
130.82
130.61
123.29
123.14
121.35
121.02
120.27
120.09
119.46
118.65
118.49
118.38
118.17
111.92
111.87
111.82
111.44
111.11
55.70
55.50
N
N
OMe
9b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

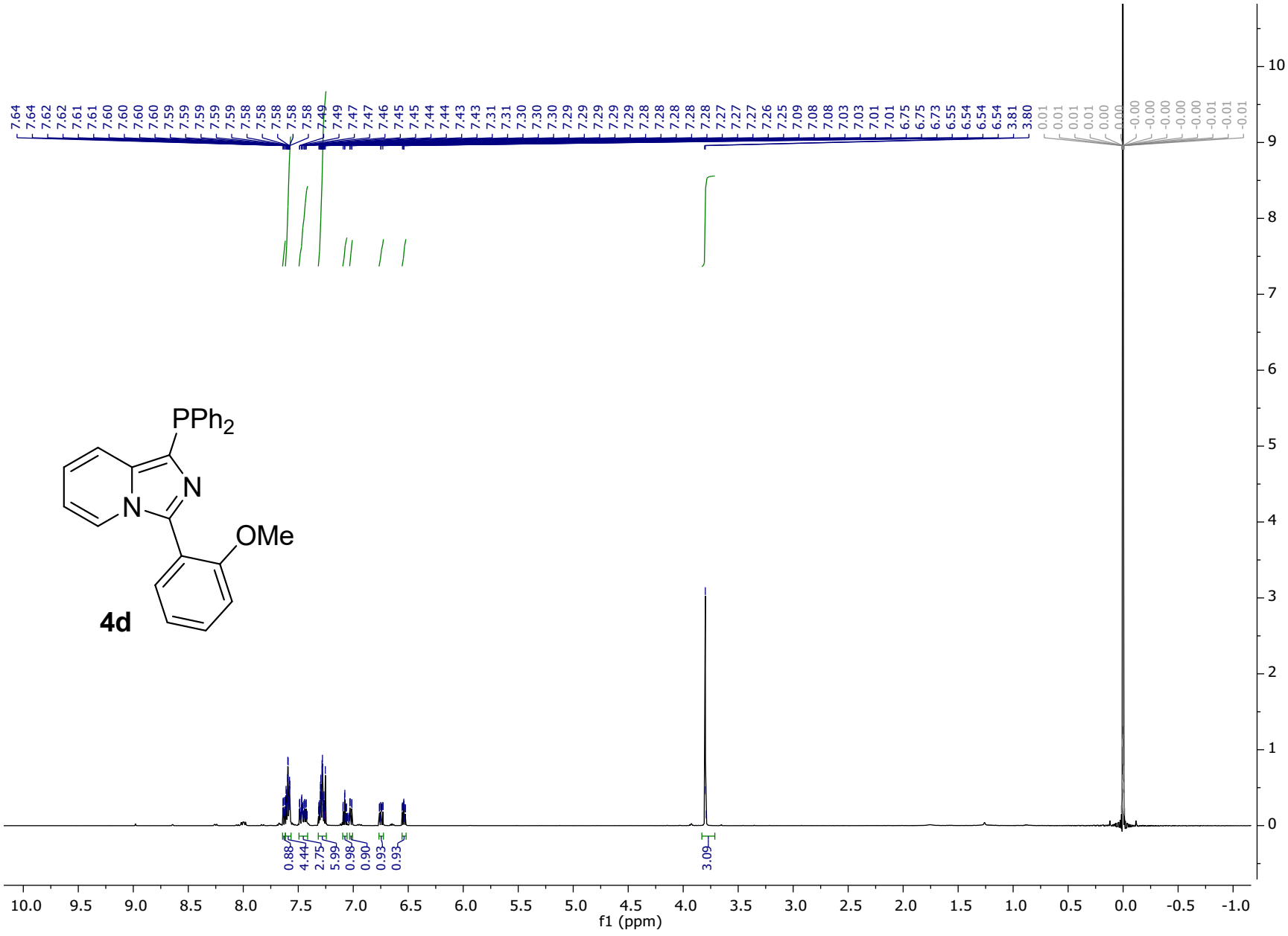

7.61 7.61 7.60 7.60 7.59 7.59 7.59 7.58 7.58 7.57 7.57 7.57 7.56 7.48 7.48 7.47 7.46 7.46 7.46 7.45 7.44 7.37 7.36 7.36 7.35 7.34 7.34 7.25 CHLOROFORM-D 7.11 7.11 7.10 7.09 7.08 7.08 7.03 7.03 7.02 7.02 6.82 6.82 6.81 6.81 6.80 6.79 6.57 6.57 6.56 6.56 6.55 6.54 6.54 3.81 3.80
0.01 0.01 0.01 0.00 0.00 0.00 -0.01 -0.01 -0.01 -0.02 -0.02
I
N
N
OMe
10b
1.18 1.14 1.00 0.93 1.03 1.01 1.16 1.01
2.68
f1 (ppm)

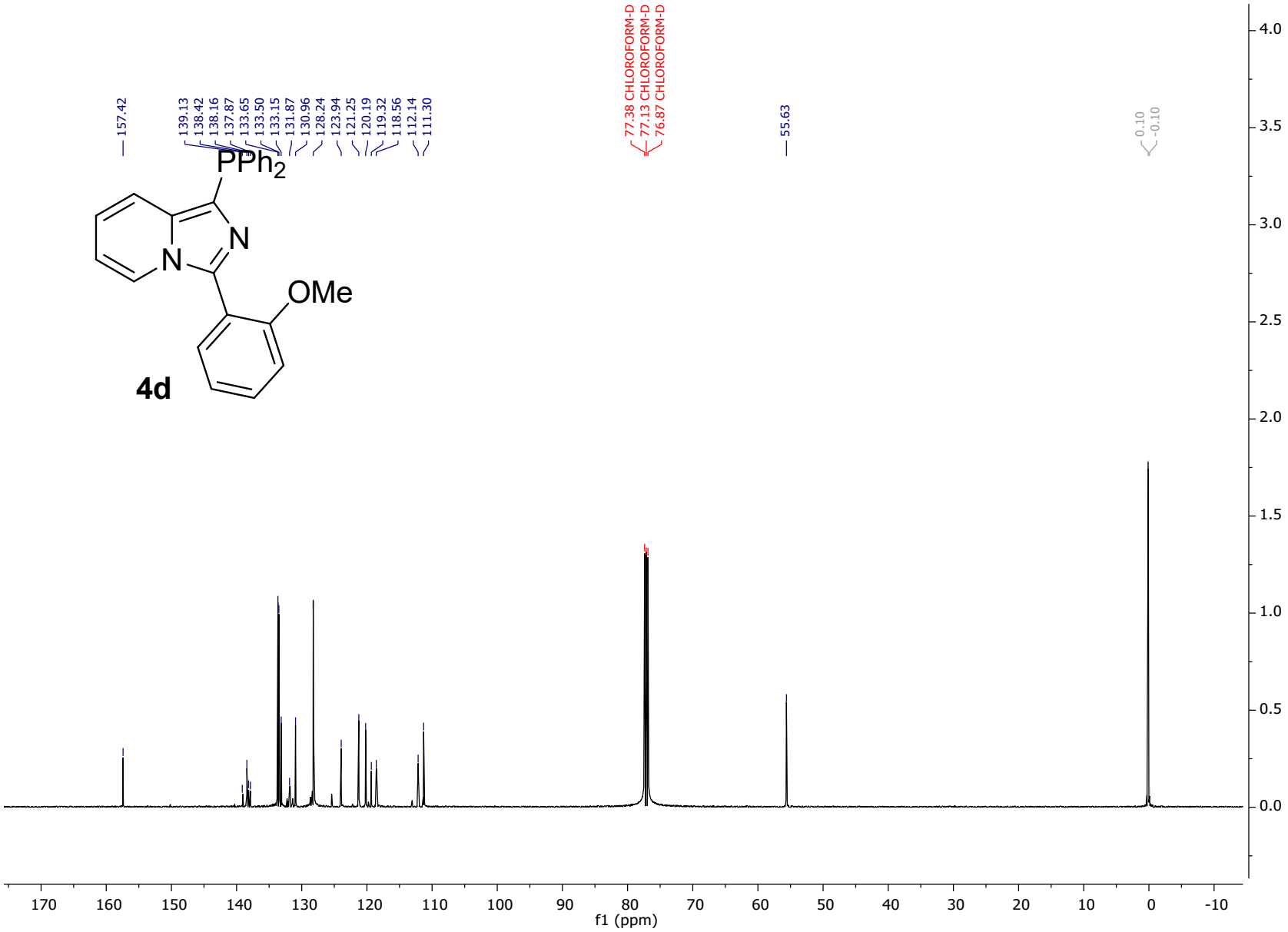

177.18
157.24
138.56
133.32
132.91
131.27
123.88
121.45
120.16
118.62
112.75
111.06
77.38 CHLOROFORM-D
77.12 CHLOROFORM-D
76.87 CHLOROFORM-D
73.17
55.54
0.86
0.29
0.16
0.02
-0.68
I
N
N
OMe
10b
f1 (ppm)

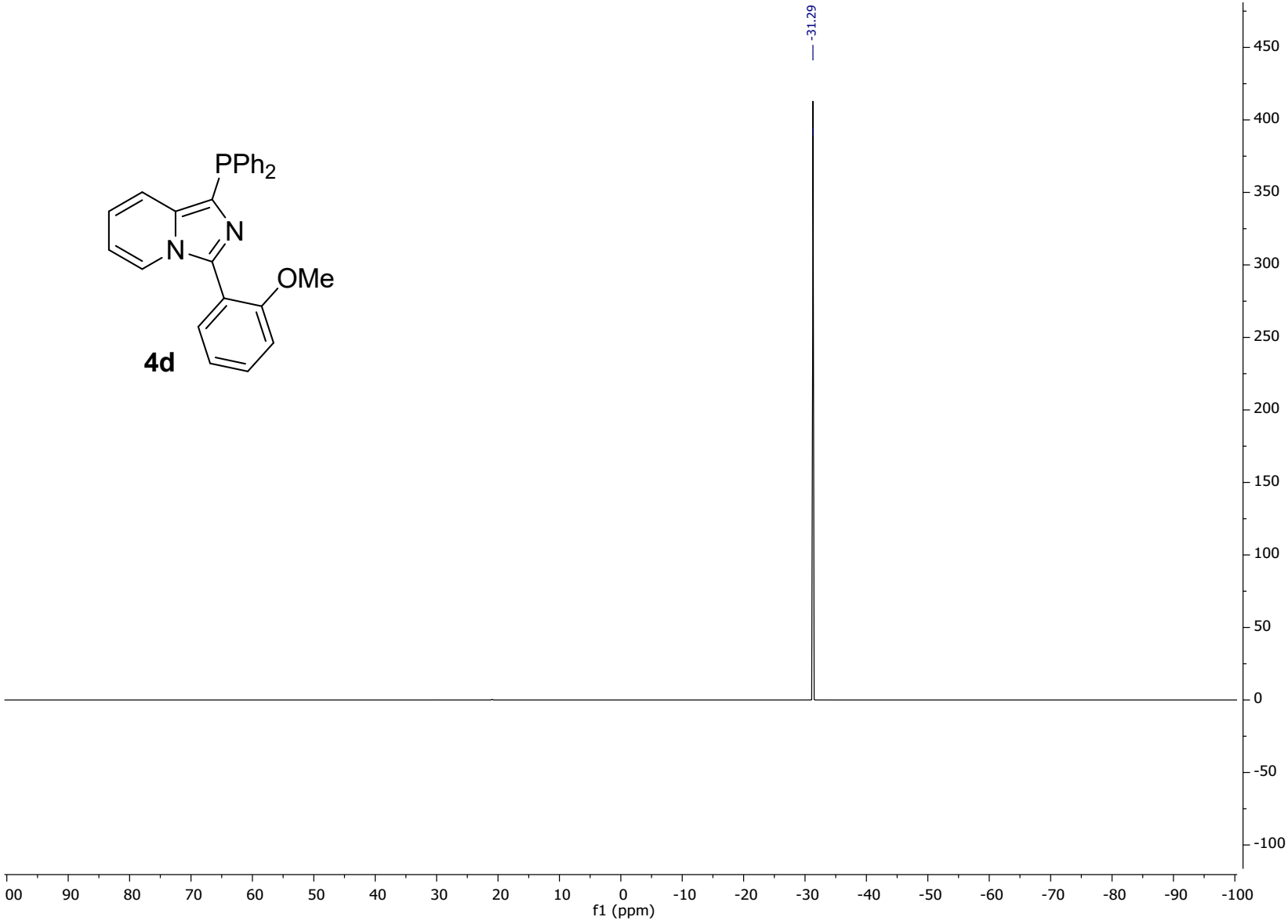

PCy2
N
N
OMe
4c
HDO
f1 (ppm)

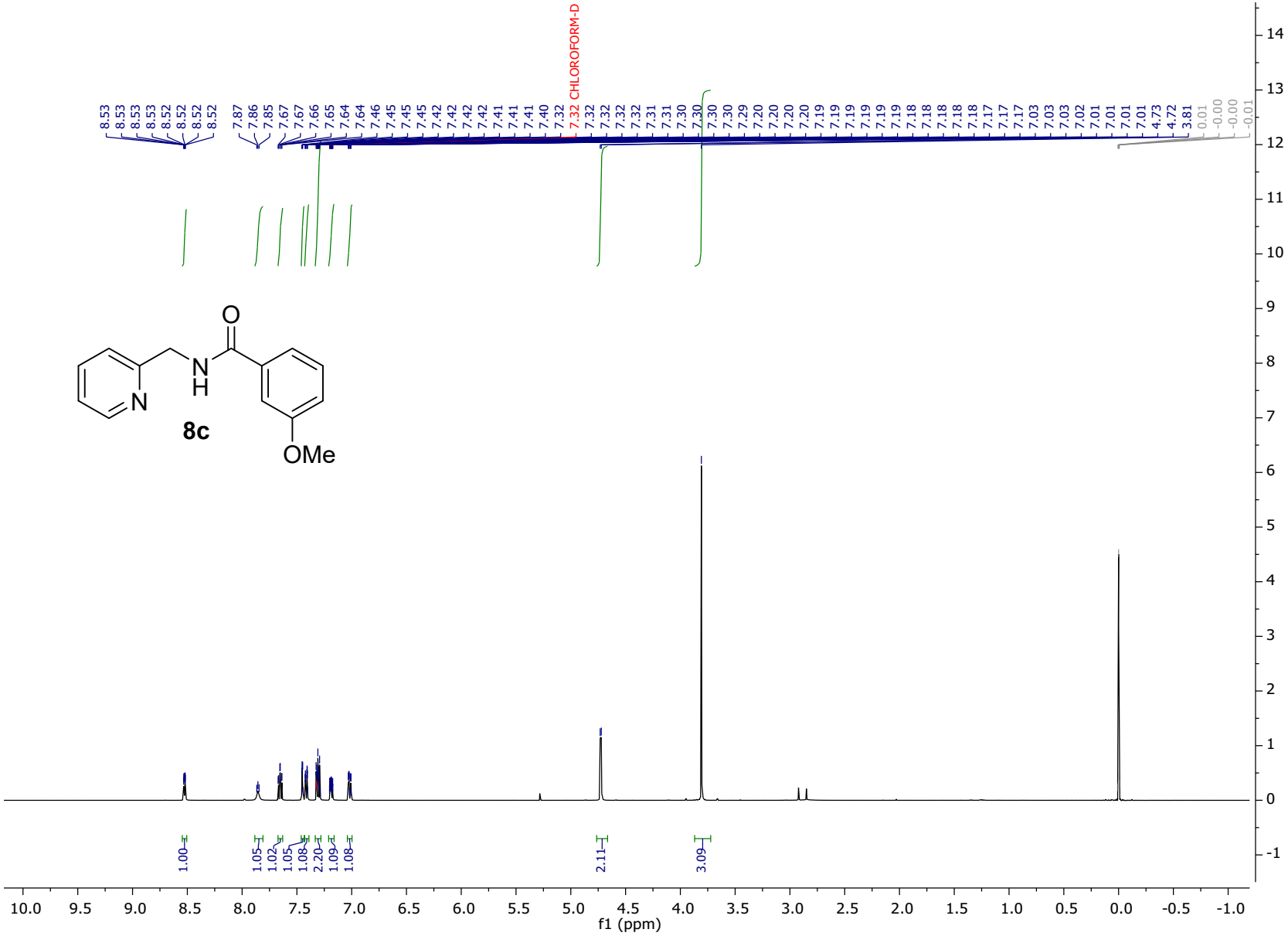

157.62
139.11
138.77
138.07
132.98
130.79
123.33
121.31
119.72
119.04
118.88
111.89
111.56
77.41 CHLOROFORM-D
77.15 CHLOROFORM-D
76.90 CHLOROFORM-D
55.69
33.02
32.97
30.84
30.71
29.57
29.51
27.28
27.18
27.06
26.99
26.68
0.08
-0.12
PCy2
N
N
OMe
4c
f1 (ppm)

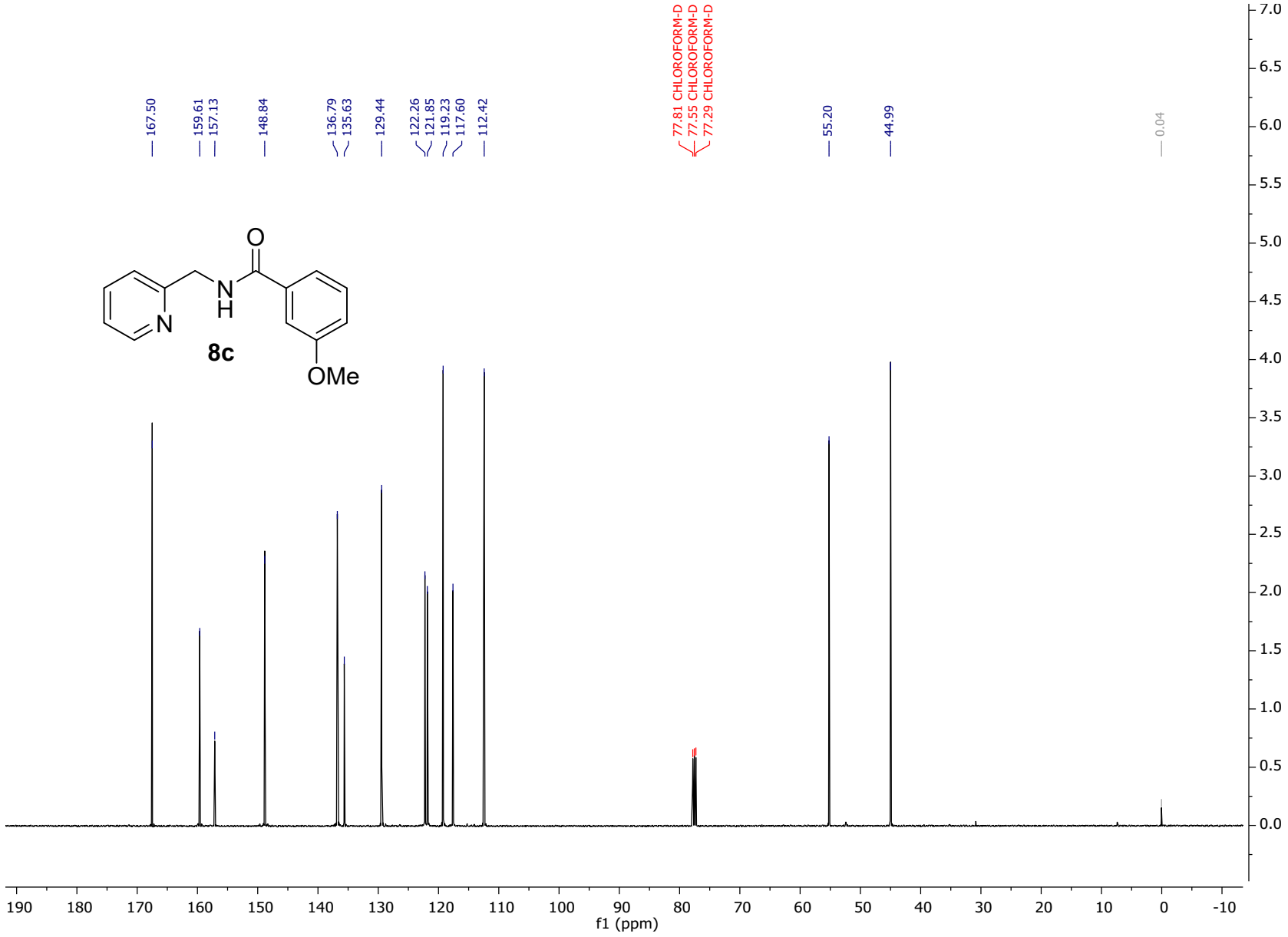

PCy2
N
N
OMe
4c
-25.93
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
-5
-10
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

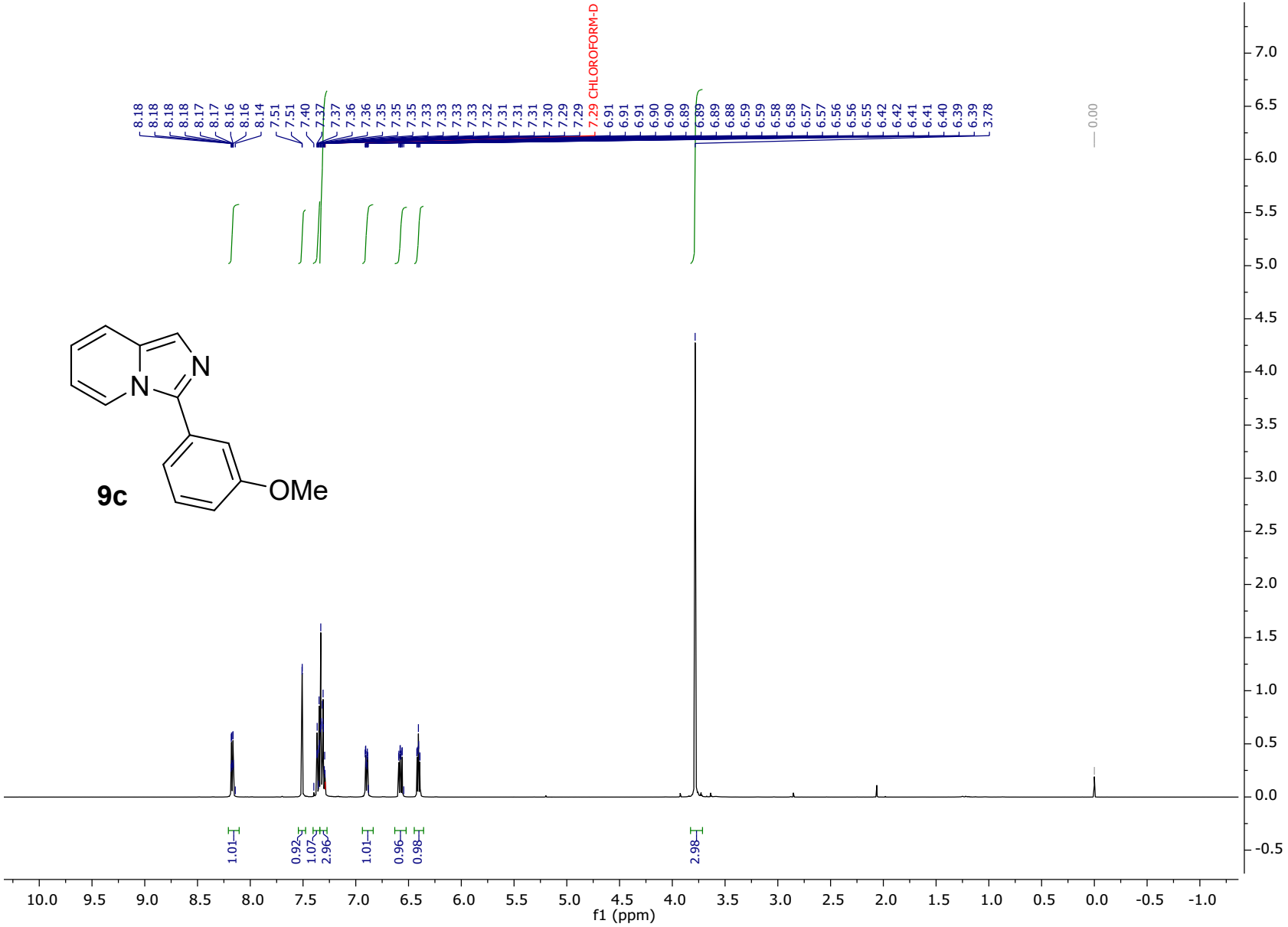

PPh2
N
N
OMe
4d
f1 (ppm)

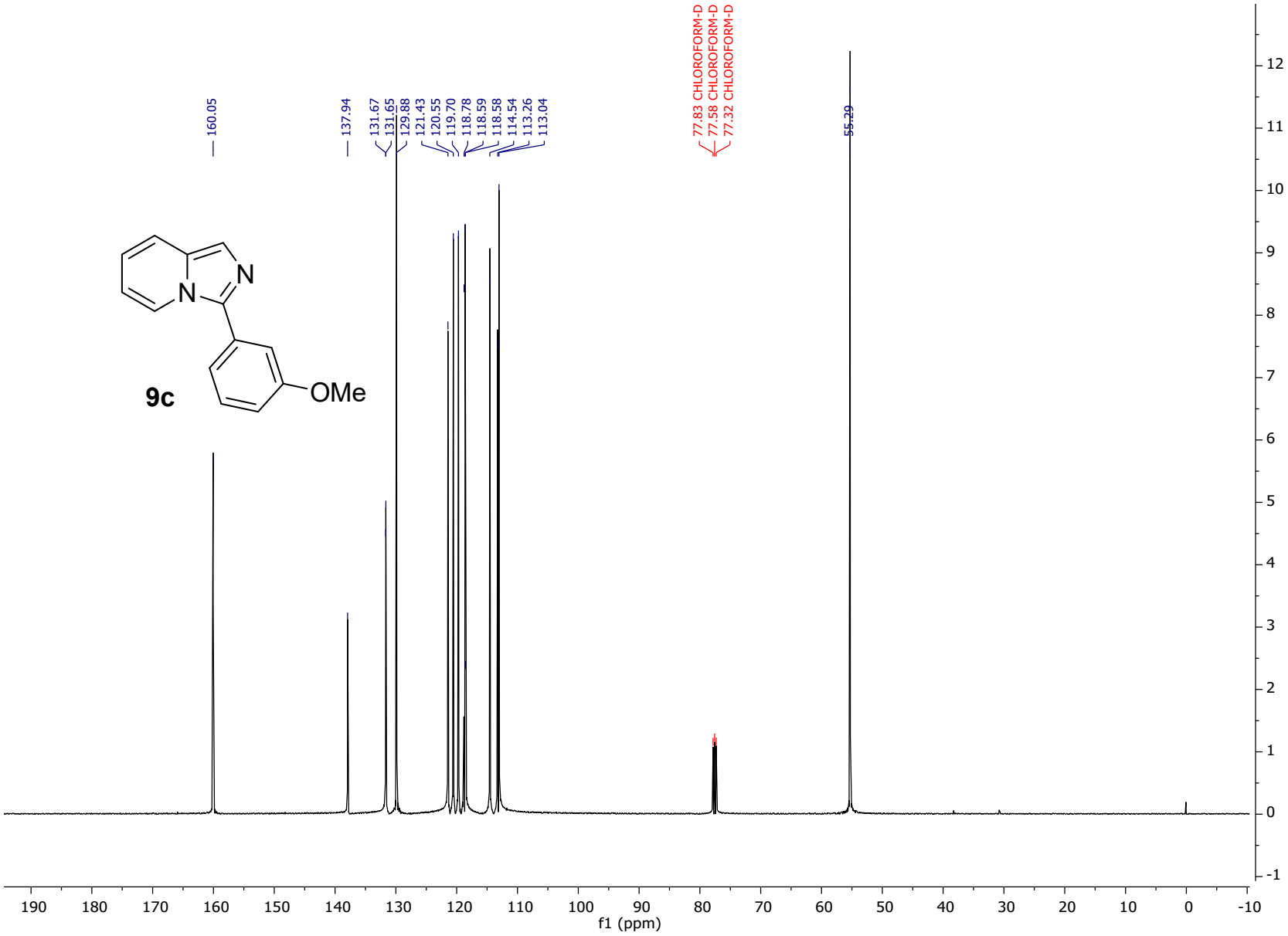

157.42
139.13
138.42
138.16
137.87
133.65
133.50
133.15
131.87
130.96
128.24
123.94
121.25
120.19
119.32
118.56
112.14
111.30
77.38 CHLOROFORM-D
77.13 CHLOROFORM-D
76.87 CHLOROFORM-D
55.63
0.10
-0.10
PPh2
N
N
OMe
4d
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

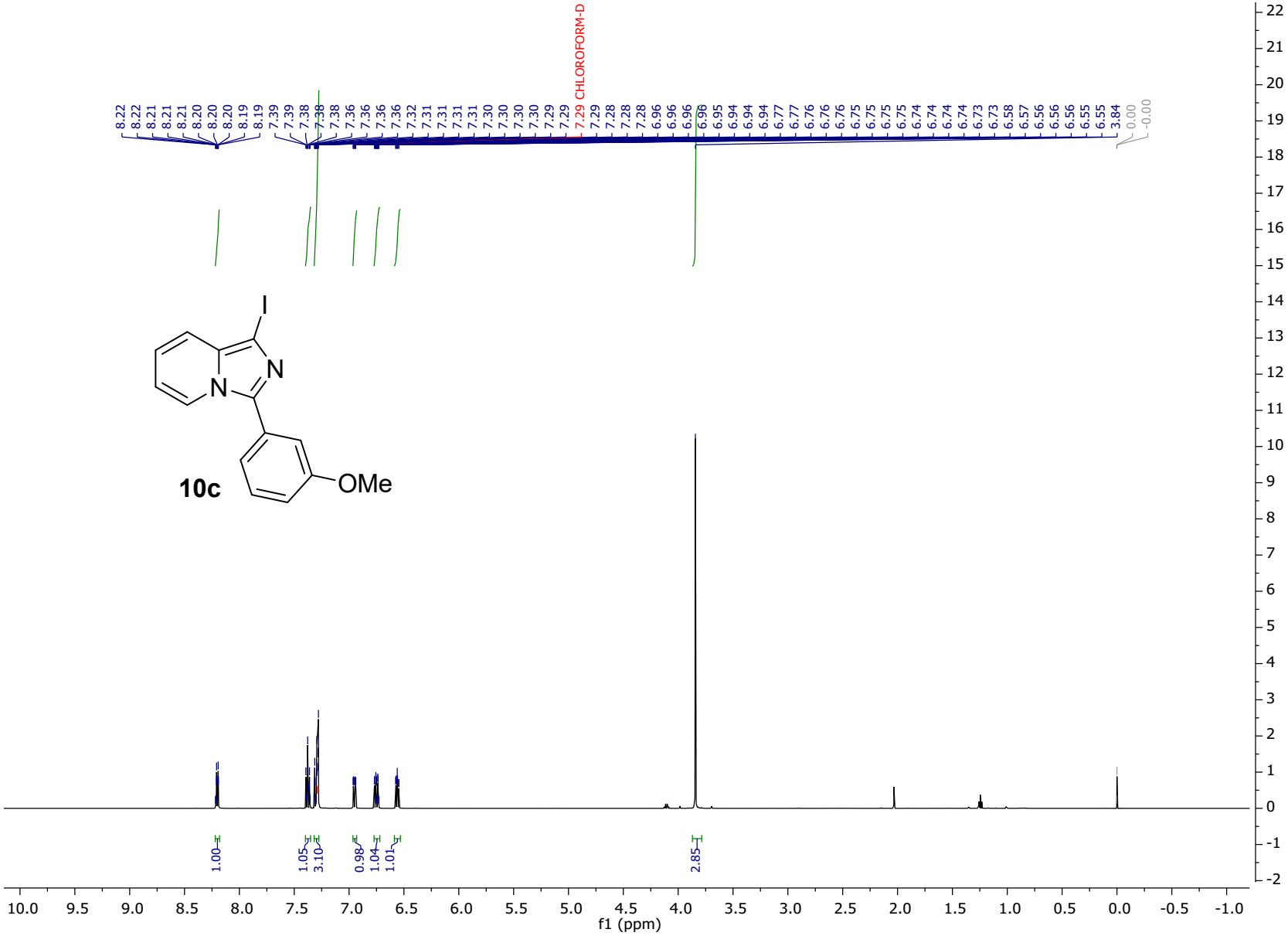

PPh2
N
N
OMe
4d
-31.29
450
400
350
300
250
200
150
100
50
0
-50
-100
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

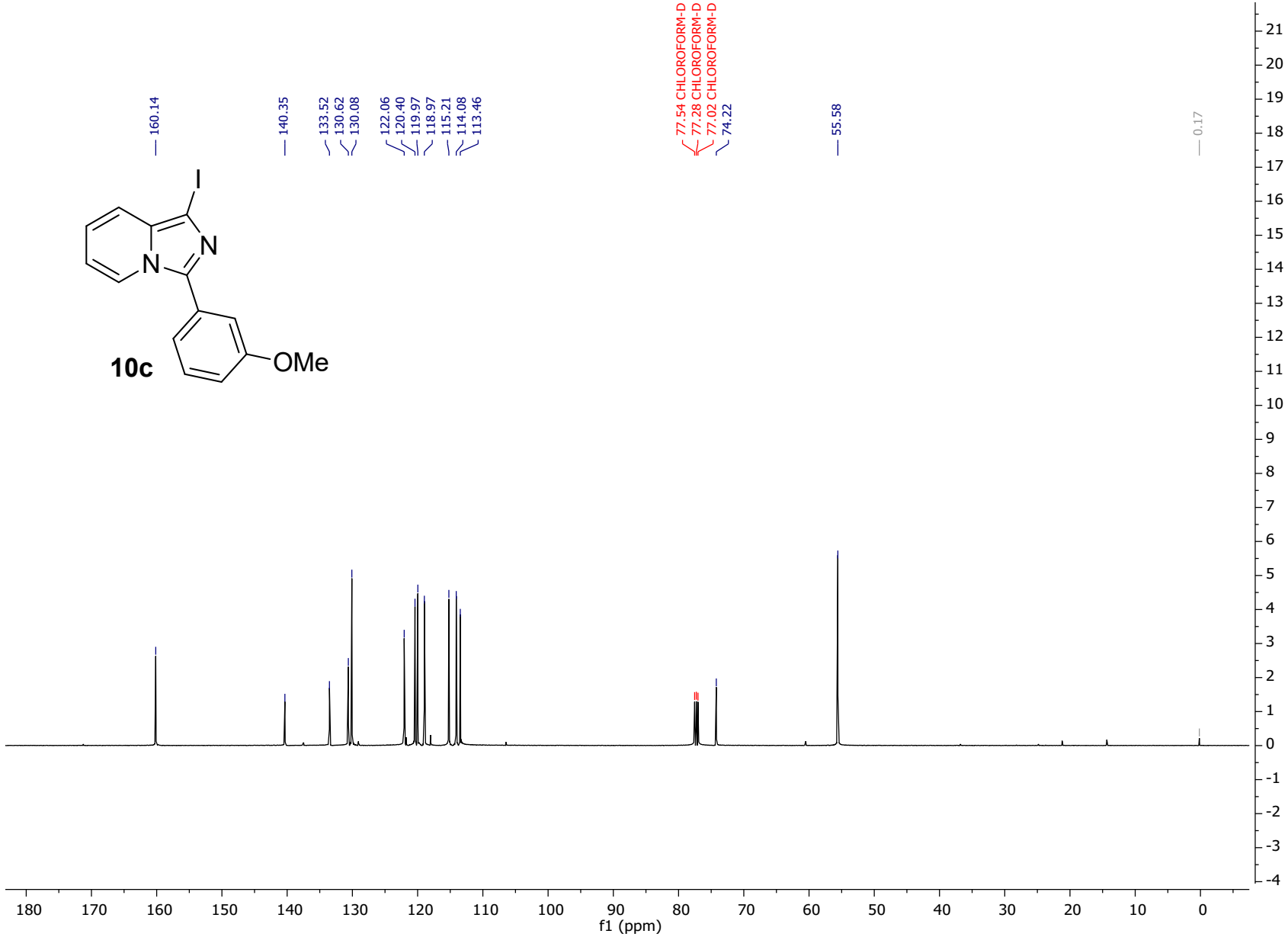

CHLOROFORM-D
8.53 8.53 8.53 8.52 8.52 8.52 8.52
7.87 7.86 7.85 7.67 7.67 7.66 7.65 7.64 7.64 7.46 7.45 7.45 7.42 7.42 7.42 7.41 7.41 7.40 7.32 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.29 7.20 7.20 7.20 7.19 7.19 7.19 7.19 7.19 7.18 7.18 7.18 7.18 7.17 7.17 7.17 7.03 7.03 7.02 7.01 7.01 7.01 4.73 4.72 3.81 0.01 -0.00 -0.00 -0.01
O
N
H
N
8c
OMe
1.00 1.05 1.02 1.05 1.08 2.20 1.09 1.08 2.11 3.09
f1 (ppm)

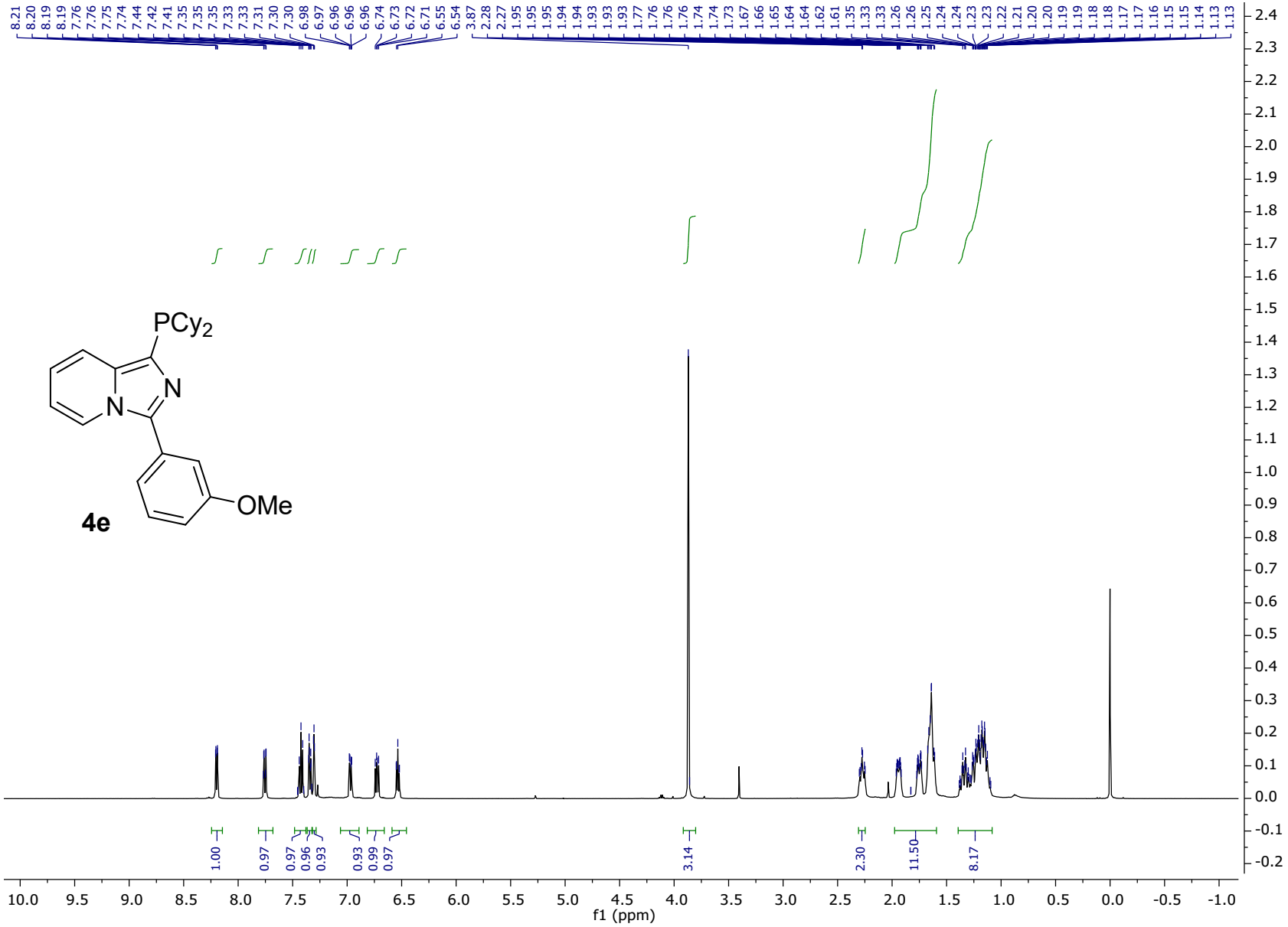

167.50
159.61
157.13
148.84
136.79
135.63
129.44
122.26
121.85
119.23
117.60
112.42
77.81 CHLOROFORM-D
77.55 CHLOROFORM-D
77.29 CHLOROFORM-D
55.20
44.99
0.04
O
N
H
N
8c
OMe
f1 (ppm)

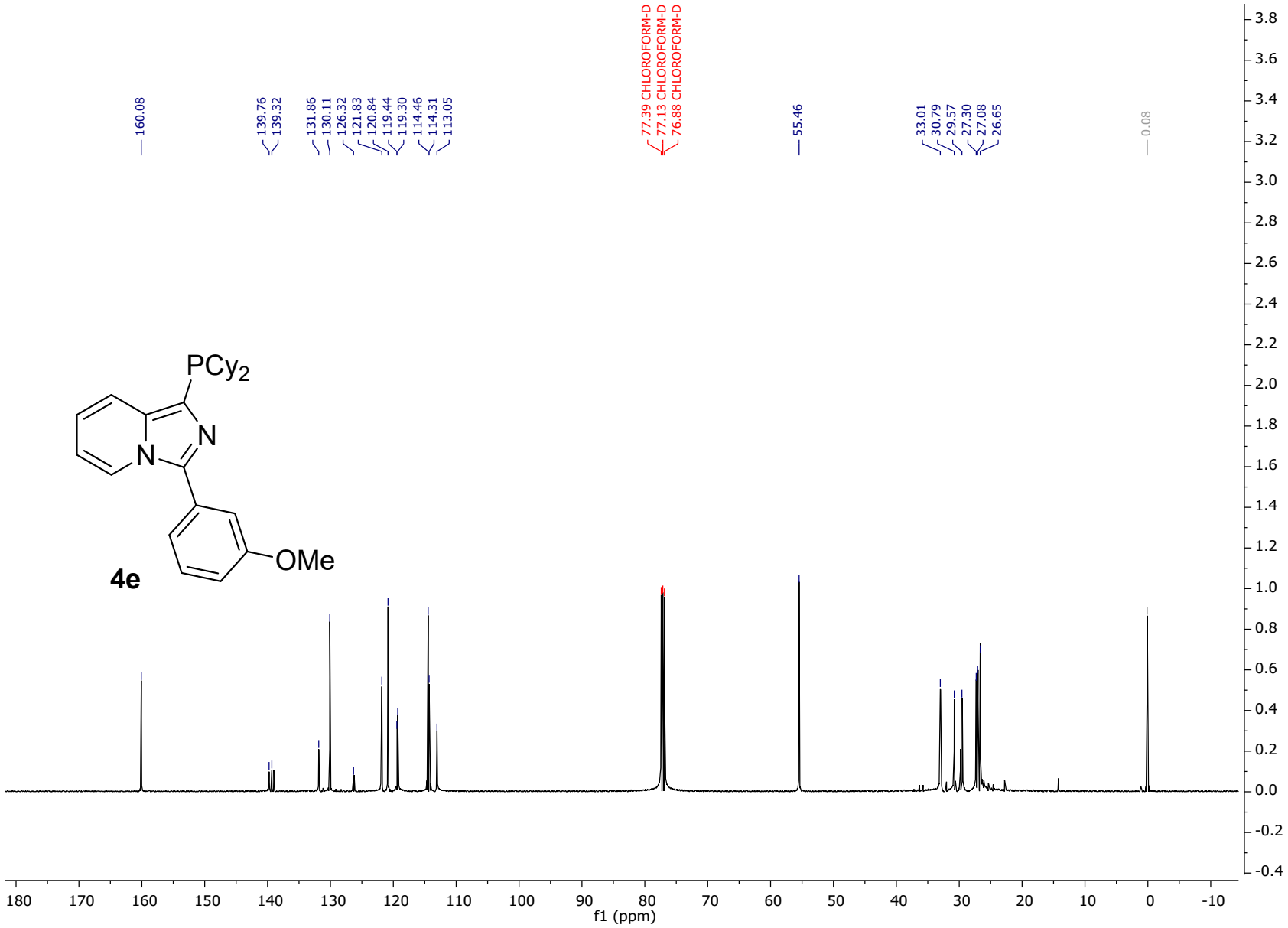

8.18 8.18 8.18 8.17 8.17 8.16 8.16 8.14 7.51 7.51 7.40 7.37 7.37 7.36 7.36 7.35 7.35 7.35 7.33 7.33 7.33 7.32 7.31 7.31 7.31 7.30 7.29 7.29 7.29 CHLOROFORM-D 6.91 6.91 6.91 6.90 6.90 6.89 6.89 6.89 6.88 6.59 6.59 6.58 6.58 6.57 6.57 6.56 6.56 6.55 6.42 6.42 6.41 6.41 6.40 6.39 6.39 3.78
0.00
N
N
OMe
9c
1.01
0.92
1.07
2.96
1.01
0.96
0.98
2.98
f1 (ppm)

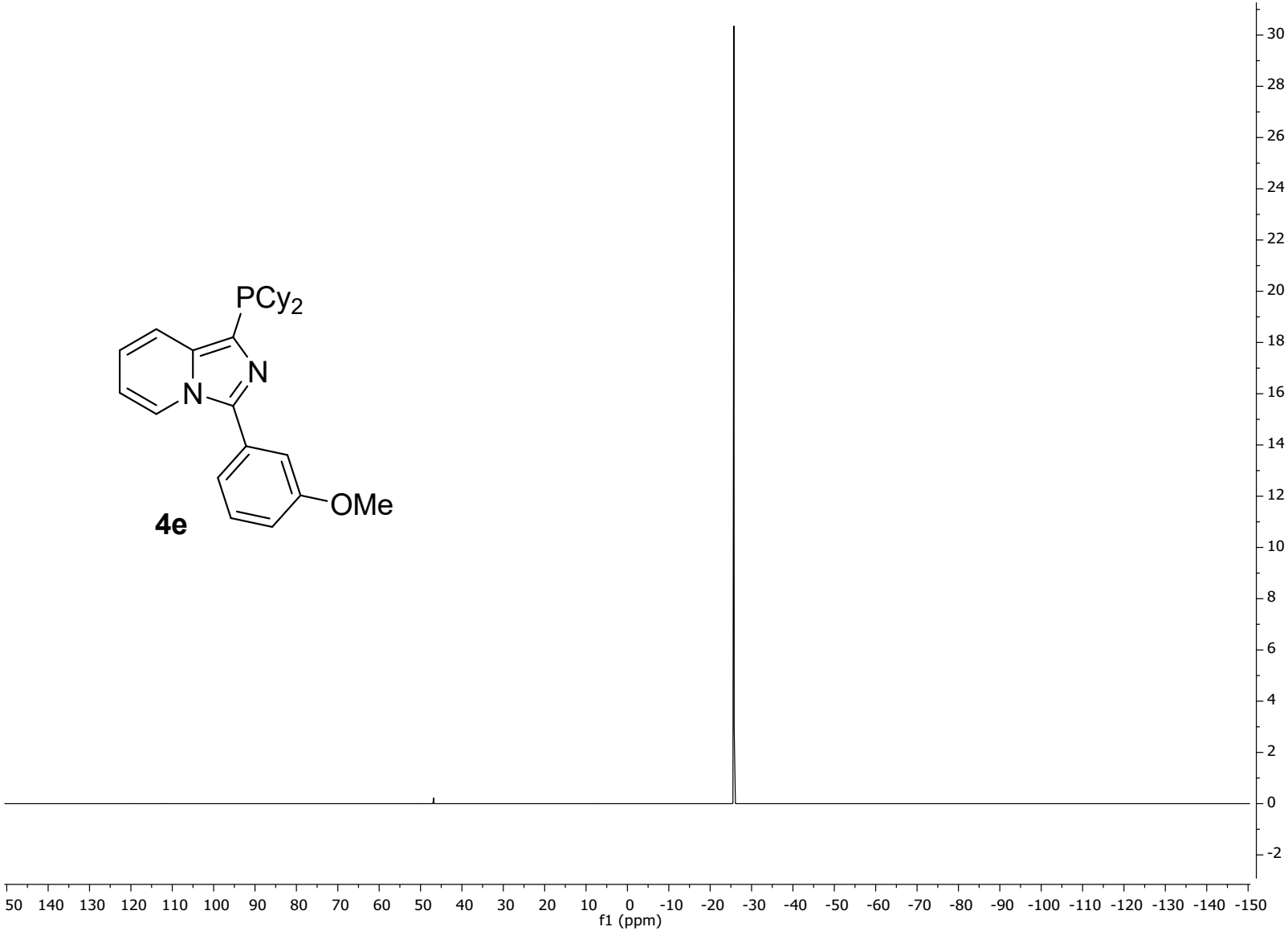

160.05
137.94
131.67
131.65
129.88
121.43
120.55
119.70
118.78
118.59
118.58
114.54
113.26
113.04
77.83 CHLOROFORM-D
77.58 CHLOROFORM-D
77.32 CHLOROFORM-D
55.29
N
N
OMe
9c
f1 (ppm)

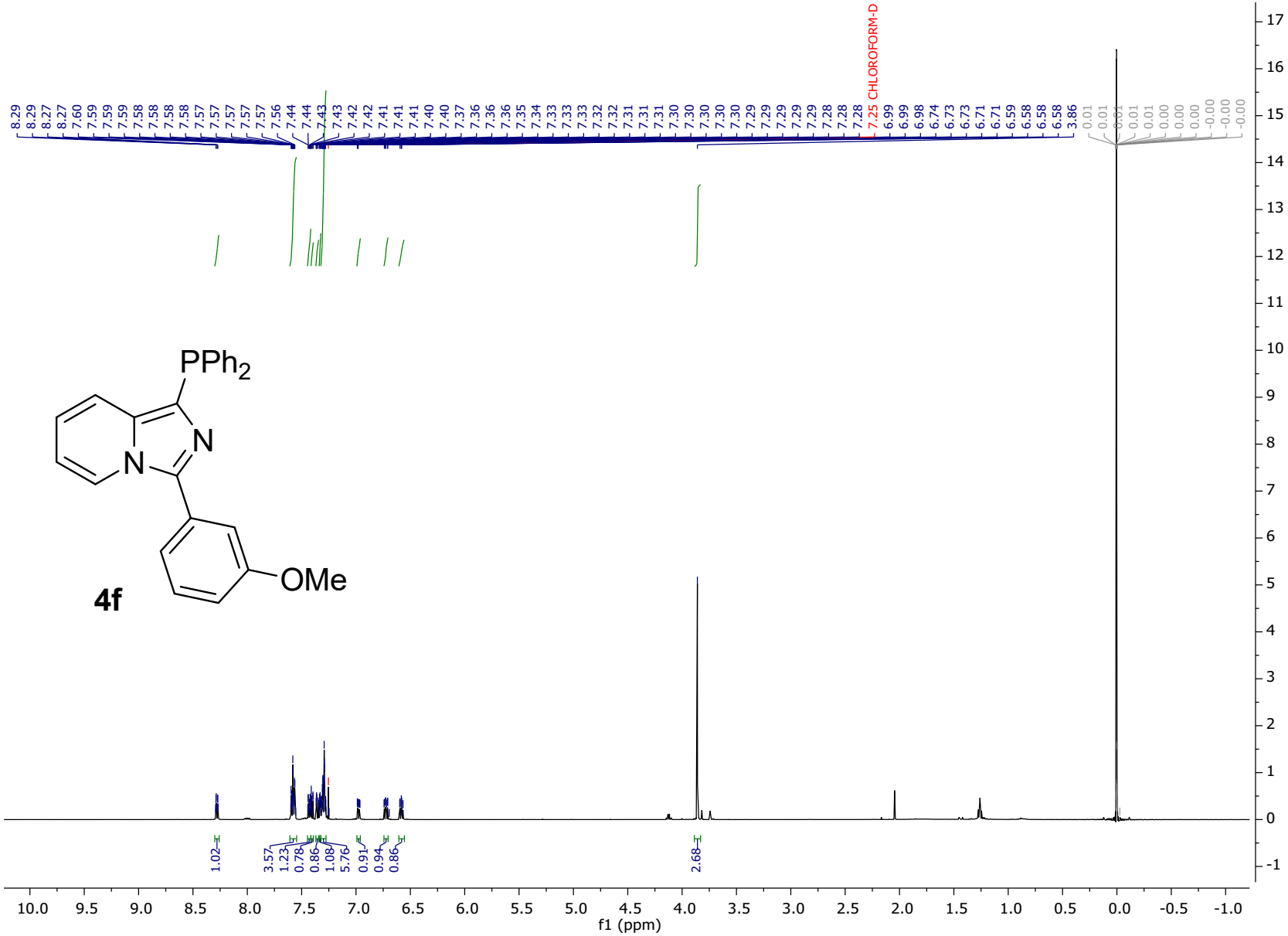

8.22 8.22 8.21 8.21 8.21 8.20 8.20 8.20 8.19 8.19 7.39 7.39 7.38 7.38 7.38 7.36 7.36 7.36 7.36 7.32 7.31 7.31 7.31 7.30 7.30 7.30 7.30 7.29 7.29 7.29 CHLOROFORM-D 7.29 7.28 7.28 7.28 6.96 6.96 6.96 6.96 6.95 6.94 6.94 6.94 6.77 6.77 6.76 6.76 6.76 6.75 6.75 6.75 6.75 6.74 6.74 6.74 6.74 6.73 6.73 6.58 6.57 6.56 6.56 6.56 6.55 6.55 3.84 0.00 -0.00
I
N
N
OMe
10c
1.00
1.05
3.10
0.98
1.04
1.01
2.85
f1 (ppm)

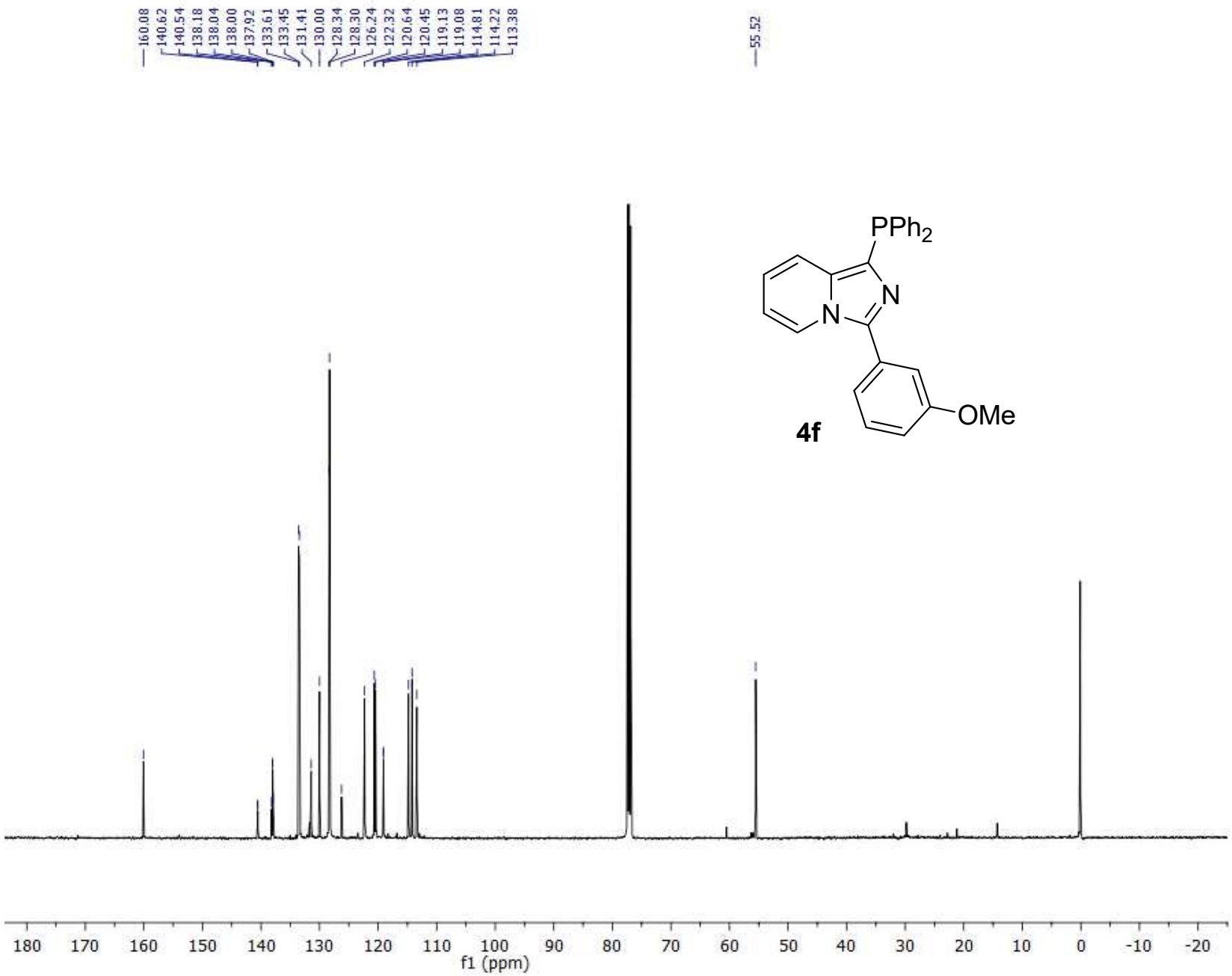

160.14
140.35
133.52
130.62
130.08
122.06
120.40
119.97
118.97
115.21
114.08
113.46
77.54 CHLOROFORM-D
77.28 CHLOROFORM-D
77.02 CHLOROFORM-D
74.22
55.58
0.17
I
N
N
OMe
10c
f1 (ppm)

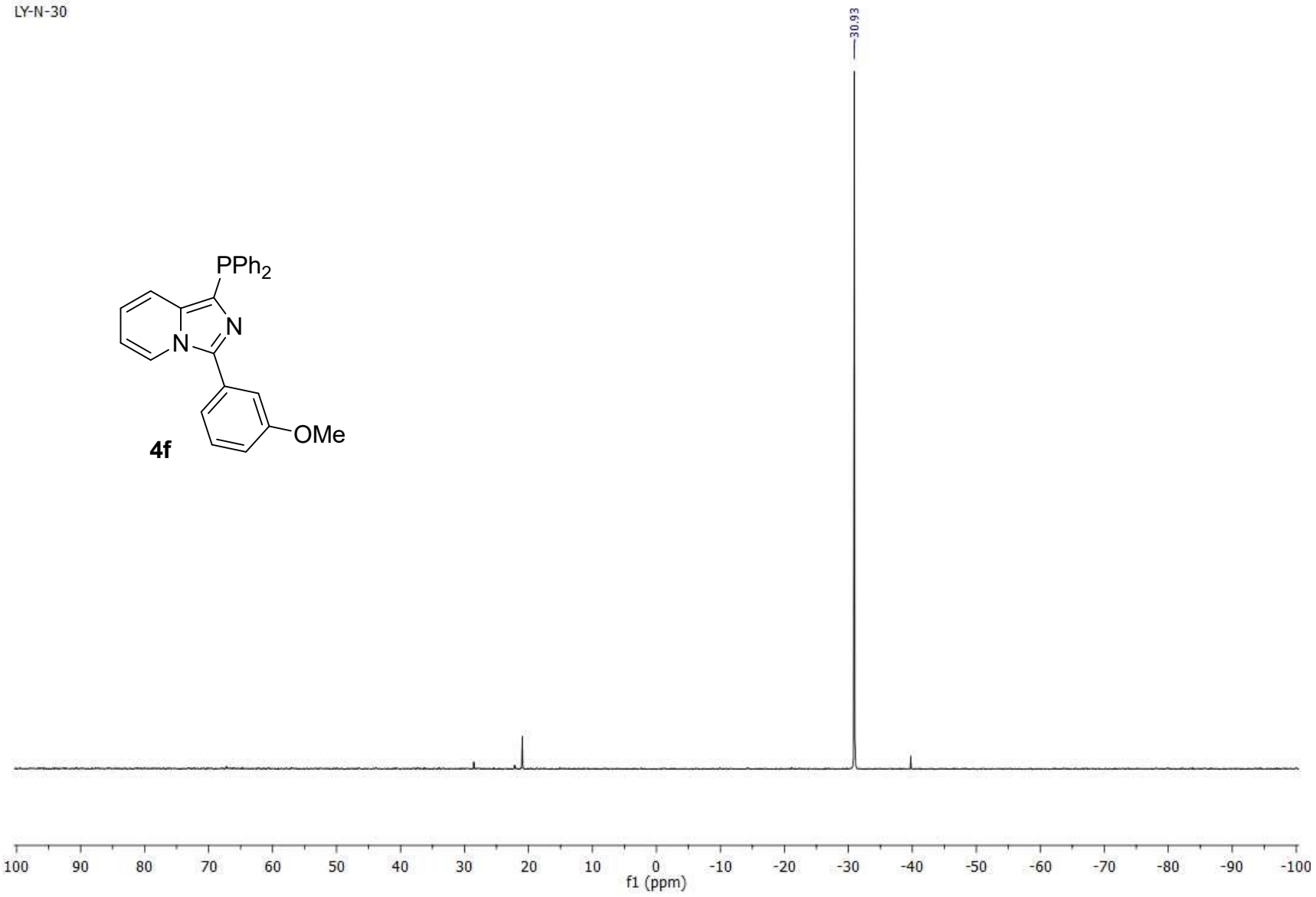

PCy2
N
N
OMe
4e
f1 (ppm)

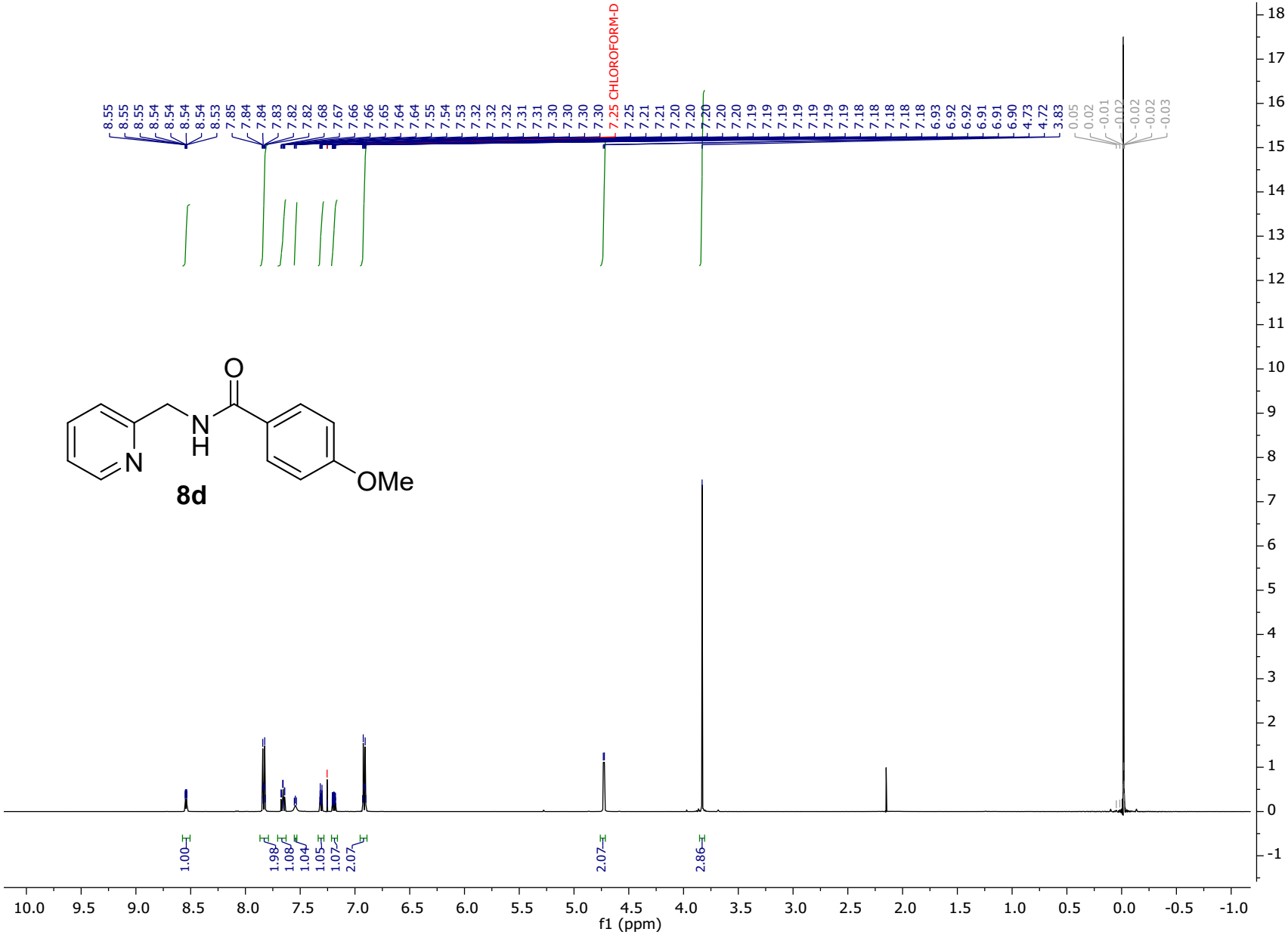

160.08
139.76
139.32
131.86
130.11
126.32
121.83
120.84
119.44
119.30
114.46
114.31
113.05
77.39 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
55.46
33.01
30.79
29.57
27.30
27.08
26.65
0.08
PCy2
N
N
OMe
4e
f1 (ppm)

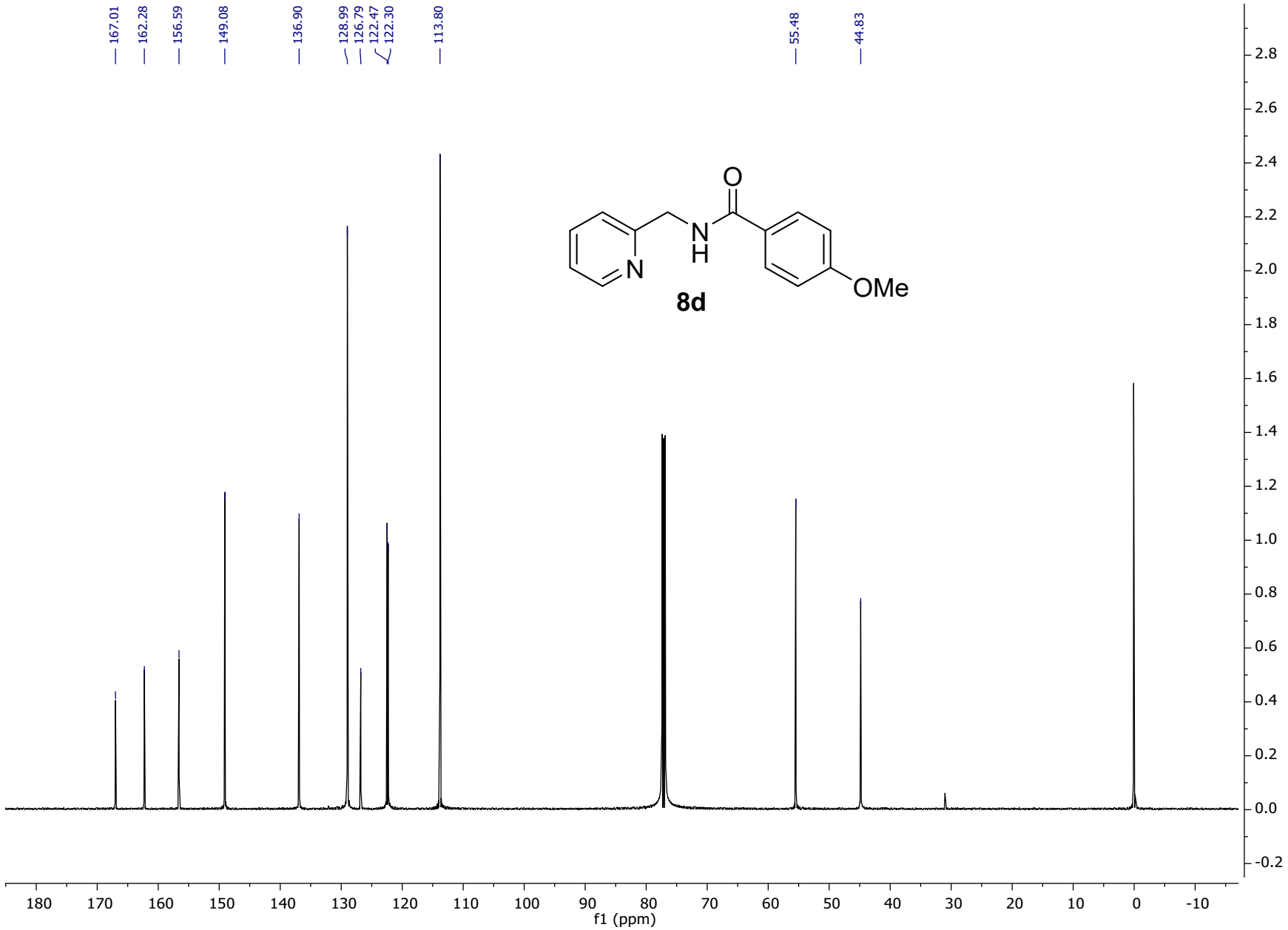

PCy2
N
N
OMe
4e
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
50 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

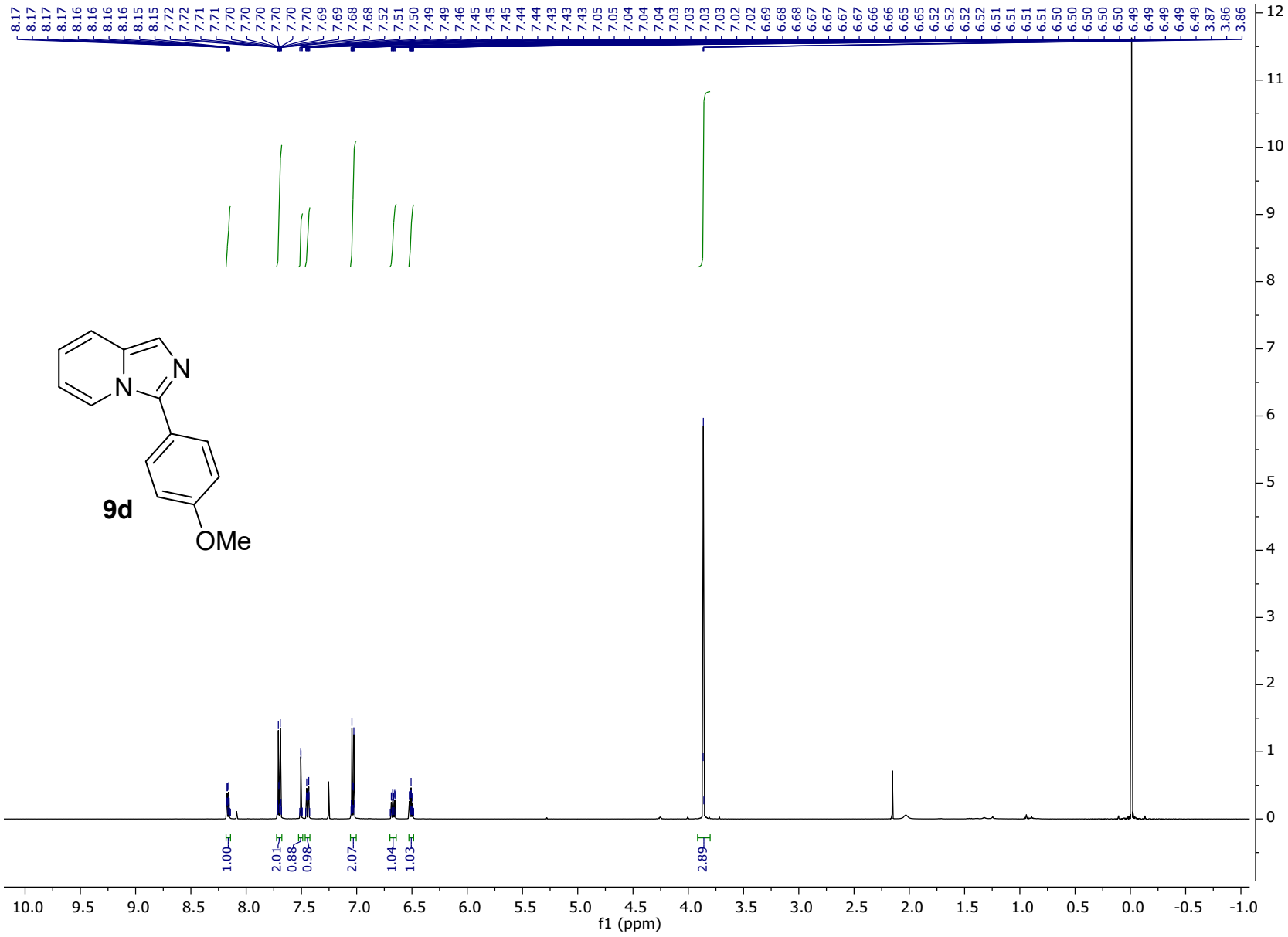

PPh2
N
N
OMe
4f
7.25 CHLOROFORM-D
1.02
3.57
1.23
0.78
0.86
1.08
5.76
0.91
0.94
0.86
2.68
f1 (ppm)

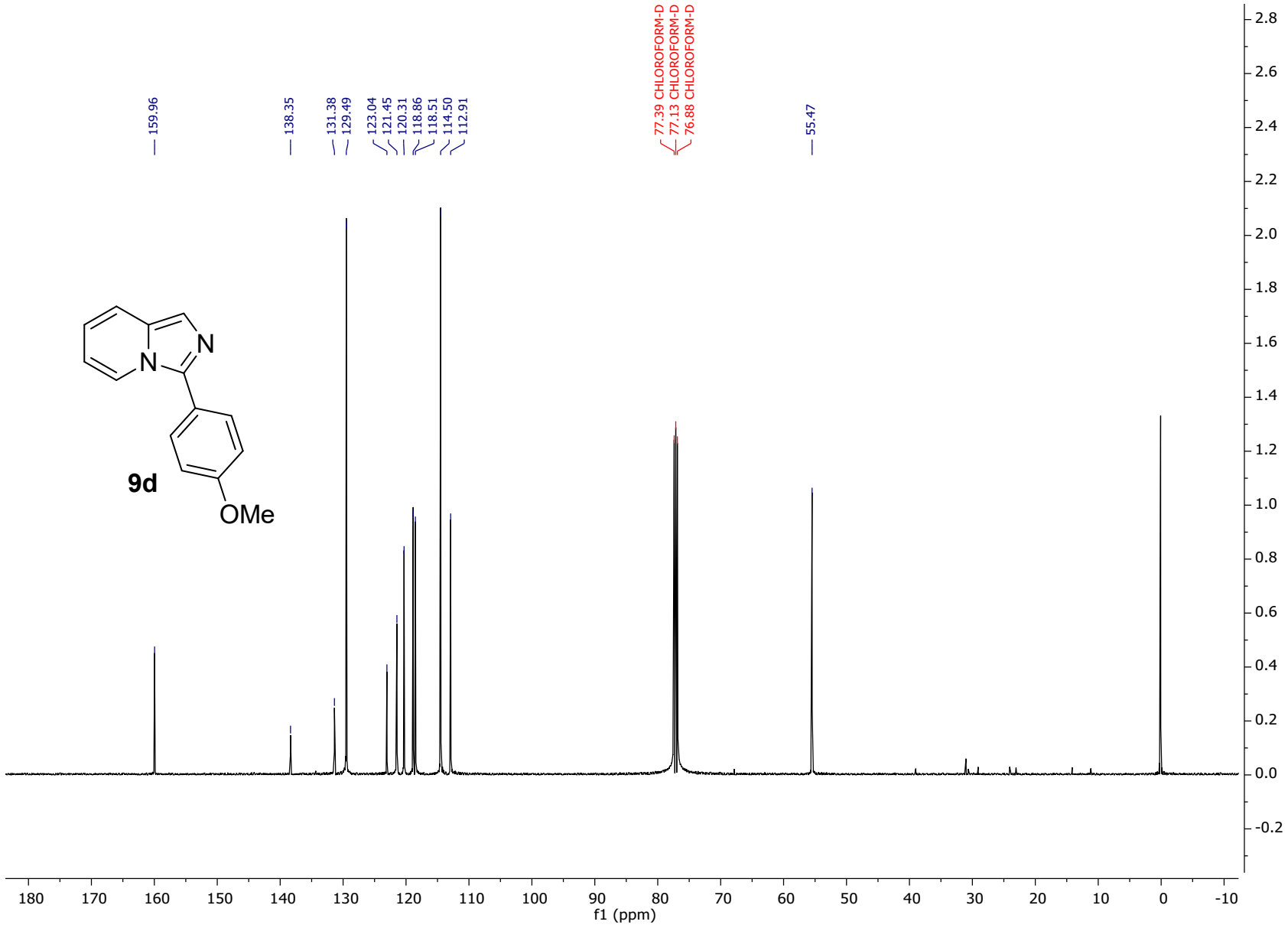

160.08
140.62
140.54
138.18
138.04
138.00
137.92
133.61
133.45
131.41
130.00
128.34
128.30
126.24
122.32
120.64
120.45
119.13
119.08
114.81
114.22
113.38
55.52
PPh2
N
N
OMe
4f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

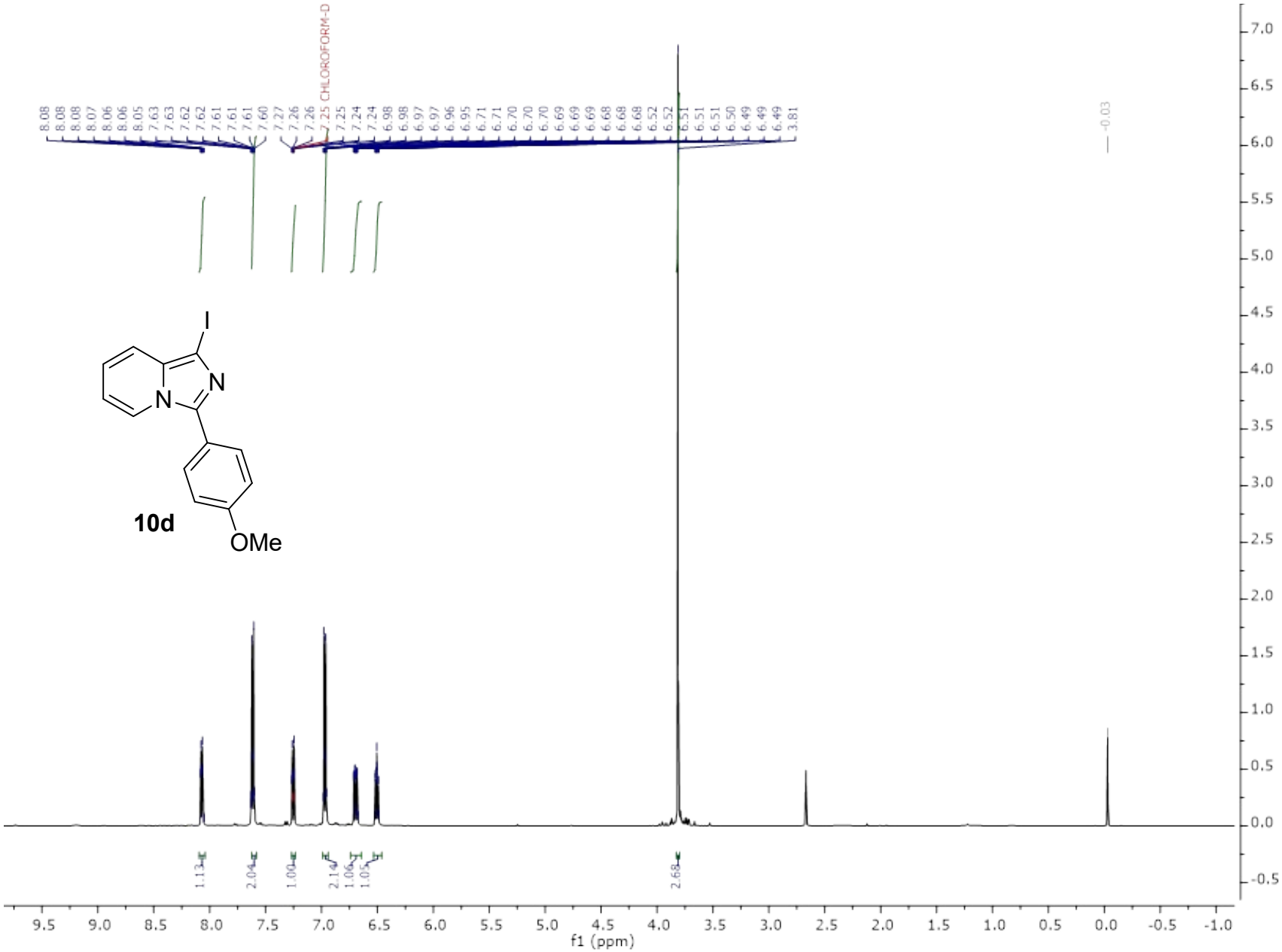

LY-N-30
30.93
PPh2
N
N
OMe
4f
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

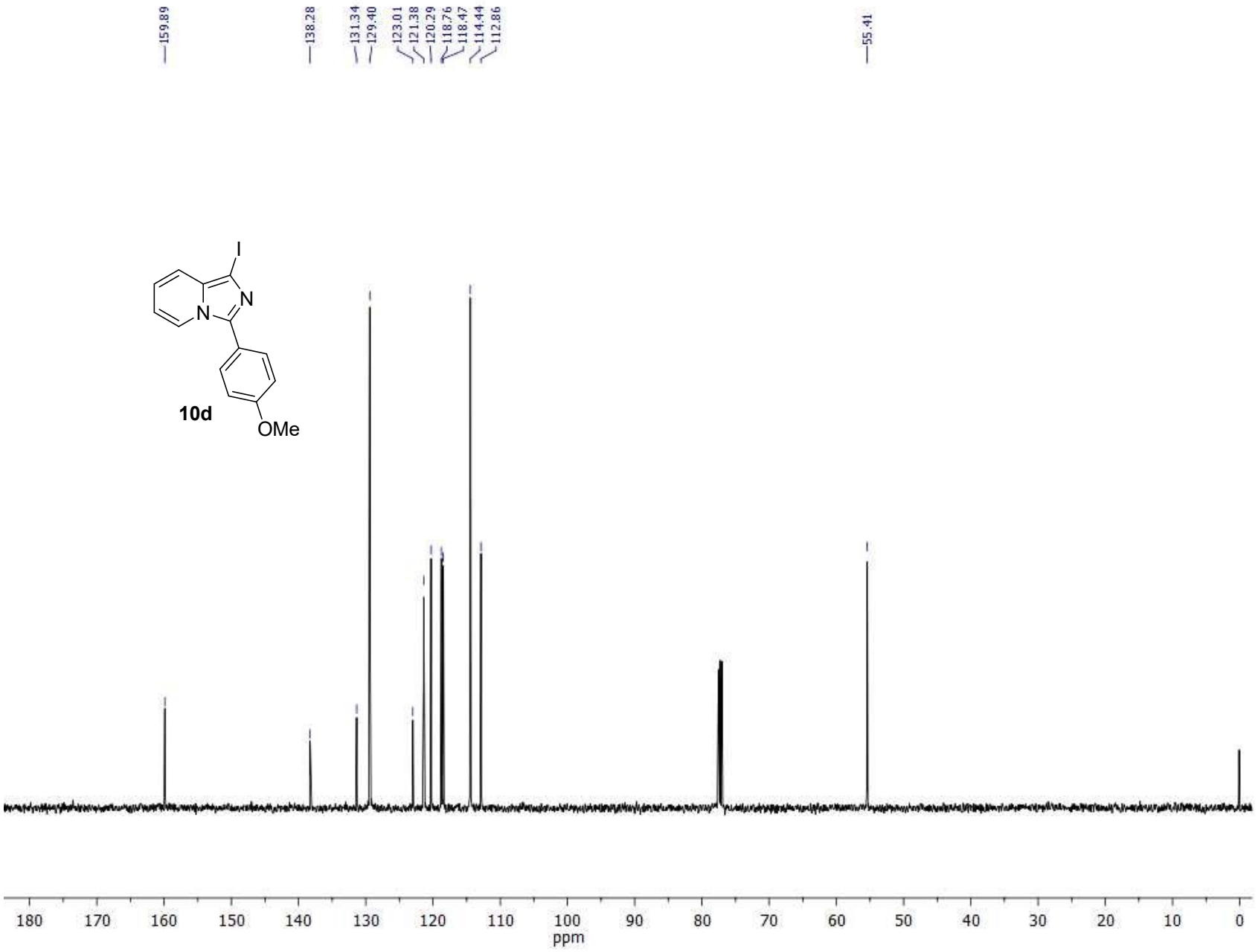

8.55 8.55 8.55 8.54 8.54 8.54 8.54 8.53 7.85 7.84 7.84 7.83 7.82 7.82 7.68 7.67 7.66 7.66 7.65 7.64 7.64 7.55 7.54 7.53 7.32 7.32 7.32 7.31 7.31 7.30 7.30 7.30 7.30 7.25 CHLOROFORM-D 7.25 7.21 7.21 7.20 7.20 7.20 7.20 7.20 7.19 7.19 7.19 7.19 7.19 7.19 7.19 7.18 7.18 7.18 7.18 7.18 6.93 6.92 6.92 6.91 6.91 6.90 4.73 4.72 3.83 0.05 0.02 -0.01 0.02 -0.02 -0.02 -0.03
O
N
H
N
OMe
8d
1.00 1.98 1.08 1.04 1.05 1.07 2.07 2.07 2.86
f1 (ppm)


167.01
162.28
156.59
149.08
136.90
128.99
126.79
122.47
122.30
113.80
55.48
44.83
O
N
H
N
OMe
8d
f1 (ppm)


9d
OMe
N
N
f1 (ppm)


159.96
138.35
131.38
129.49
123.04
121.45
120.31
118.86
118.51
114.50
112.91
77.39 CHLOROFORM-D
77.13 CHLOROFORM-D
76.88 CHLOROFORM-D
55.47
N
N
9d
OMe
f1 (ppm)


8.08
8.08
8.08
8.07
8.06
8.06
8.05
7.63
7.63
7.62
7.62
7.61
7.61
7.61
7.60
7.27
7.26
7.26
7.25 CHLOROFORM-D
7.25
7.24
7.24
6.98
6.98
6.97
6.97
6.96
6.95
6.71
6.71
6.70
6.70
6.70
6.69
6.69
6.69
6.68
6.68
6.68
6.52
6.52
6.51
6.51
6.51
6.50
6.49
6.49
6.49
3.81
-0.03
I
N
N
10d
OMe
1.13
2.04
1.00
2.14
1.06
1.05
2.68
f1 (ppm)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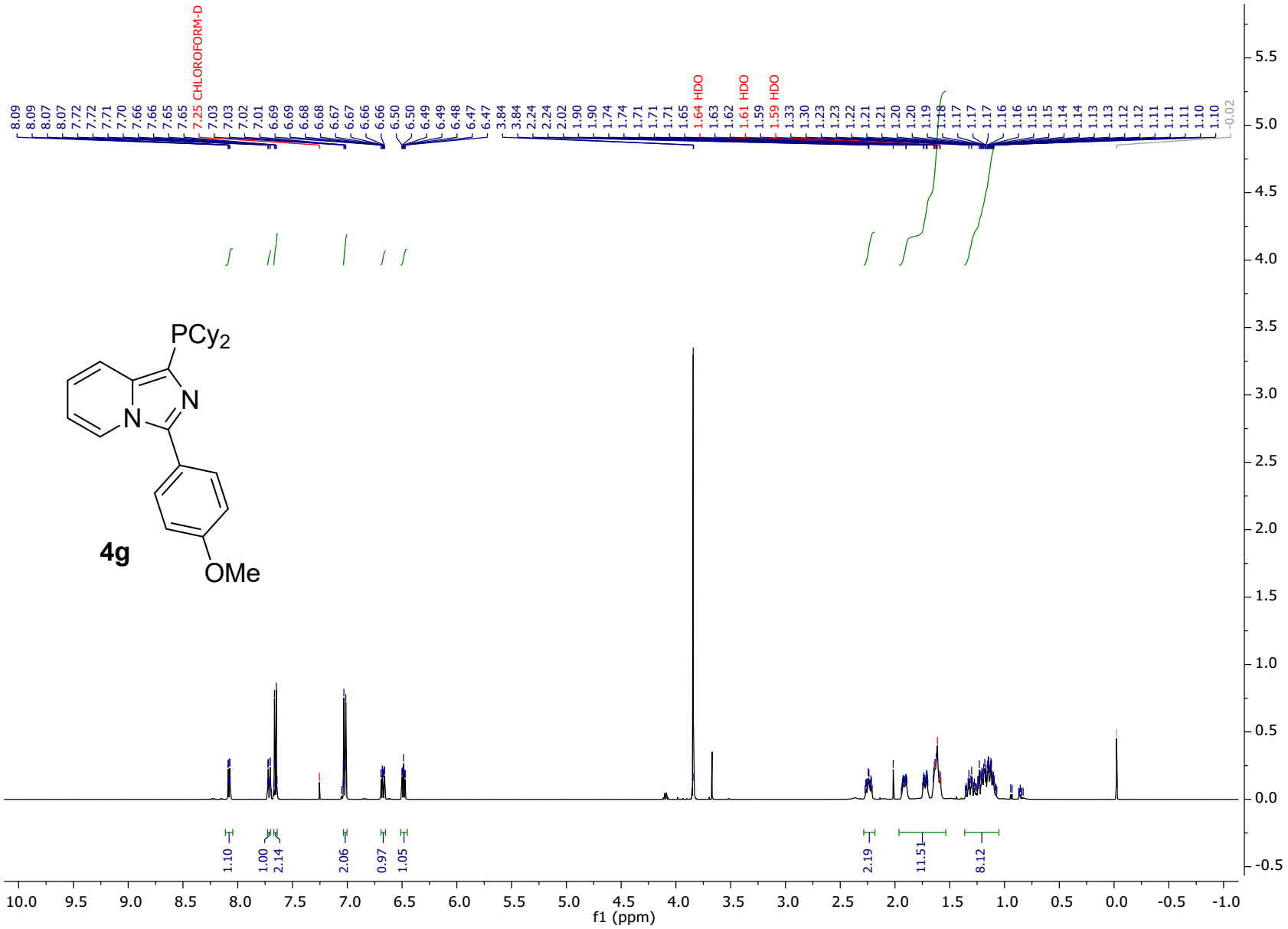
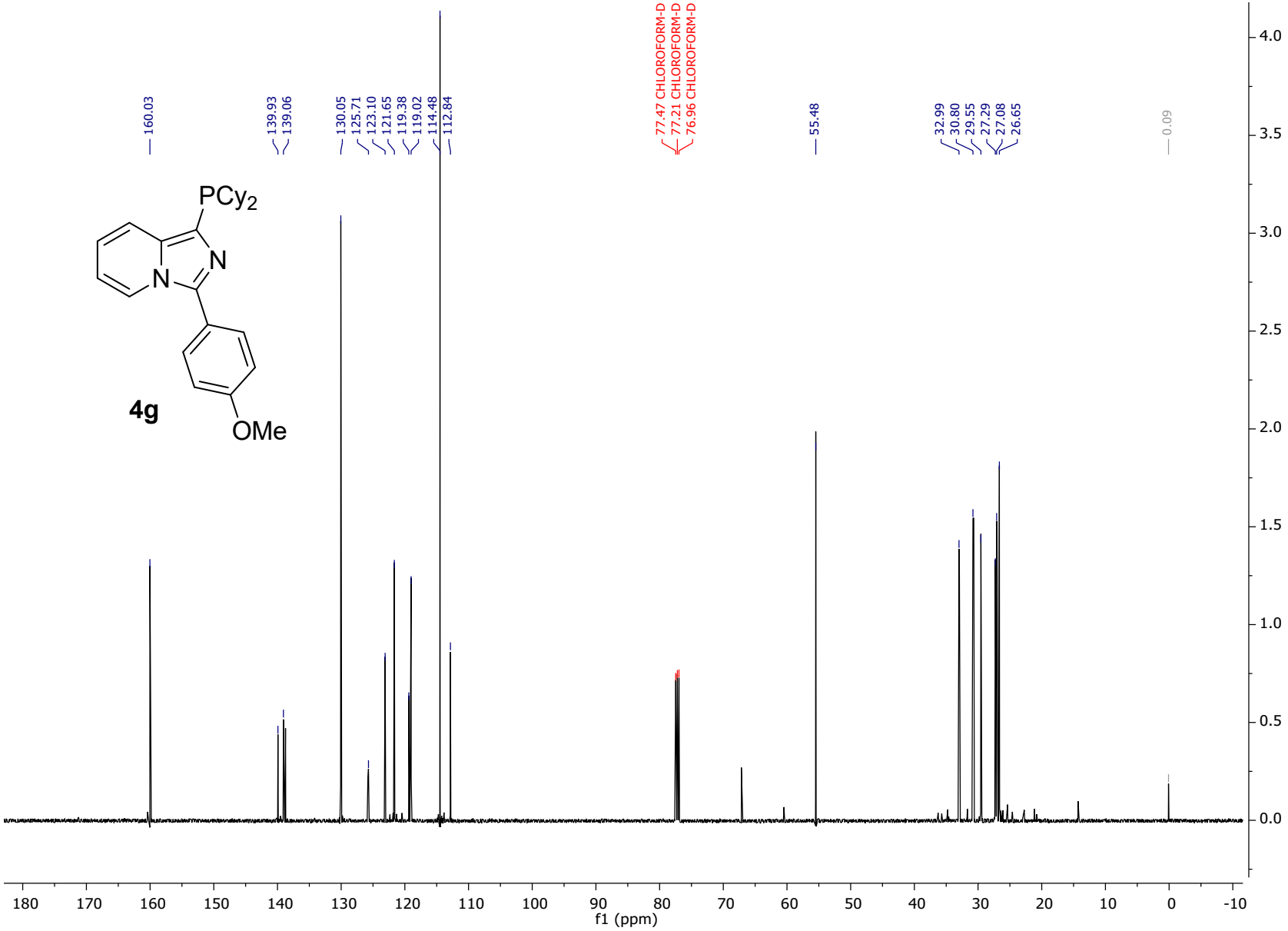
138.28
131.34
129.40
123.01
121.38
120.29
118.76
118.47
114.44
112.86
55.41
I
N
N
OMe
10d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


PCy2
N
N
OMe
4g
7.25 CHLOROFORM-D
1.64 HDO
1.61 HDO
1.59 HDO
1.10
1.00
2.14
2.06
0.97
1.05
2.19
11.51
8.12
f1 (ppm)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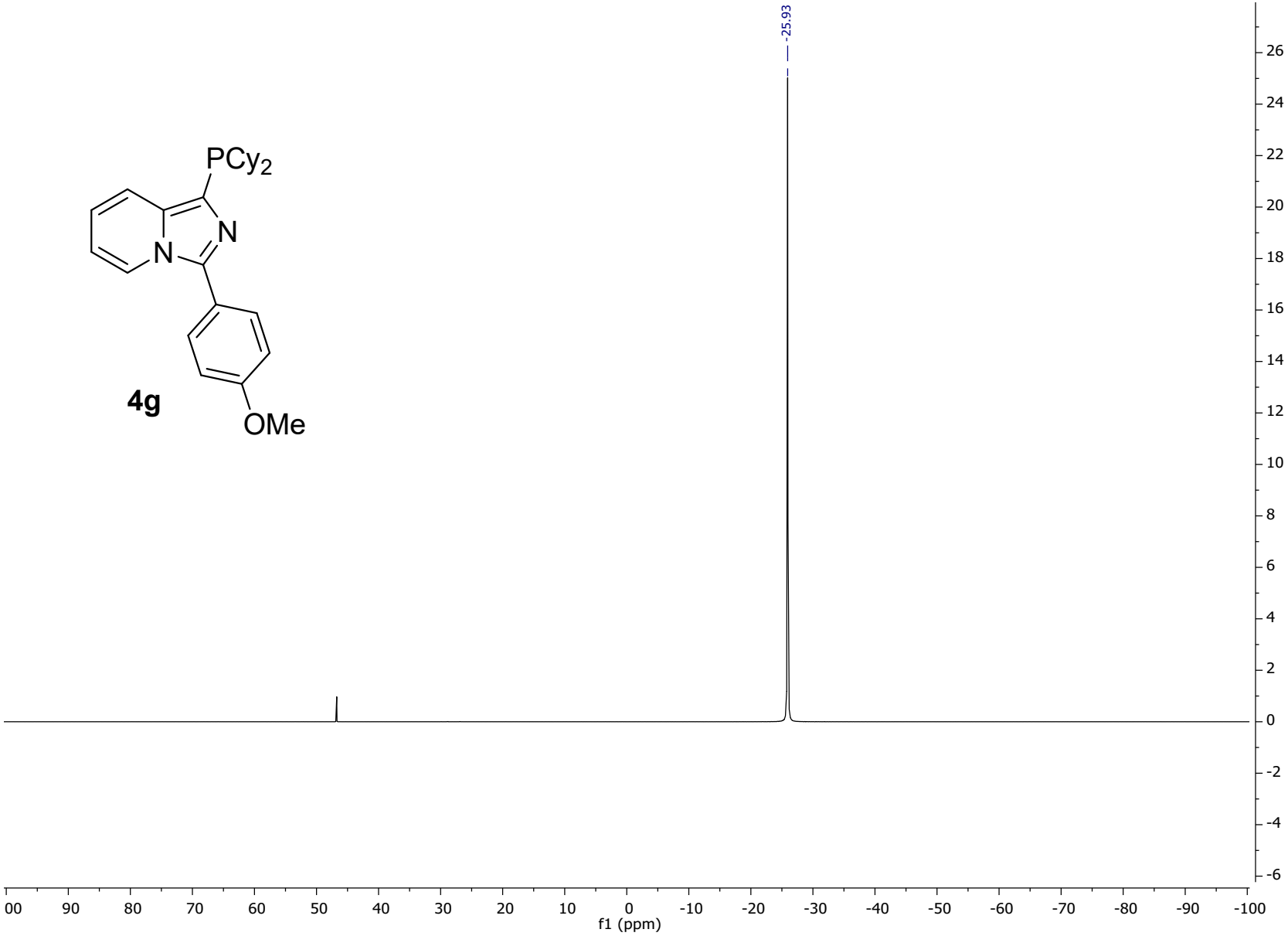
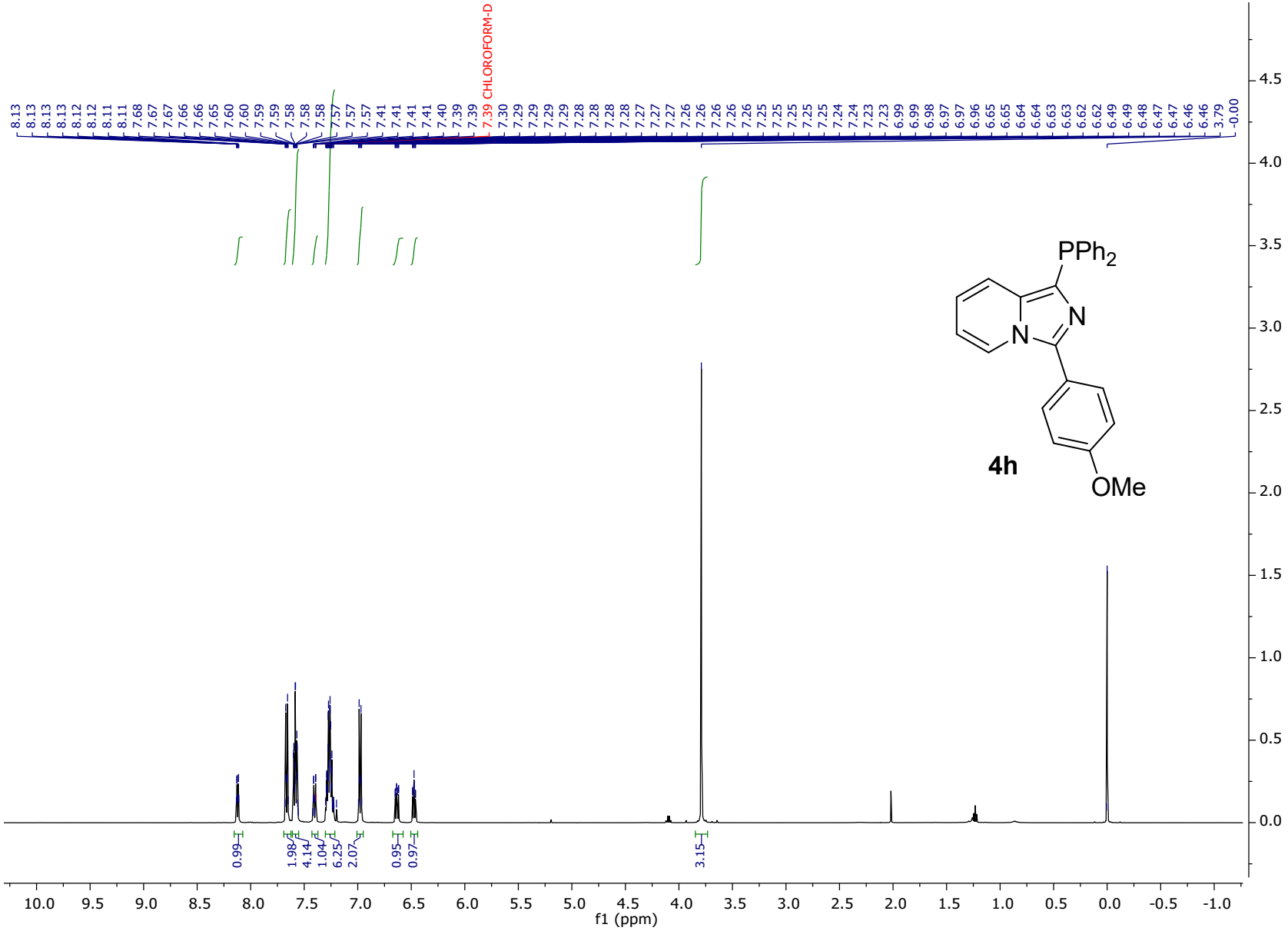
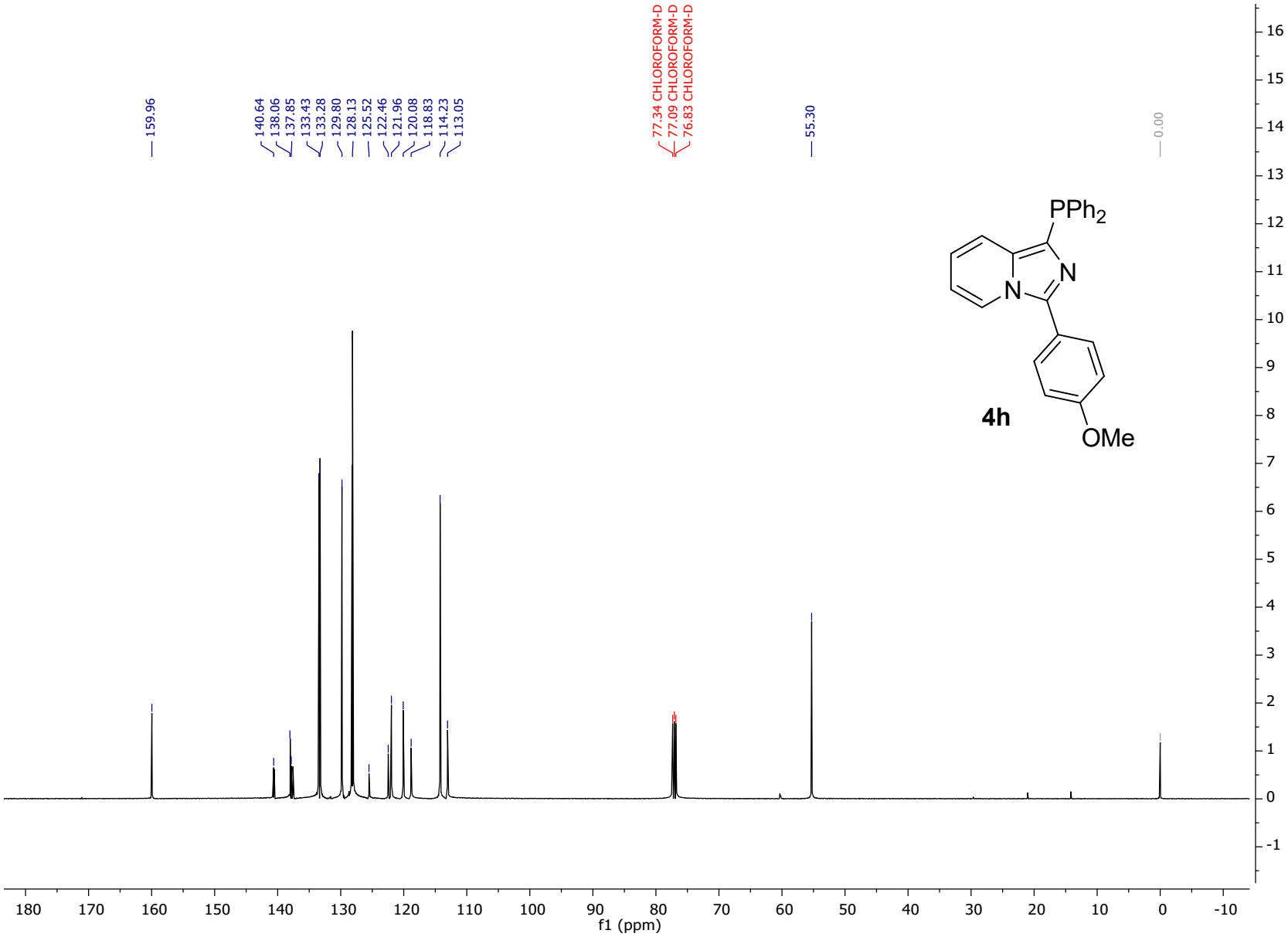
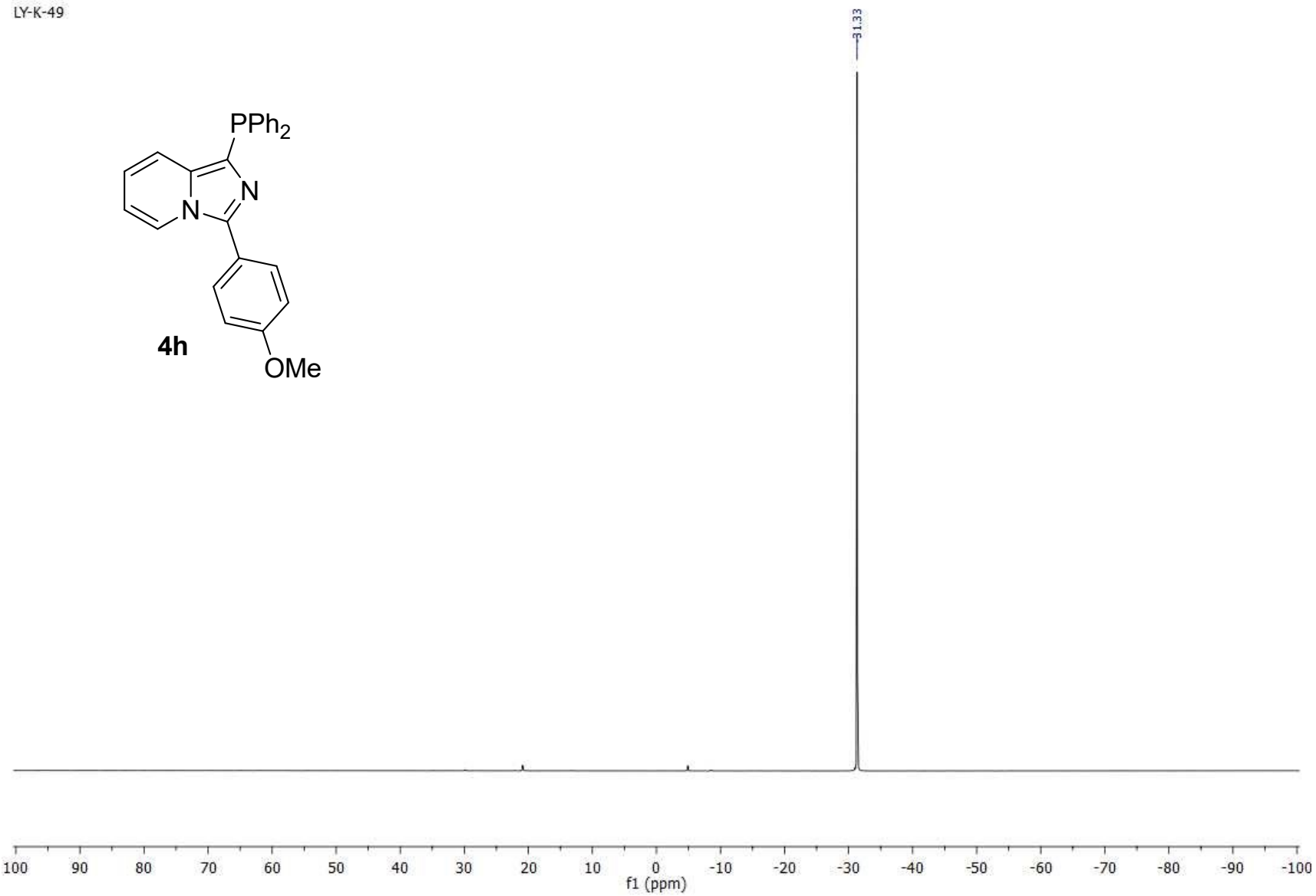
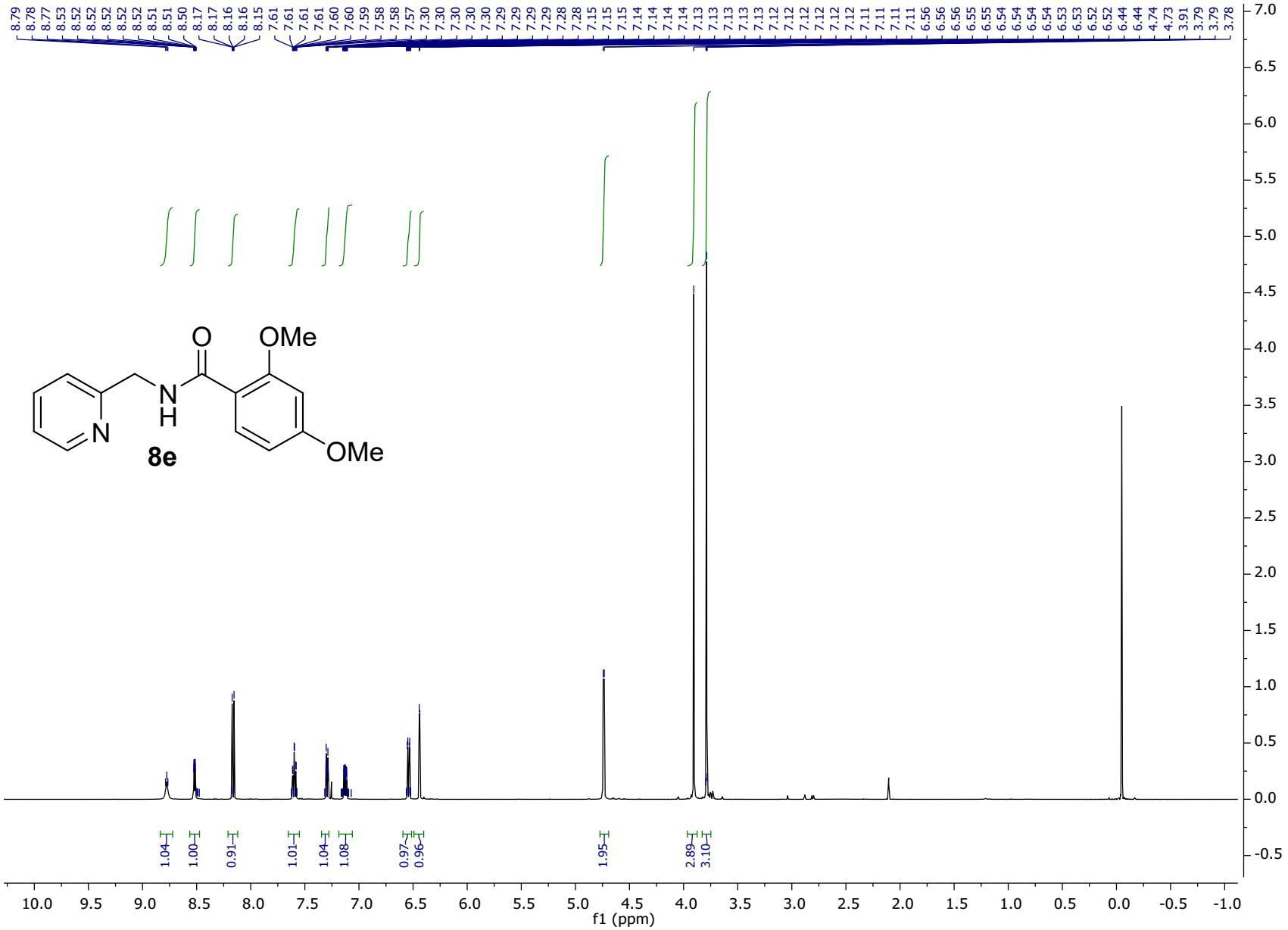
139.93
139.06
130.05
125.71
123.10
121.65
119.38
119.02
114.48
112.84
77.47 CHLOROFORM-D
77.21 CHLOROFORM-D
76.96 CHLOROFORM-D
55.48
32.99
30.80
29.55
27.29
27.08
26.65
0.09
PCy2
N
N
4g
OMe
f1 (ppm)

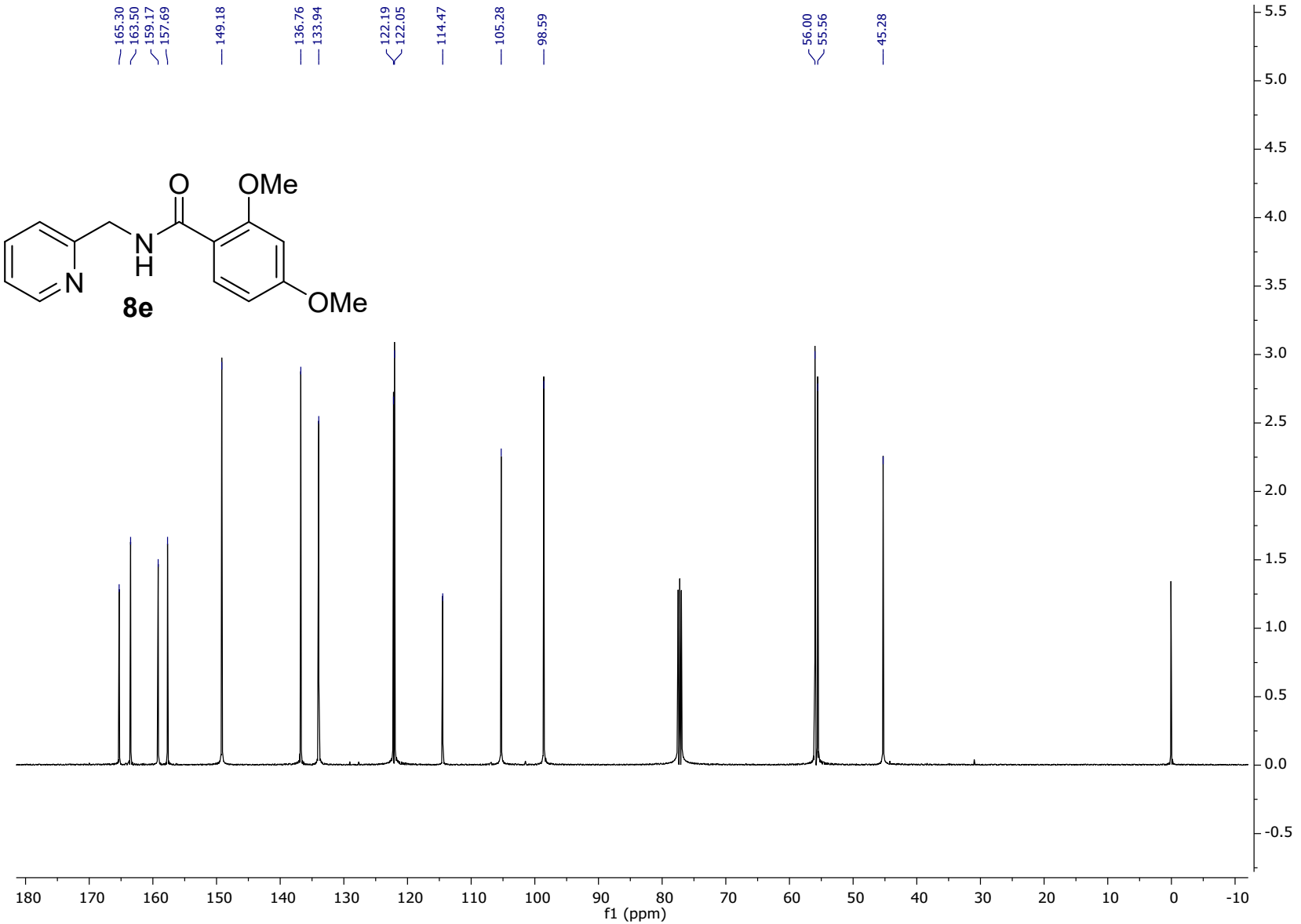

PCy2
N
N
4g
OMe
-25.93
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
-4
-6
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

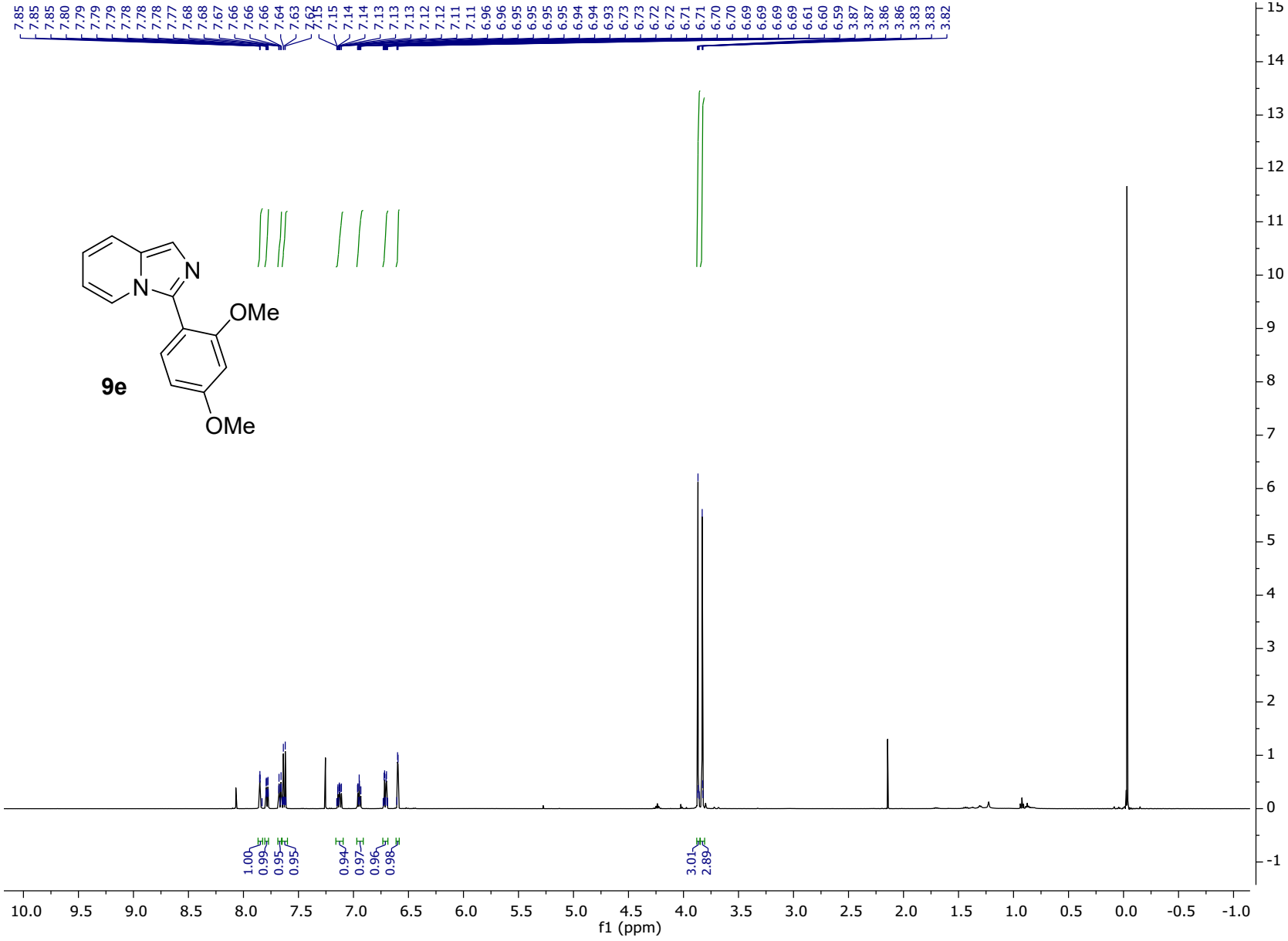

CHLOROFORM-D
PPh2
N
N
4h
OMe
0.99
1.98
4.14
1.04
6.25
2.07
0.95
0.97
3.15
f1 (ppm)

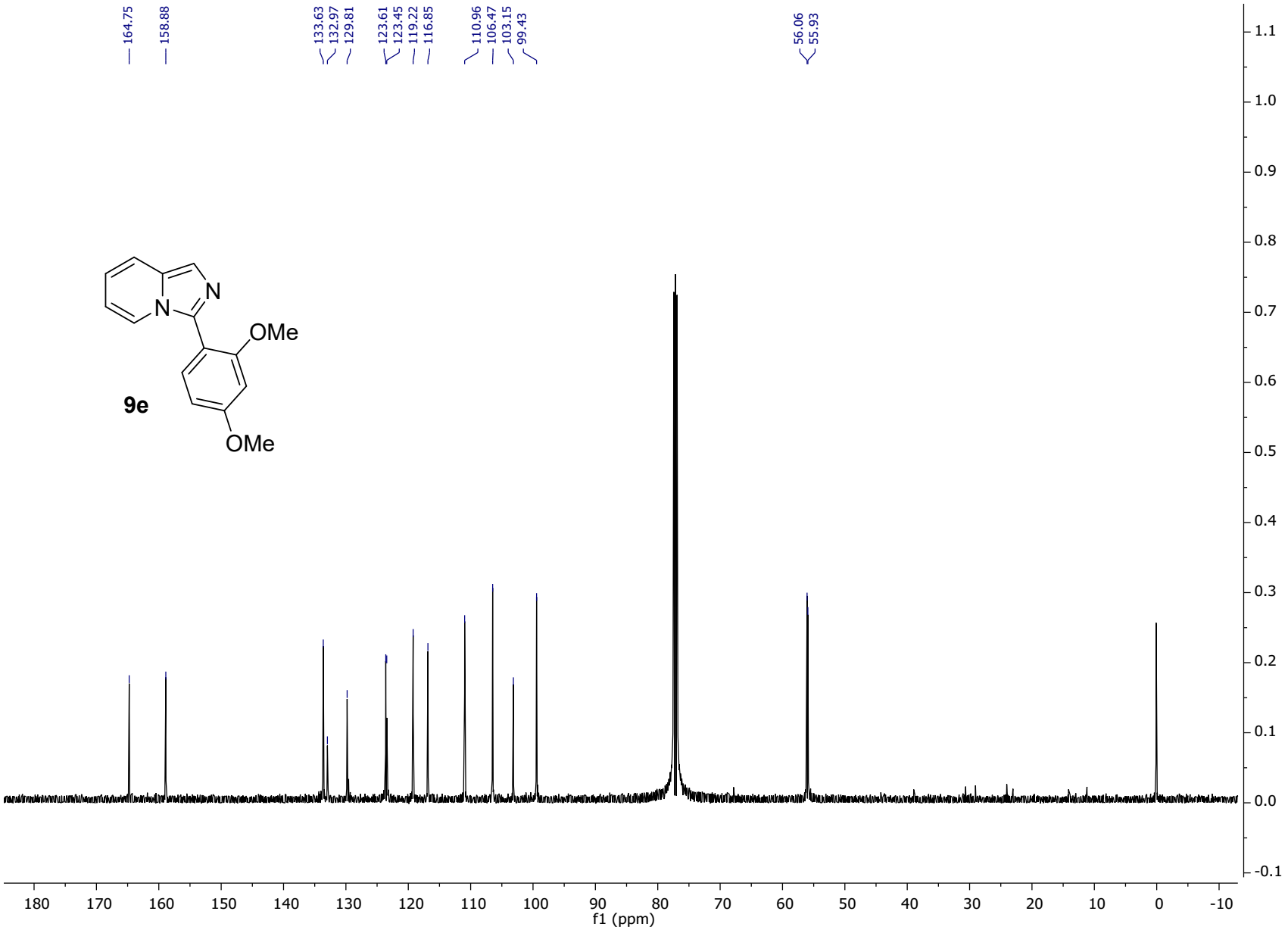

159.96
140.64
138.06
137.85
133.43
133.28
129.80
128.13
125.52
122.46
121.96
120.08
118.83
114.23
113.05
77.34 CHLOROFORM-D
77.09 CHLOROFORM-D
76.83 CHLOROFORM-D
55.30
0.00
PPh2
N
N
4h
OMe
f1 (ppm)

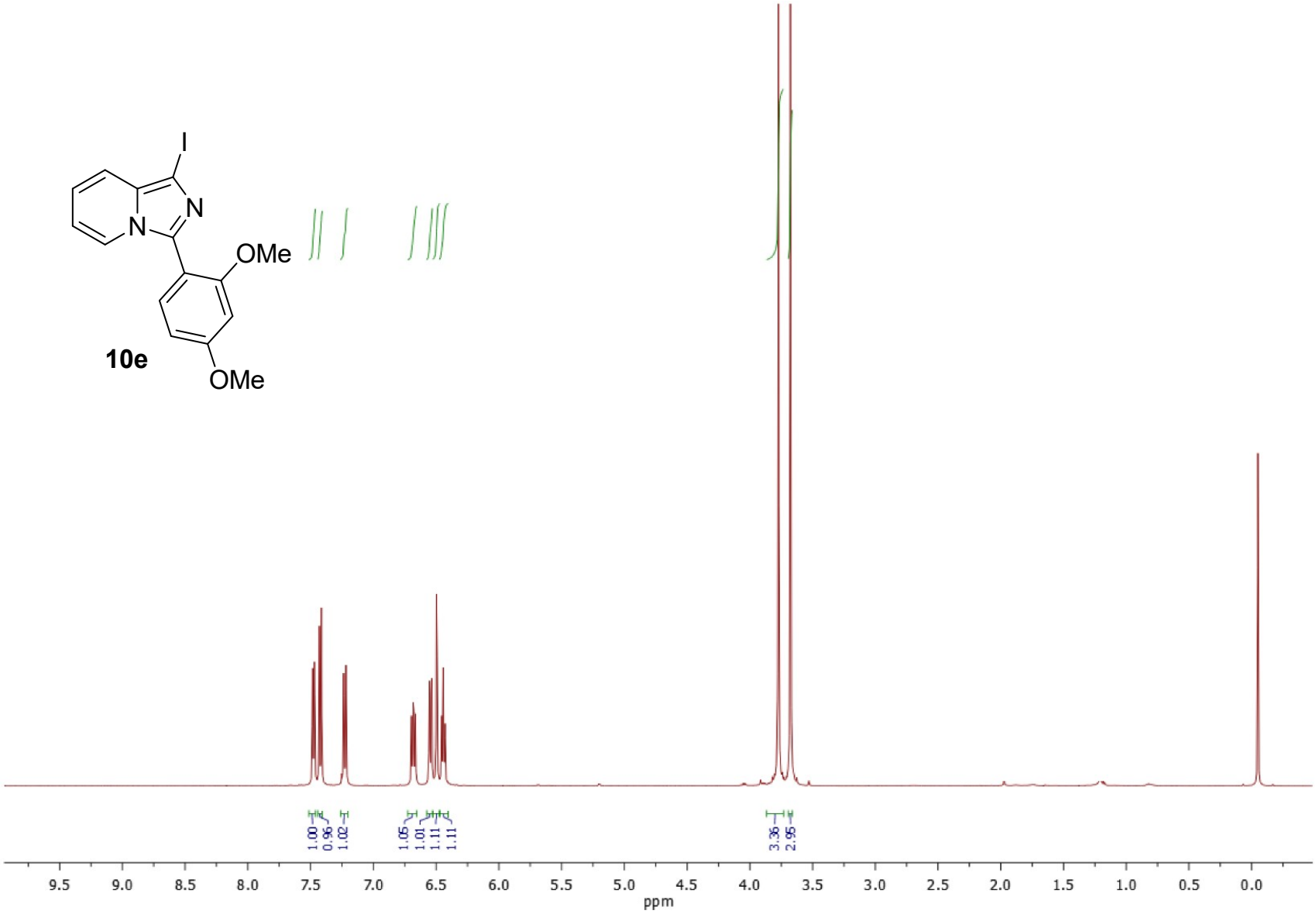

LY-K-49
31.33
PPh2
N
N
OMe
4h
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

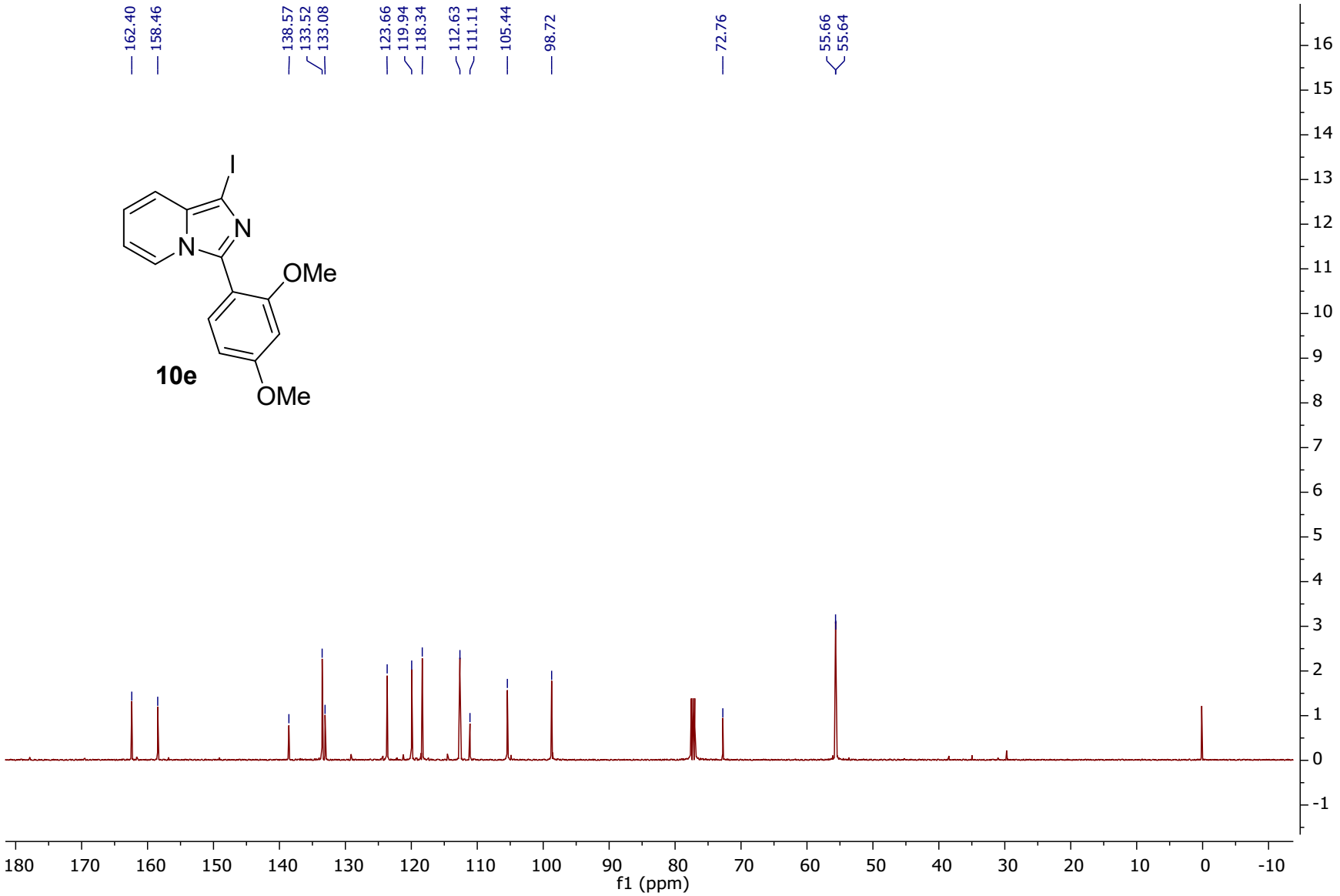

O
OMe
N
H
N
OMe
8e
f1 (ppm)

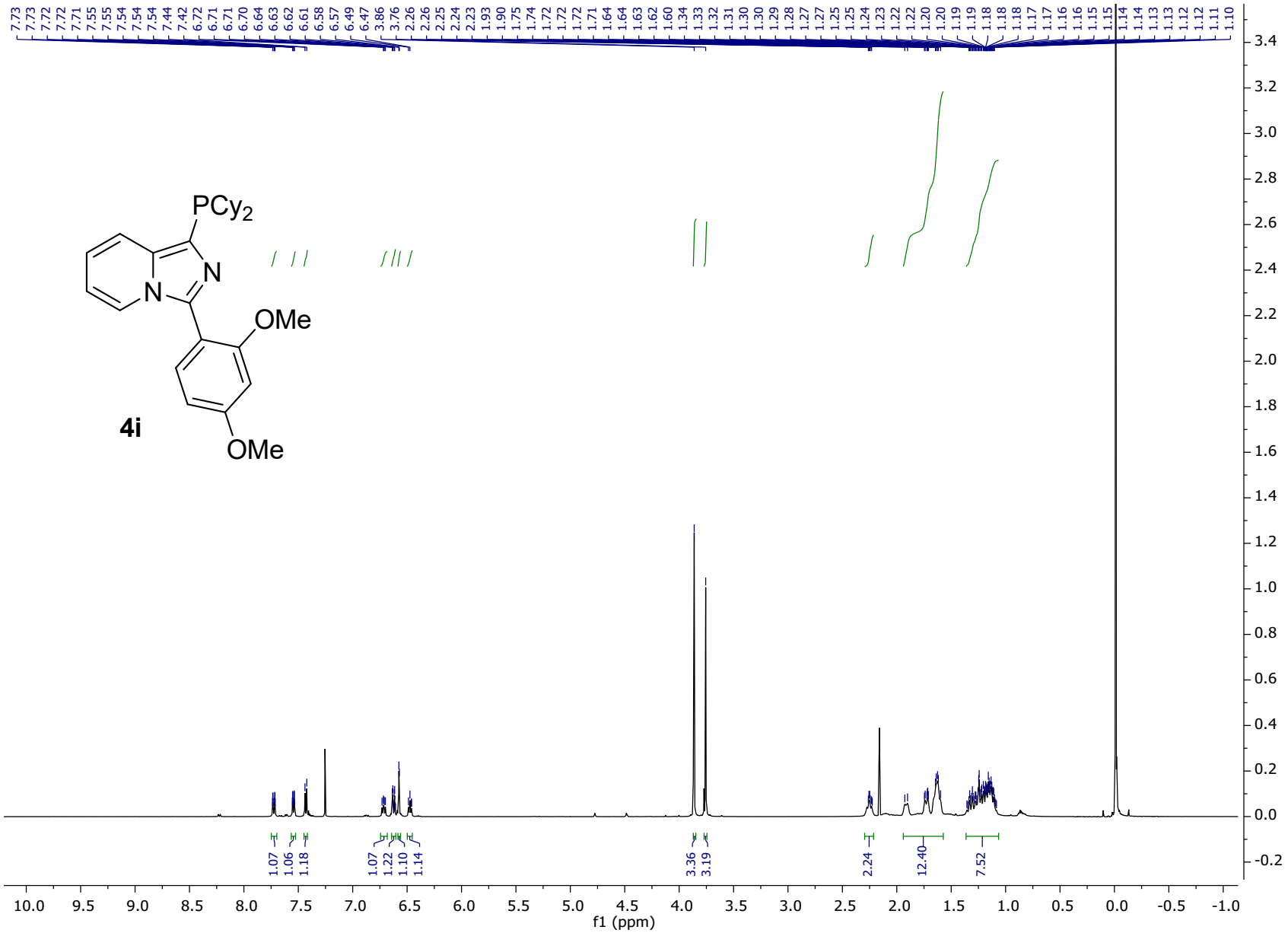

165.30
163.50
159.17
157.69
149.18
136.76
133.94
122.19
122.05
114.47
105.28
98.59
56.00
55.56
45.28
O
OMe
N
H
N
OMe
8e
f1 (ppm)

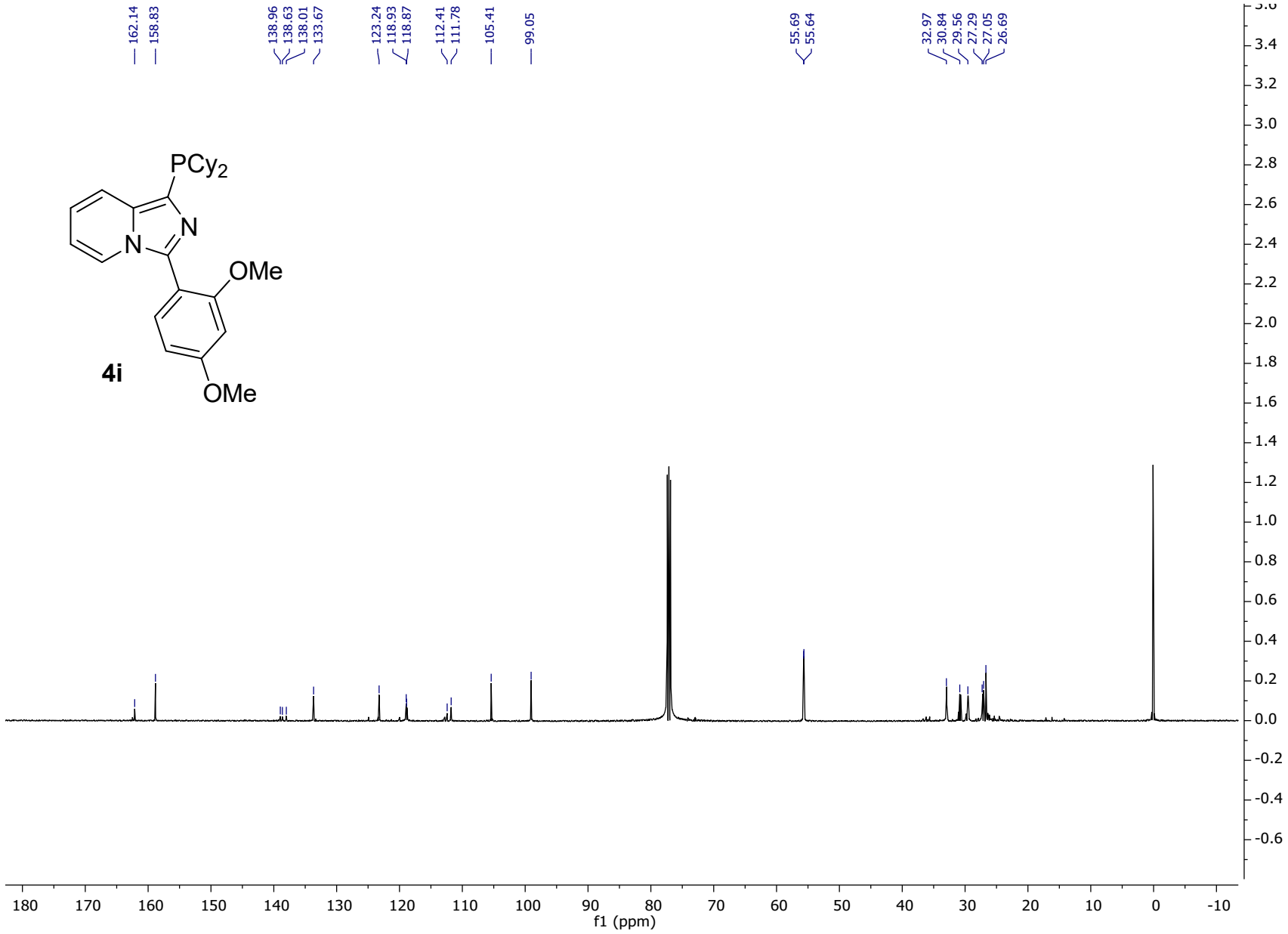

7.85 7.85 7.85 7.80 7.79 7.79 7.79 7.78 7.78 7.78 7.77 7.68 7.68 7.67 7.66 7.66 7.66 7.64 7.63 7.62 7.62 7.15 7.14 7.14 7.13 7.13 7.12 7.12 7.11 7.11 6.96 6.96 6.95 6.95 6.95 6.95 6.94 6.94 6.93 6.73 6.73 6.72 6.72 6.71 6.71 6.70 6.70 6.69 6.69 6.69 6.69 6.61 6.60 6.59 3.87 3.87 3.86 3.86 3.83 3.83 3.82
N
N
OMe
OMe
9e
1.00 0.99 0.95 0.95 0.94 0.97 0.96 0.98 3.01 2.89
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1


164.75
158.88
133.63
132.97
129.81
123.61
123.45
119.22
116.85
110.96
106.47
103.15
99.43
56.06
55.93
N
N
OMe
OMe
9e
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

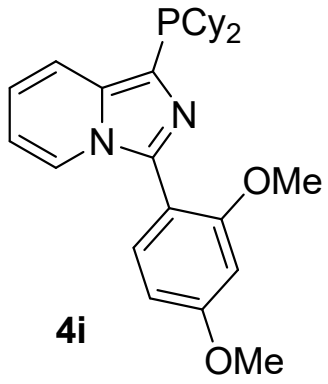

I
N
N
OMe
OMe
10e
1.00
0.96
1.02
1.05
1.01
1.11
1.11
3.36
2.95
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


162.40
158.46
138.57
133.52
133.08
123.66
119.94
118.34
112.63
111.11
105.44
98.72
72.76
55.66
55.64
I
N
N
OMe
OMe
10e
f1 (ppm)


PCy2
N
N
OMe
OMe
4i
f1 (ppm)

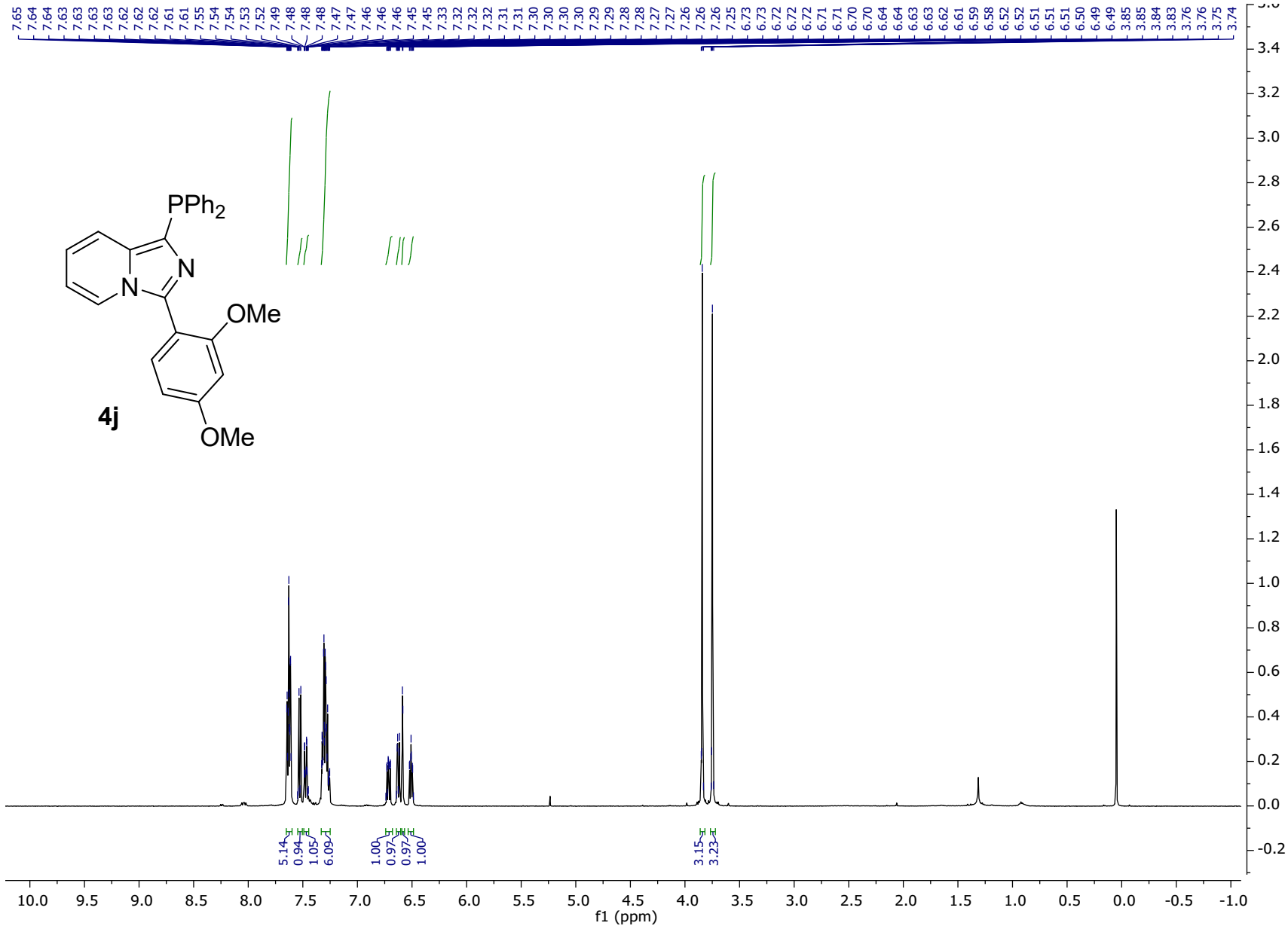

162.14
158.83
138.96
138.63
138.01
133.67
123.24
118.93
118.87
112.41
111.78
105.41
99.05
55.69
55.64
32.97
30.84
29.56
27.29
27.05
26.69
PCy2
N
N
OMe
OMe
4i
f1 (ppm)

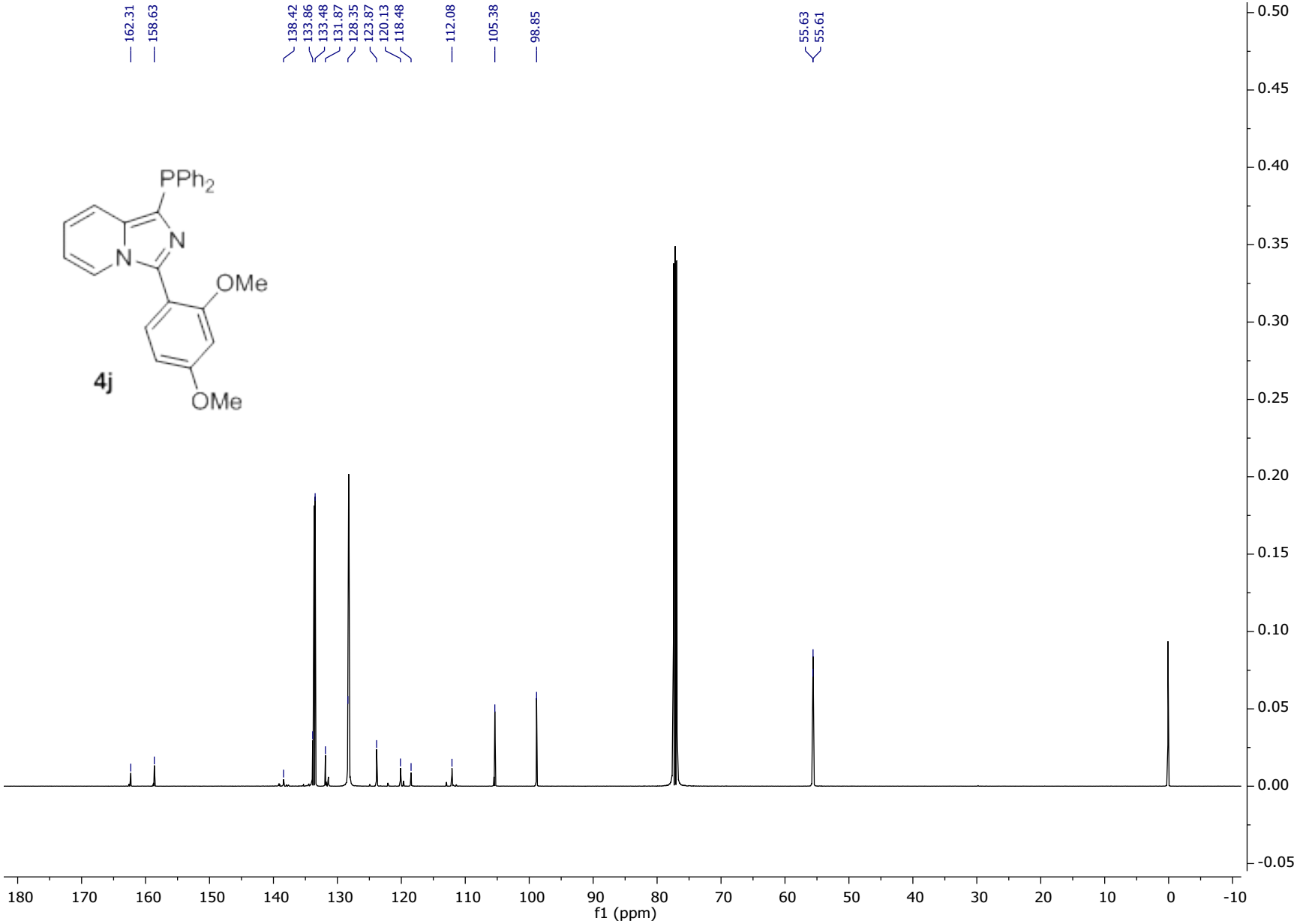
LY-K-59-2

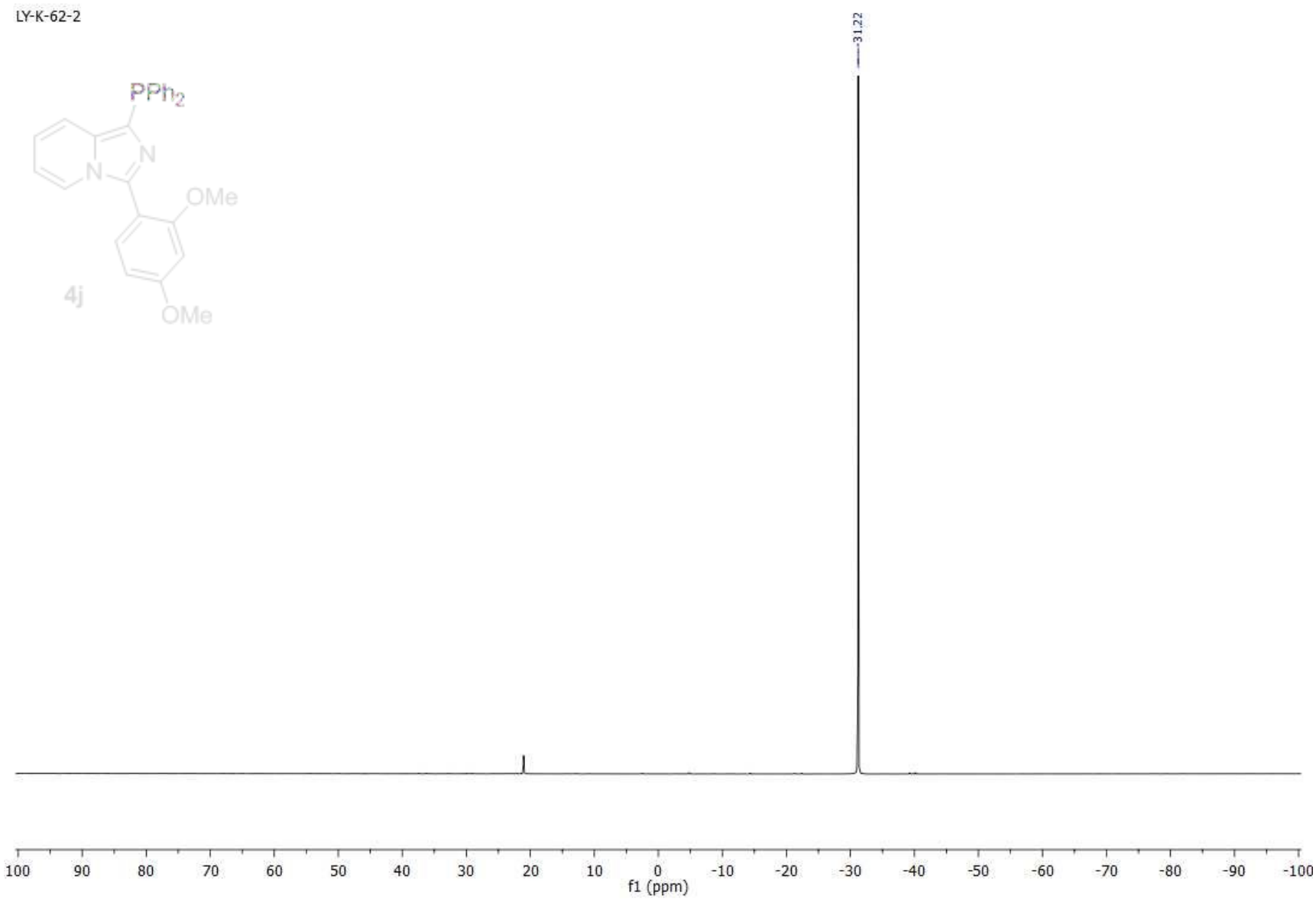

PCy2
N
N
OMe
OMe

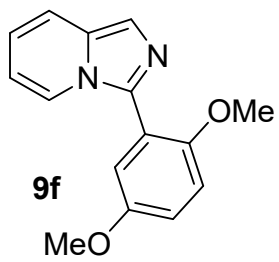
4i

25.99
120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120
f1 (ppm)


PPh2
N
N
OMe
OMe
4j
f1 (ppm)

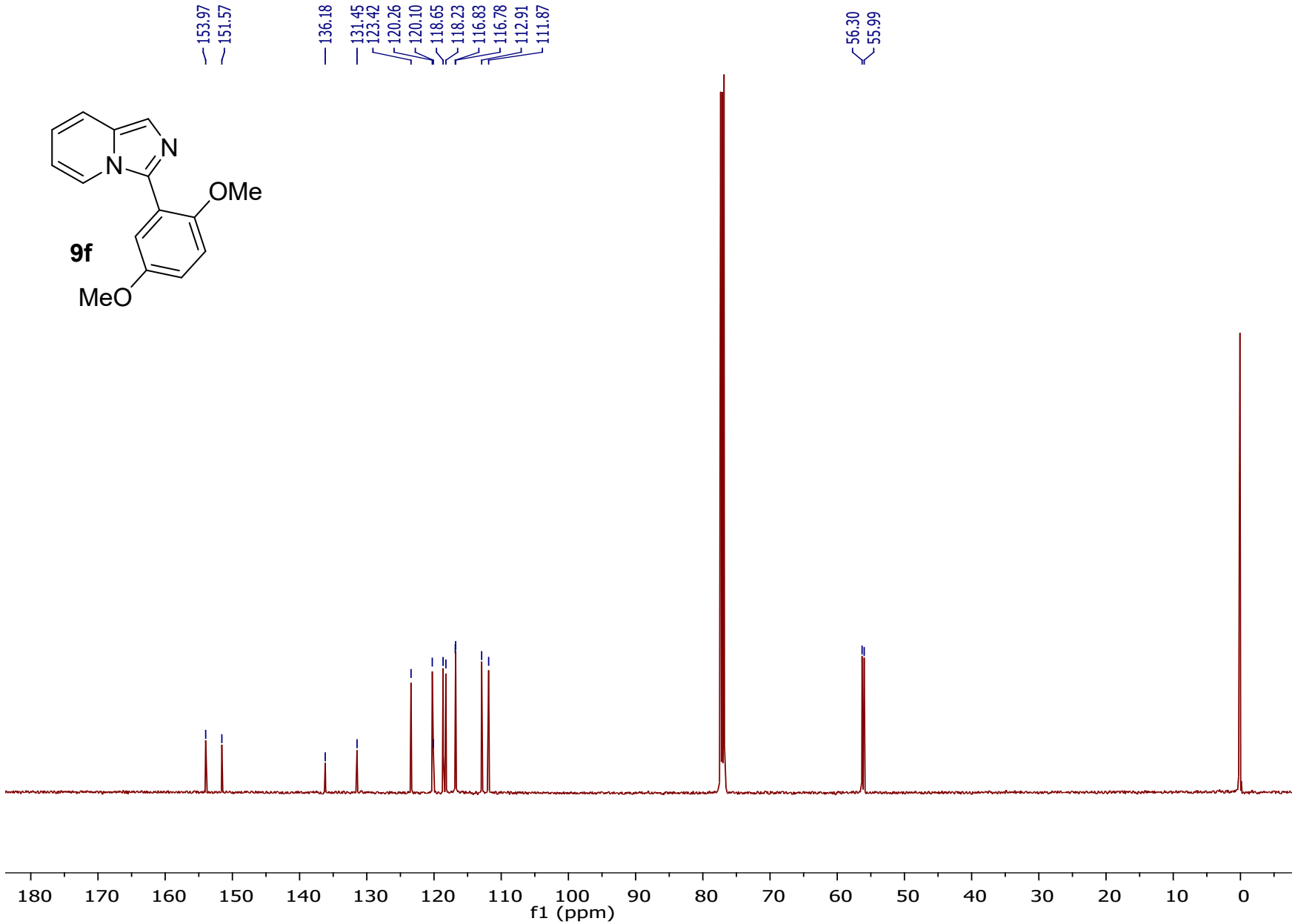

162.31
158.63
138.42
133.86
133.48
131.87
128.35
123.87
120.13
118.48
112.08
105.38
98.85
55.63
55.61
PPh2
N
N
OMe
OMe
4j
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
-0.05
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

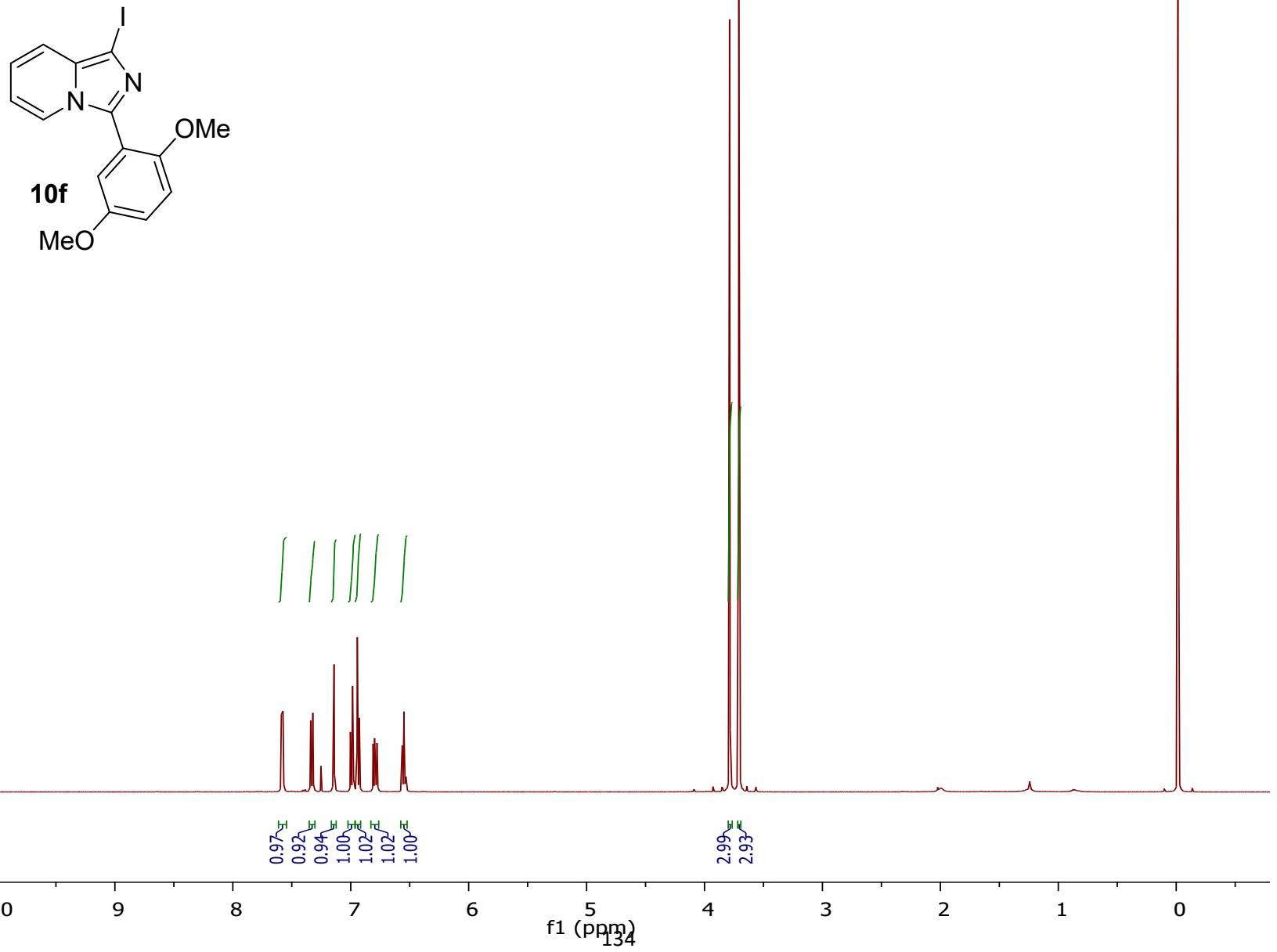

LY-K-62-2
PPh2
N
N
OMe
4j
OMe
31.22
100
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

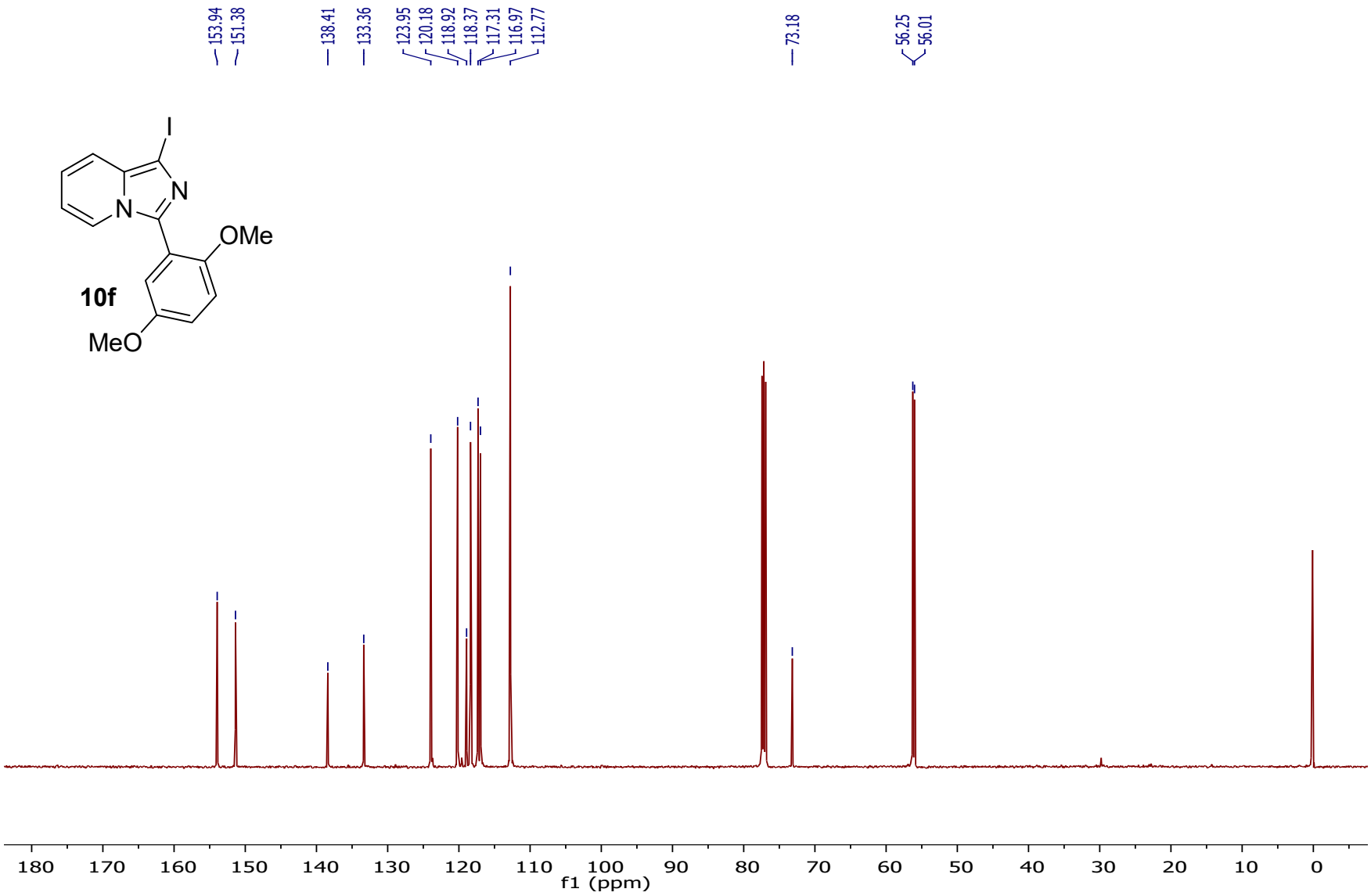

N
N
OMe
MeO

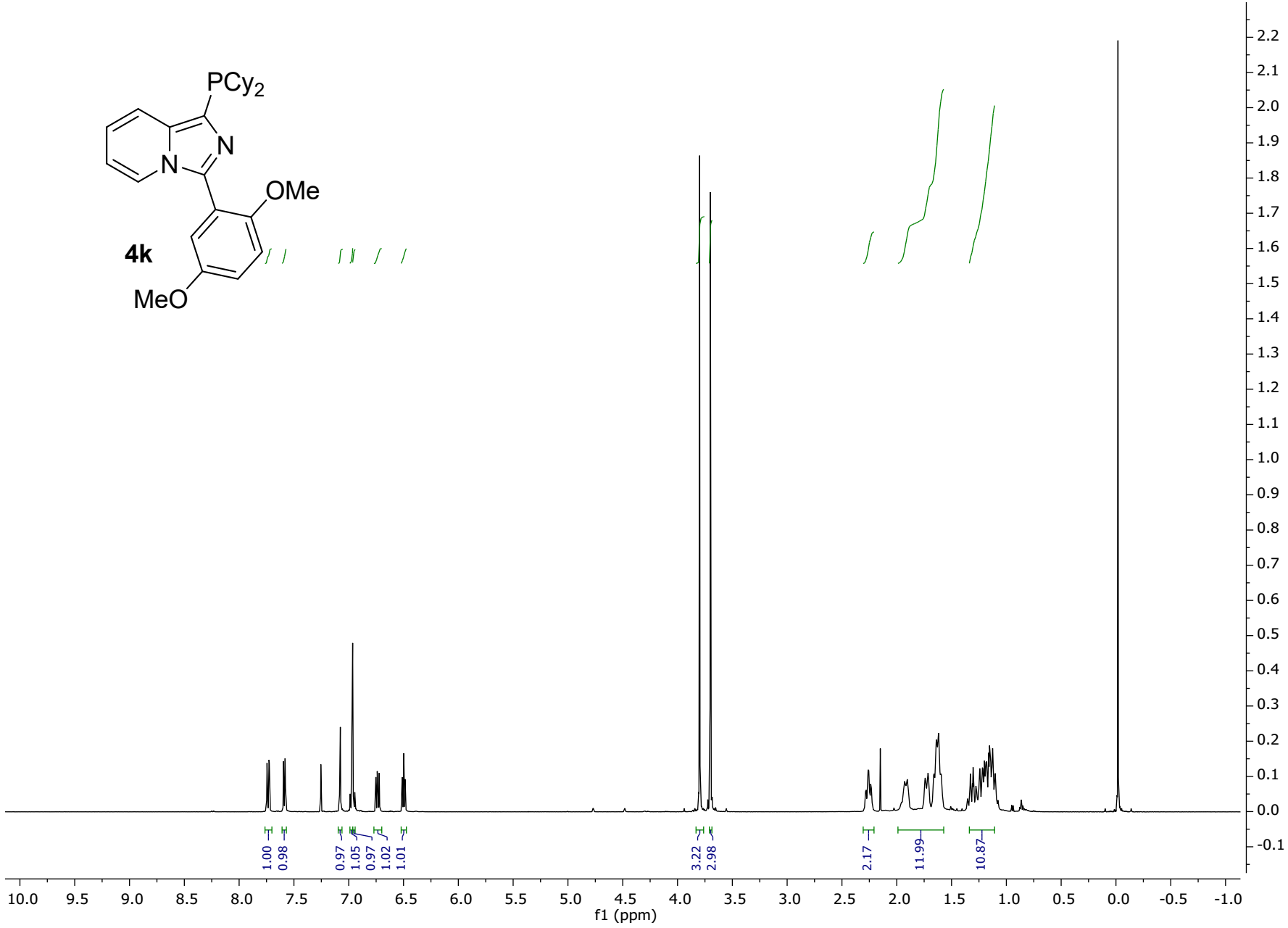
9f

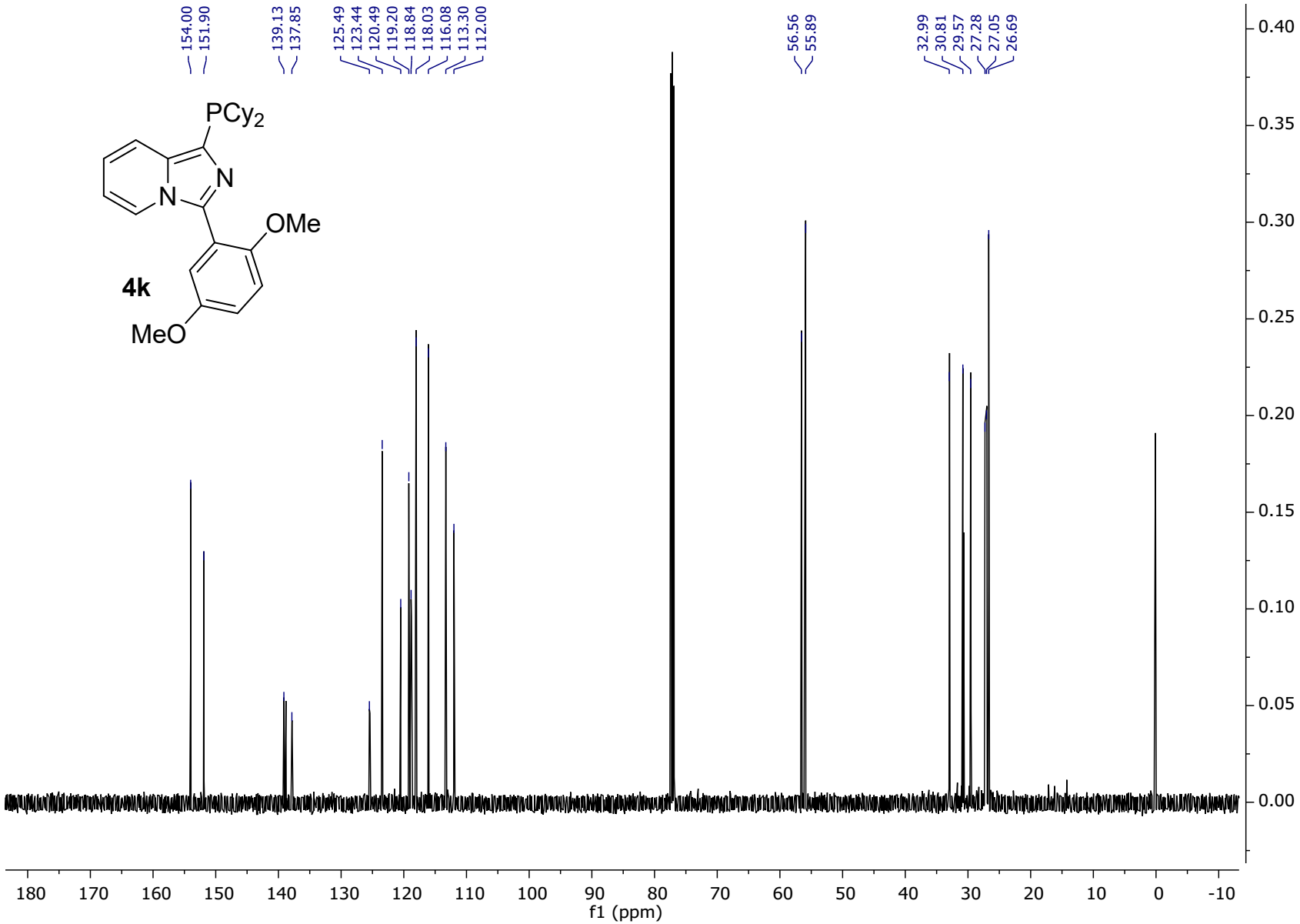
1.00
0.92
1.03
0.99
2.17
1.06
1.05
3.23
3.15
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

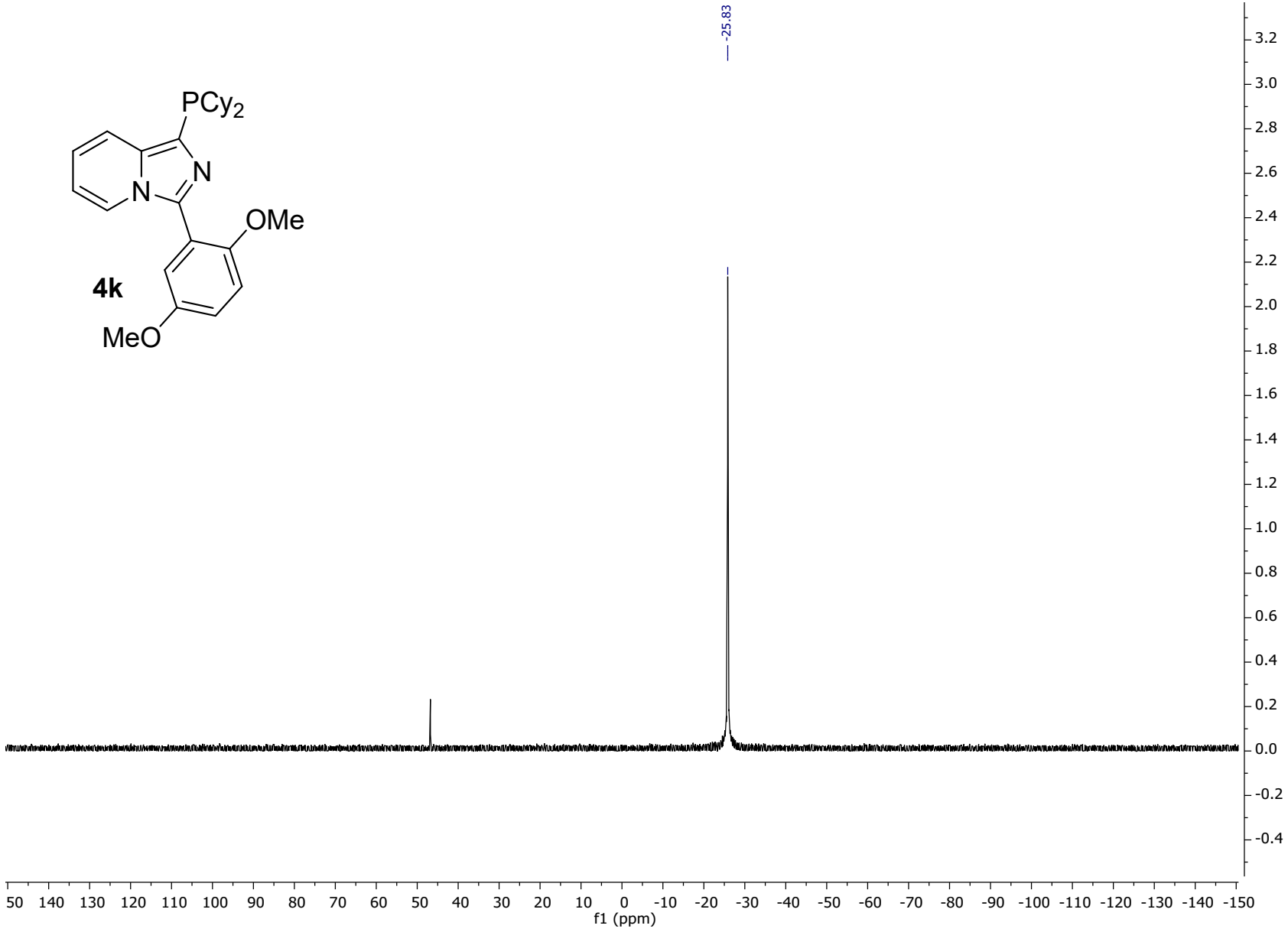

153.97
151.57
136.18
131.45
123.42
120.26
120.10
118.65
118.23
116.83
116.78
112.91
111.87
56.30
55.99
N
N
OMe
MeO
9f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

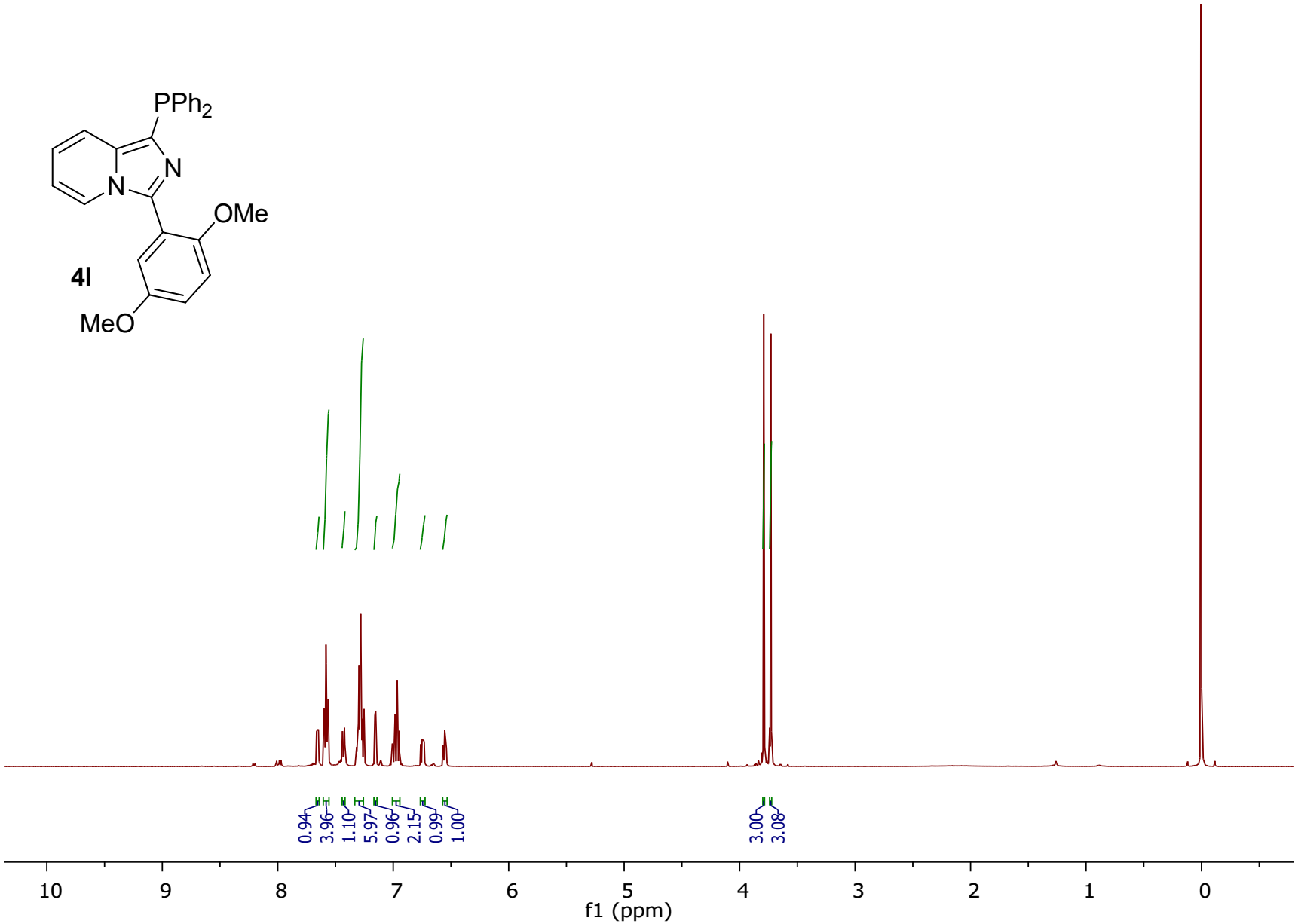

I
N
N
OMe
10f
MeO
0.97
0.92
0.94
1.00
1.02
1.02
1.00
2.99
2.93
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

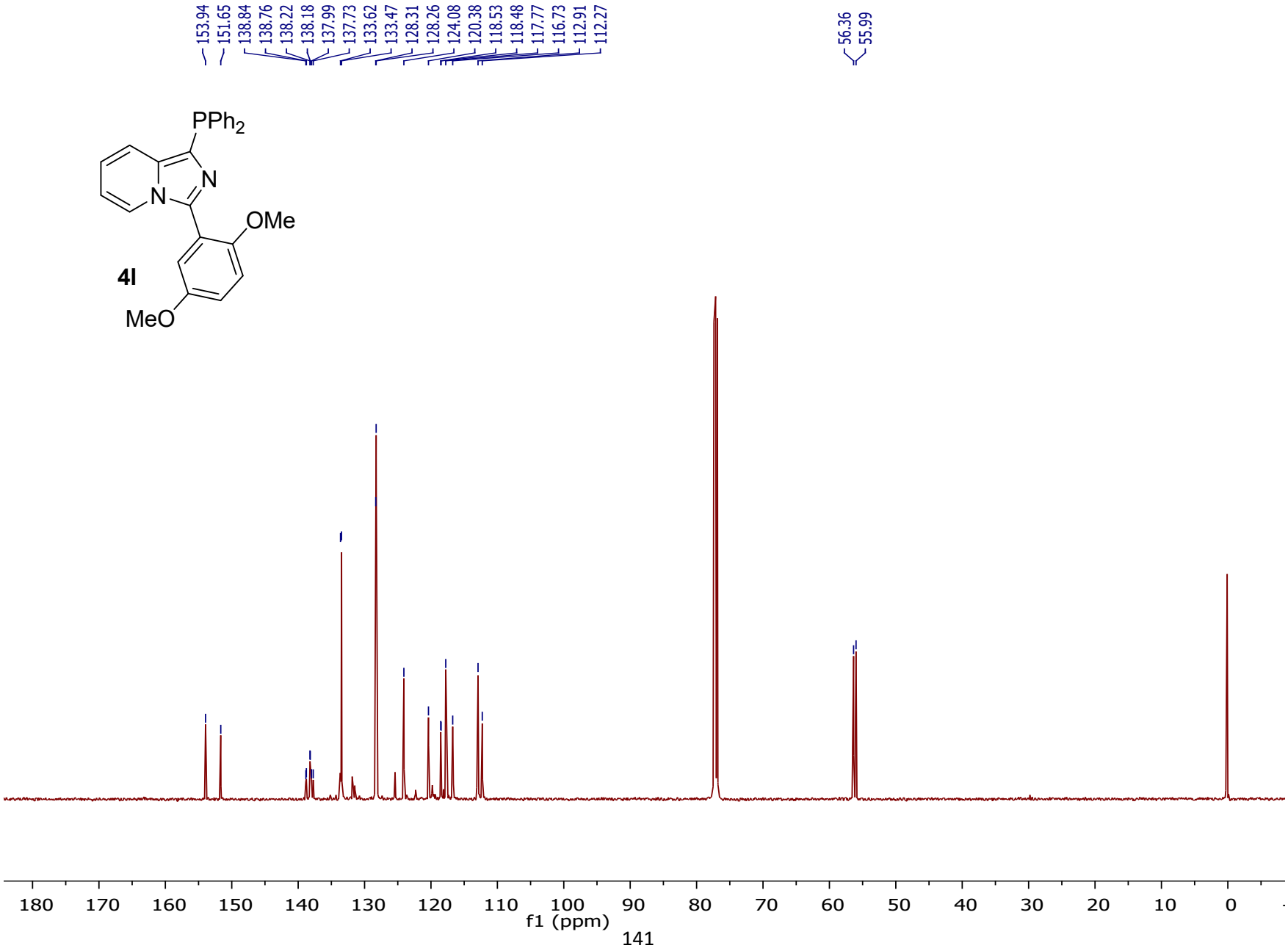

153.94
151.38
138.41
133.36
123.95
120.18
118.92
118.37
117.31
116.97
112.77
73.18
56.25
56.01
I
N
N
OMe
MeO
10f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


PCy2
N
N
OMe
4k
MeO
1.00
0.98
0.97
1.05
0.97
1.02
1.01
3.22
2.98
2.17
11.99
10.87
f1 (ppm)

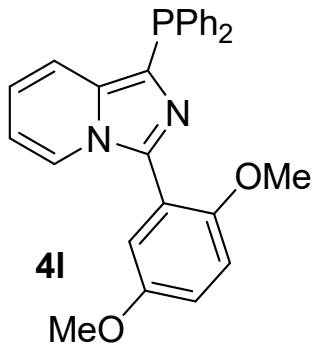

154.00
151.90
139.13
137.85
125.49
123.44
120.49
119.20
118.84
118.03
116.08
113.30
112.00
56.56
55.89
32.99
30.81
29.57
27.28
27.05
26.69
PCy2
N
N
OMe
4k
MeO
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


PCy2
N
N
OMe
4k
MeO
-25.83
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
50 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)


PPh2
N
N
OMe
4l
MeO
0.94
3.96
1.10
5.97
0.96
2.15
0.99
1.00
3.00
3.08
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

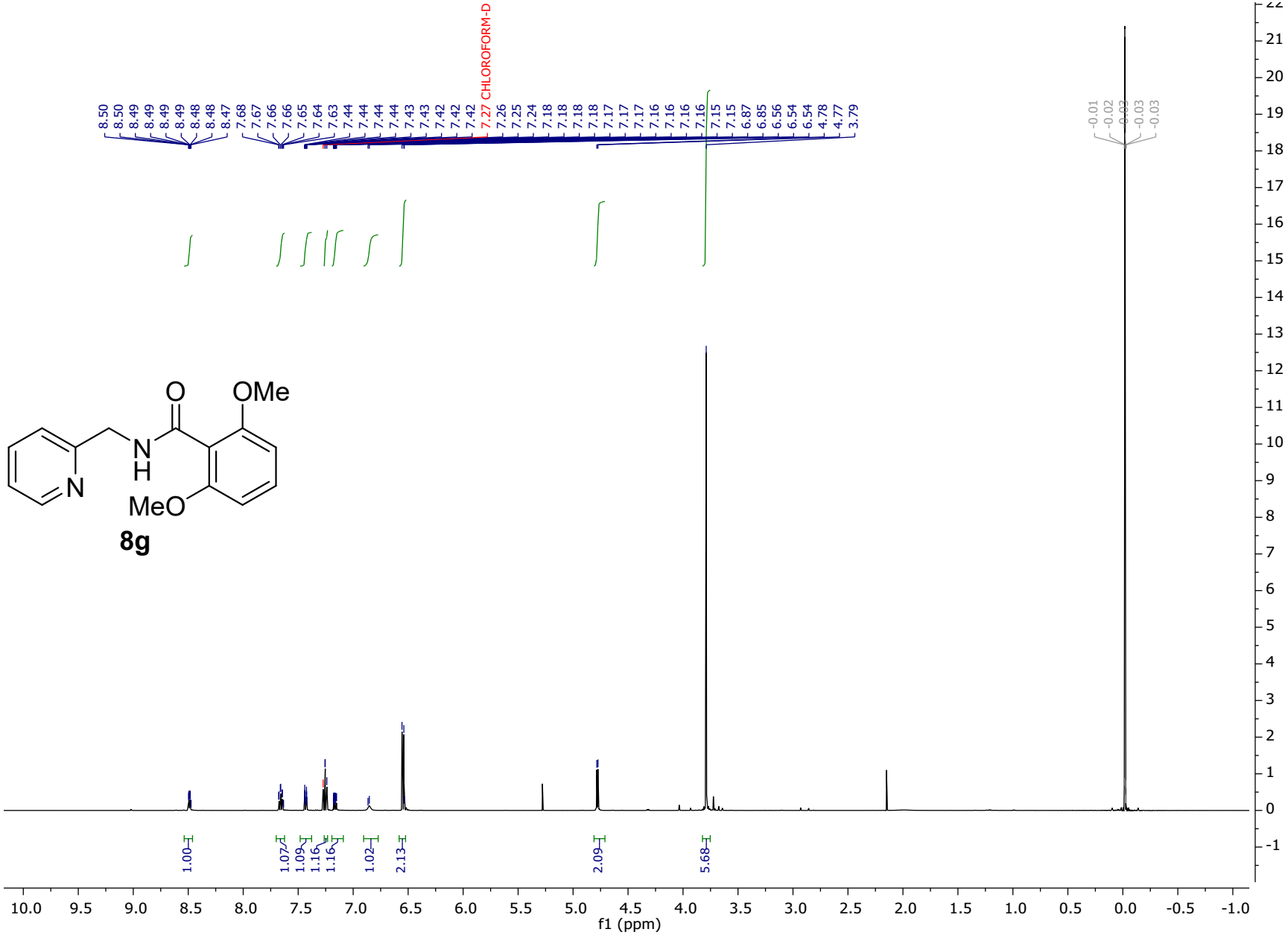

153.94
151.65
138.84
138.76
138.22
138.18
137.99
137.73
133.62
133.47
128.31
128.26
124.08
120.38
118.53
118.48
117.77
116.73
112.91
112.27
56.36
55.99
PPh2
N
N
OMe
MeO
4l
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

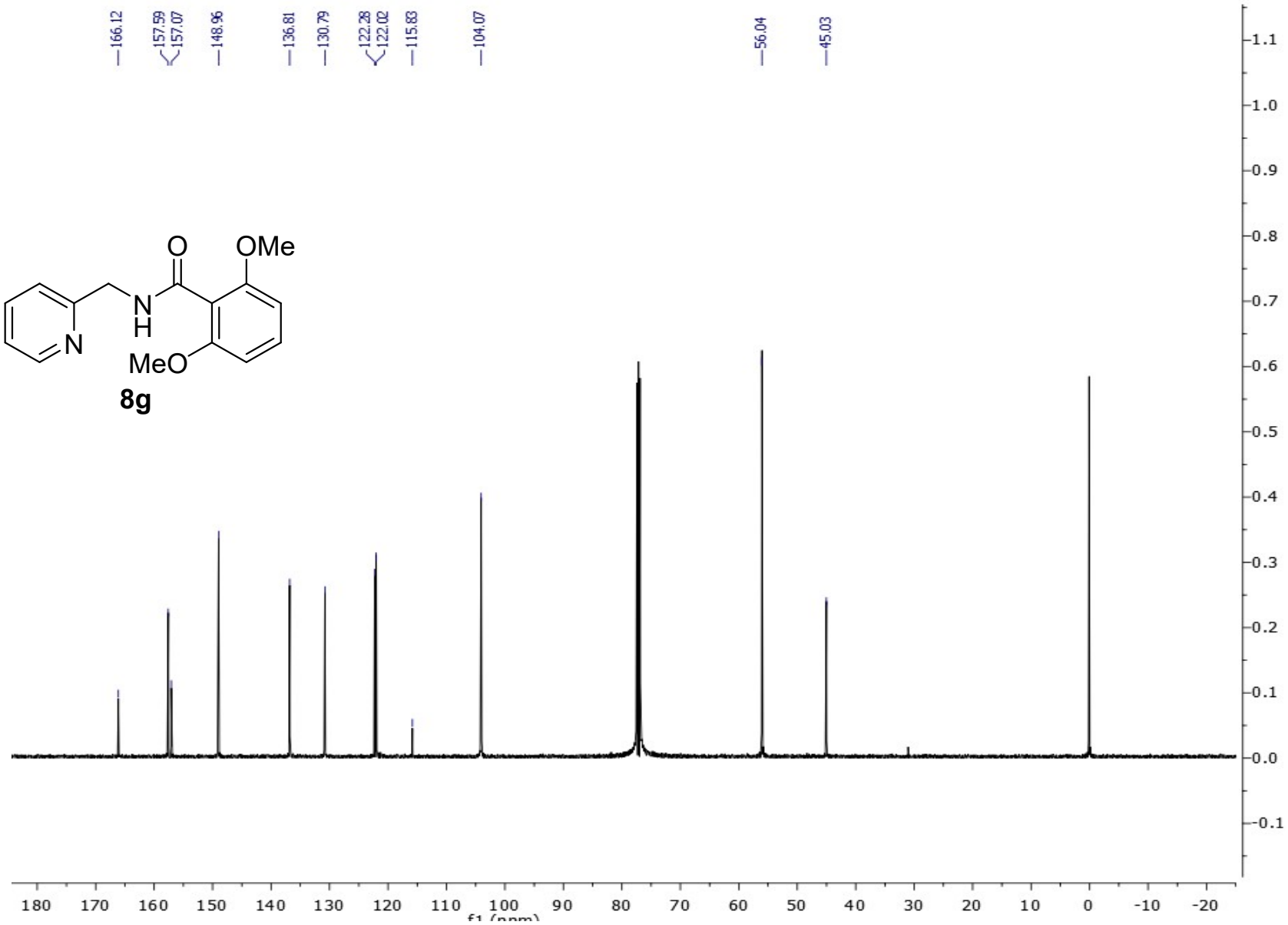
-N-28a

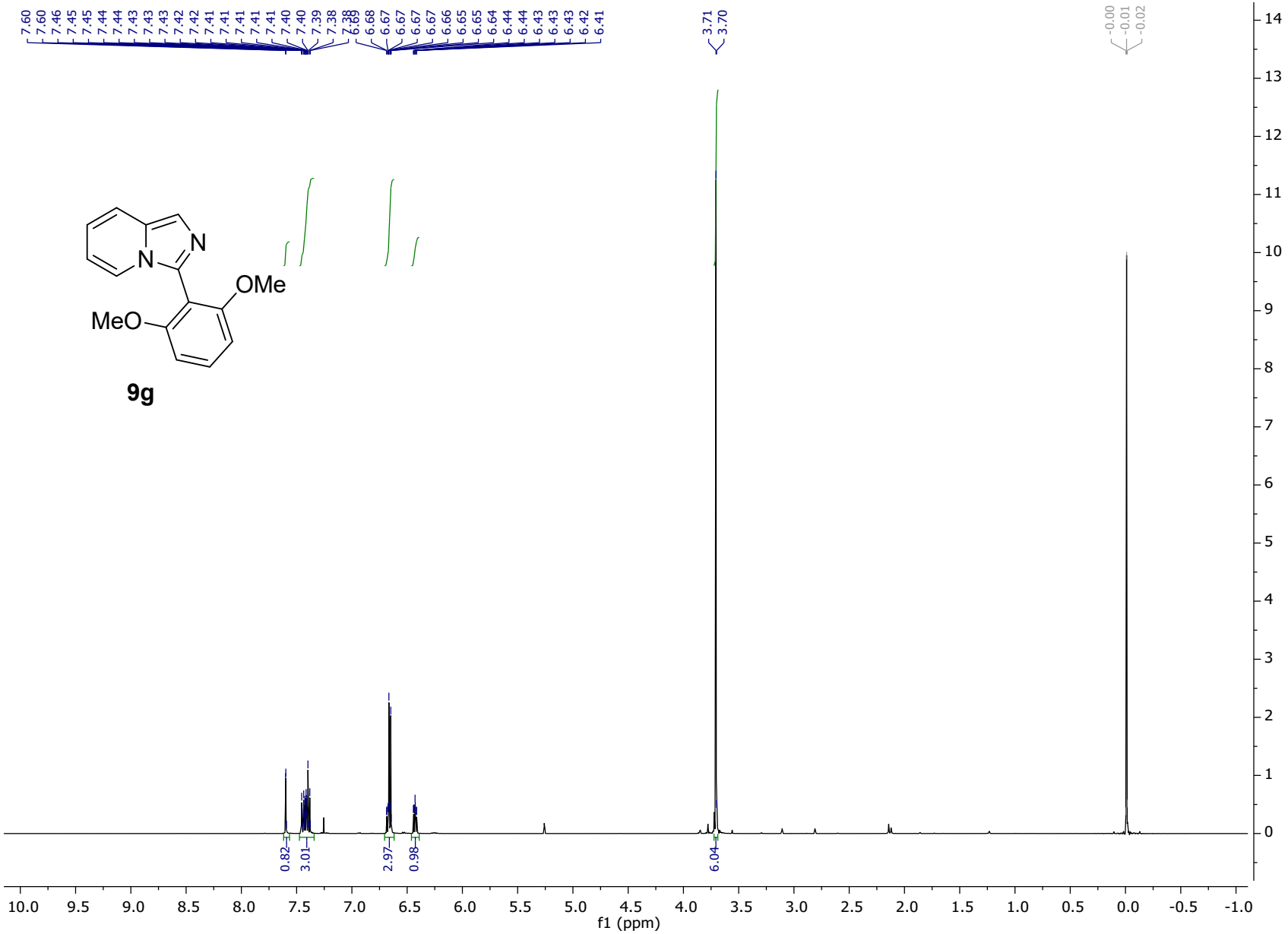

PPh2
N
N
OMe
MeO

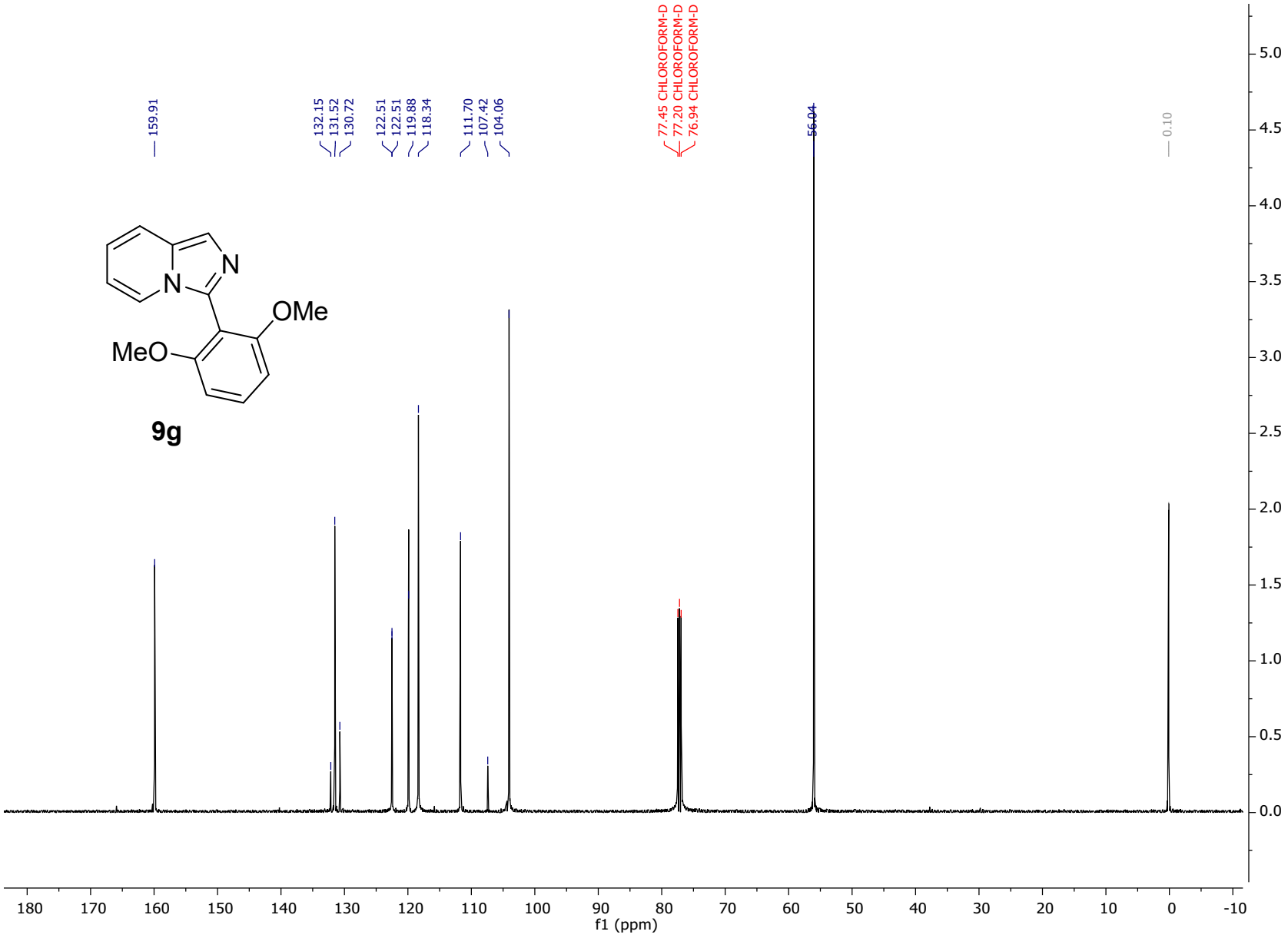
4l

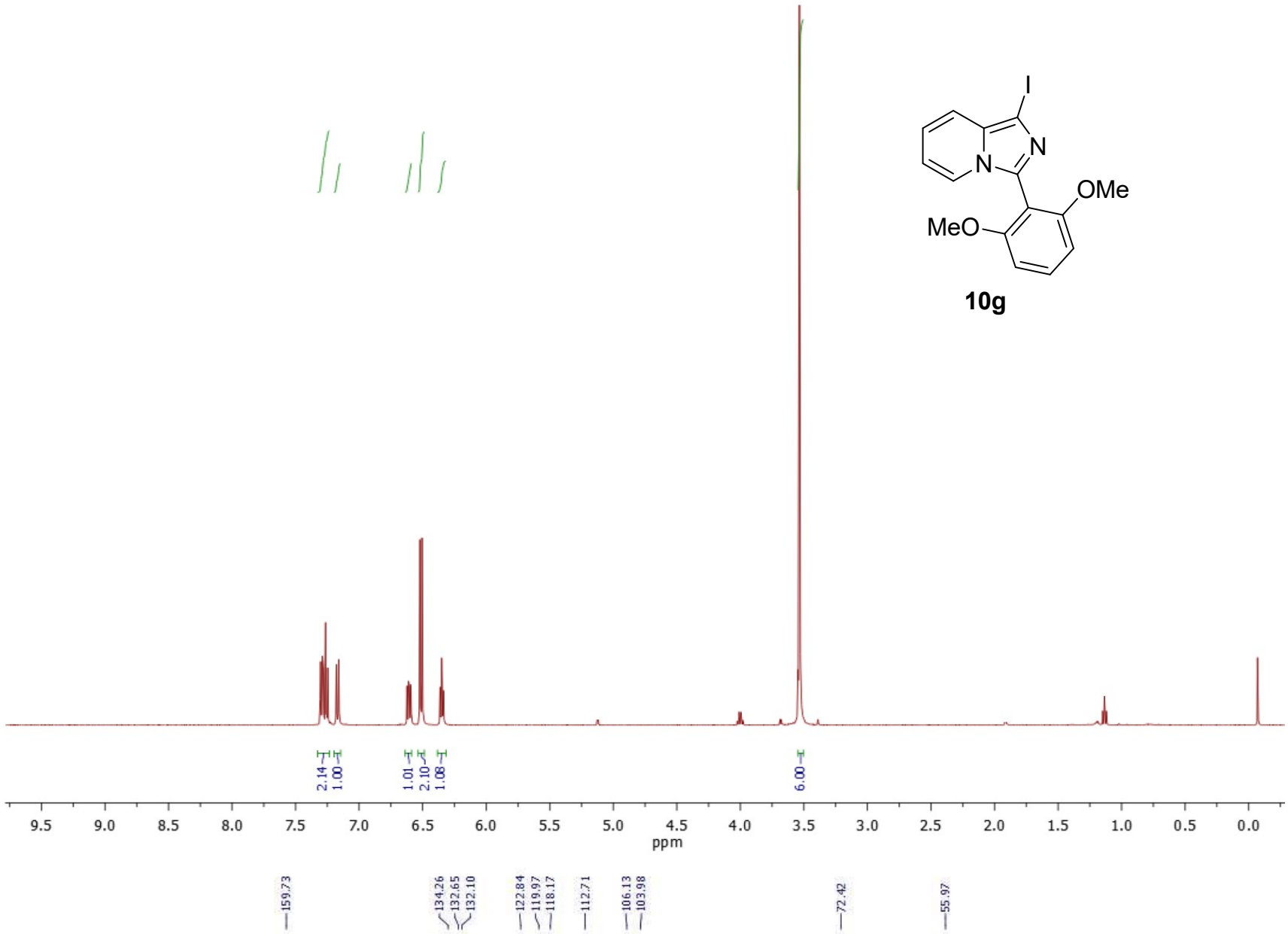
-30.83
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
f1 (ppm)

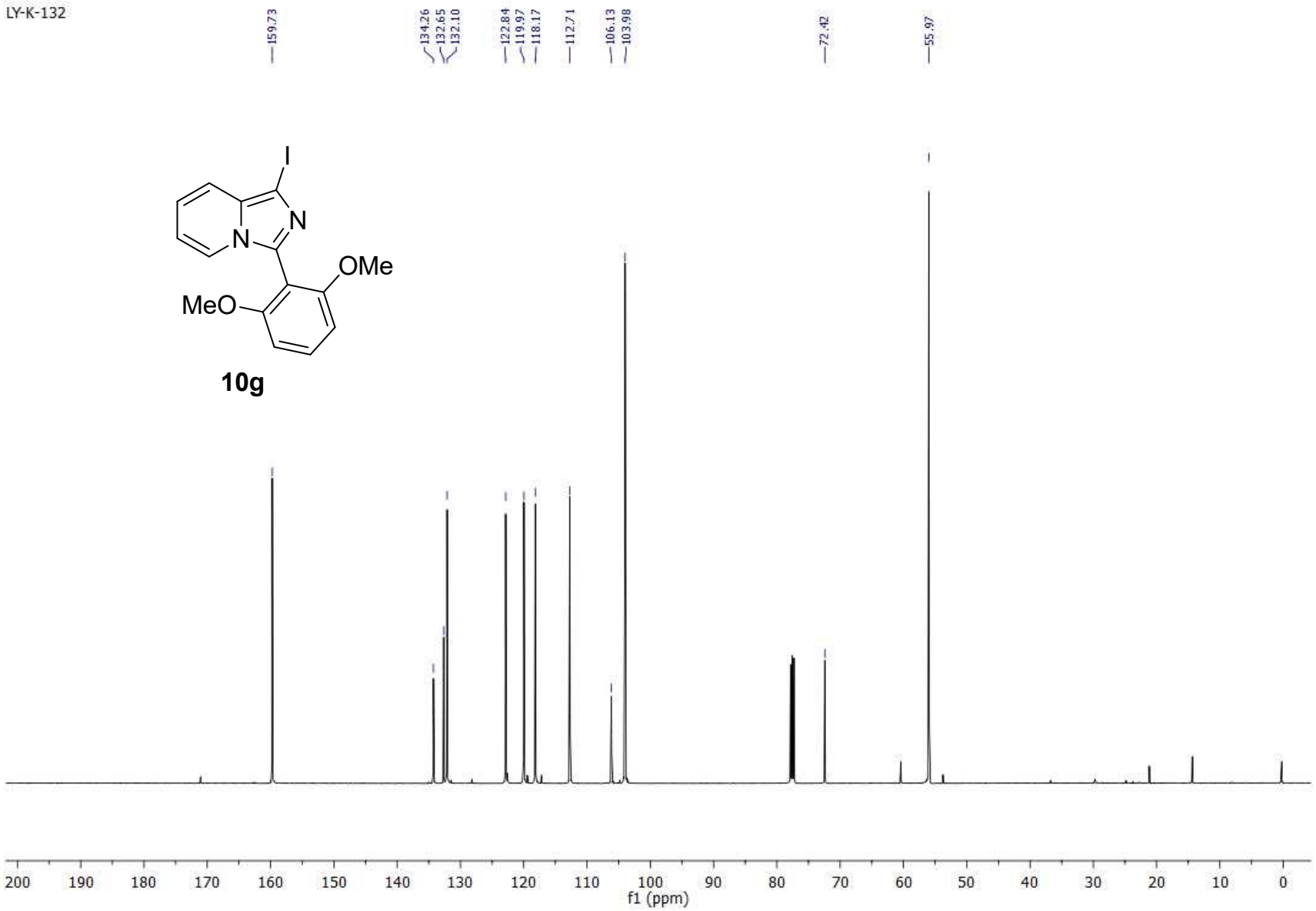

8.50 8.50 8.49 8.49 8.49 8.49 8.48 8.48 8.47 7.68 7.67 7.66 7.66 7.65 7.64 7.63 7.44 7.44 7.44 7.44 7.43 7.43 7.42 7.42 7.42 7.27 CHLOROFORM-D 7.26 7.25 7.24 7.18 7.18 7.18 7.18 7.17 7.17 7.17 7.16 7.16 7.16 7.16 7.15 7.15 6.87 6.85 6.56 6.54 6.54 4.78 4.77 3.79
-0.01 -0.02 0.03 -0.03 -0.03
O
OMe
N
H
N
MeO
8g
1.00 1.07 1.09 1.16 1.16 1.02 2.13 2.09 5.68
f1 (ppm)

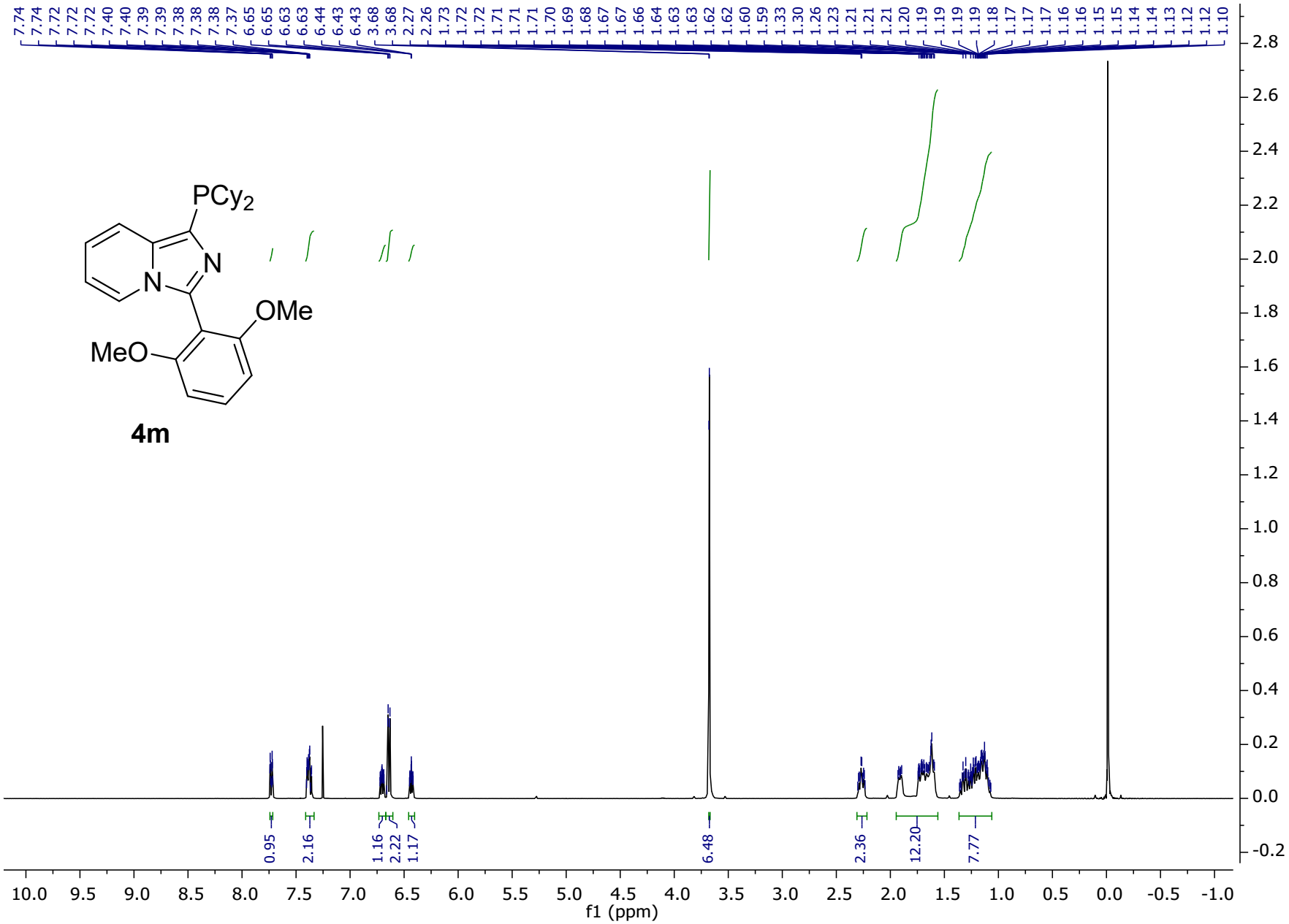

166.12
157.59
157.07
148.96
136.81
130.79
122.28
122.02
115.83
104.07
56.04
45.03
O
OMe
N
H
N
MeO
8g
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

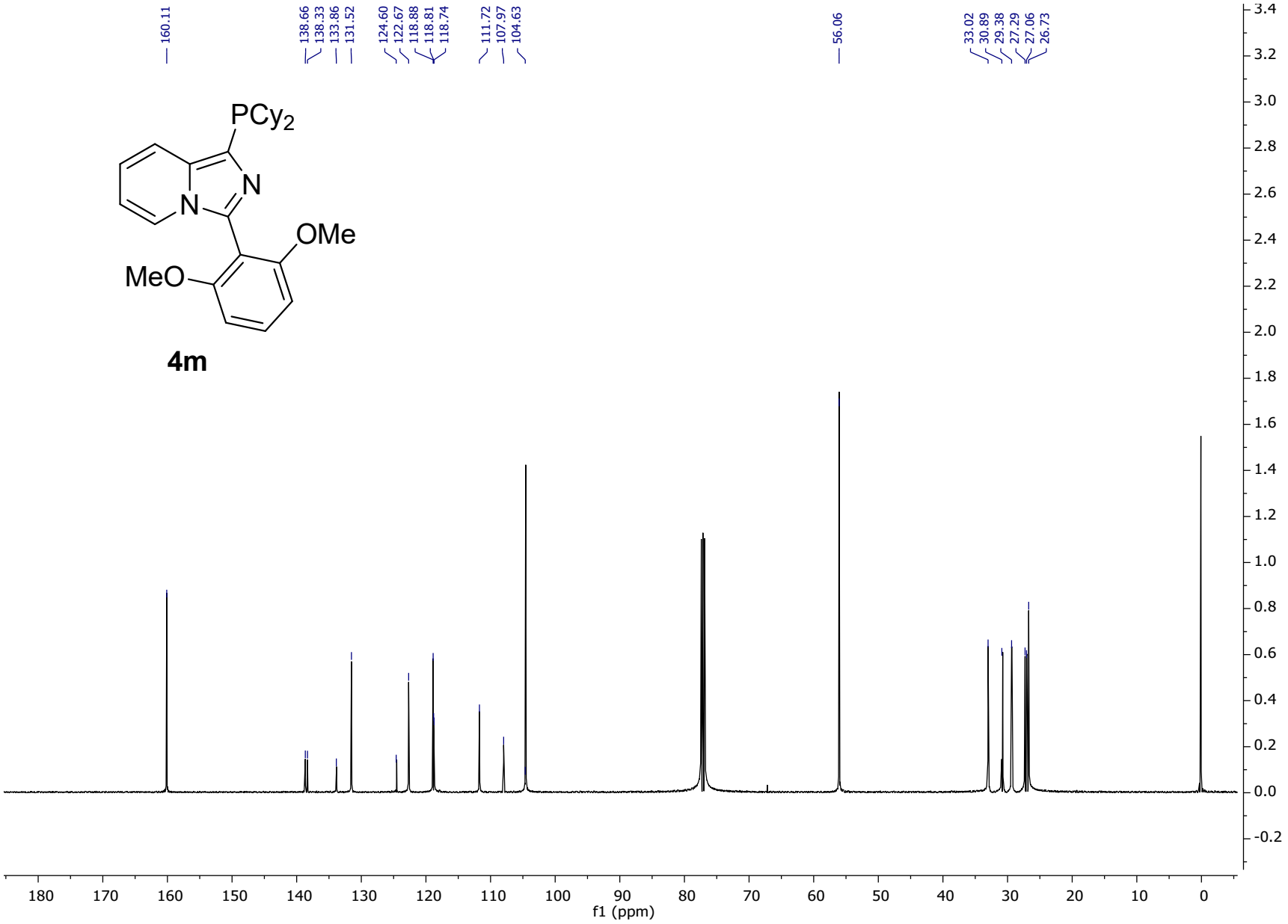

7.60
7.60
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.43
7.42
7.42
7.41
7.41
7.41
7.41
7.41
7.40
7.40
7.39
7.38
6.68
6.68
6.67
6.67
6.67
6.67
6.66
6.65
6.64
6.44
6.44
6.43
6.43
6.43
6.42
6.41
3.71
3.70
-0.00
-0.01
-0.02
N
N
OMe
MeO
9g
0.82
3.01
2.97
0.98
6.04
f1 (ppm)

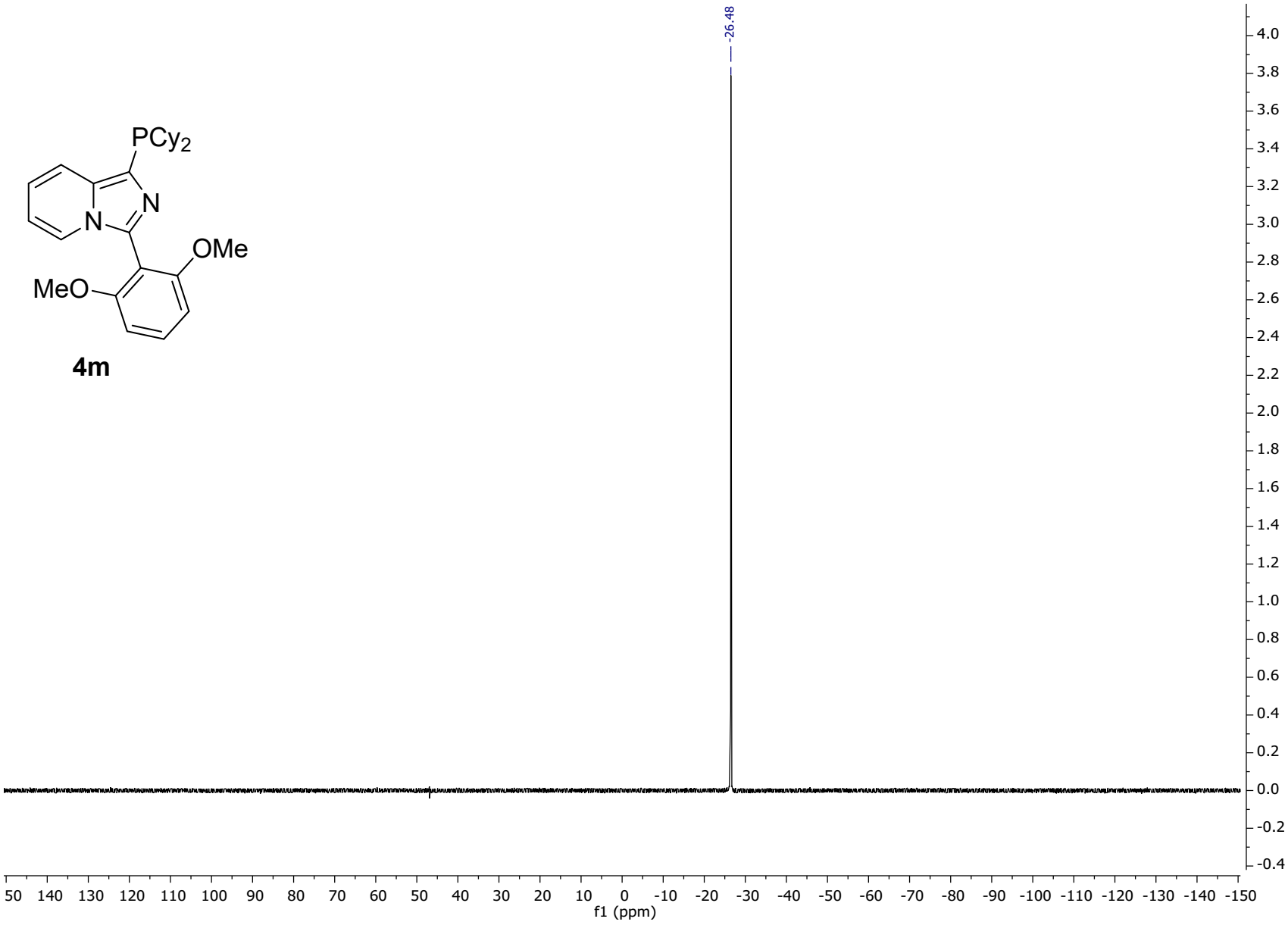

159.91
132.15
131.52
130.72
122.51
122.51
119.88
118.34
111.70
107.42
104.06
77.45 CHLOROFORM-D
77.20 CHLOROFORM-D
76.94 CHLOROFORM-D
56.04
0.10
N
N
OMe
MeO
9g
f1 (ppm)


I
N
N
OMe
MeO
10g
2.14
1.00
1.01
2.10
1.08
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
159.73
134.26
132.65
132.10
122.84
119.97
118.17
112.71
106.13
103.98
72.42
55.97

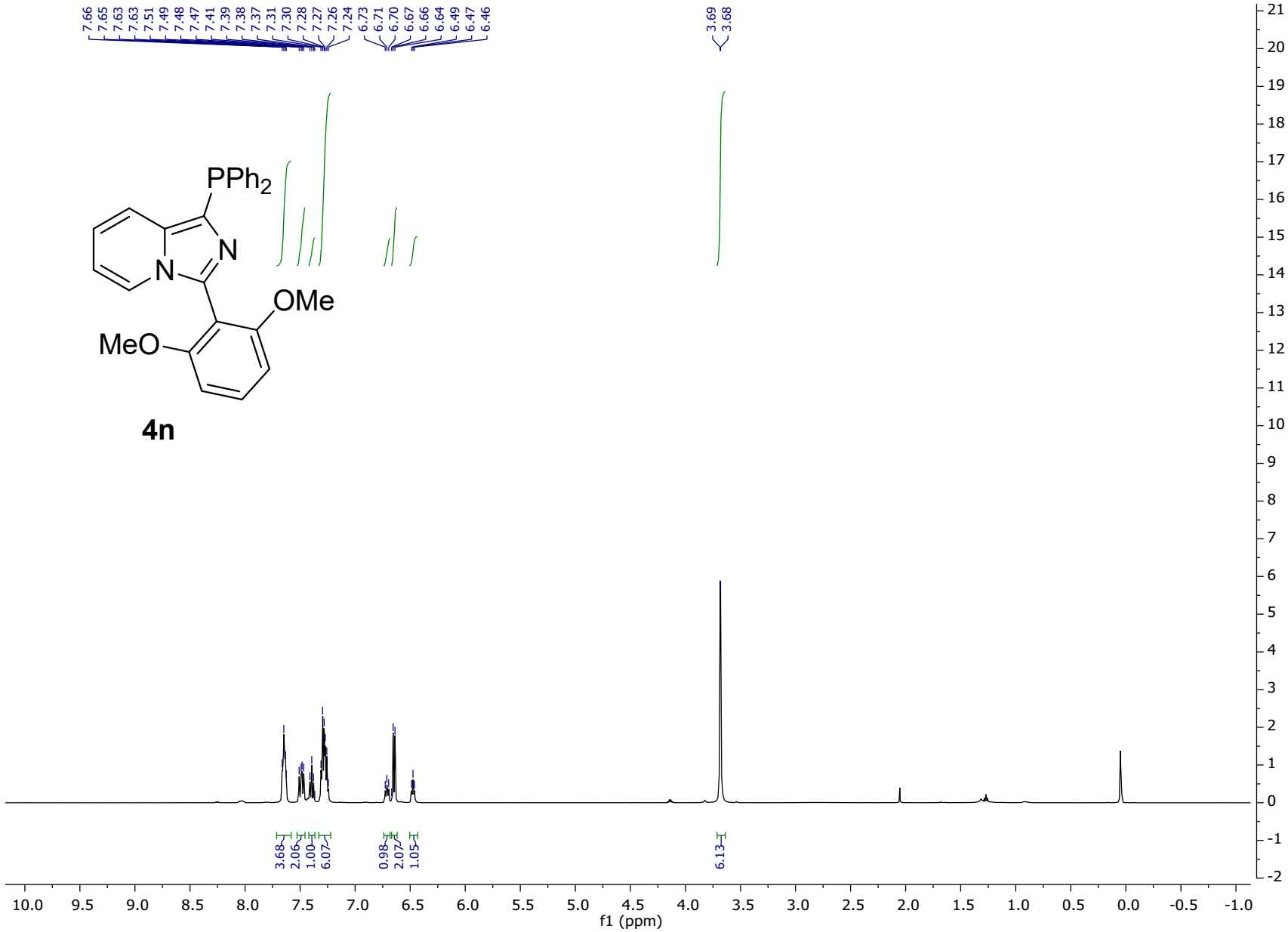

LY-K-132
159.73
134.26
132.65
132.10
122.84
119.97
118.17
112.71
106.13
103.98
72.42
55.97
I
N
N
OMe
MeO
10g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

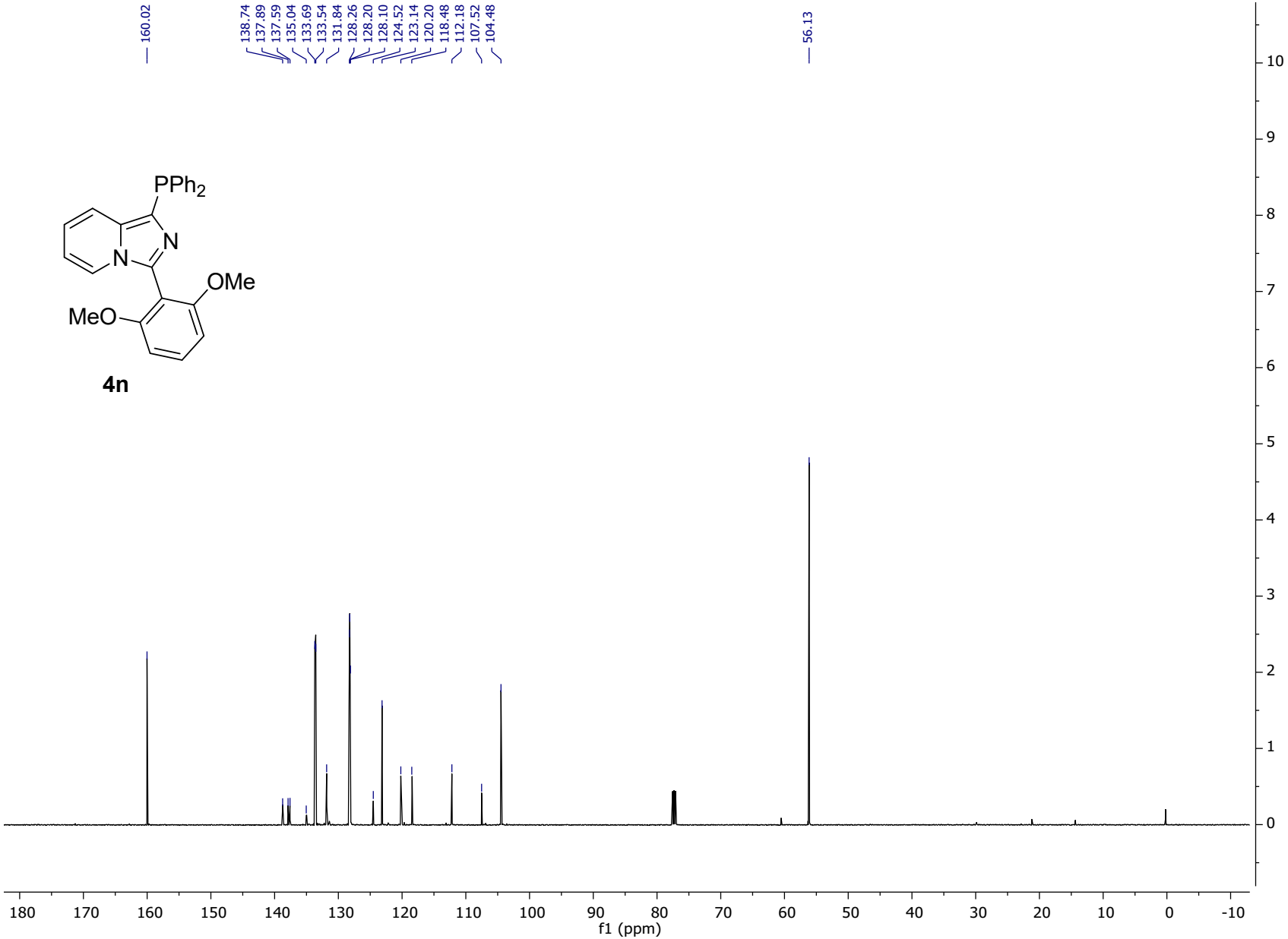

PCy2
N
N
OMe
MeO
4m
f1 (ppm)

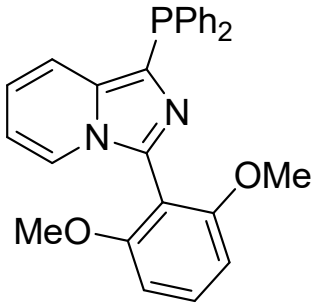

160.11
138.66
138.33
133.86
131.52
124.60
122.67
118.88
118.81
118.74
111.72
107.97
104.63
56.06
33.02
30.89
29.38
27.29
27.06
26.73
PCy2
N
N
OMe
MeO
4m
f1 (ppm)


PCy2
N
N
OMe
MeO
-26.48
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
50 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150
f1 (ppm)

4m

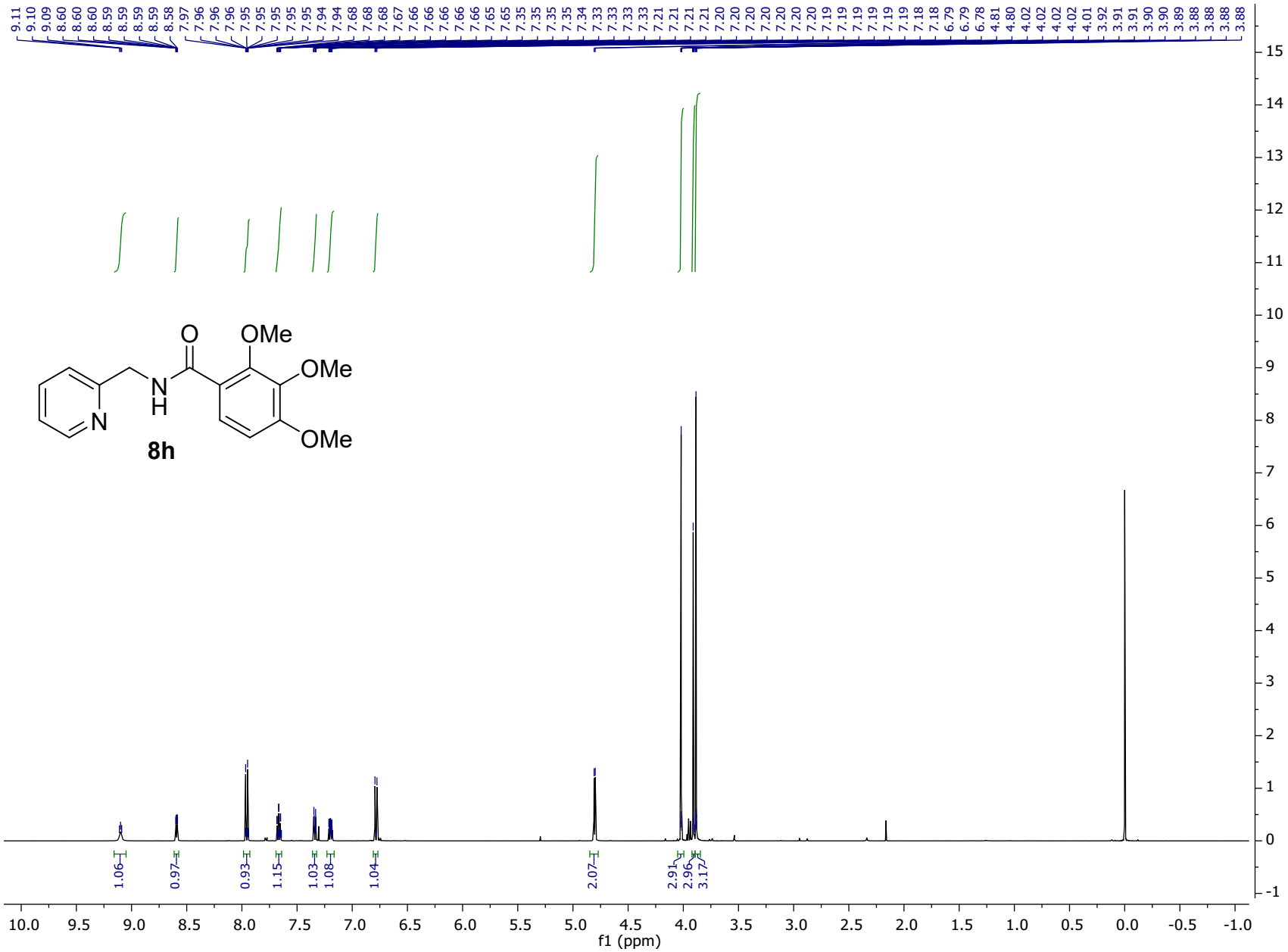

7.66
7.65
7.63
7.63
7.51
7.49
7.48
7.47
7.41
7.39
7.38
7.37
7.31
7.30
7.28
7.27
7.26
7.24
6.73
6.71
6.70
6.67
6.66
6.64
6.49
6.47
6.46
3.69
3.68
PPh2
N
N
OMe
MeO
4n
3.68
2.06
1.00
6.07
0.98
2.07
1.05
6.13
f1 (ppm)

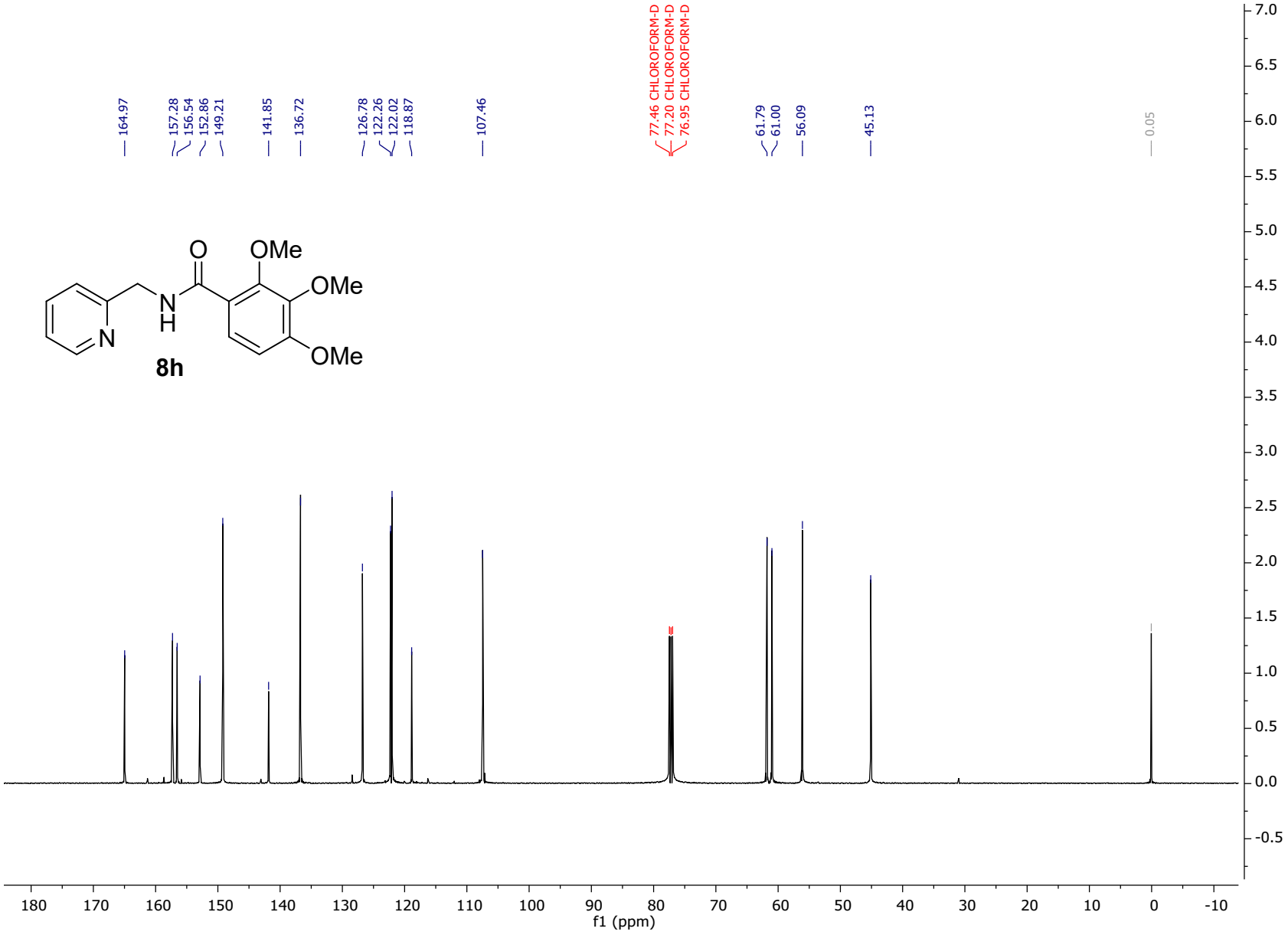

160.02
138.74
137.89
137.59
135.04
133.69
133.54
131.84
128.26
128.20
128.10
124.52
123.14
120.20
118.48
112.18
107.52
104.48
56.13
PPh2
N
N
OMe
MeO
4n
f1 (ppm)


PPh2
N
N
OMe
MeO

4n

-31.87
2500
2000
1500
1000
500
0
00 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100
f1 (ppm)


9.11 9.10 9.09 8.60 8.60 8.60 8.59 8.59 8.59 8.59 8.58 7.97 7.96 7.96 7.96 7.95 7.95 7.95 7.95 7.94 7.94 7.68 7.68 7.68 7.67 7.66 7.66 7.66 7.66 7.66 7.65 7.65 7.35 7.35 7.35 7.34 7.33 7.33 7.33 7.33 7.21 7.21 7.21 7.20 7.20 7.20 7.20 7.20 7.20 7.20 7.19 7.19 7.19 7.19 7.19 7.18 7.18 6.79 6.79 6.78 4.81 4.80 4.02 4.02 4.02 4.02 4.01 3.92 3.91 3.91 3.90 3.90 3.89 3.88 3.88 3.88 3.88
O
OMe
OMe
N
H
N
OMe
8h
1.06
0.97
0.93
1.15
1.03
1.08
1.04
2.07
2.91
2.96
3.17
f1 (ppm)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141.85
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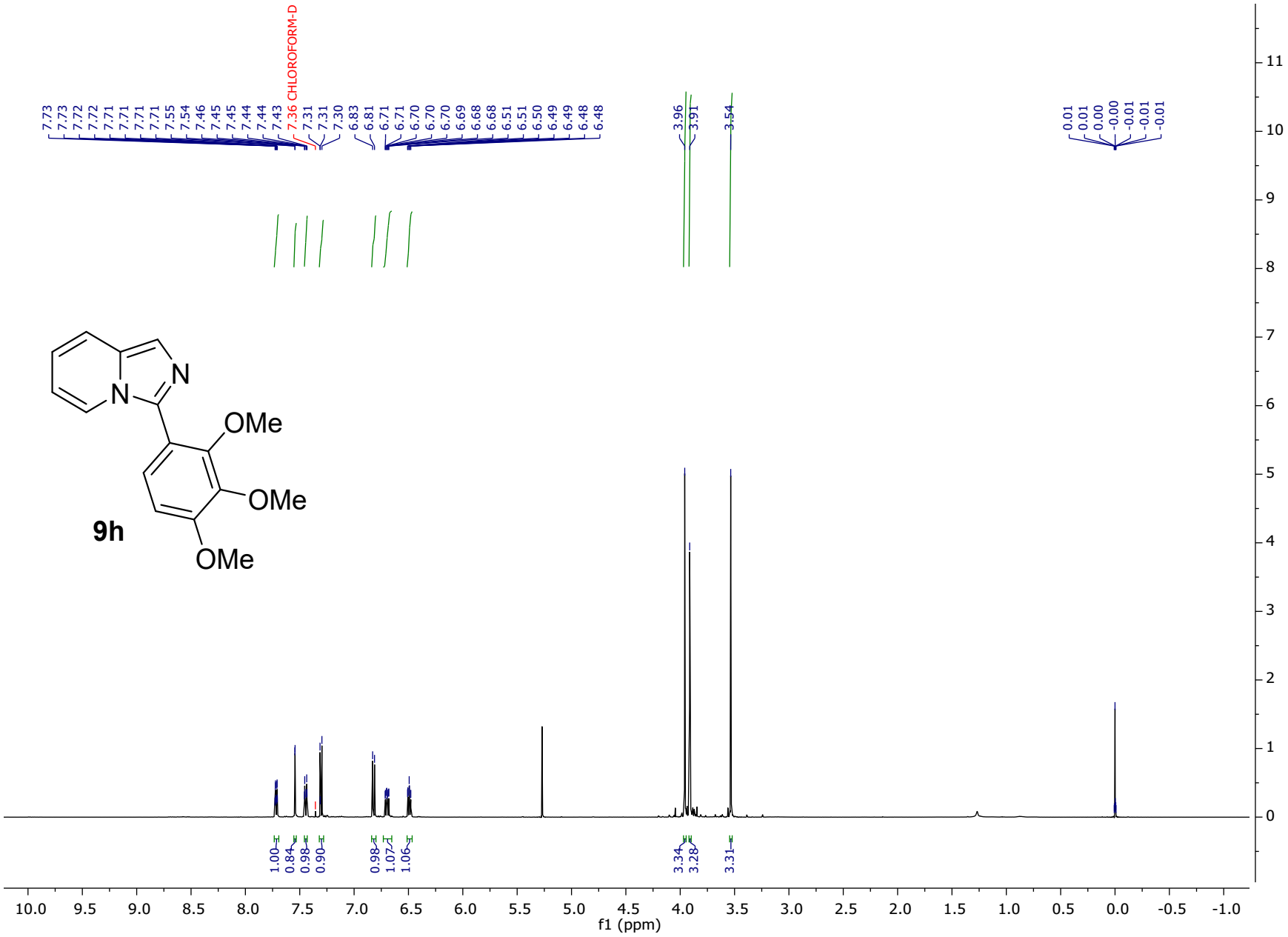
126.78
122.26
122.02
118.87
107.46
77.46 CHLOROFORM-D
77.20 CHLOROFORM-D
76.95 CHLOROFORM-D
61.79
61.00
56.09
45.13
0.05
O
OMe
OMe
OMe
N
H
N
8h
f1 (ppm)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7.73
7.72
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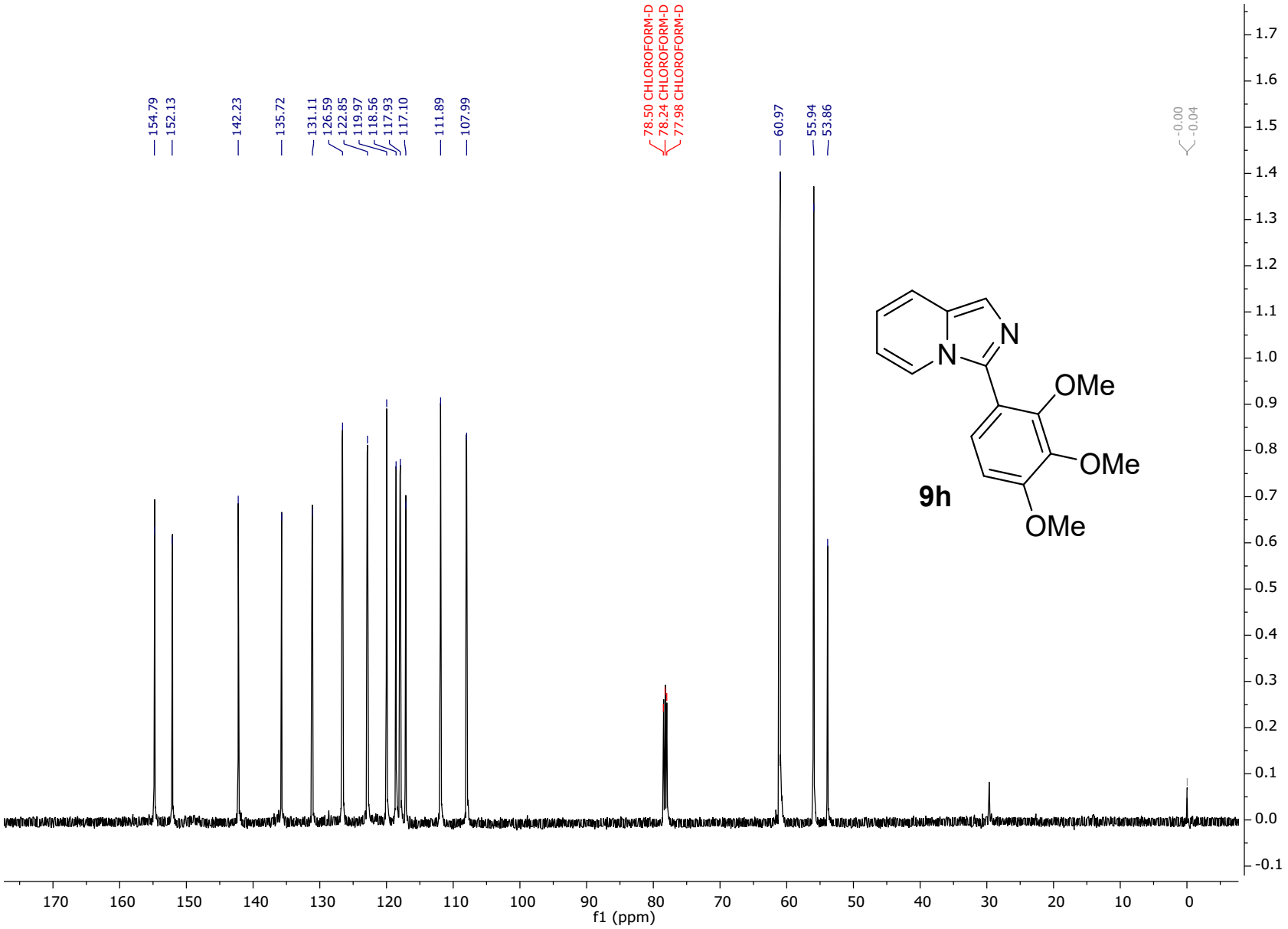
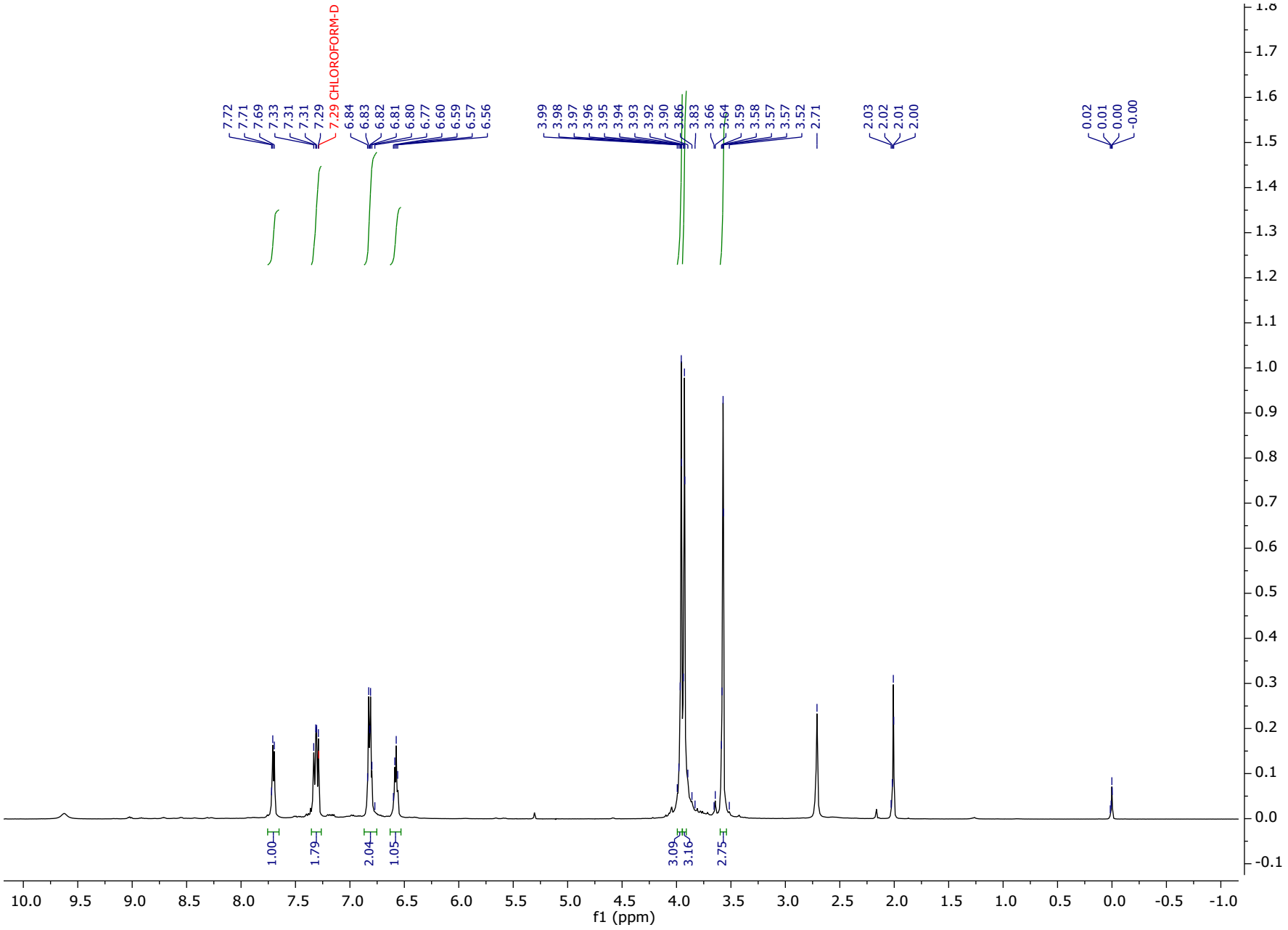
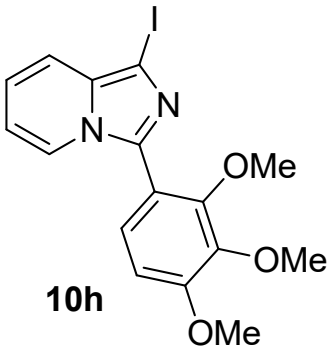
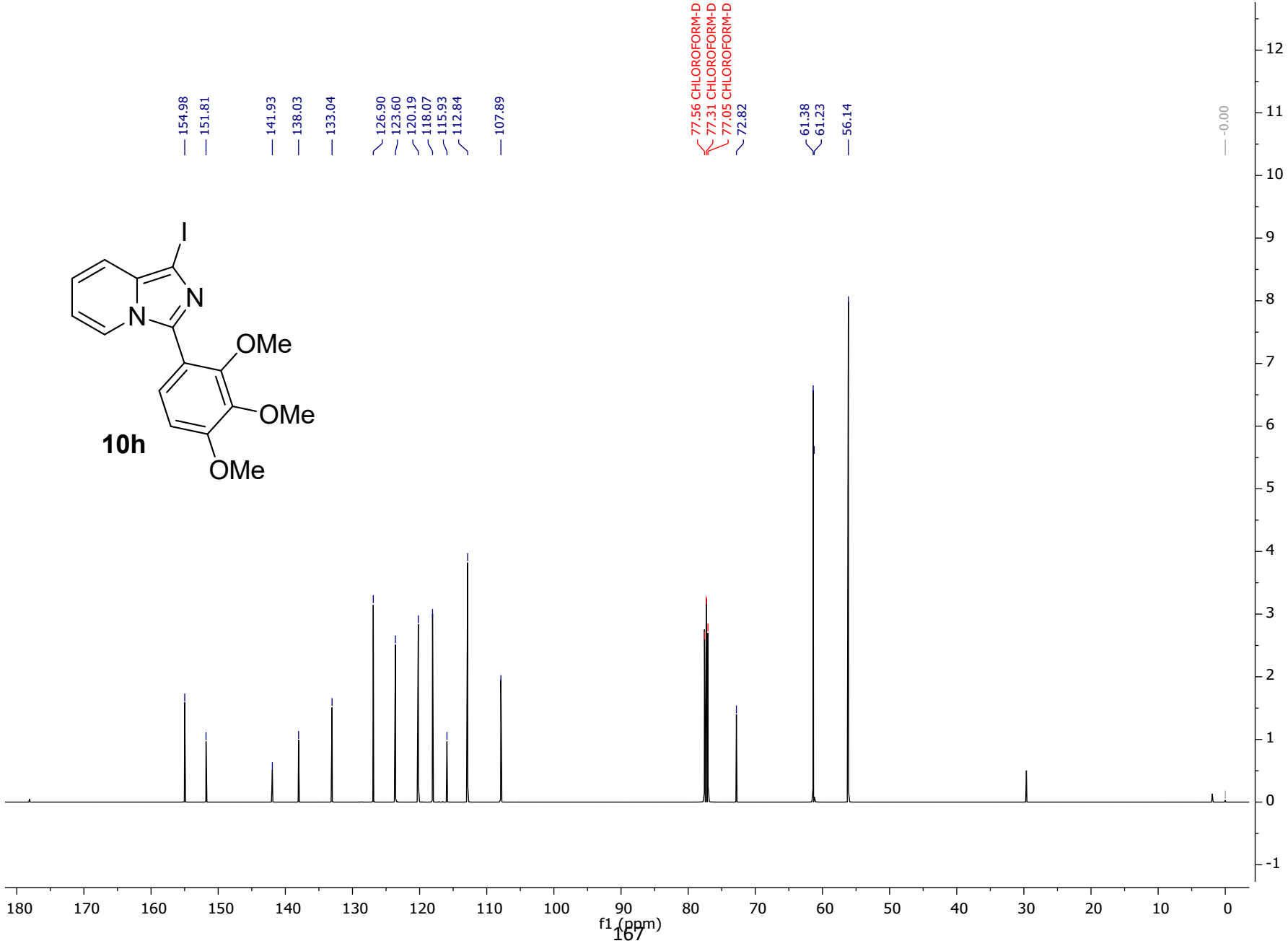
7.71
7.71
7.55
7.54
7.46
7.45
7.45
7.44
7.44
7.43
7.36 CHLOROFORM-D
7.31
7.31
7.30
6.83
6.81
6.71
6.71
6.70
6.70
6.70
6.69
6.68
6.68
6.51
6.51
6.50
6.49
6.49
6.48
6.48
3.96
3.91
3.54
0.01
0.01
0.00
-0.00
-0.01
-0.01
-0.01
N
N
OMe
OMe
OMe
9h
1.00
0.84
0.98
0.90
0.98
1.07
1.06
3.34
3.28
3.31
f1 (ppm)


154.79
152.13
142.23
135.72
131.11
126.59
122.85
119.97
118.56
117.93
117.10
111.89
107.99
78.50 CHLOROFORM-D
78.24 CHLOROFORM-D
77.98 CHLOROFORM-D
60.97
55.94
53.86
-0.00
-0.04
N
N
OMe
OMe
OMe
9h
f1 (ppm)


7.72
7.71
7.69
7.33
7.31
7.31
7.29
7.29 CHLOROFORM-D
6.84
6.83
6.82
6.81
6.80
6.77
6.60
6.59
6.57
6.56
3.99
3.98
3.97
3.96
3.95
3.94
3.93
3.92
3.90
3.86
3.83
3.66
3.64
3.59
3.58
3.57
3.57
3.52
2.71
2.03
2.02
2.01
2.00
0.02
0.01
0.00
-0.00
1.00
1.79
2.04
1.05
3.09
3.16
2.75
f1 (ppm)



10h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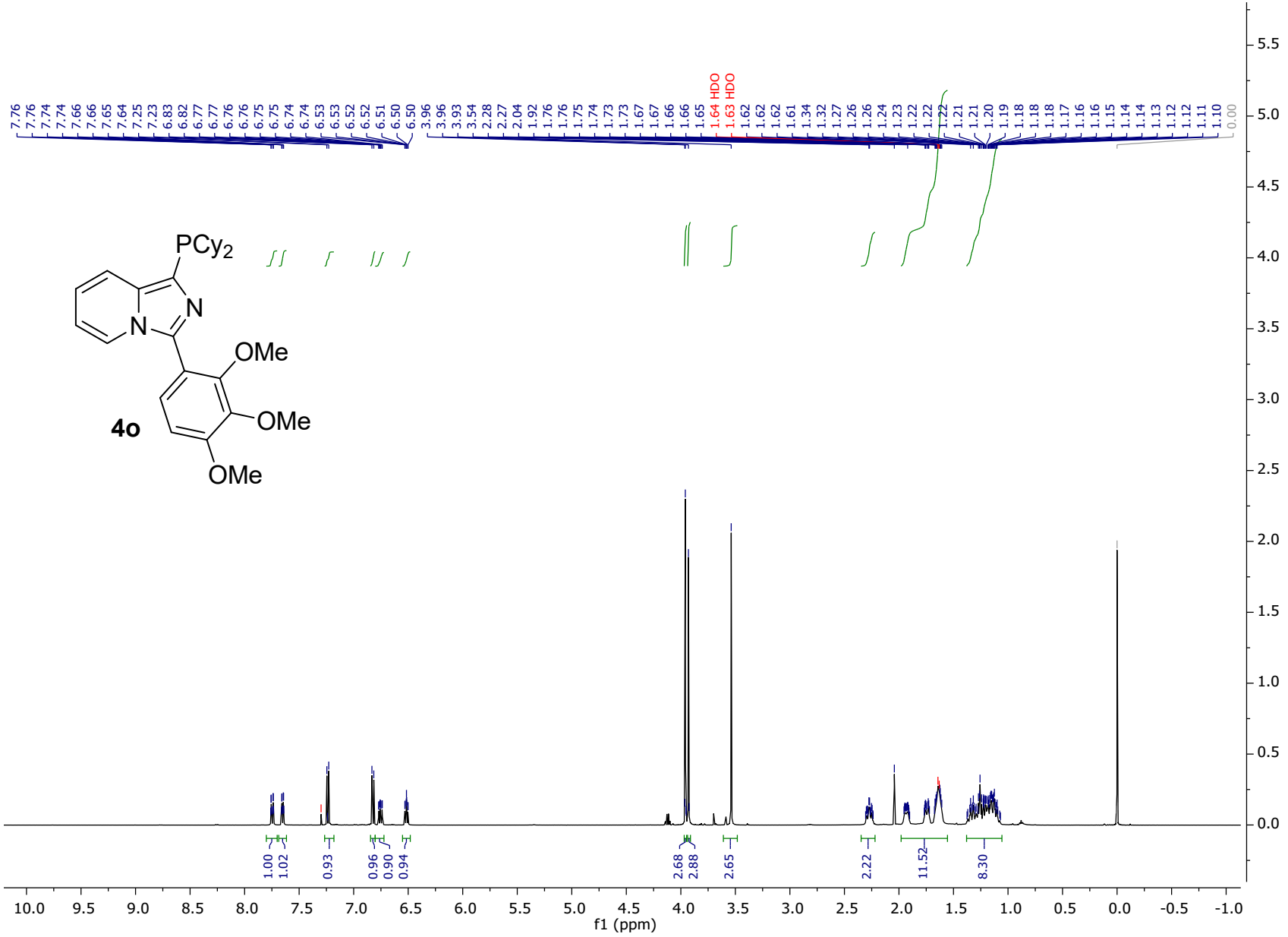
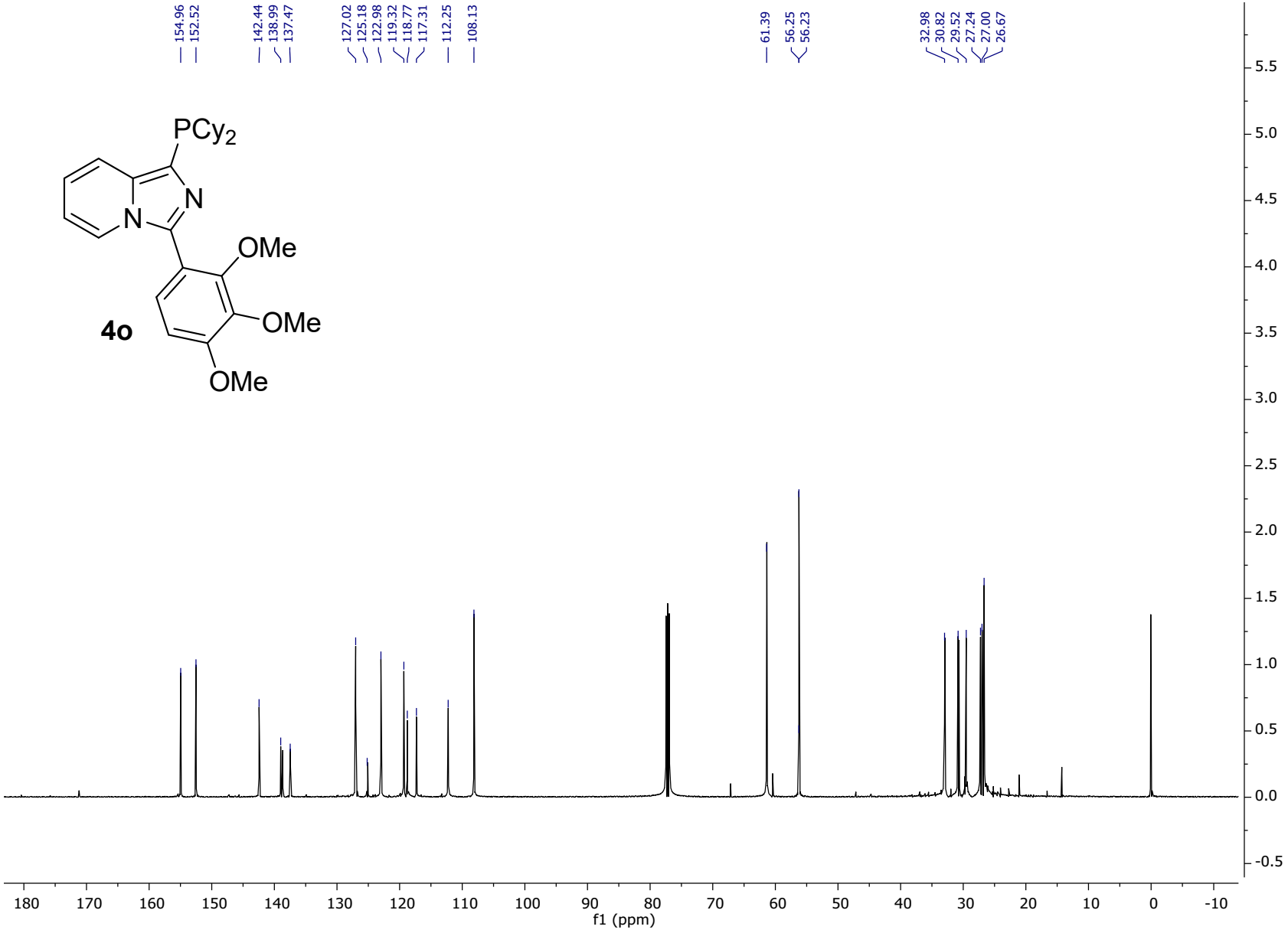
138.03
133.04
126.90
123.60
120.19
118.07
115.93
112.84
107.89
77.56 CHLOROFORM-D
77.31 CHLOROFORM-D
77.05 CHLOROFORM-D
72.82
61.38
61.23
56.14
-0.00
I
N
N
OMe
OMe
OMe
10h
f1 (ppm)


PCy2
N
N
OMe
OMe
OMe
4o
f1 (ppm)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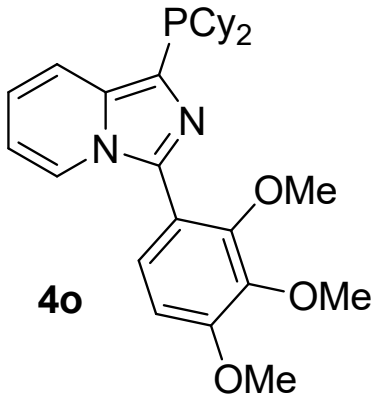
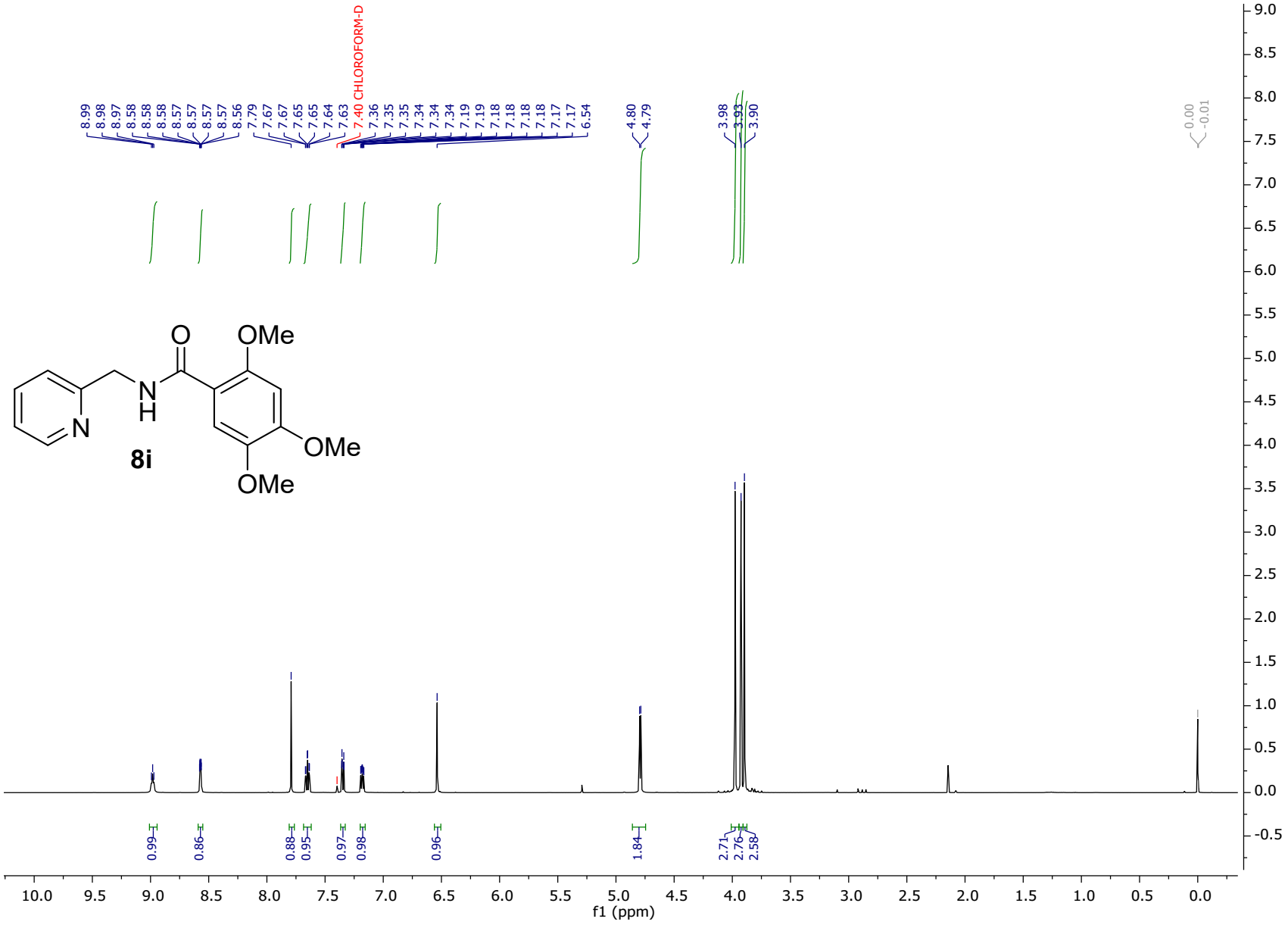
152.52
142.44
138.99
137.47
127.02
125.18
122.98
119.32
118.77
117.31
112.25
108.13
61.39
56.25
56.23
32.98
30.82
29.52
27.24
27.00
26.67
PCy2
N
N
OMe
OMe
OMe
4o
f1 (ppm)


PCy2
N
N
OMe
OMe
OMe

4o

-26.45
32
30
28
26
24
22
20
18
16
14
12
10
8
6
4
2
0
-2
-4
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)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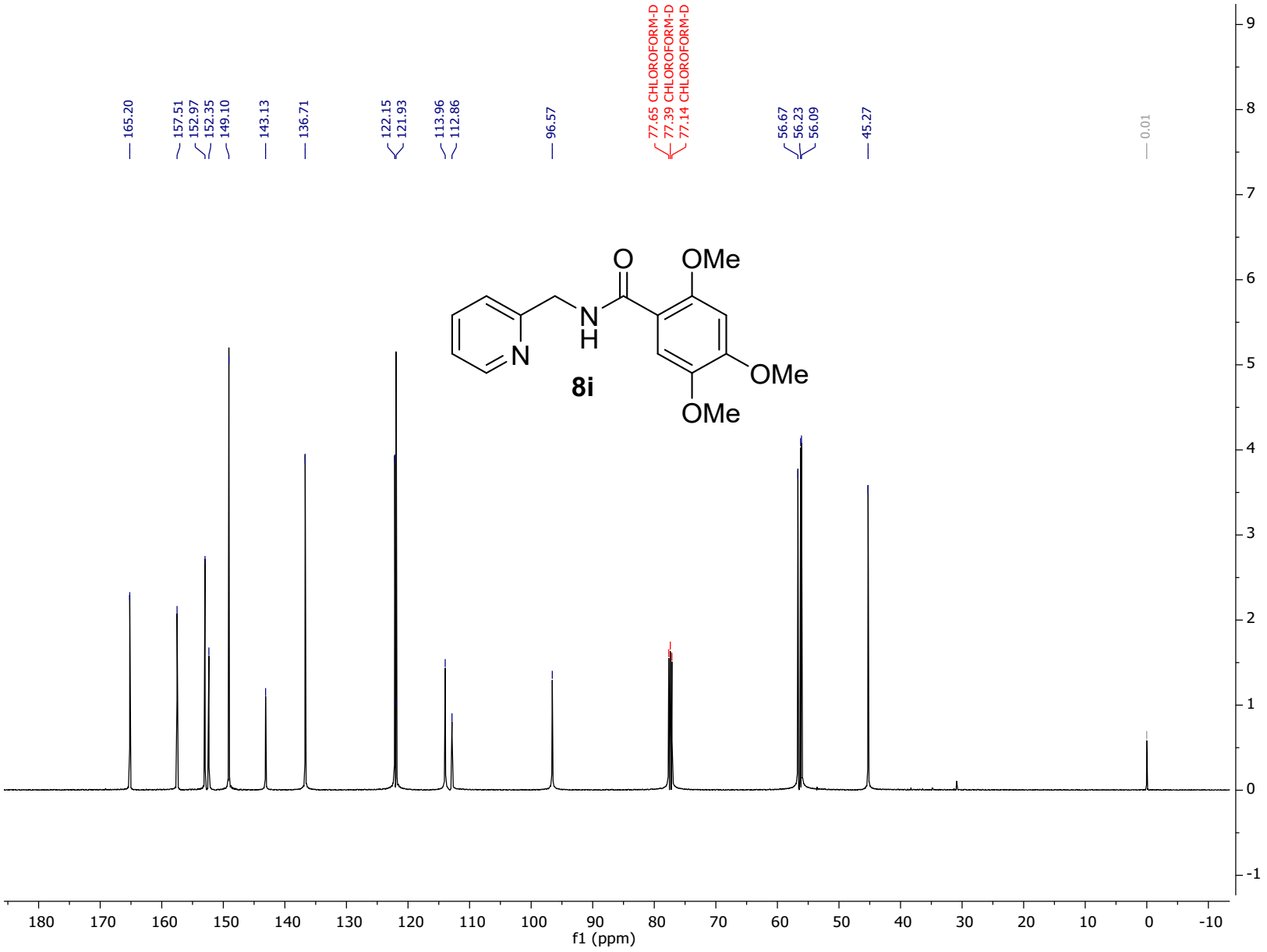
8.98
8.97
8.58
8.58
8.58
8.57
8.57
8.57
8.57
8.56
7.79
7.67
7.67
7.65
7.65
7.64
7.63
7.40 CHLOROFORM-D
7.36
7.35
7.35
7.34
7.34
7.34
7.19
7.19
7.18
7.18
7.18
7.18
7.17
7.17
6.54
4.80
4.79
3.98
3.93
3.90
0.00
-0.01
O
OMe
N
H
N
OMe
OMe
8i
0.99
0.86
0.88
0.95
0.97
0.98
0.96
1.84
2.71
2.76
2.58
f1 (ppm)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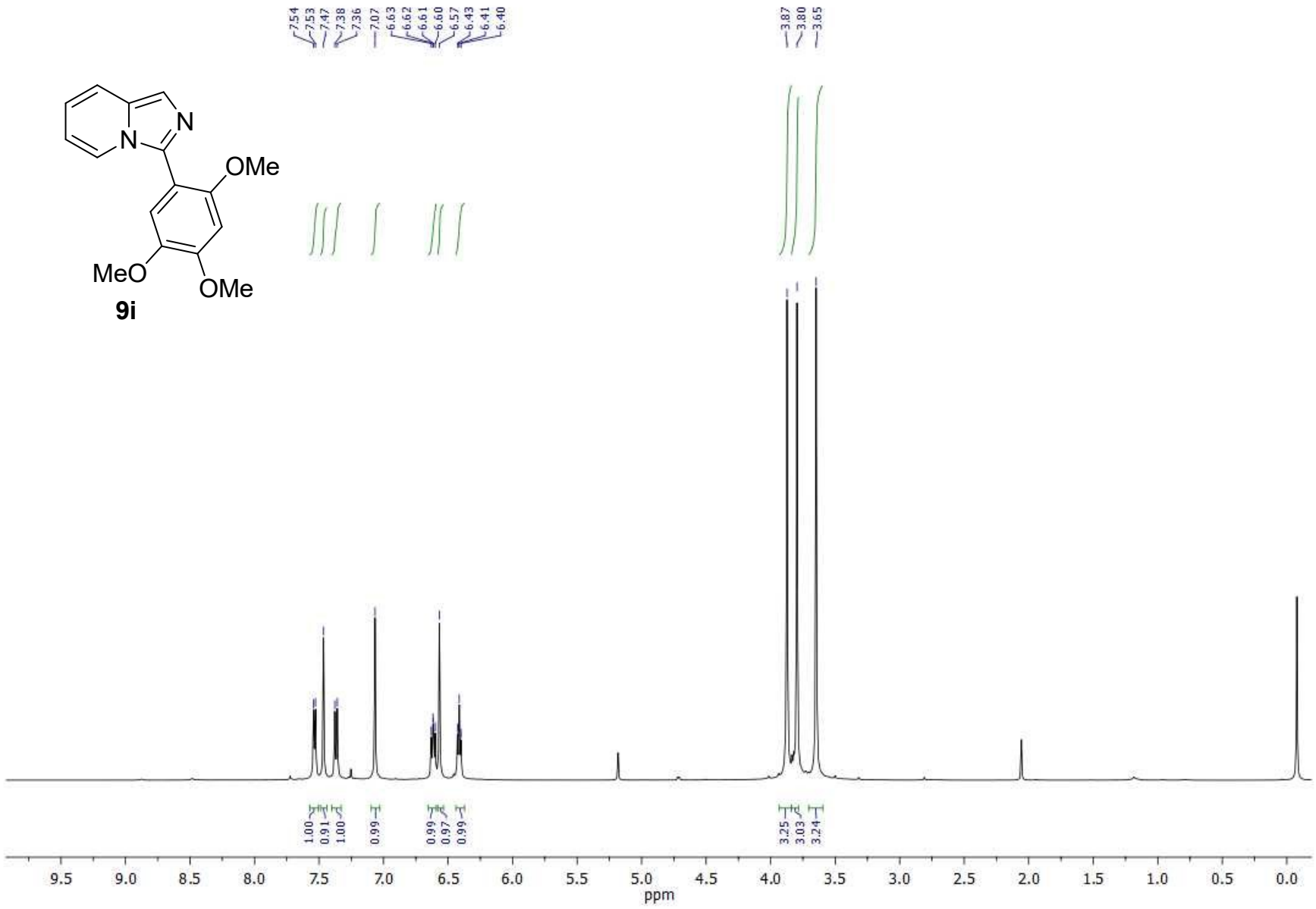
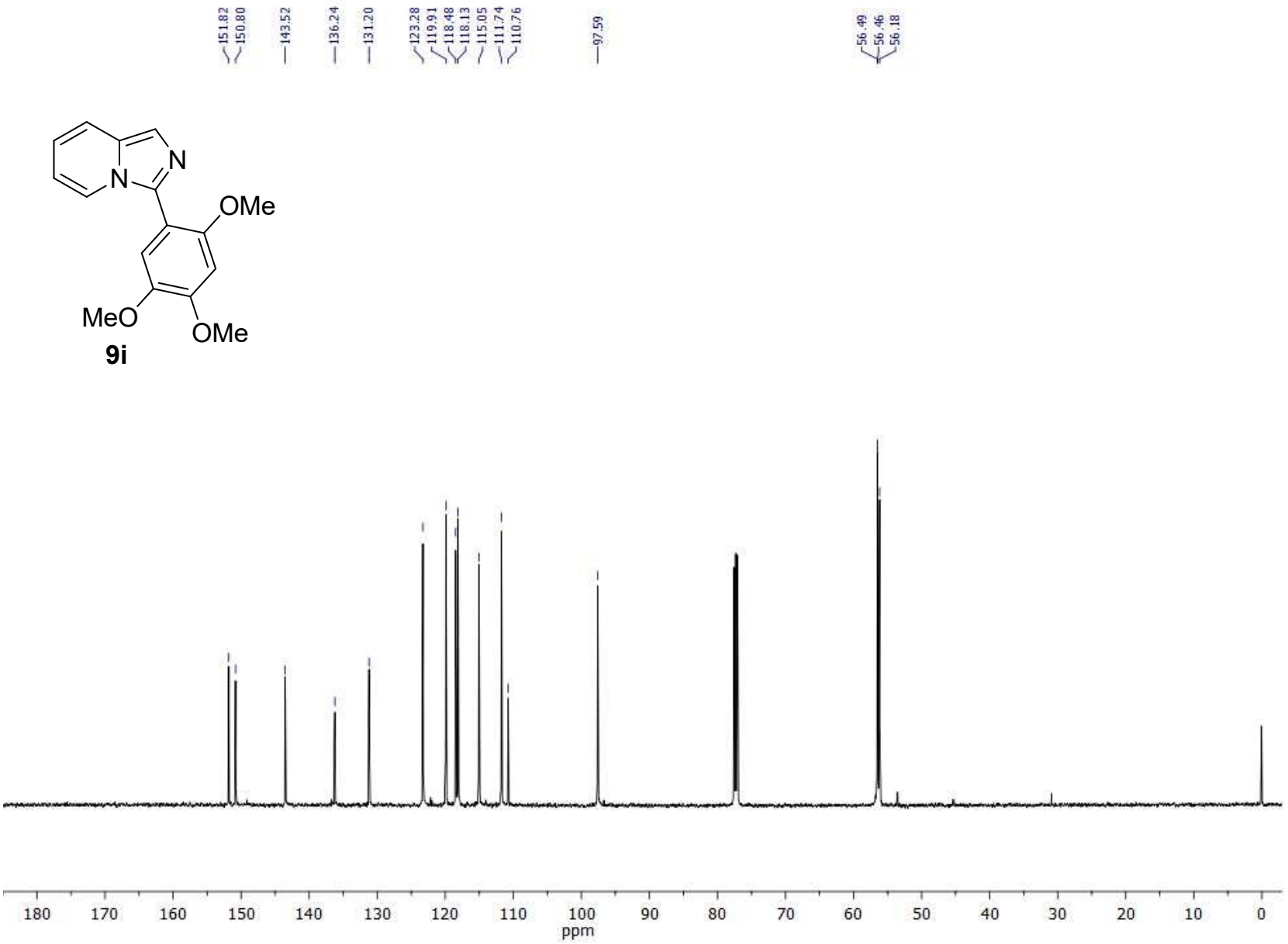
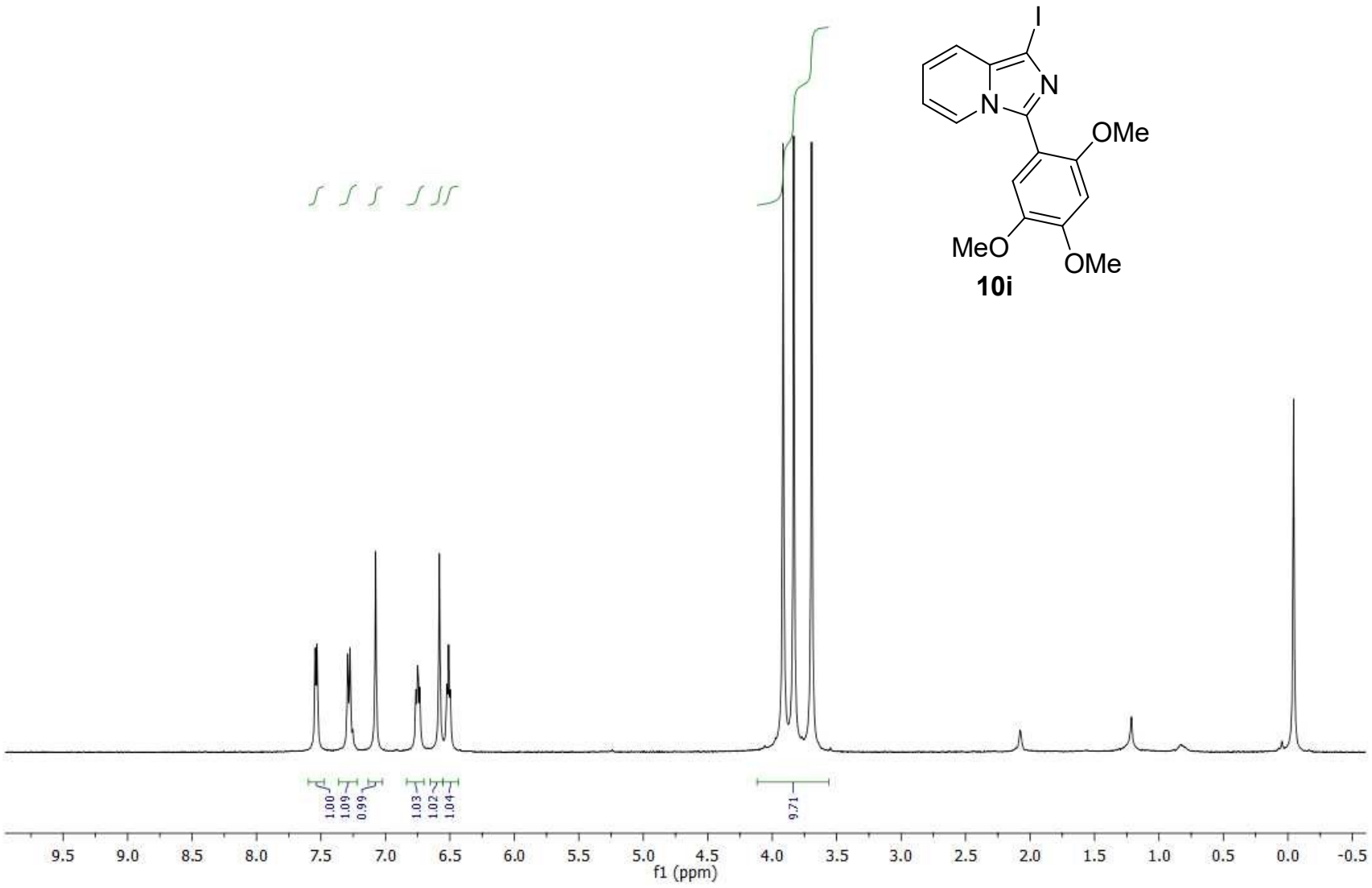
157.51
152.97
152.35
149.10
143.13
136.71
122.15
121.93
113.96
112.86
96.57
77.65 CHLOROFORM-D
77.39 CHLOROFORM-D
77.14 CHLOROFORM-D
56.67
56.23
56.09
45.27
0.01
O
OMe
N
H
N
OMe
OMe
8i
f1 (ppm)

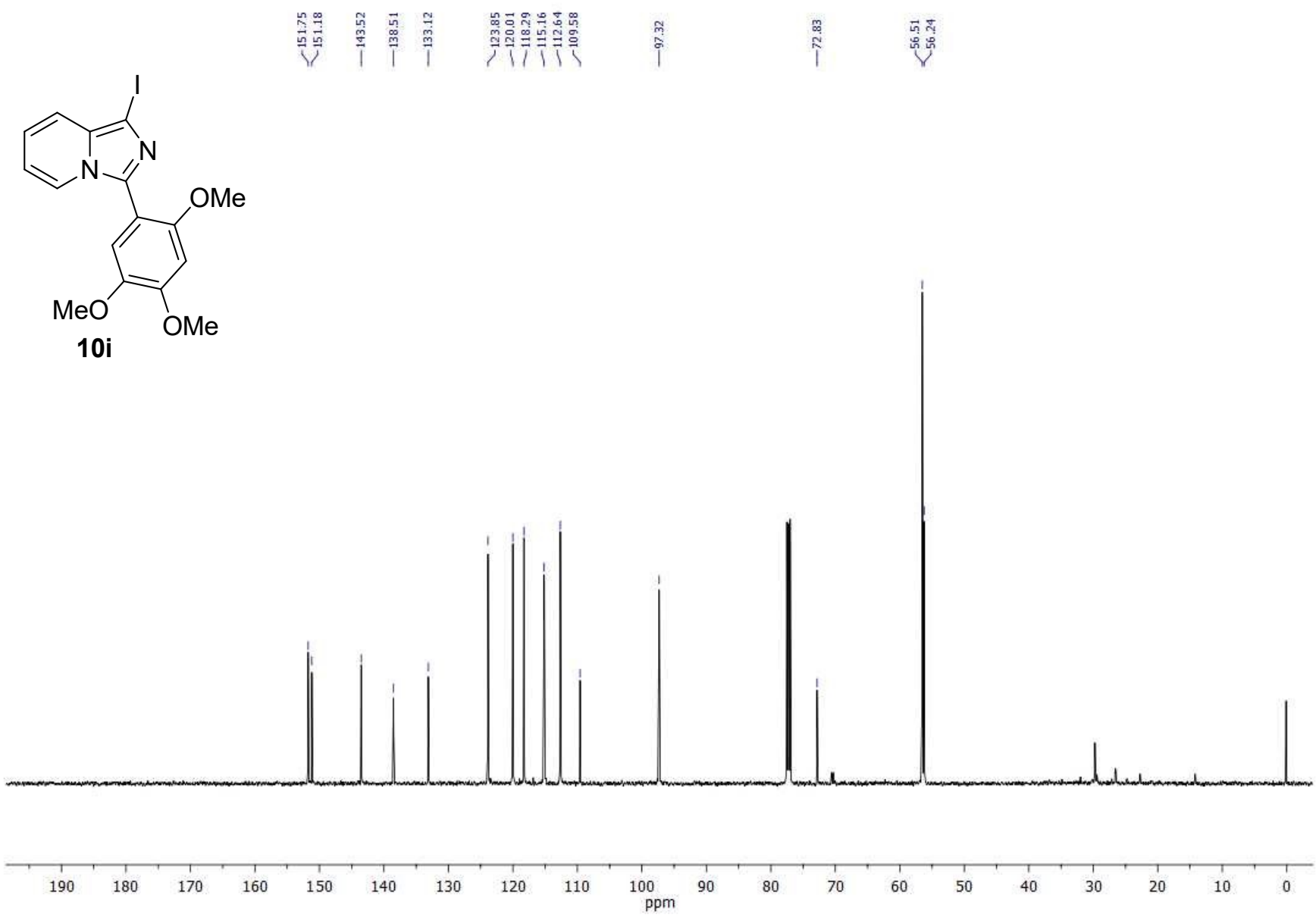

7.54
7.53
7.47
7.38
7.36
7.07
6.63
6.62
6.61
6.60
6.57
6.43
6.41
6.40
3.87
3.80
3.65
N
N
OMe
MeO
OMe
1.00
0.91
1.00
0.99
0.99
0.97
0.99
3.25
3.03
3.24
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

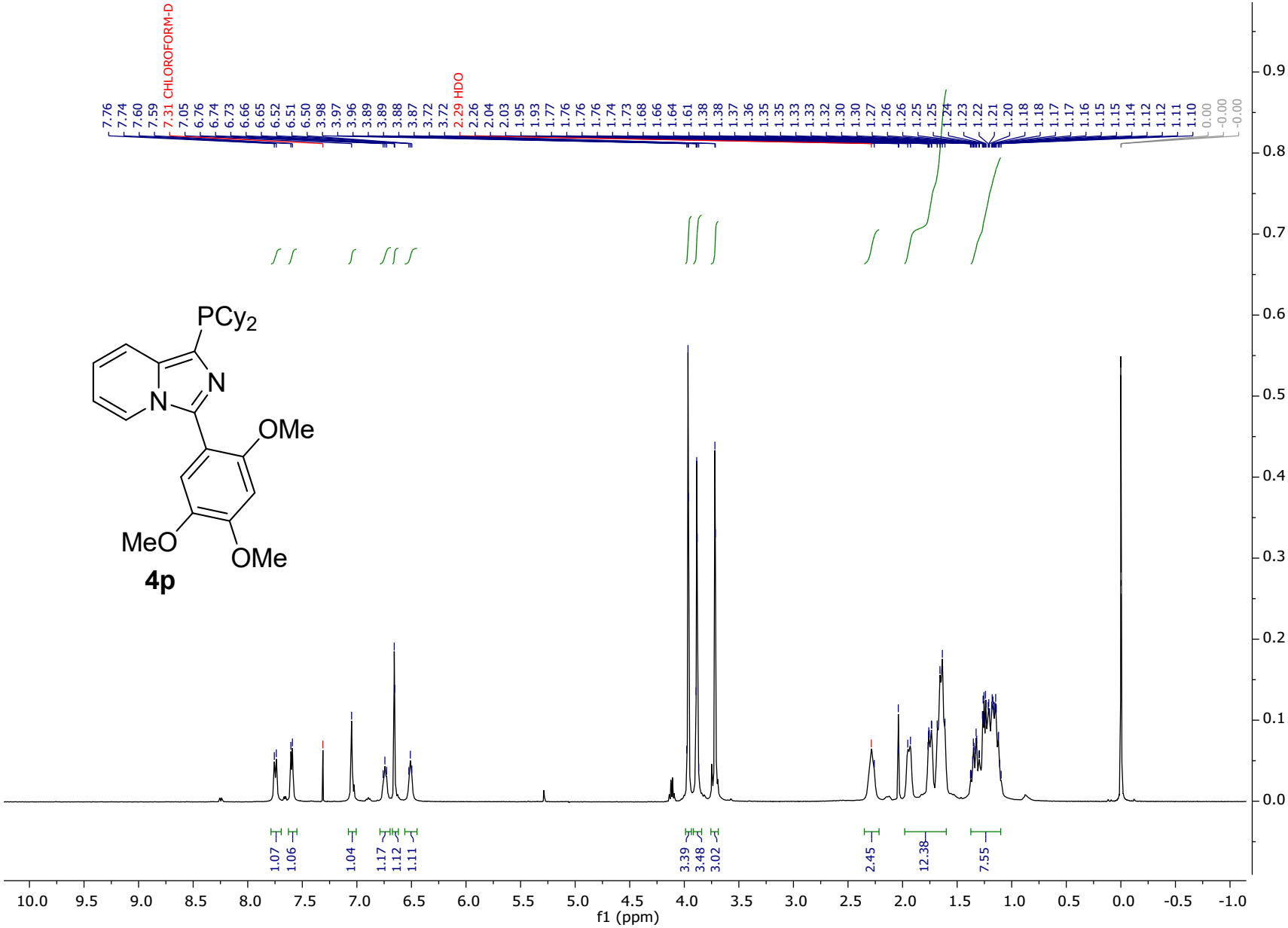
9i

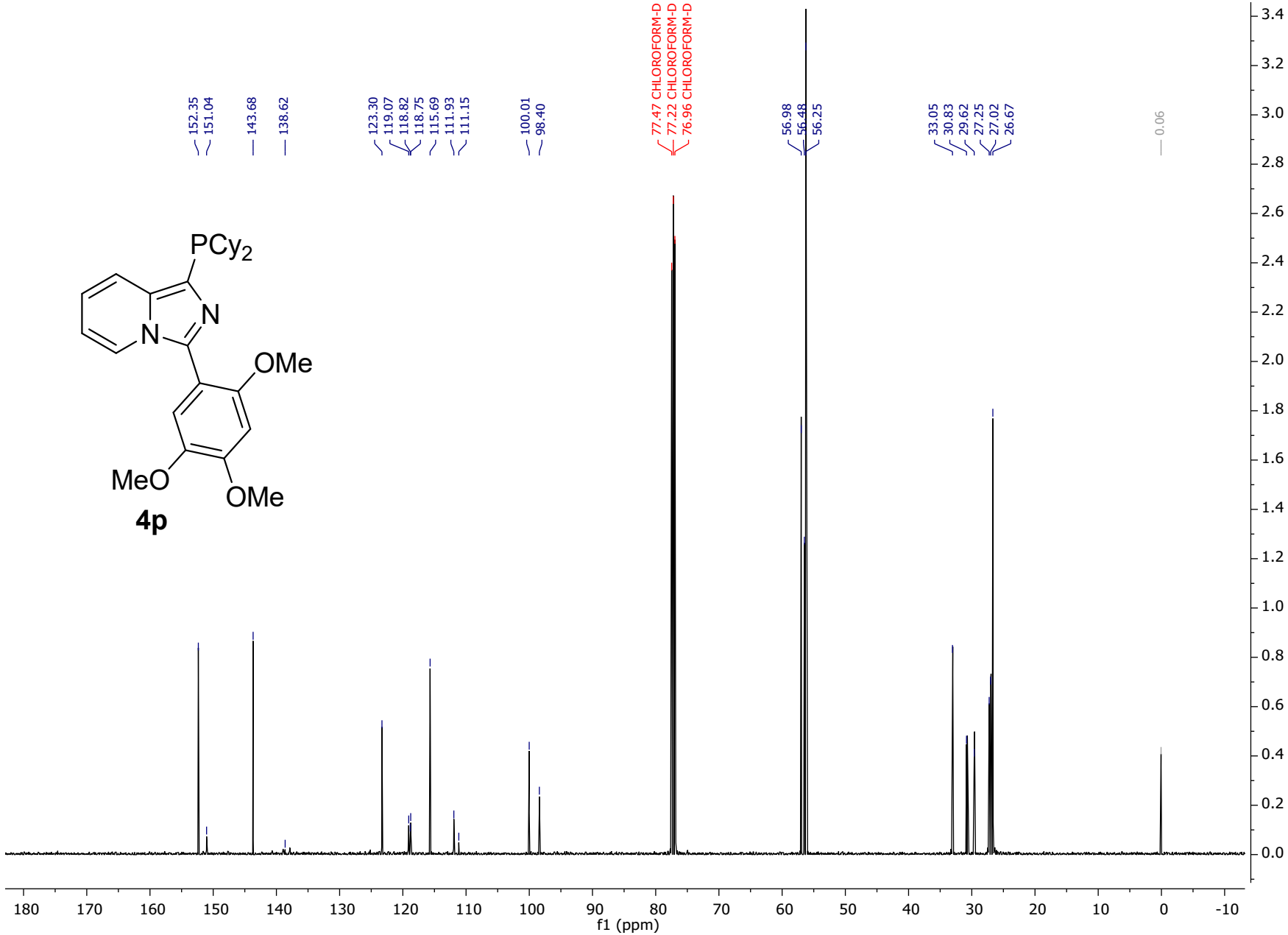

151.82
150.80
143.52
136.24
131.20
123.28
119.91
118.48
118.13
115.05
111.74
110.76
97.59
56.49
56.46
56.18
N
N
OMe
MeO
OMe
9i
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

LY-K-111


I
N
N
OMe
MeO
OMe
10i
1.00
1.09
0.99
1.03
1.02
1.04
9.71
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


151.75
151.18
143.52
138.51
133.12
123.85
120.01
118.29
115.16
112.64
109.58
97.32
72.83
56.51
56.24
I
N
N
OMe
MeO
OMe
10i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


7.76 7.74 7.60 7.59 7.31 CHLOROFORM-D 7.05 6.76 6.74 6.73 6.66 6.65 6.52 6.51 6.50 3.98 3.97 3.96 3.89 3.89 3.88 3.87 3.72 3.72 2.29 HDO 2.26 2.04 2.03 1.95 1.93 1.77 1.76 1.76 1.76 1.74 1.73 1.68 1.66 1.64 1.61 1.38 1.38 1.37 1.36 1.35 1.35 1.33 1.33 1.32 1.30 1.30 1.27 1.26 1.26 1.25 1.25 1.24 1.23 1.22 1.21 1.20 1.18 1.18 1.17 1.17 1.16 1.15 1.15 1.14 1.12 1.12 1.11 1.10 0.00 -0.00 -0.00
PCy2
N
N
OMe
MeO
OMe
4p
1.07 1.06 1.04 1.17 1.12 1.11 3.39 3.48 3.02 2.45 12.38 7.55
f1 (ppm)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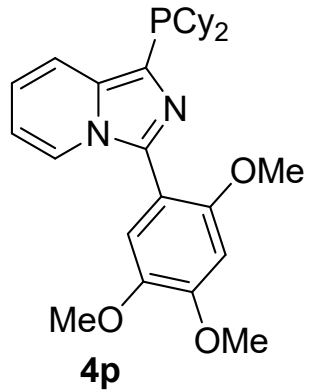
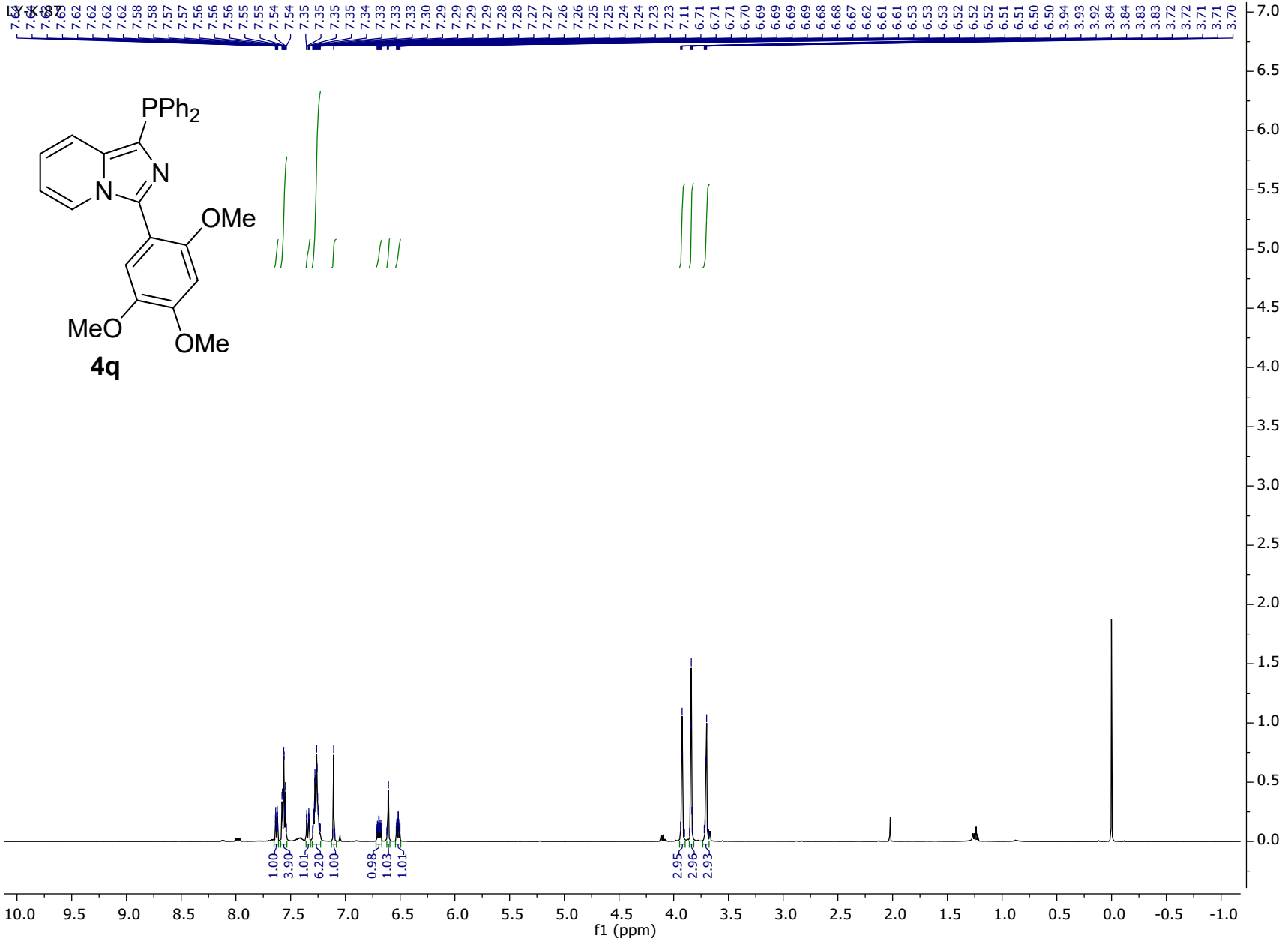
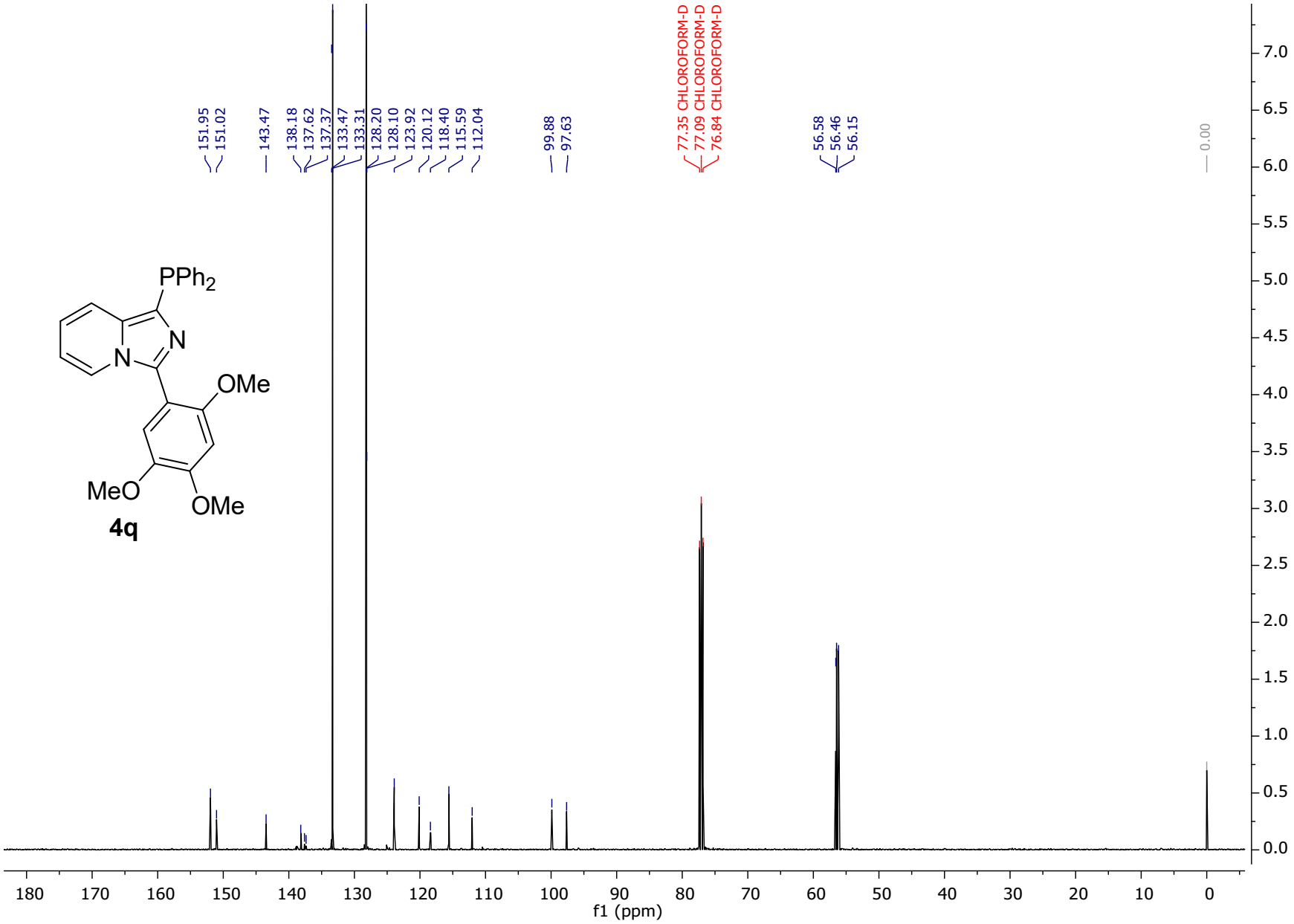
138.62
123.30
119.07
118.82
118.75
115.69
111.93
111.15
100.01
98.40
77.47 CHLOROFORM-D
77.22 CHLOROFORM-D
76.96 CHLOROFORM-D
56.98
56.48
56.25
33.05
30.83
29.62
27.25
27.02
26.67
0.06
PCy2
N
N
OMe
MeO
OMe
4p
f1 (ppm)


PCy2
N
N
OMe
MeO
OMe

4p

-25.85
450
400
350
300
250
200
150
100
50
0
-50
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
f1 (ppm)


PPh2
N
N
OMe
MeO
OMe
4q
f1 (ppm)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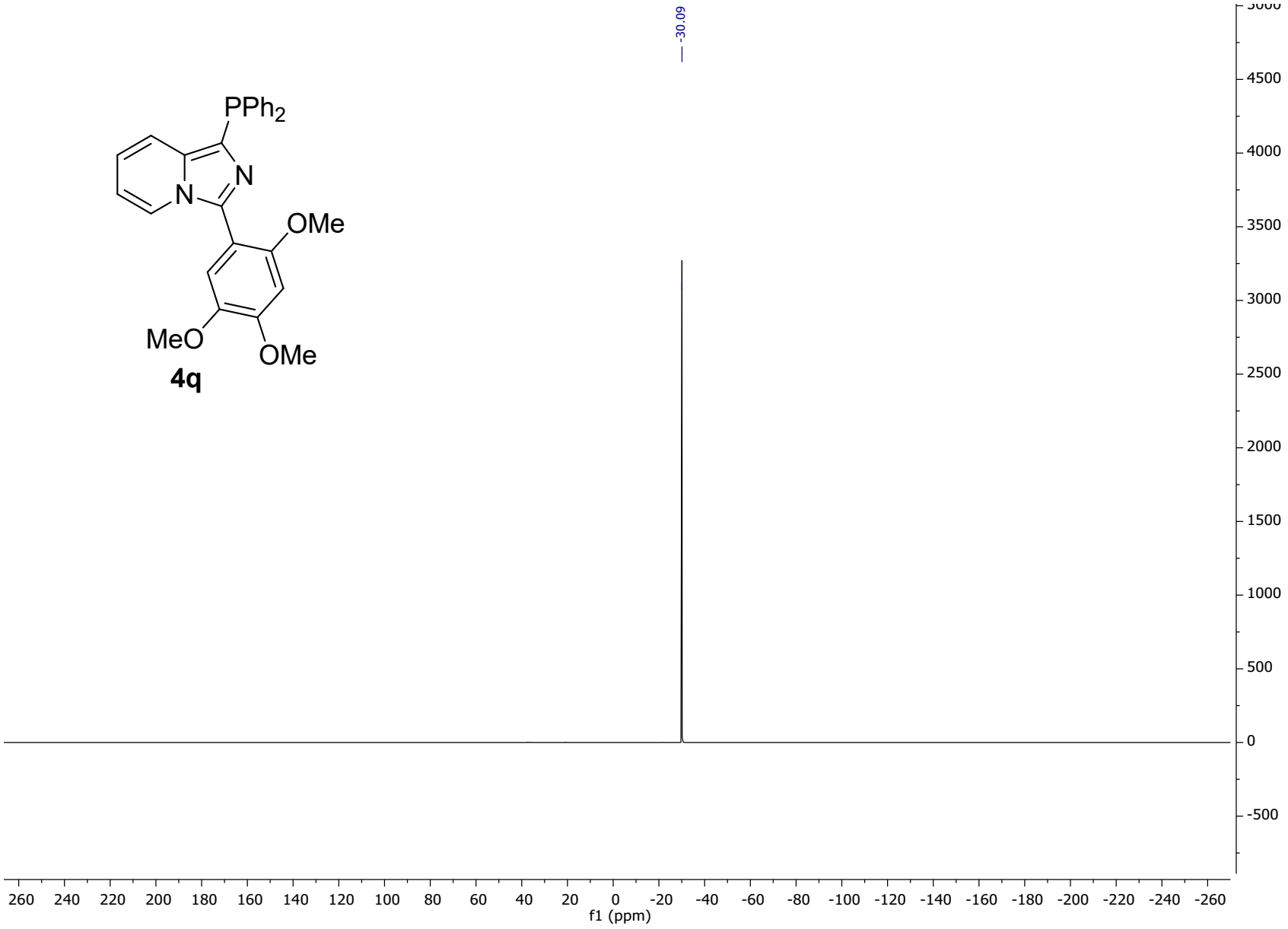
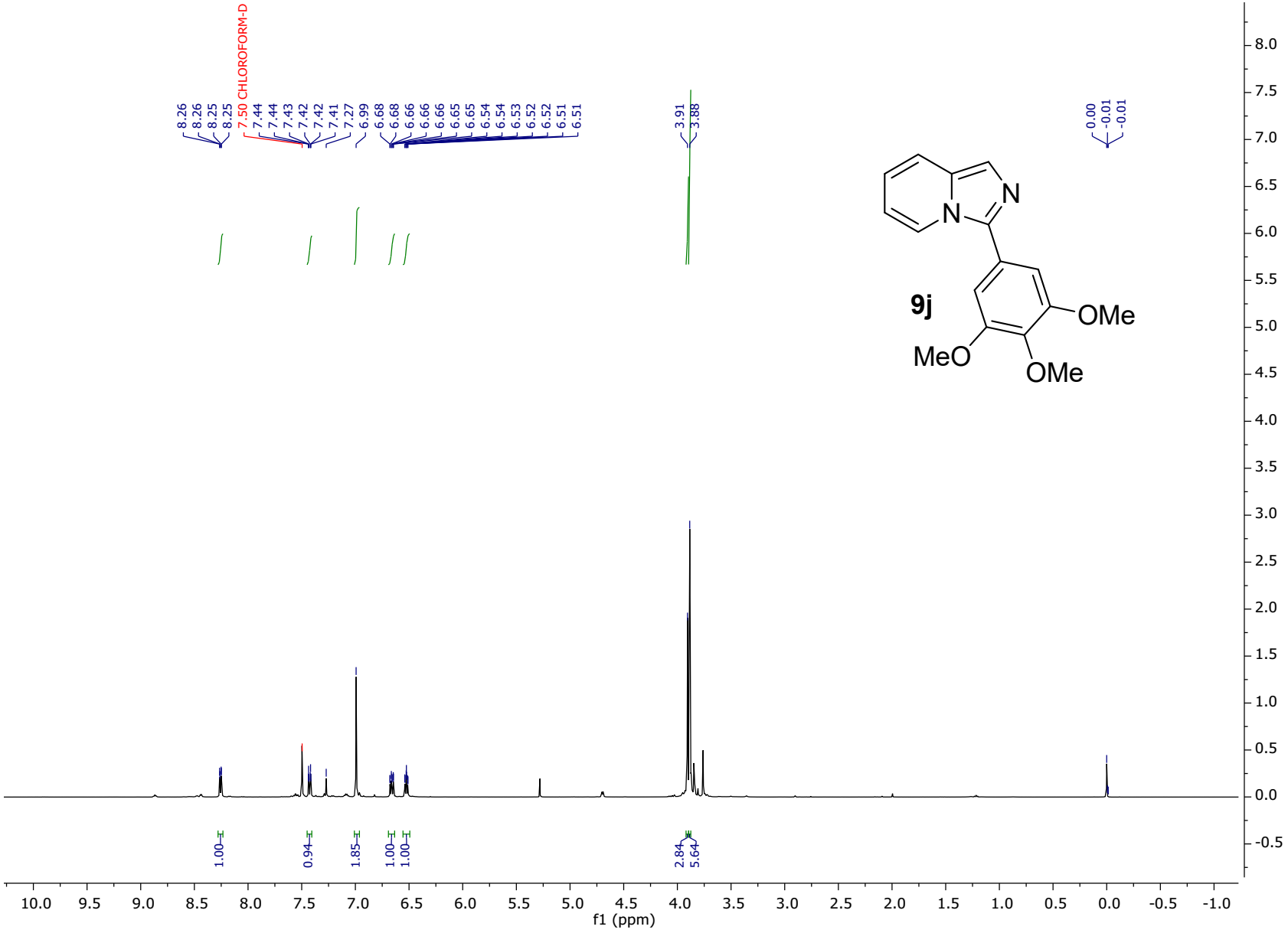
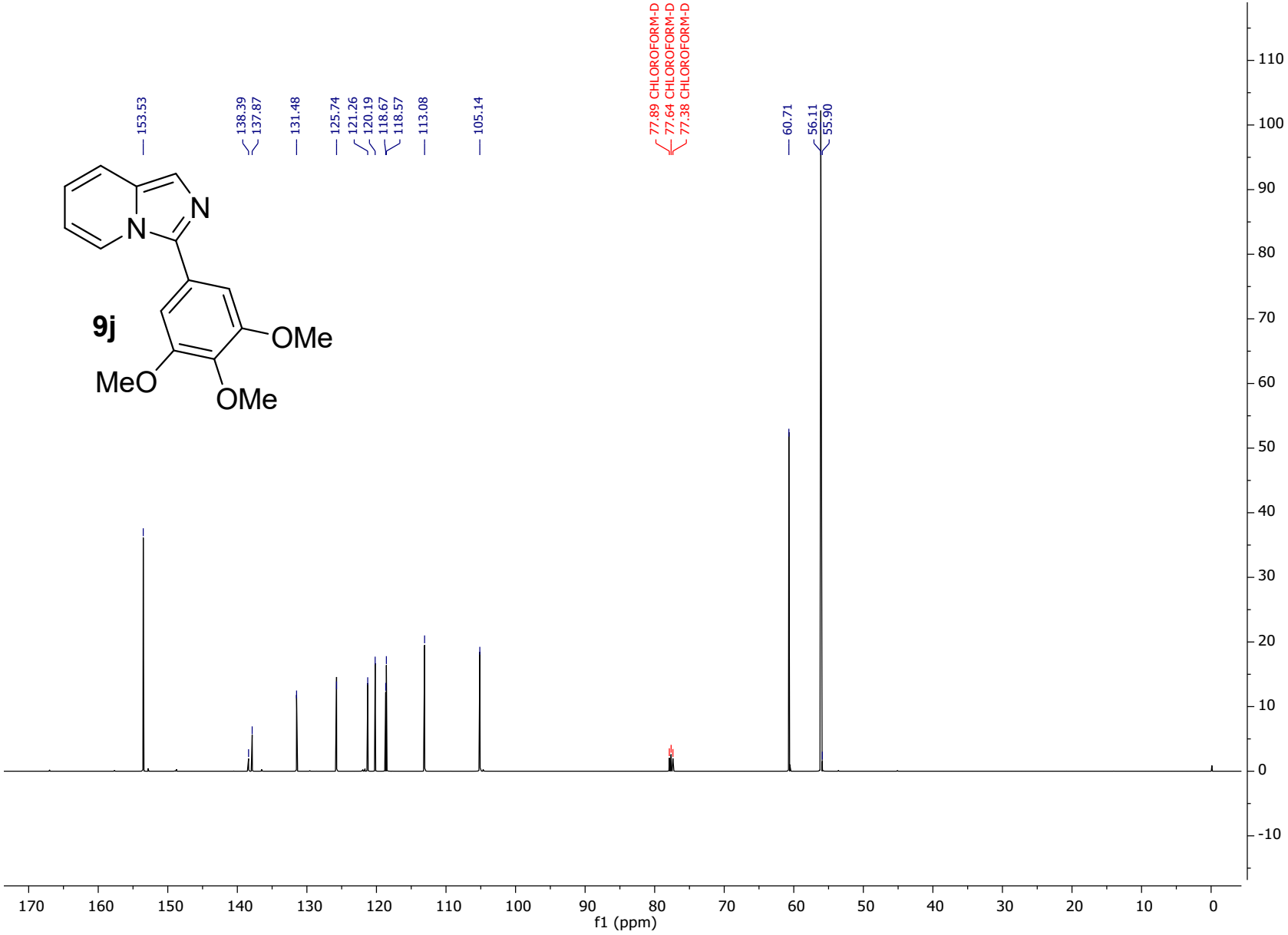
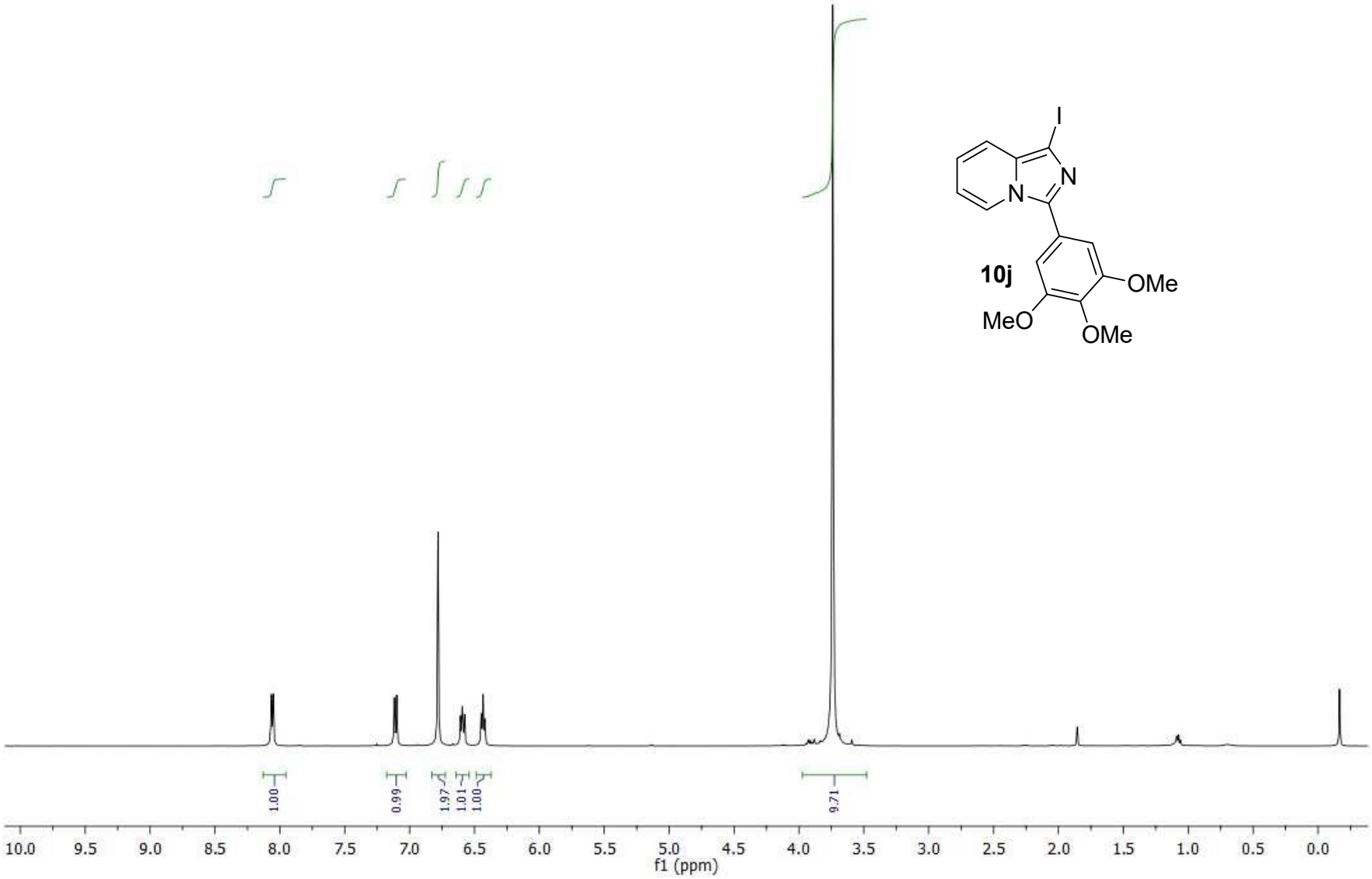
138.18
137.62
137.37
133.47
133.31
128.20
128.10
123.92
120.12
118.40
115.59
112.04
99.88
97.63
77.35 CHLOROFORM-D
77.09 CHLOROFORM-D
76.84 CHLOROFORM-D
56.58
56.46
56.15
0.00
PPh2
N
N
OMe
MeO
OMe
4q
f1 (ppm)

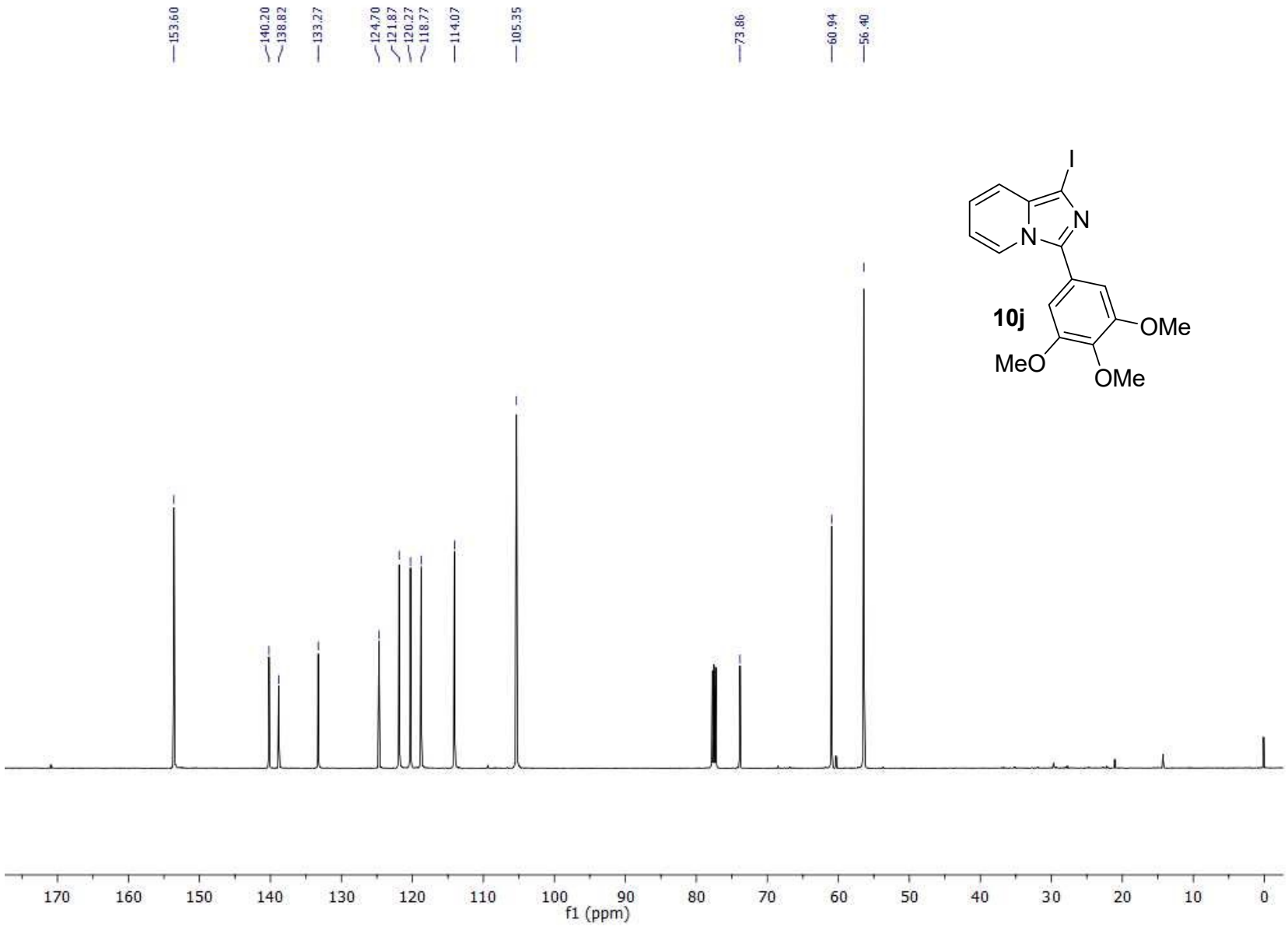

PPh2
N
N
OMe
MeO
OMe
4q
-30.09
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260
f1 (ppm)

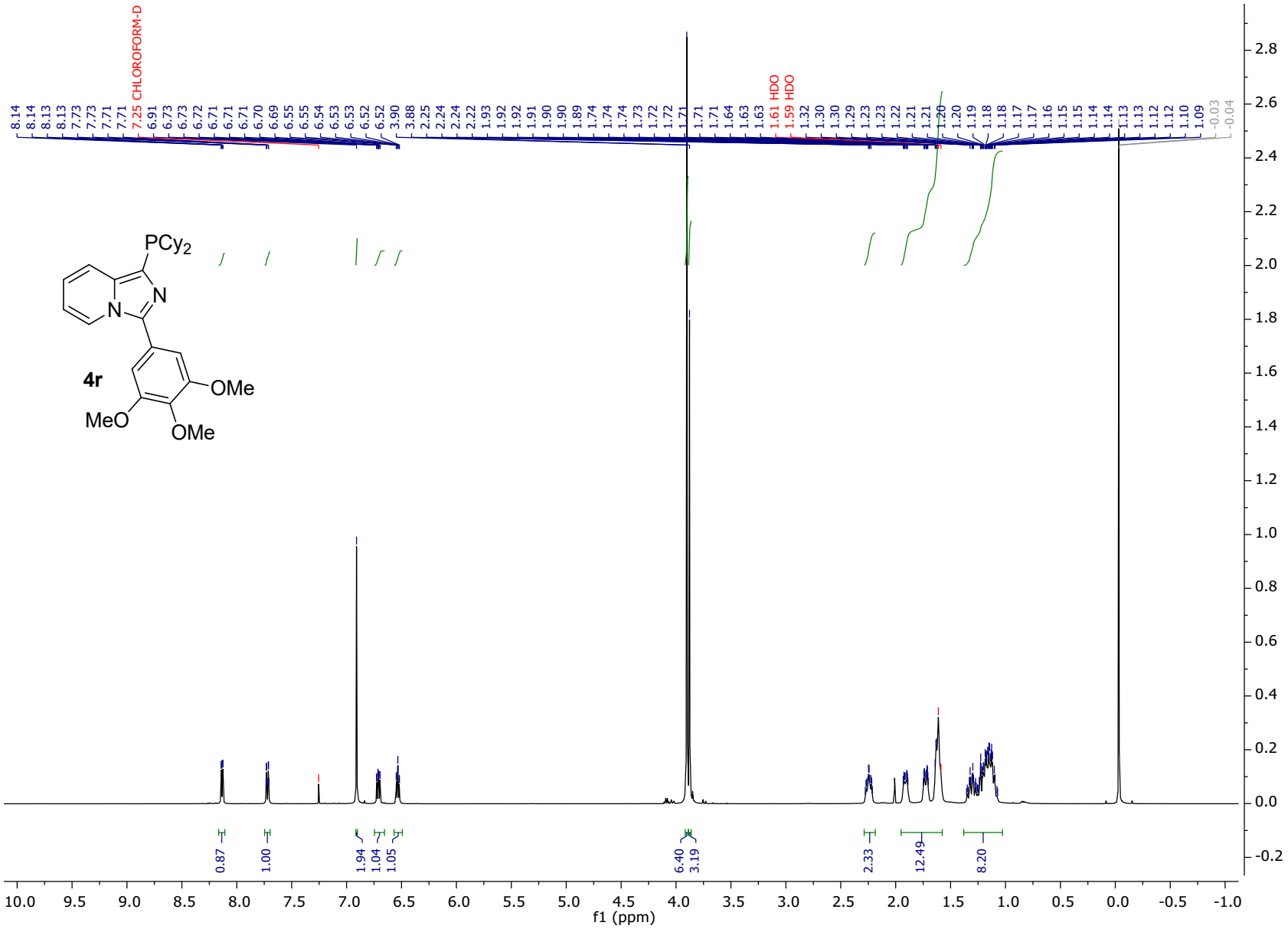

8.26
8.26
8.25
8.25
7.50 CHLOROFORM-D
7.44
7.44
7.43
7.42
7.42
7.41
7.27
6.99
6.68
6.68
6.66
6.66
6.66
6.65
6.65
6.54
6.54
6.53
6.52
6.52
6.51
6.51
3.91
3.88
0.00
-0.01
-0.01
N
N
9j
OMe
MeO
OMe
1.00
0.94
1.85
1.00
1.00
2.84
5.64
f1 (ppm)

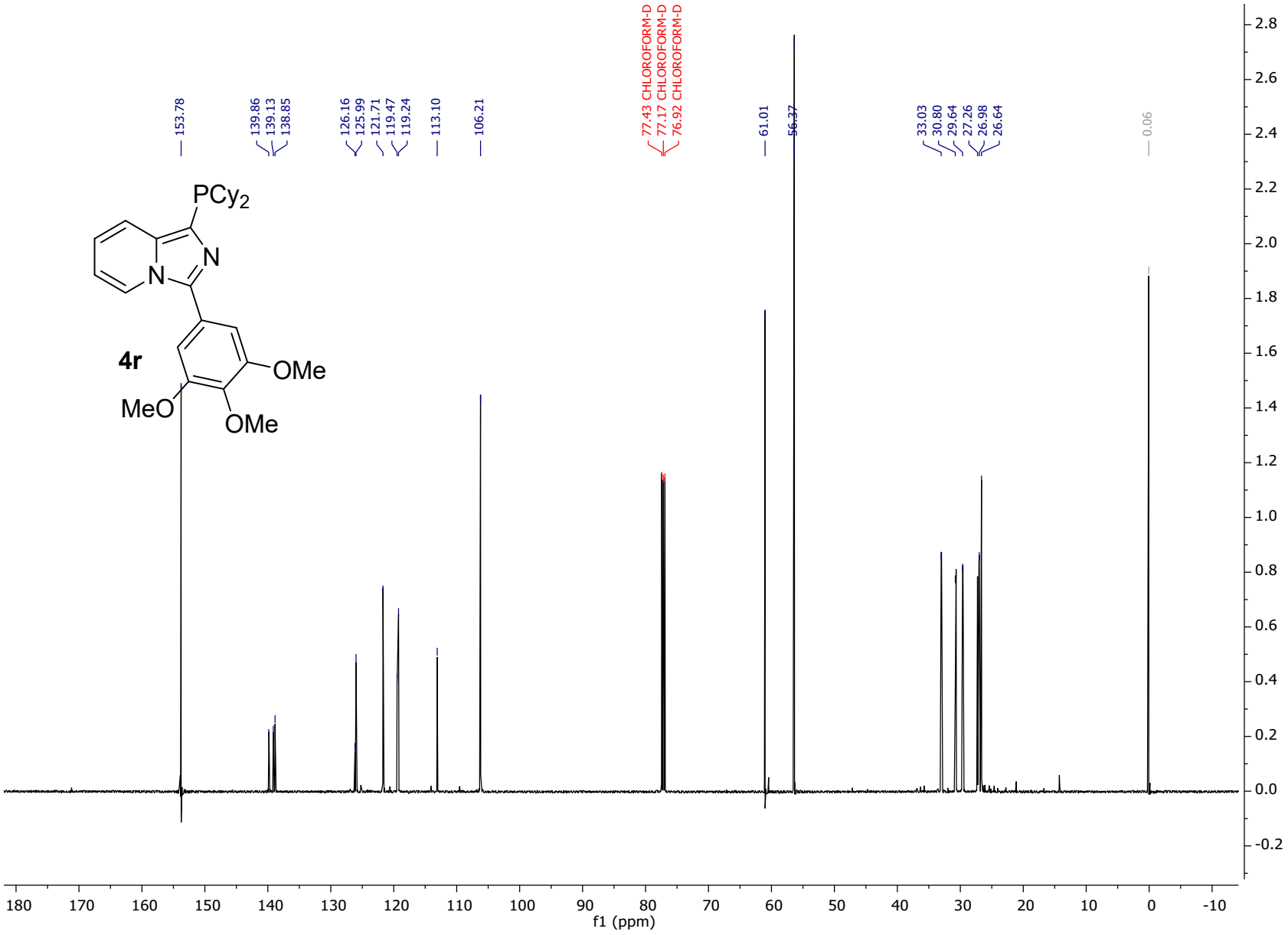

153.53
138.39
137.87
131.48
125.74
121.26
120.19
118.67
118.57
113.08
105.14
77.89 CHLOROFORM-D
77.64 CHLOROFORM-D
77.38 CHLOROFORM-D
60.71
56.11
55.90
9j
N
N
OMe
MeO
OMe
f1 (ppm)

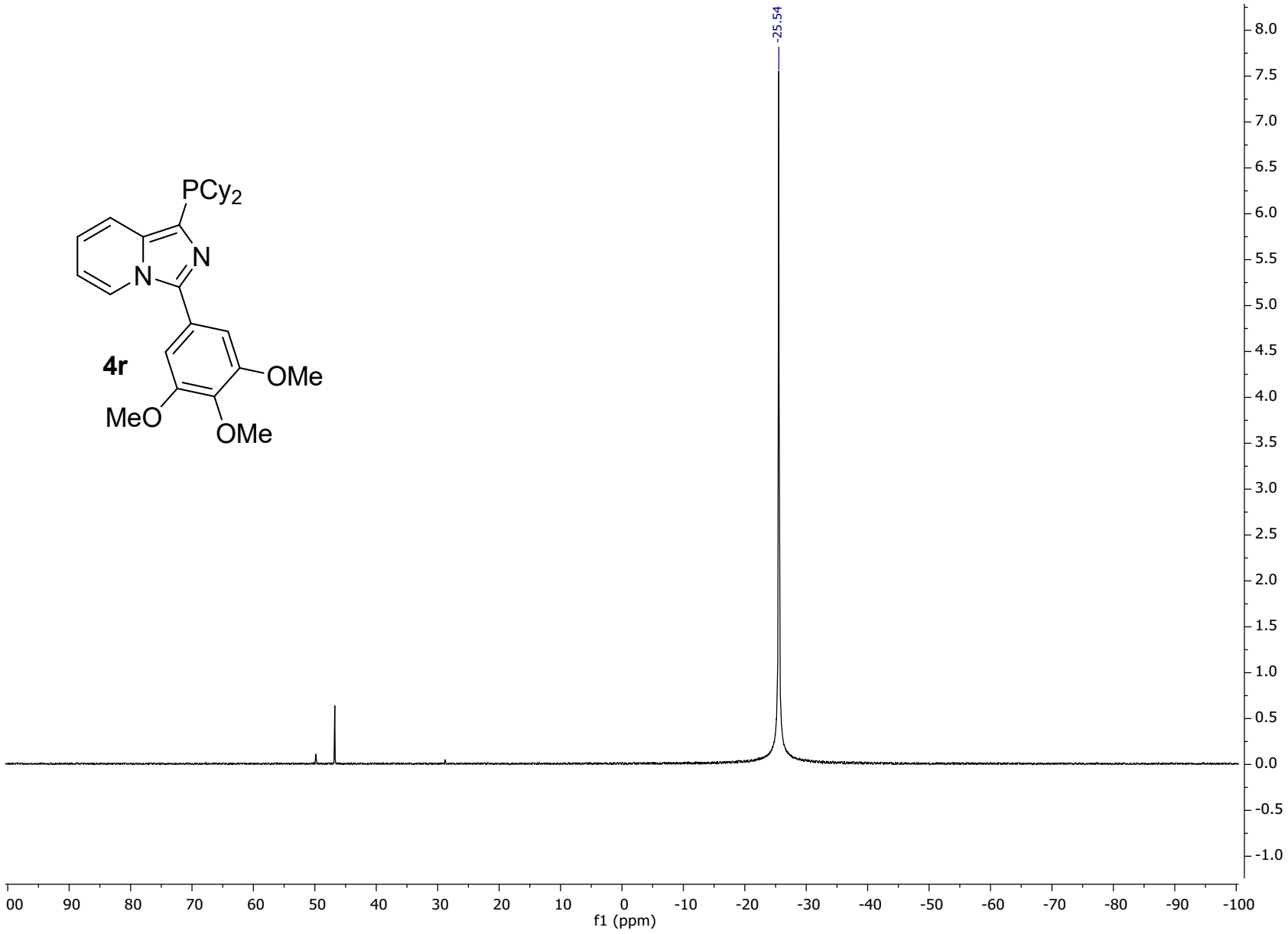
LY-N-4

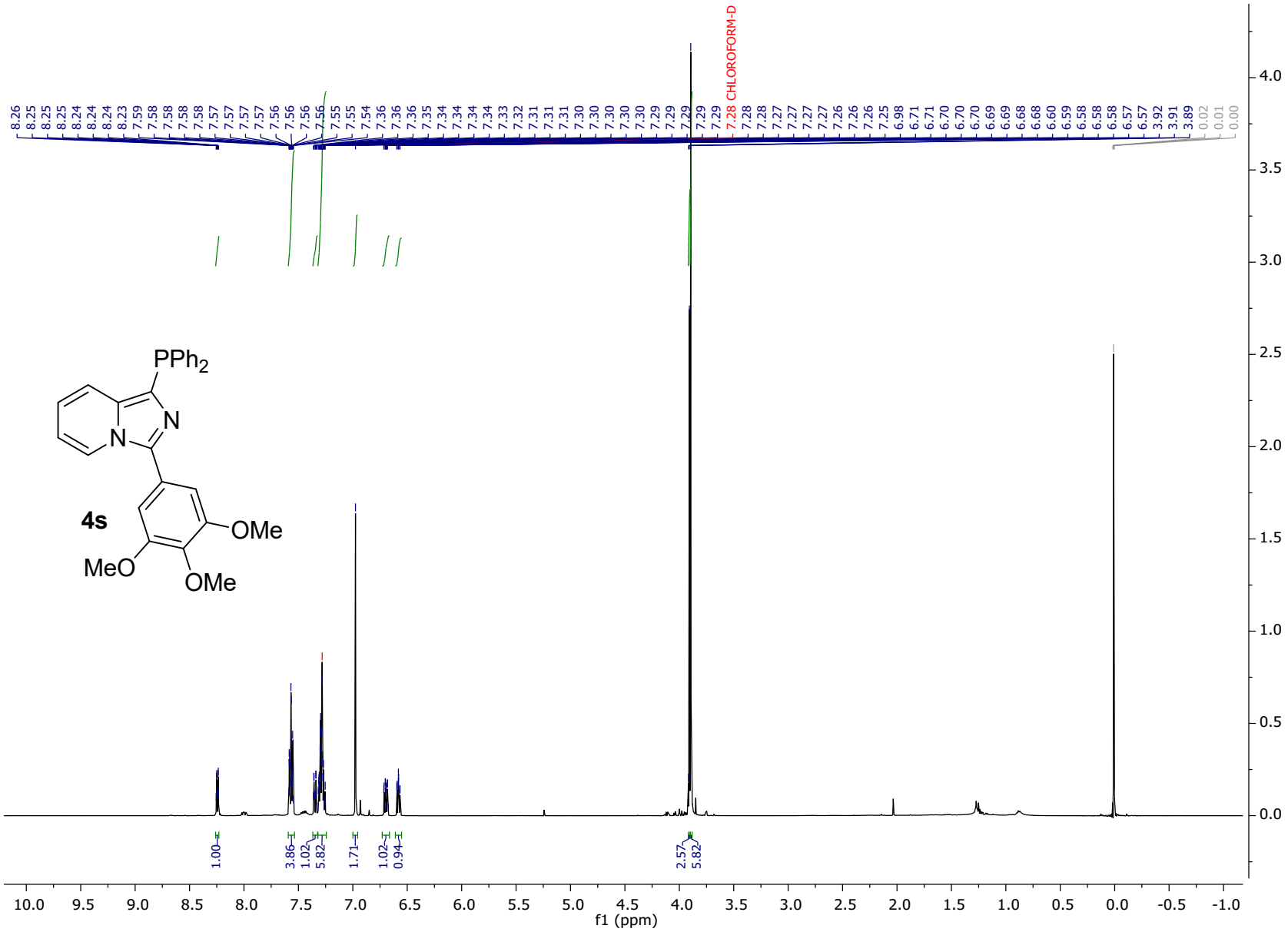

I
N
N
10j
OMe
MeO
OMe
1.00
0.99
1.97
1.01
1.00
9.71
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

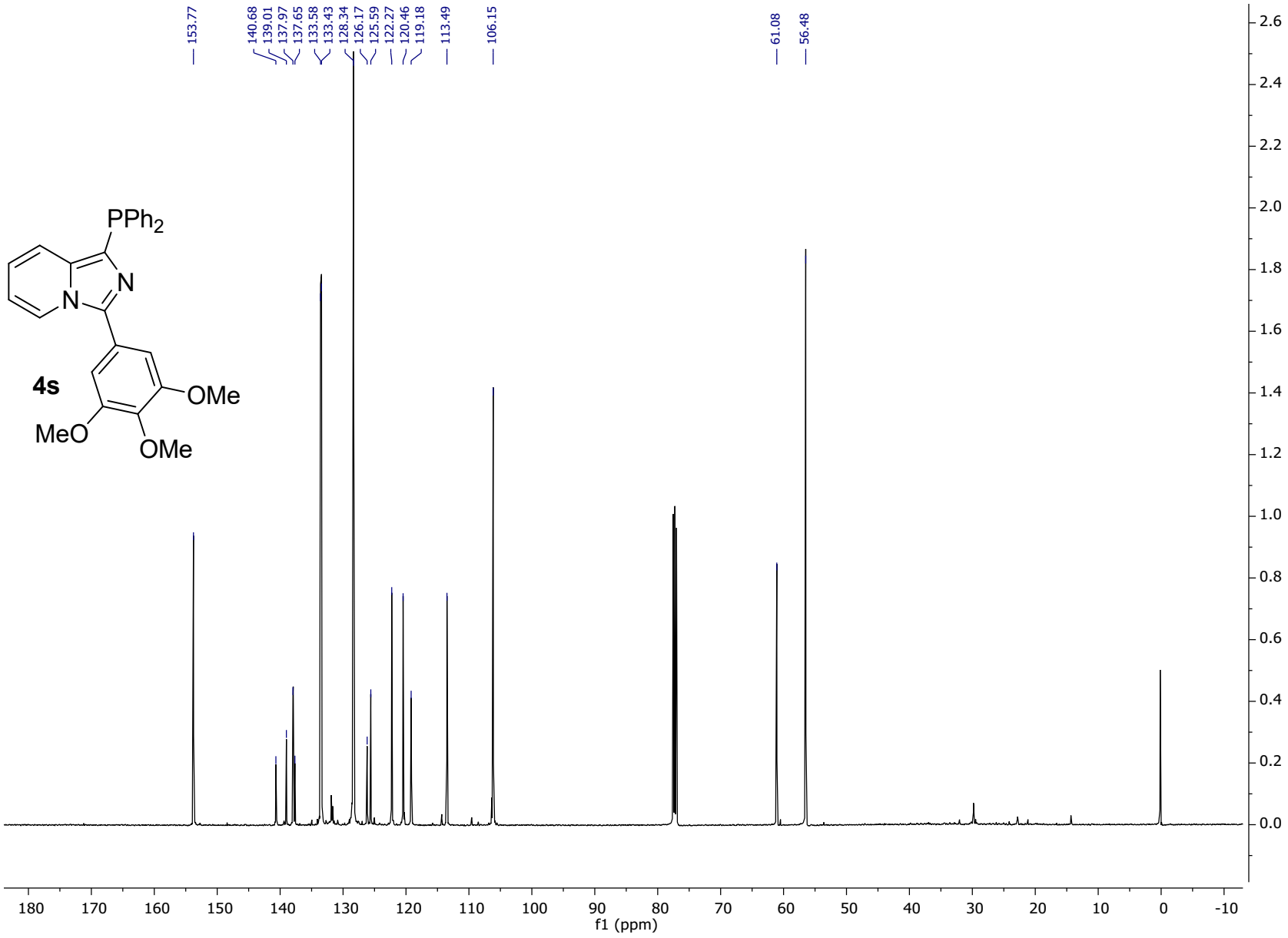

153.60
140.20
138.82
133.27
124.70
121.87
120.27
118.77
114.07
105.35
73.86
60.94
56.40
I
N
N
10j
OMe
MeO
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

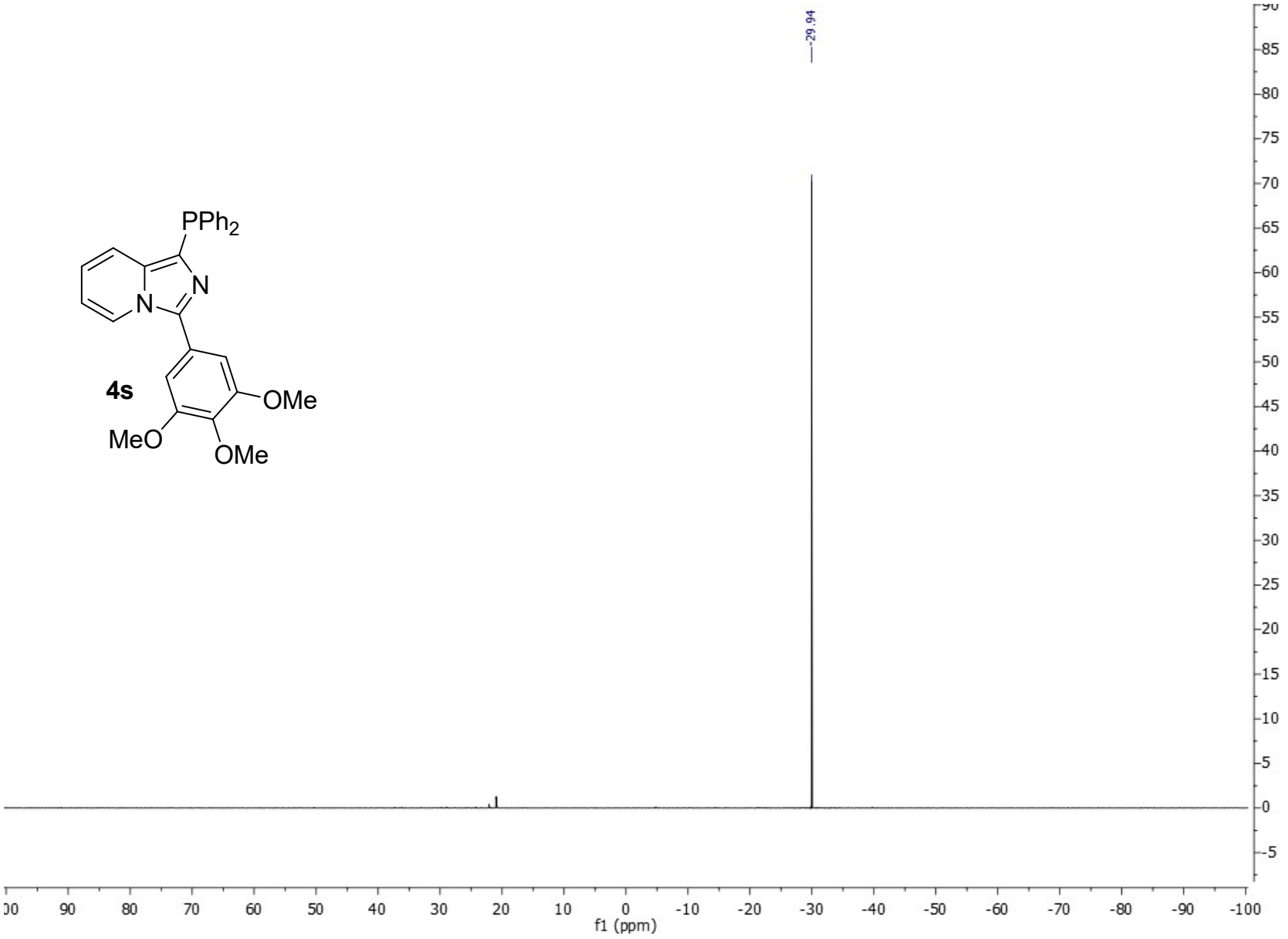

PCy2
N
N
4r
OMe
MeO
OMe
CHLOROFORM-D
HDO
HDO
0.87
1.00
1.94
1.04
1.05
6.40
3.19
2.33
12.49
8.20
f1 (ppm)

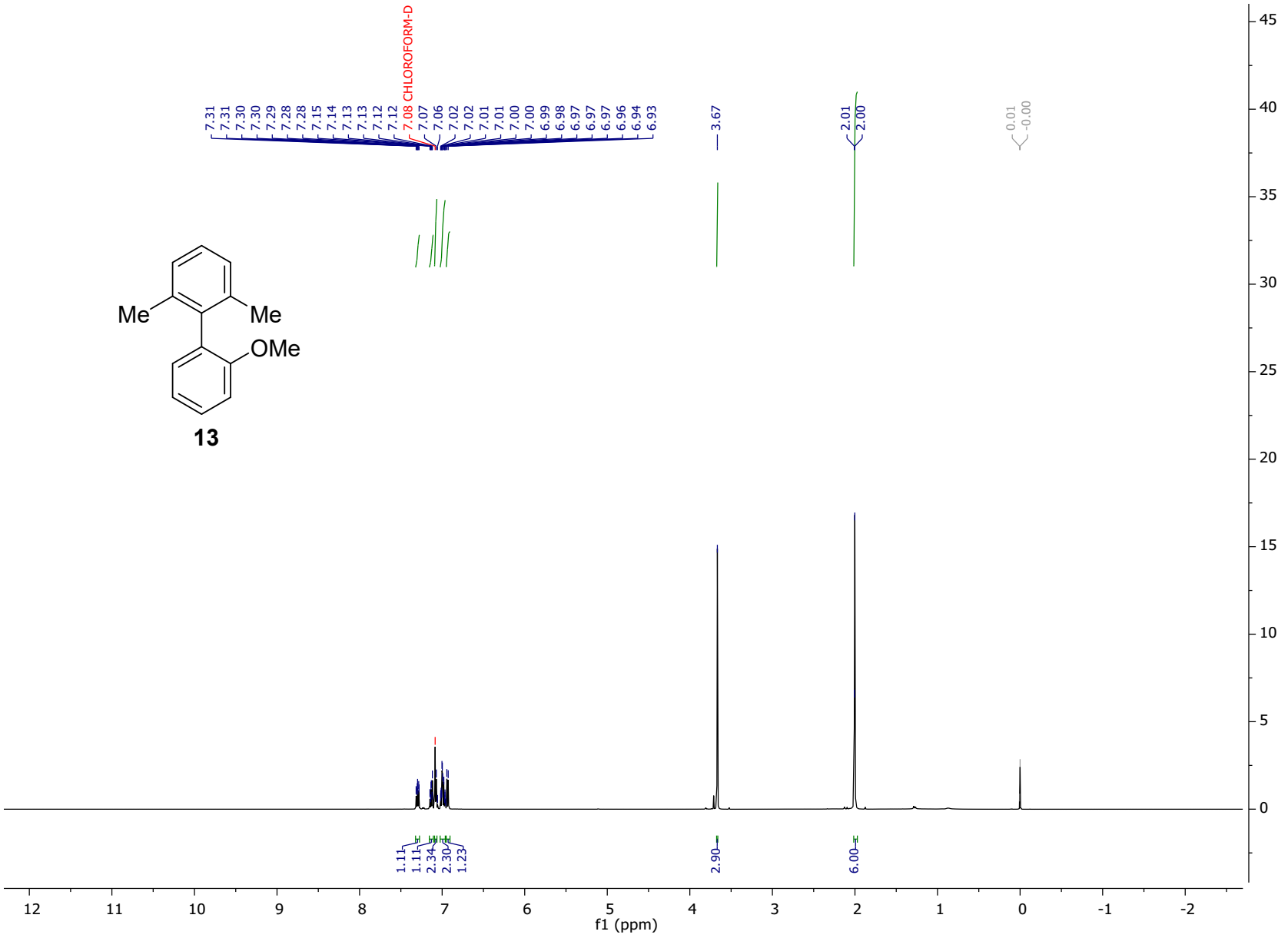

153.78
139.86
139.13
138.85
126.16
125.99
121.71
119.47
119.24
113.10
106.21
77.43 CHLOROFORM-D
77.17 CHLOROFORM-D
76.92 CHLOROFORM-D
61.01
56.37
33.03
30.80
29.64
27.26
26.98
26.64
0.06
PCy2
N
N
4r
OMe
MeO
OMe
f1 (ppm)

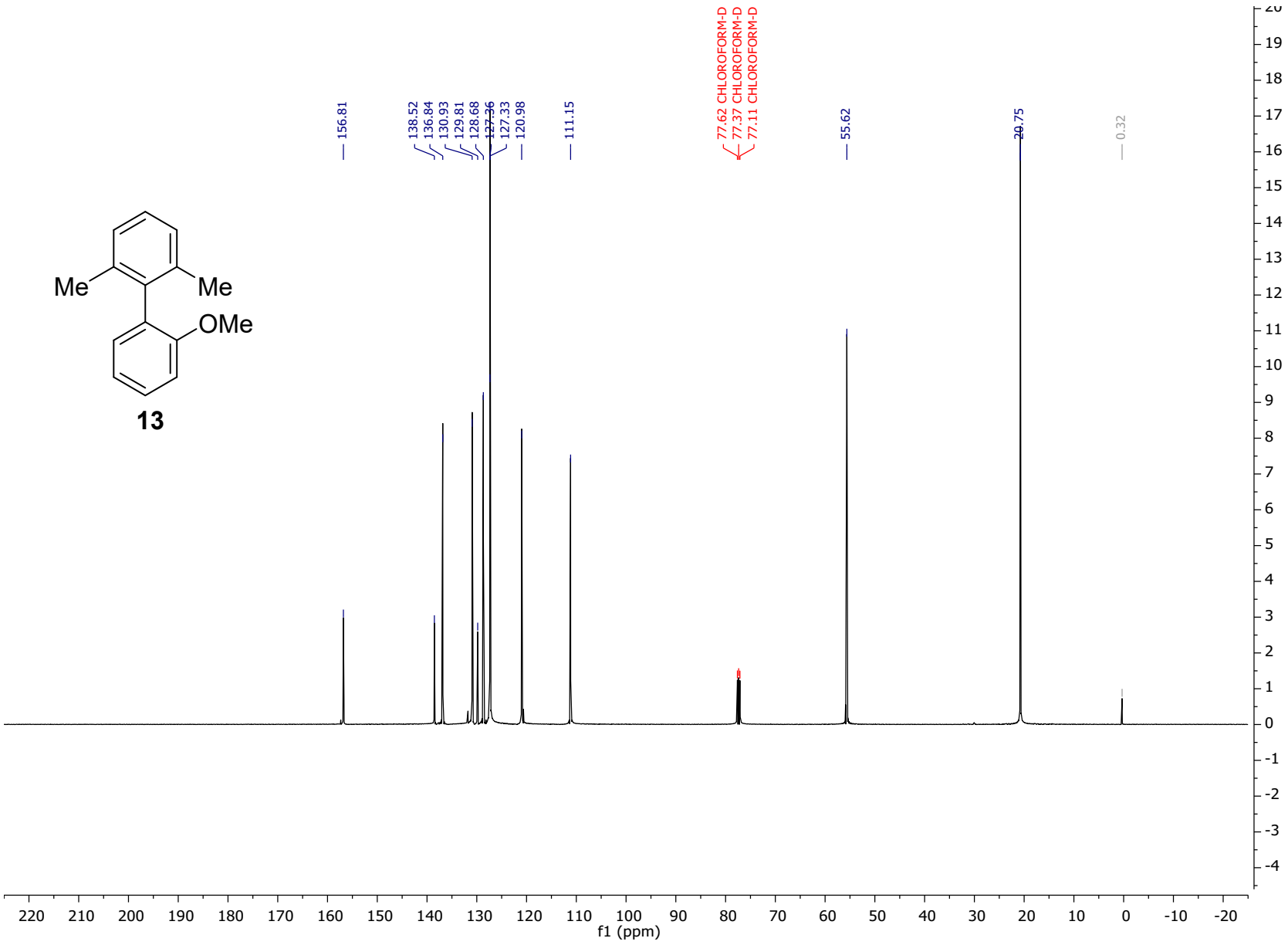

PCy2
N
N
4r
OMe
MeO
OMe
-25.54
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
00
90
80
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
f1 (ppm)

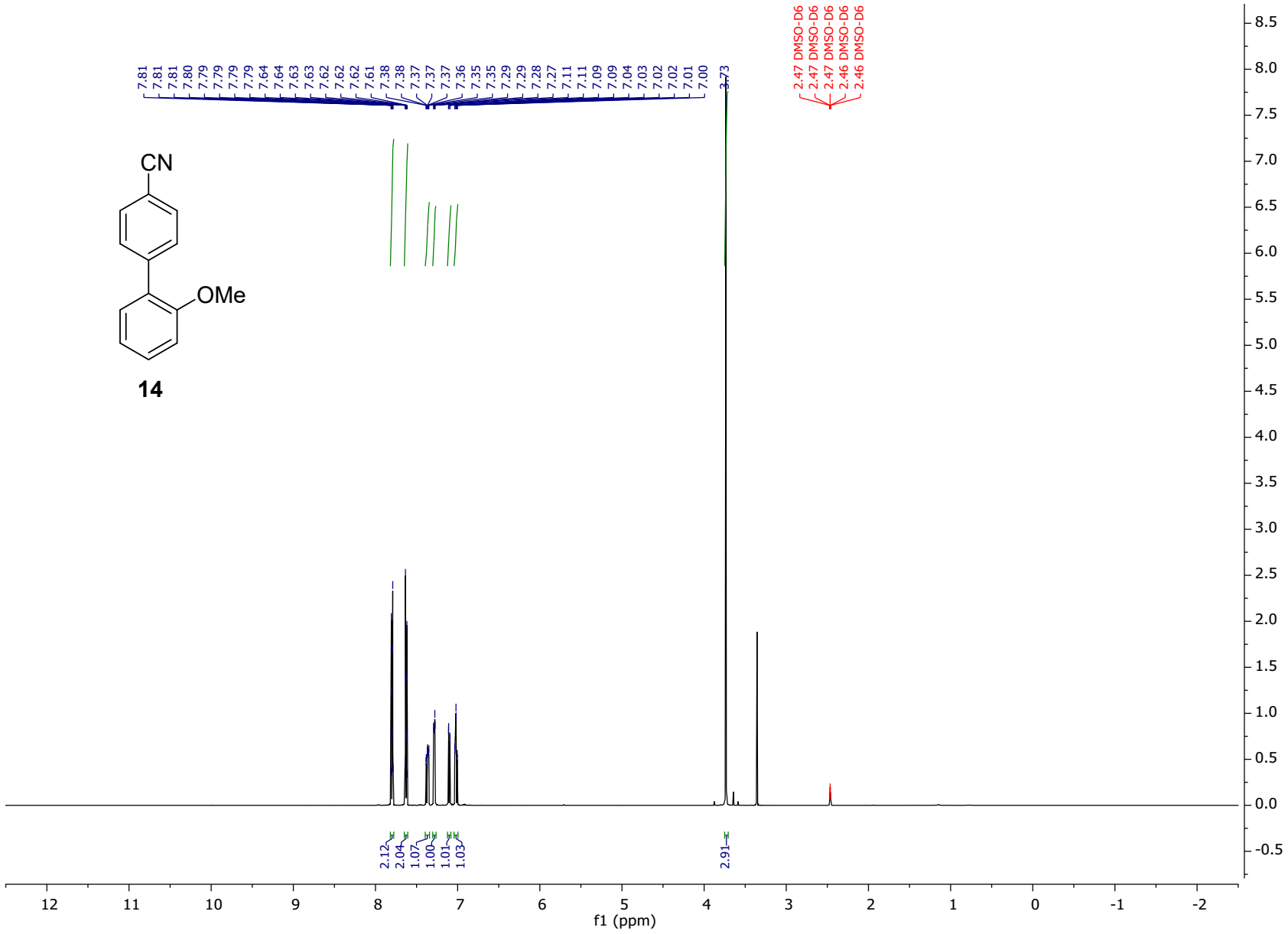

PPh2
N
N
4s
OMe
MeO
OMe
CHLOROFORM-D
1.00
3.86
1.02
5.82
1.71
1.02
0.94
2.57
5.82
f1 (ppm)

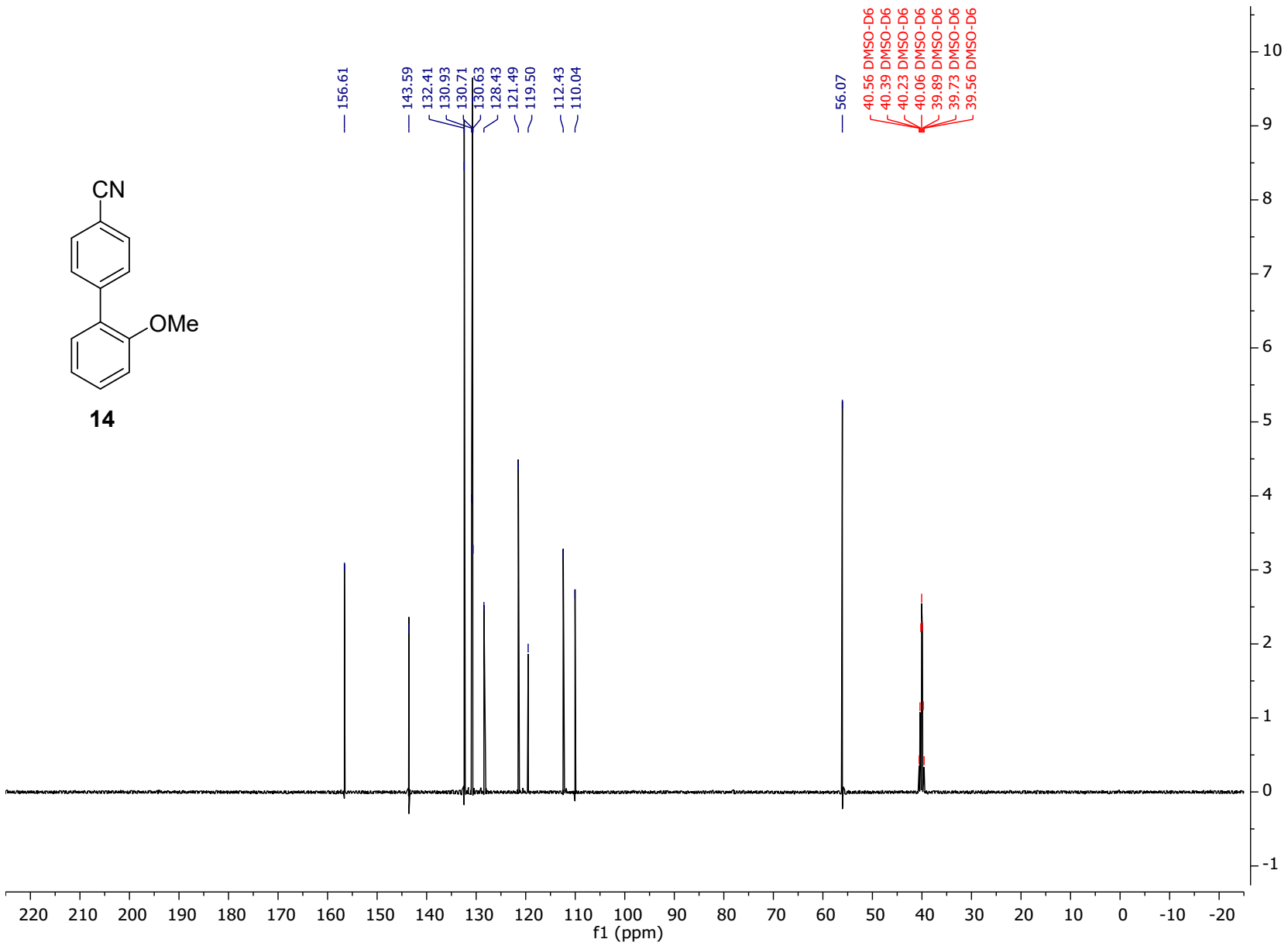

153.77
140.68
139.01
137.97
137.65
133.58
133.43
128.34
126.17
125.59
122.27
120.46
119.18
113.49
106.15
61.08
56.48
PPh2
N
N
4s
OMe
MeO
OMe
f1 (ppm)

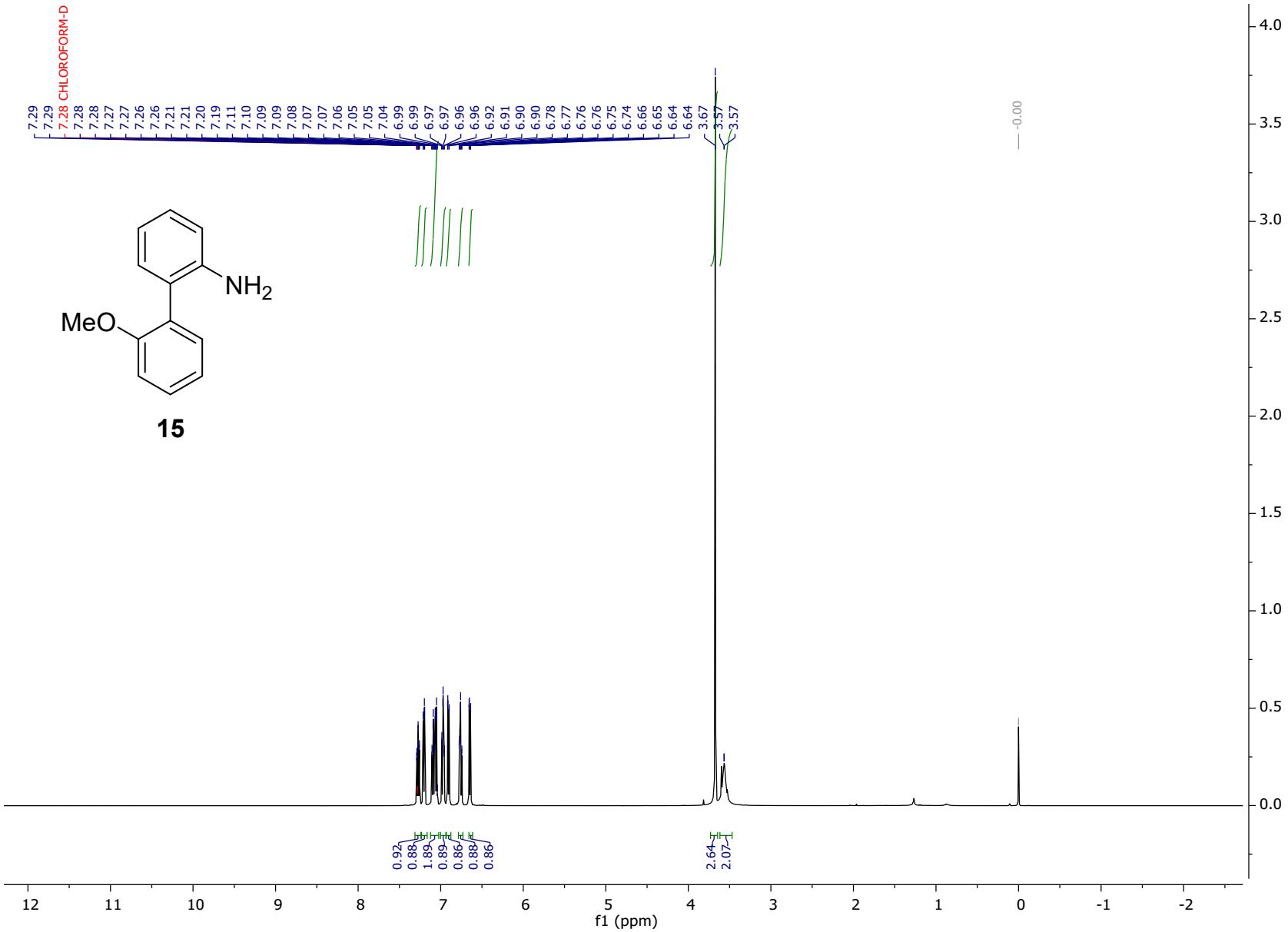

PPh2
N
N
4s
OMe
MeO
OMe
-29.94
f1 (ppm)

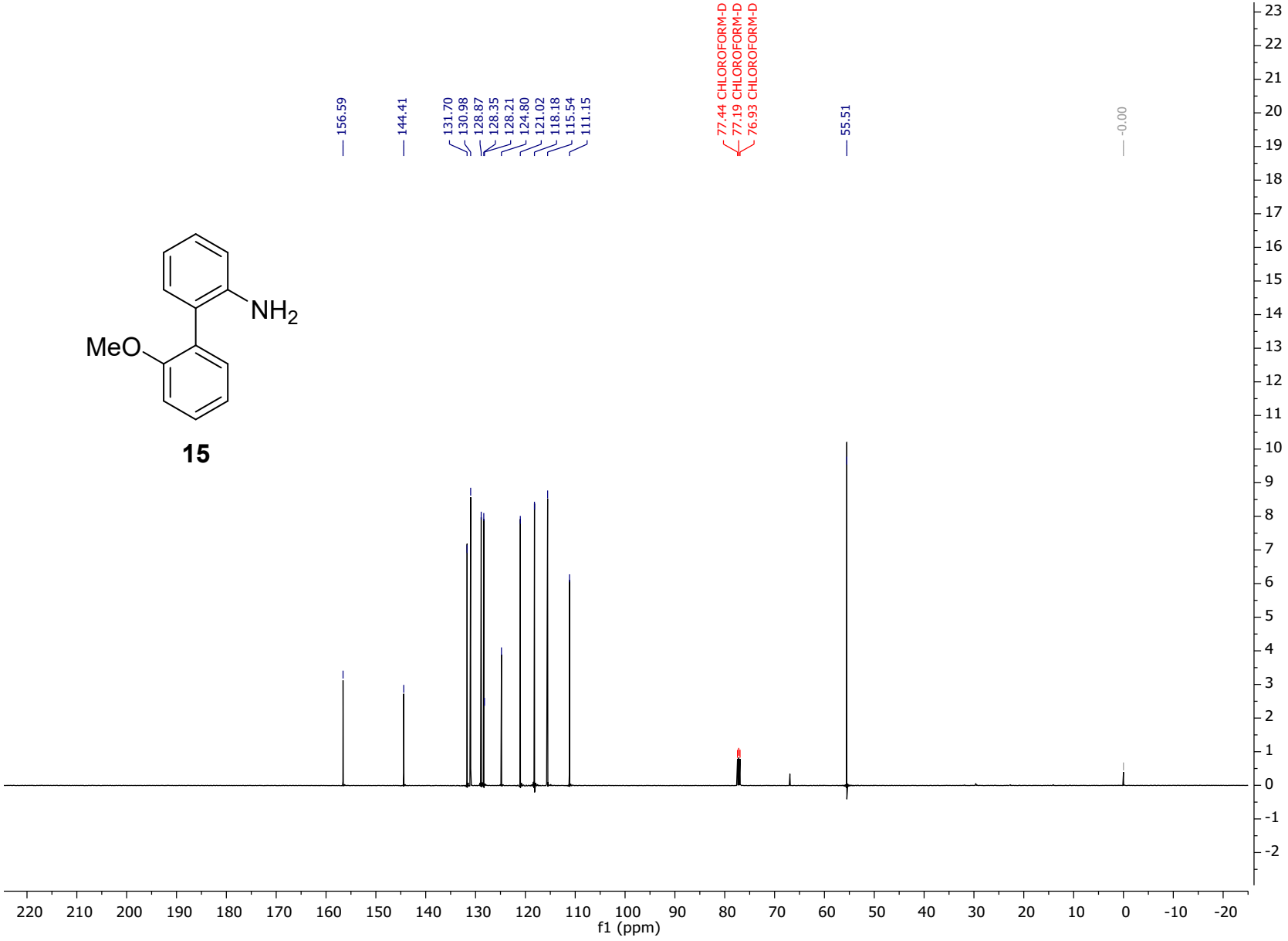

7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.15
7.14
7.13
7.13
7.12
7.12
7.08 CHLOROFORM-D
7.07
7.06
7.02
7.02
7.01
7.01
7.00
7.00
6.99
6.98
6.97
6.97
6.97
6.96
6.94
6.93
3.67
2.01
2.00
0.01
-0.00
Me
Me
OMe
13
1.11
1.11
2.34
2.30
1.23
2.90
6.00
f1 (ppm)

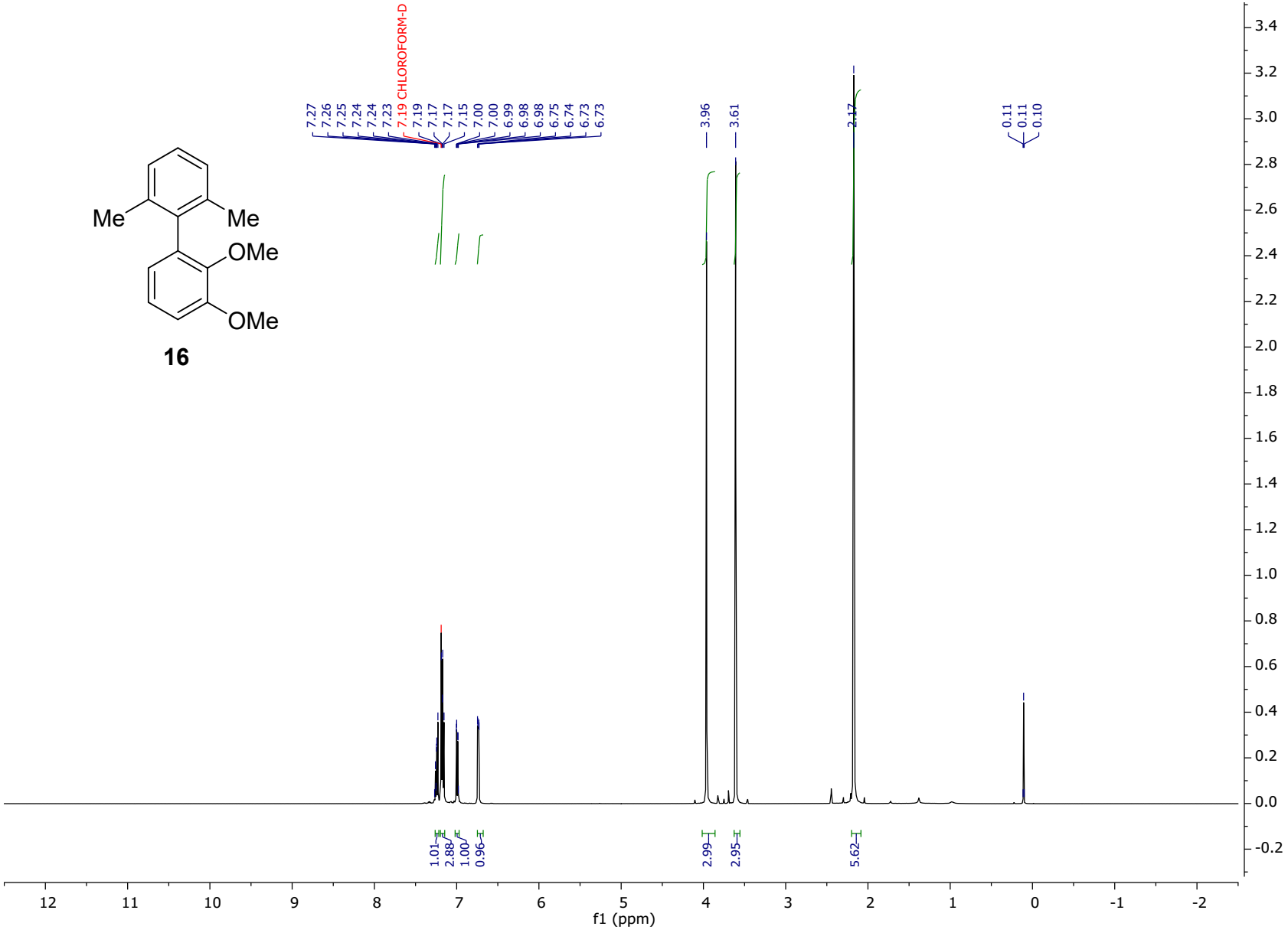

Me
Me
OMe
13
156.81
138.52
136.84
130.93
129.81
128.68
127.36
127.33
120.98
111.15
77.62 CHLOROFORM-D
77.37 CHLOROFORM-D
77.11 CHLOROFORM-D
55.62
20.75
0.32
f1 (ppm)

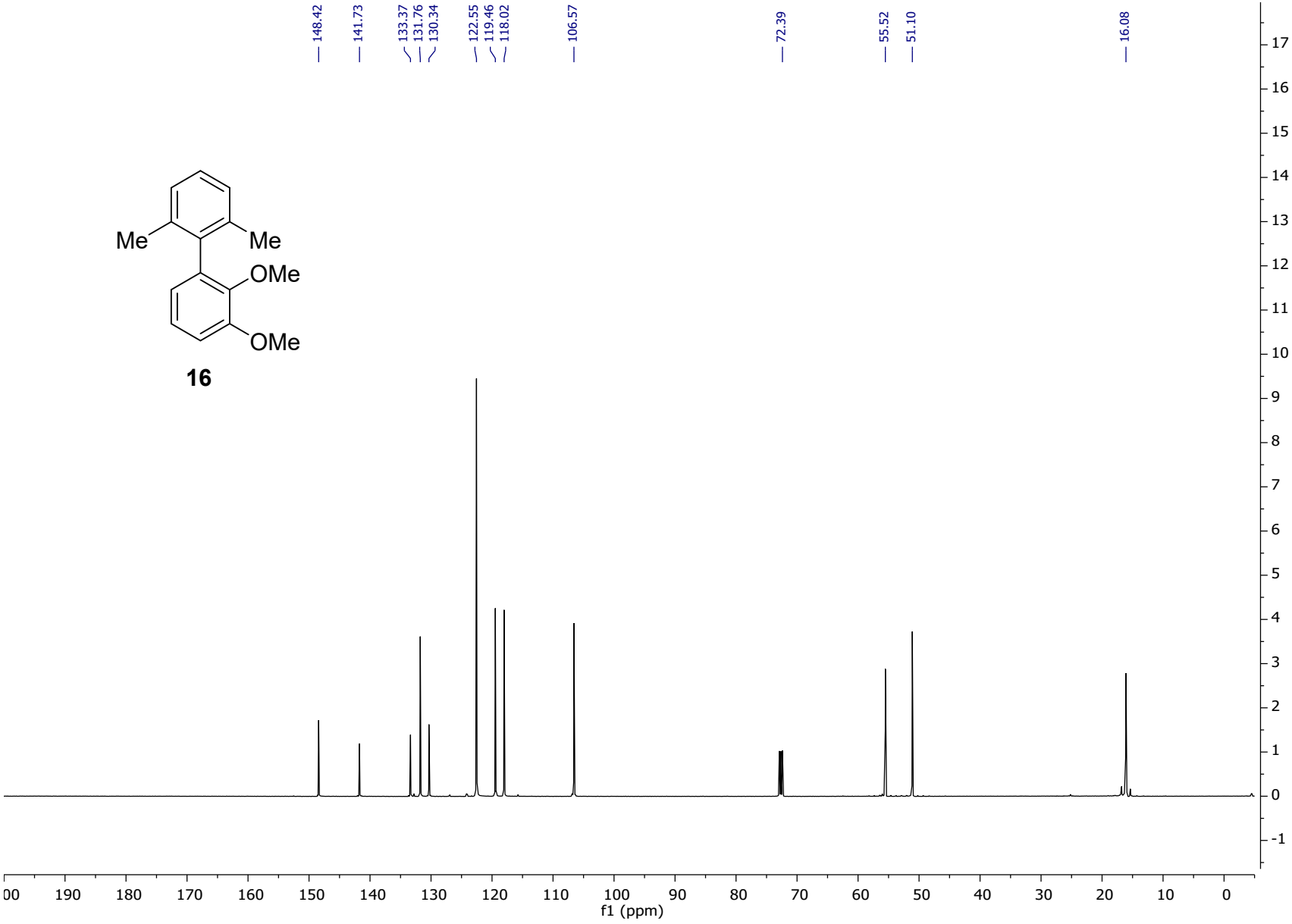

CN
OMe
14
f1 (ppm)

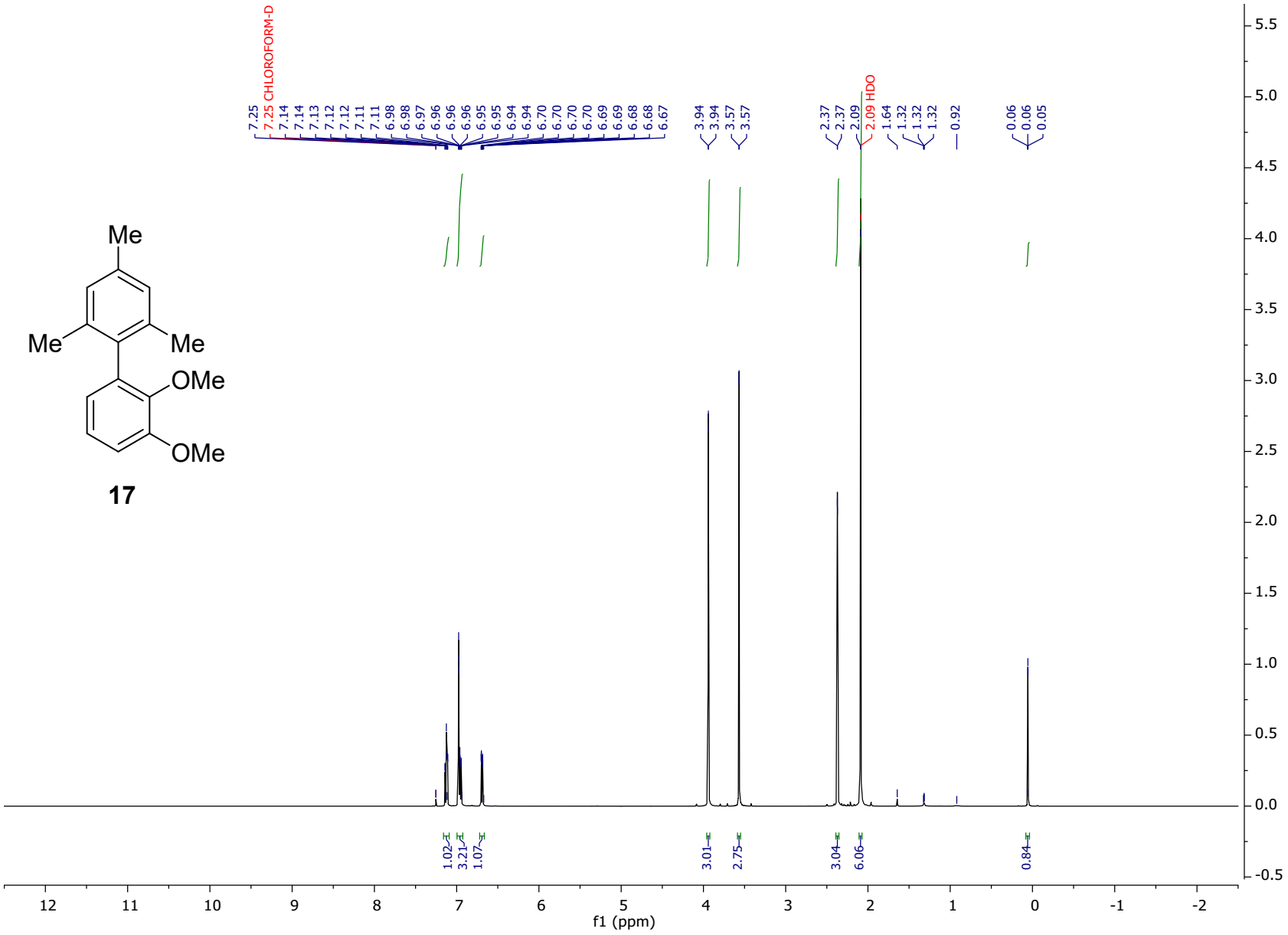

CN
OMe
14
156.61
143.59
132.41
130.93
130.71
130.63
128.43
121.49
119.50
112.43
110.04
56.07
40.56 DMSO-D6
40.39 DMSO-D6
40.23 DMSO-D6
40.06 DMSO-D6
39.89 DMSO-D6
39.73 DMSO-D6
39.56 DMSO-D6
f1 (ppm)

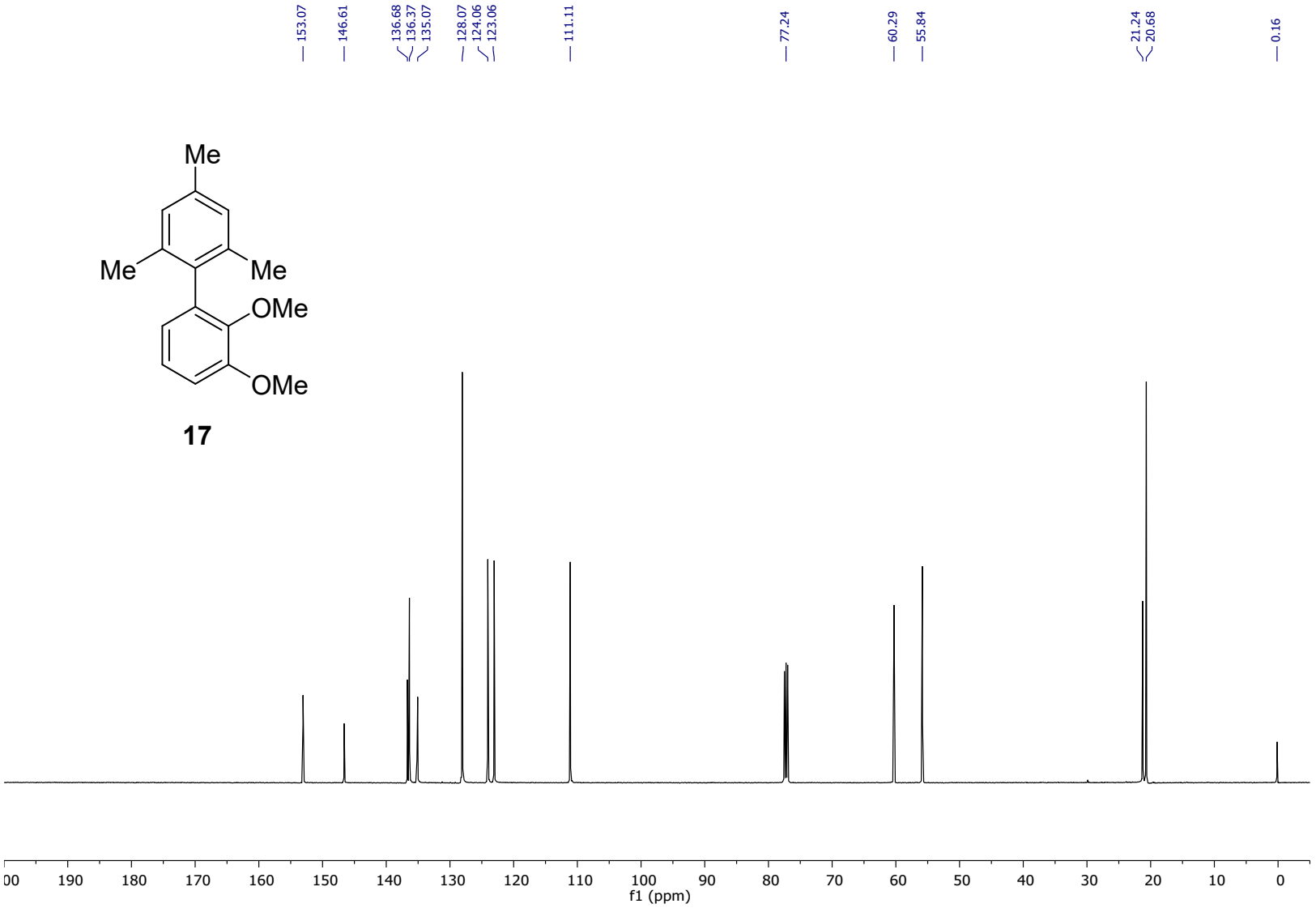

7.29
7.29
7.28 CHLOROFORM-D
7.28
7.28
7.27
7.27
7.26
7.26
7.21
7.21
7.20
7.19
7.11
7.10
7.09
7.09
7.08
7.07
7.07
7.06
7.05
7.05
7.04
6.99
6.99
6.97
6.97
6.96
6.96
6.92
6.91
6.90
6.90
6.78
6.77
6.76
6.76
6.75
6.74
6.66
6.65
6.64
6.64
3.67
3.57
3.57
-0.00
NH2
MeO
15
0.92
0.88
1.89
0.89
0.86
0.88
0.86
2.64
2.07
f1 (ppm)

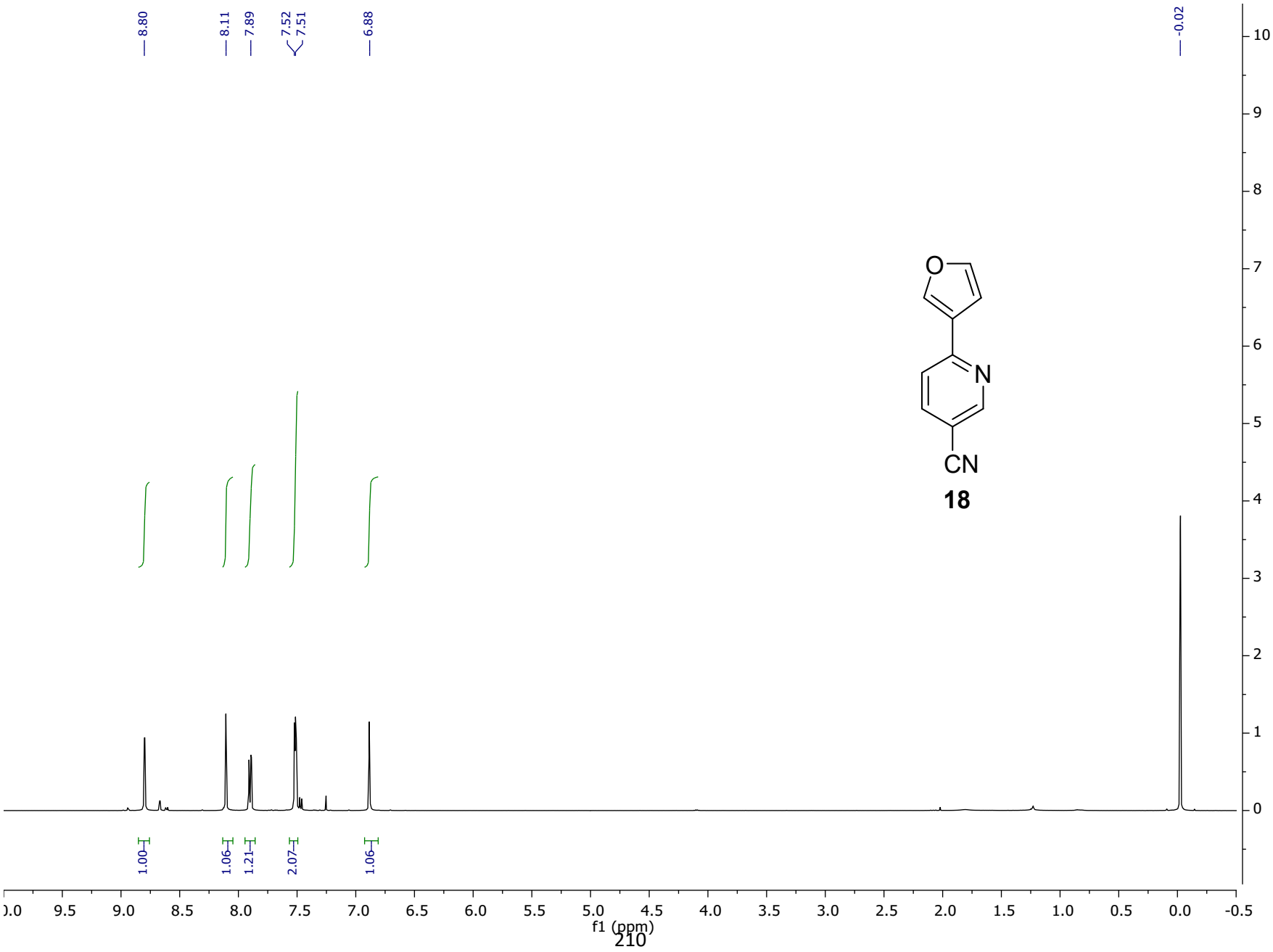

156.59
144.41
131.70
130.98
128.87
128.35
128.21
124.80
121.02
118.18
115.54
111.15
77.44 CHLOROFORM-D
77.19 CHLOROFORM-D
76.93 CHLOROFORM-D
55.51
-0.00
NH2
MeO
15
f1 (ppm)

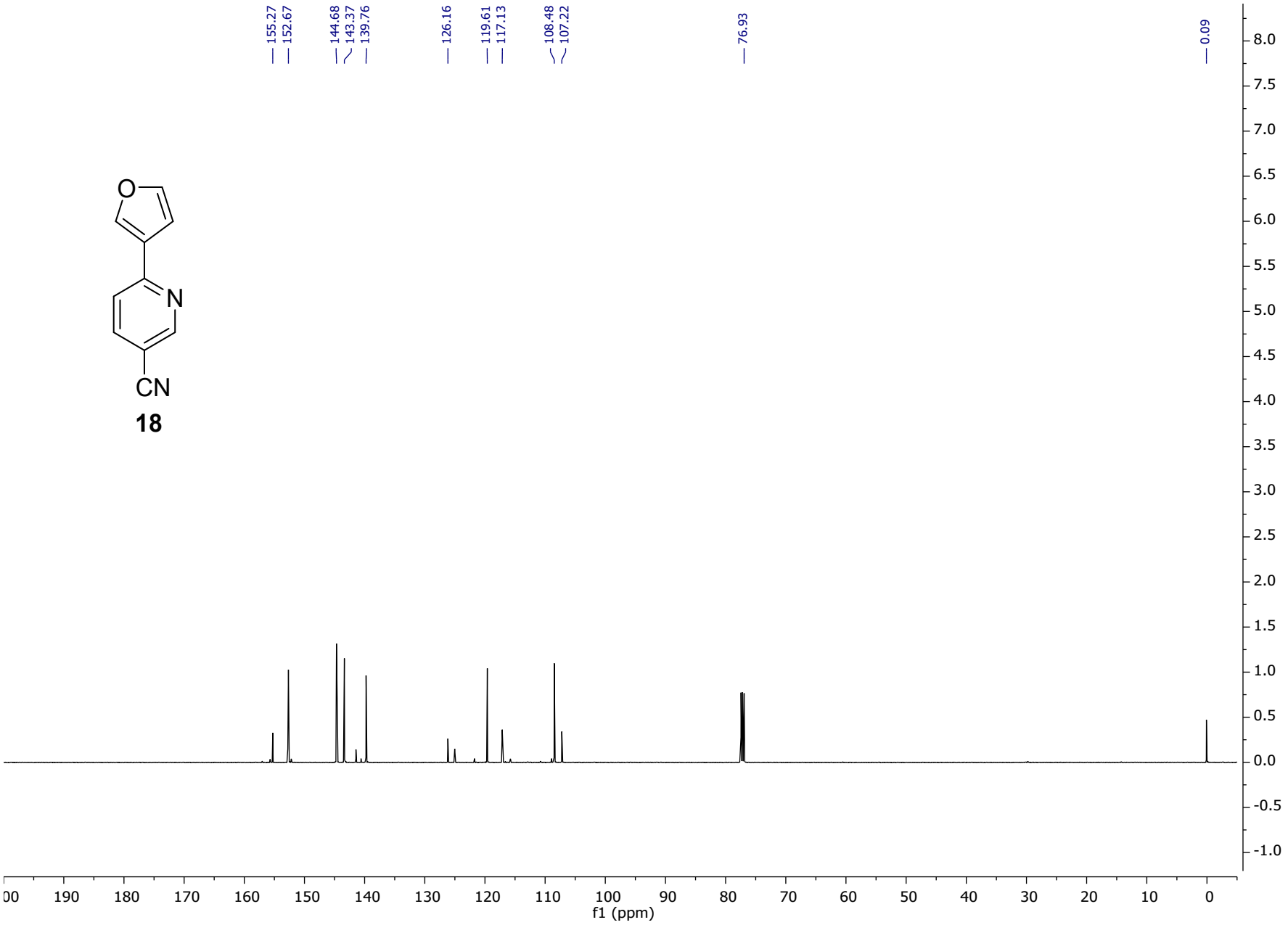

Me
Me
OMe
OMe
16
7.27
7.26
7.25
7.24
7.24
7.23
7.19 CHLOROFORM-D
7.19
7.17
7.17
7.15
7.00
7.00
6.99
6.98
6.98
6.75
6.74
6.73
6.73
3.96
3.61
2.17
0.11
0.11
0.10
1.01
2.88
1.00
0.96
2.99
2.95
5.62
f1 (ppm)

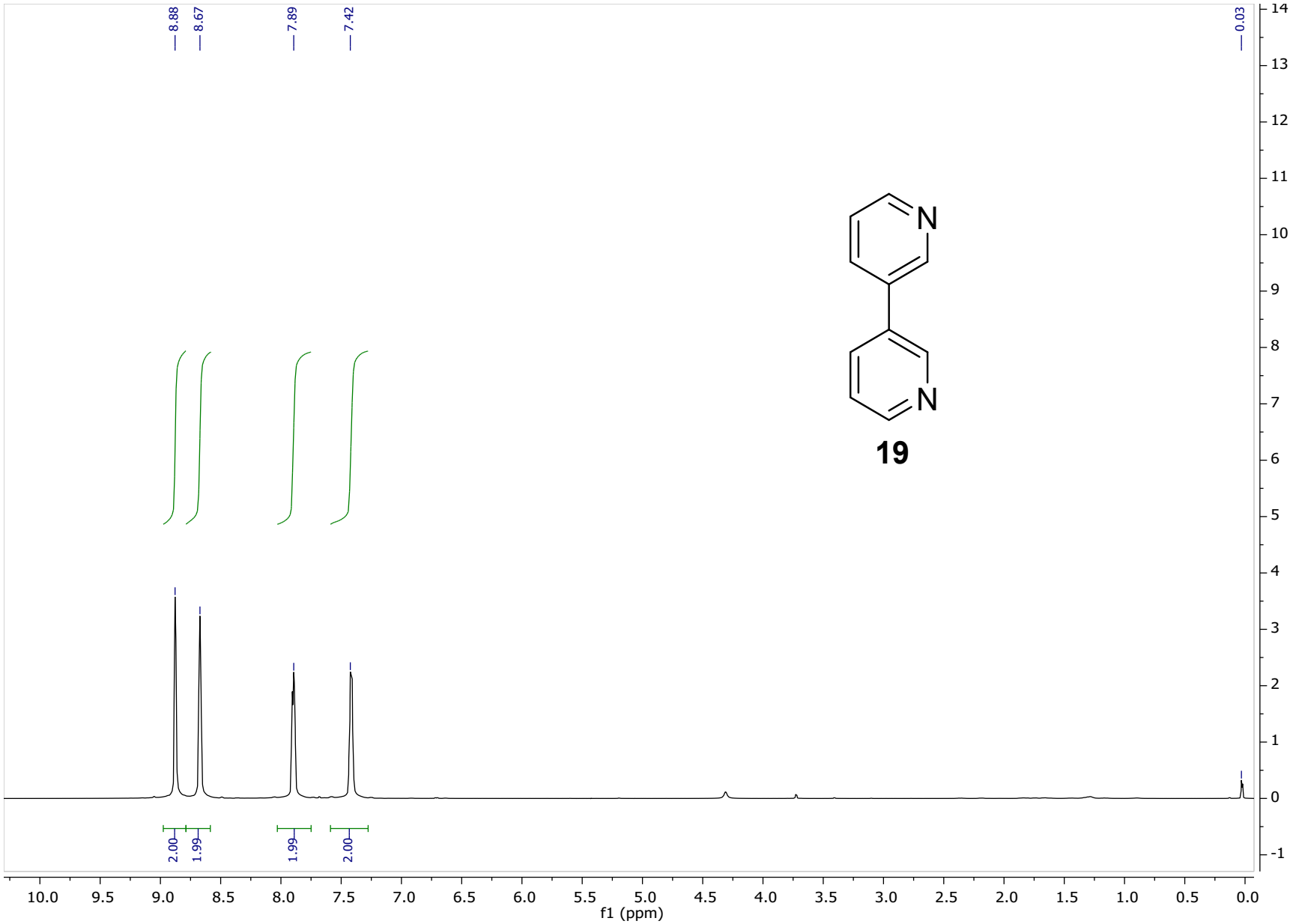

148.42
141.73
133.37
131.76
130.34
122.55
119.46
118.02
106.57
72.39
55.52
51.10
16.08
Me
Me
OMe
OMe
16
f1 (ppm)

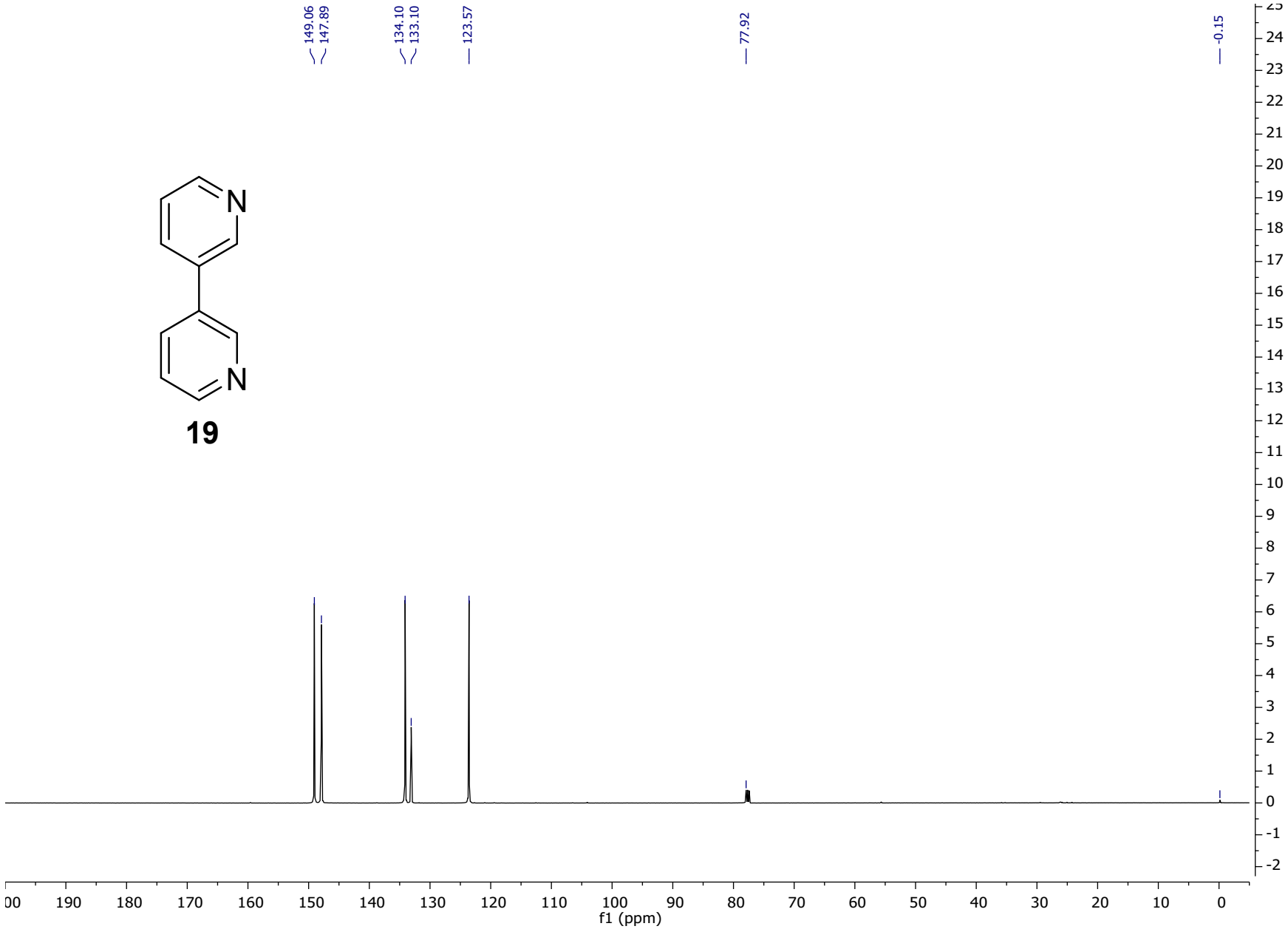

Me
Me
Me
OMe
OMe
17
7.25 CHLOROFORM-D
7.25 7.14 7.14 7.13 7.12 7.12 7.11 7.11 6.98 6.98 6.97 6.96 6.96 6.96 6.95 6.95 6.94 6.94 6.70 6.70 6.70 6.69 6.69 6.68 6.68 6.67
3.94 3.94 3.57 3.57
2.37 2.37 2.09 2.09 HDO 1.64 1.32 1.32 1.32 0.92
0.06 0.06 0.05
1.02 3.21 1.07 3.01 2.75 3.04 6.06 0.84
f1 (ppm)

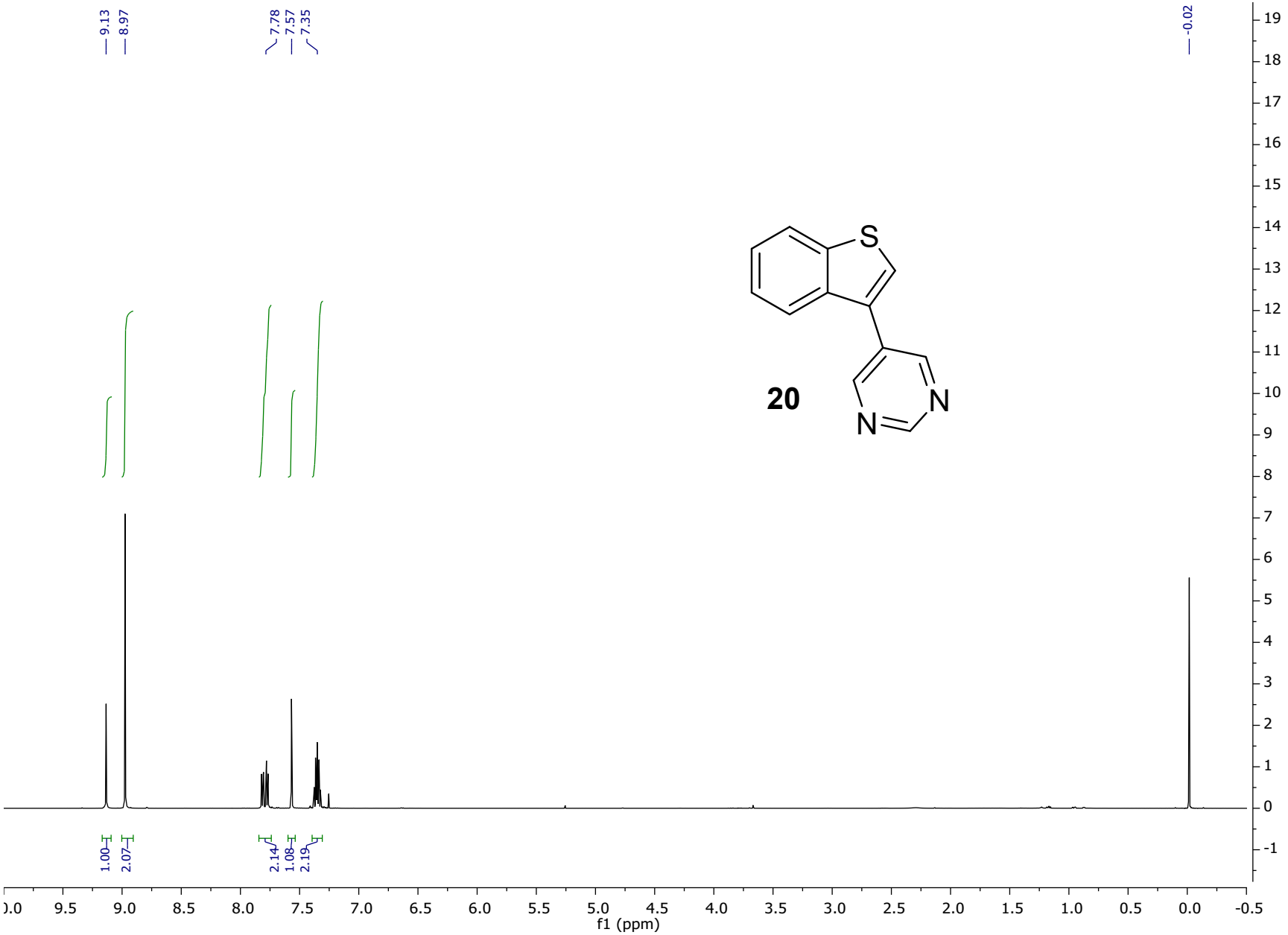

153.07
146.61
136.68
136.37
135.07
128.07
124.06
123.06
111.11
77.24
60.29
55.84
21.24
20.68
0.16
Me
Me
Me
OMe
OMe
17
f1 (ppm)

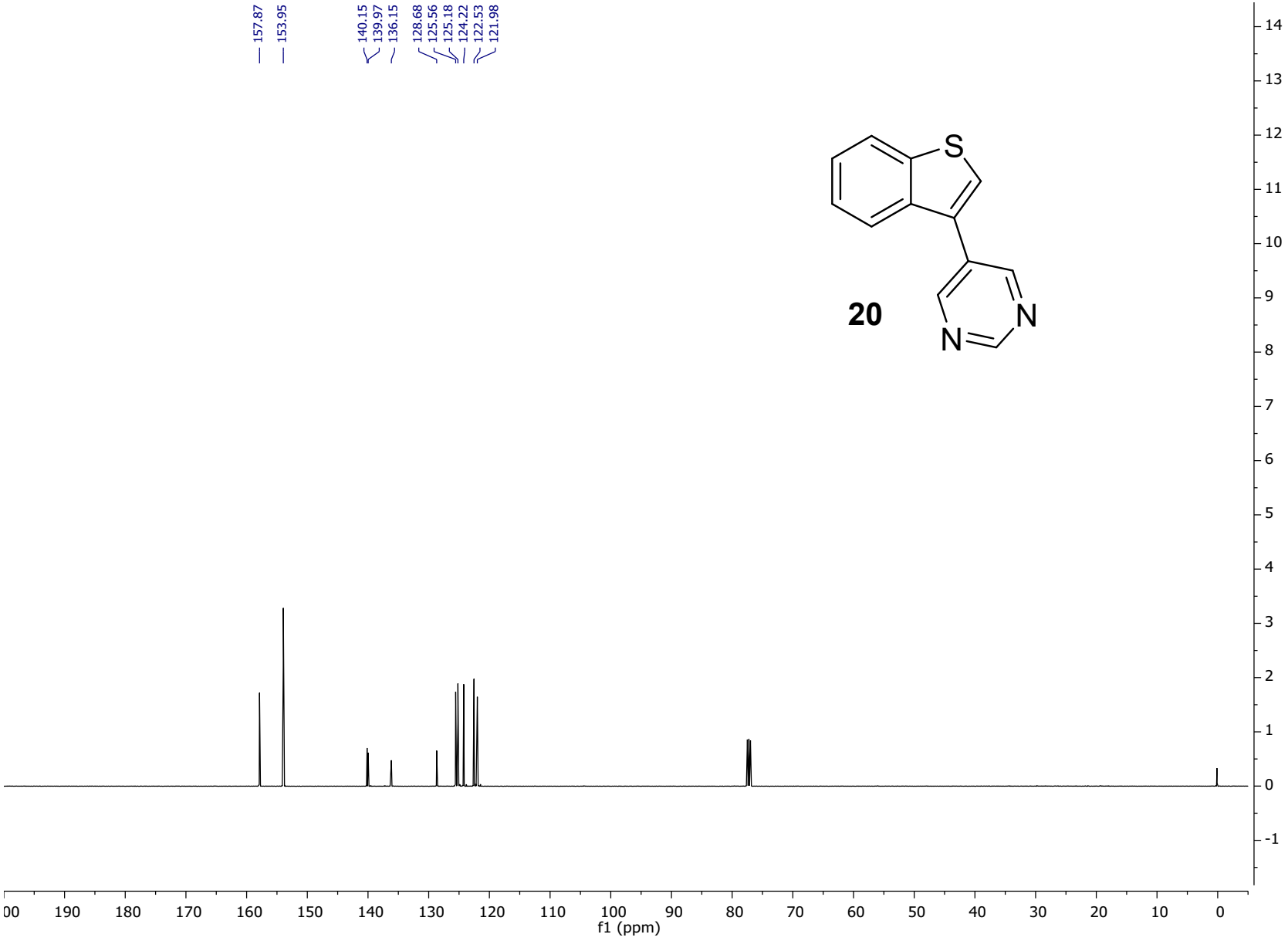

8.80
8.11
7.89
7.52
7.51
6.88
-0.02
1.00
1.06
1.21
2.07
1.06
f1 (ppm)
O
N
CN
18

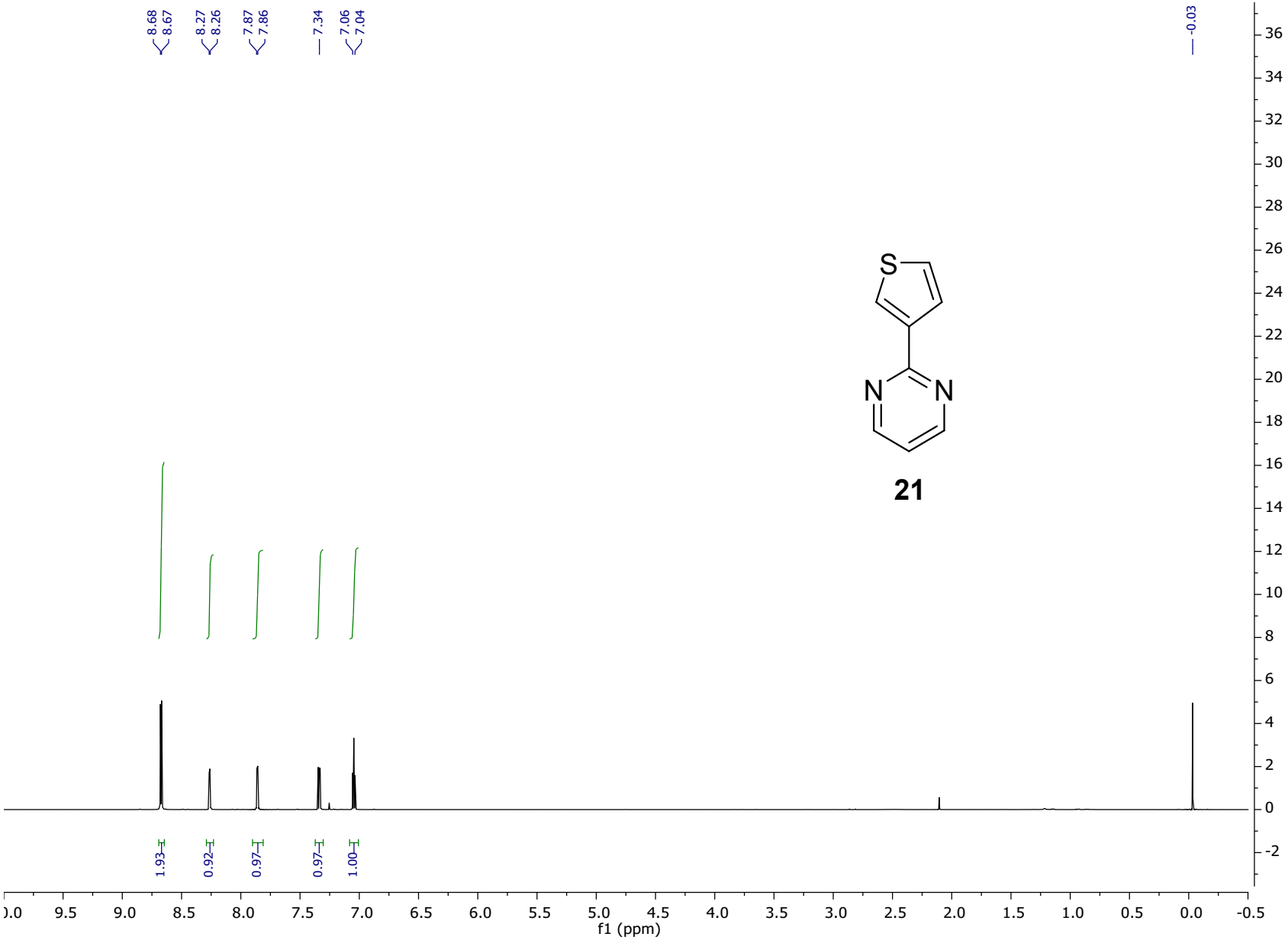

155.27
152.67
144.68
143.37
139.76
126.16
119.61
117.13
108.48
107.22
76.93
0.09
O
N
CN
18
f1 (ppm)

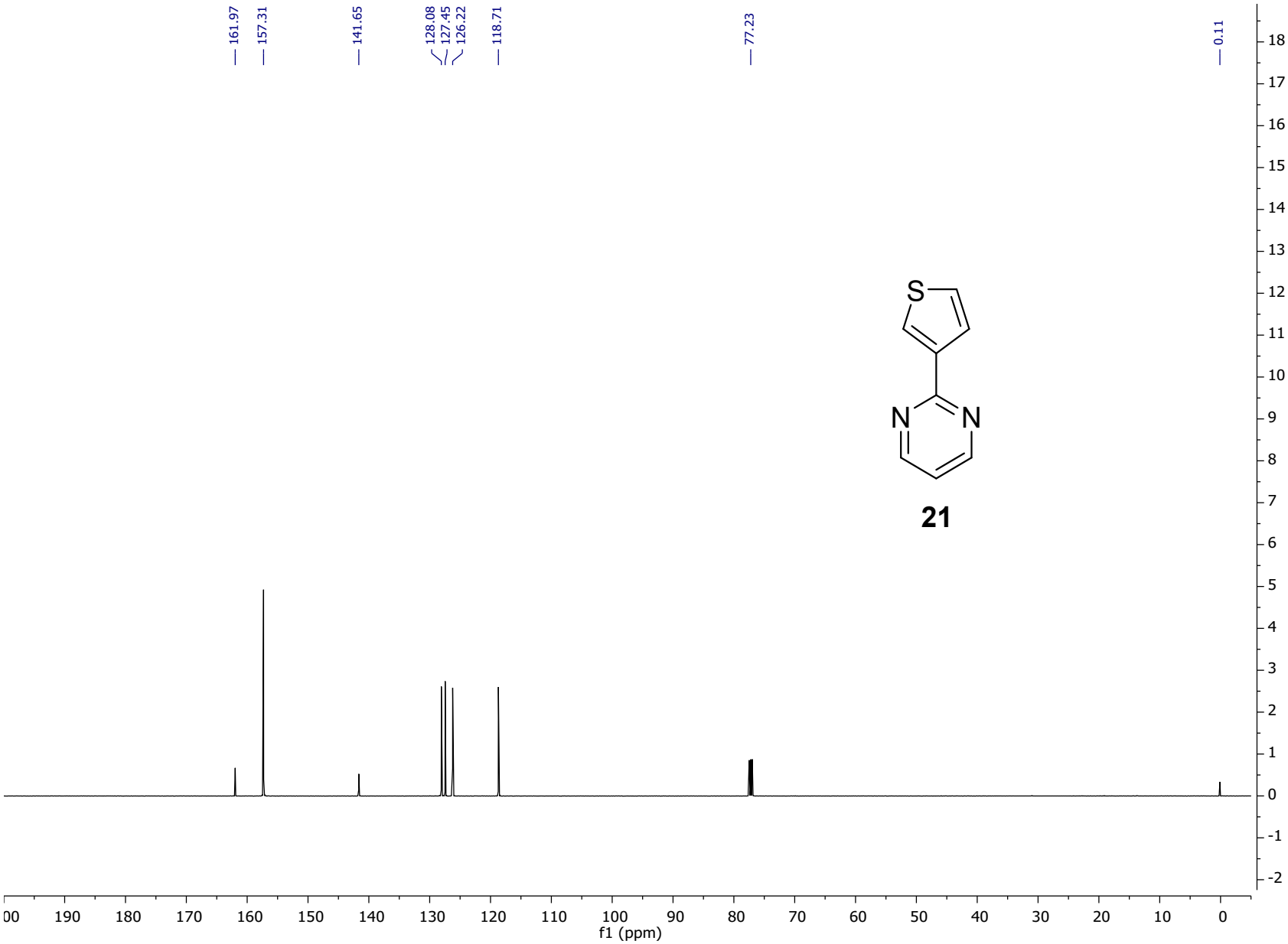

8.88
8.67
7.89
7.42
0.03
N
N
19
2.00
1.99
1.99
2.00
f1 (ppm)


149.06
147.89
134.10
133.10
123.57
77.92
-0.15
N
N
19
f1 (ppm)


9.13
8.97
7.78
7.57
7.35
-0.02
S
N
N
20
1.00
2.07
2.14
1.08
2.19
f1 (ppm)


157.87
153.95
140.15
139.97
136.15
128.68
125.56
125.18
124.22
122.53
121.98
S
N
N
20
f1 (ppm)


8.68
8.67
8.27
8.26
7.87
7.86
7.34
7.06
7.04
-0.03
S
N
N
21
1.93
0.92
0.97
0.97
1.00
f1 (ppm)


161.97
157.31
141.65
128.08
127.45
126.22
118.71
77.23
0.11
S
N
N
21
f1 (ppm)