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Supporting Information

Palladium-Catalyzed Regioselective Direct C-H Bond Alkoxycarbonylation of 2-Arylimidazo[1,2-a]pyridines

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Contents

1. General Information

All commercially available chemicals and reagents were purchased from Merck or Sigma or commercial distributors and were used without further purification. 2-aryl-imidazo[1,2-a]pyridines were synthesized according to the literature[1]. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 F_{254} plates. The products were purified by preparative column chromatography on silica gel (0.063–0.200 mm, Merck). ^{1}HNMR (500 MHz) and ^{13}CNMR (125 MHz) spectra were recorded on an Inova Varian 500 Advanced instrument in $CDCl_3$ or Methanol-d_4. Electron ionization (EI) mass spectra were obtained using an Agilent 5975C VL MSD (ion source: EI+, 70 eV, 230 °C).

2. General Procedure for Synthesis of alkoxycarbonylated Imidazo[1,2-a]pyridines:

A 10 mL microwave vial was charged with the 2-aryl-imidazo[1,2-a]pyridine derivative (0.2 mmol, 1.0 equiv.), alcohol (0.2 mL), $W(CO)_6$ (50 mol-%), $Pd(OAc)_2$ (10 mol-%), $Cu(OAc)_2$ (0.4 mmol, 2.0 eq.) and DCE (1.5 mL) in air. The reaction vessel was then sealed and immersed in an oil bath, which was preheated at 110 °C, for 16h. After this time, the mixture was cooled to room temperature and then diluted with ethyl acetate and filtered. The residue was purified by column chromatography (n-hexane/EtOAc, 10:3) to yield the desired product.

3.Spectral data

3.1. Ethyl 2-(*p*-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3aa)[2]

Pale yellow solid (88 %, 49.2 mg), mp 77-79 °C. ^{1}HNMR (500 MHz, $CDCl_3$) δ 9.40 (d, *J* = 7.1 Hz, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.02 (t, *J* = 7.0 Hz, 1H), 4.32 (q, *J* = 7.1 Hz, 2H), 2.42 (s, 3H), 1.25 (t, *J* = 7.0 Hz, 3H). ^{13}CNMR (125 MHz, $CDCl_3$) δ 161.2, 153.6, 147, 138.6, 131.3, 130.1, 128.3, 128.3, 127.9, 117.4, 114, 111.8, 60.4, 21.4, 14.1. MS (IE) m/z (relative intensity %) 280 (M^+, 58), 251 (17), 208 (100), 111 (58), 112 (54), 82 (13). IR $\nu_{(C=O)}$ 1679.8 cm^{-1}

3.2. Ethyl 2-phenyl imidazo[1,2-a] pyridine-3-carboxylate (3ba)[2]

Pale yellow solid (89 %, 47.3 mg), mp 71-73 °C. ^{1}H NMR (500 MHz, CD_3OD) δ 9.41 (d, *J* = 6.9 Hz, 1H), 7.71-7.65 (m, 3H), 7.58 (t, *J* = 7.9 Hz, 1H), 7.48-7.42 (m, 3H), 7.18 (t, *J* = 7.0 Hz, 1H), 4.26 (q, *J* = 7.1 Hz, 2H), 1.17 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 160.7, 152.6, 146.7, 133.9, 129.9, 128.9, 128.6, 128.1, 127.3, 116.1, 114.5, 111.9, 60.3, 12.9. MS (IE) m/z (relative intensity %) 266 (M^+, 29), 194 (58), 115 (14), 89 (51), 78 (100), 63 (14). IR $\nu_{(C=O)}$ 1674.1 cm^{-1}

3.3. Ethyl 2-(4-methoxyphenyl)imidazo[1,2-a]pyridine-3-carboxylate (3ca)

Yellow solid (67 %, 39.6 mg), mp 103-105 °C. ^{1}H NMR (500 MHz, CD_3OD) δ 9.41 (d, *J* = 7.0 Hz, 1H), 7.71–7.64 (m, 3H), 7.58 (t, *J* = 7.9 Hz, 0H), 7.16 (t, *J* = 7.0 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 2H), 4.30 (q, *J* = 7.1 Hz, 2H), 3.88 (s, 3H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 160.8, 160.5, 152.6, 146.7, 131.3, 131, 128.8, 128.2, 126, 115.9, 114.3, 112.7, 60.3, 54.4, 13. MS (IE) m/z (relative intensity %) 296 (M^+, 100), 267 (21), 251 (18), 224 (78), 209 (42), 78 (20). IR $\nu_{(C=O)}$ 1683.5 cm^{-1}. $C_{17}H_{16}N_2O_3$ (296.32): calcd. C 68.91, H 5.44, N 9.45; found C 68.60, H 5.47, N 9.49.

3.4. Ethyl 2-(4-chlorophenyl)imidazo[1,2-a]pyridine-3-carboxylate (3da)[3]

Yellow solid (71 %, 42.6 mg) mp 106-108 °C. ^{1}H NMR (500 MHz, CD_3OD) δ 9.38 (d, *J* = 7.0 Hz, 1H), 7.71–7.64 (m, 3H), 7.58 (t, *J* = 7.9 Hz, 1H), 7.44 (d, *J* = 8.2 Hz, 2H), 7.17 (t, *J* = 6.9 Hz, 1H), 4.28 (q, *J* = 7.1 Hz, 2H), 1.20 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 160.5, 151.2, 146.8, 134.6, 132.6, 131.5, 129, 128.2, 127.5, 116.2, 114.7, 112, 60.5, 12.9. MS (IE) m/z (relative intensity %) 302 (M+2, 14), 300 (M^+, 39), 271 (20), 230 (30), 228 (100), 192 (43), 78 (34), 69 (49). IR $\nu_{(C=O)}$ 1668.3 cm^{-1}

3.5. Ethyl 2-(3-bromophenyl)imidazo[1,2-a]pyridine-3-carboxylate (3ea)[3]

Yellow solid (85 %, 58.5 mg), mp 99-101°C.^{1}H NMR (500 MHz, $CDCl_3$) δ 9.44 (d, *J* = 7.0 Hz, 1H), 7.94 (s, 1H), 7.75 (d, *J* = 9.0 Hz, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.9 Hz, 1H), 7.32 (t, *J* = 7.9 Hz, 1H), 7.07 (t, *J* = 7.0 Hz, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 1.27 (t, *J* = 8.2 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8, 151.6, 147, 136.3, 133.3, 131.6, 129.2, 128.8, 128.4, 128.3, 121.4, 117.5, 114.4, 112.1, 60.7, 14.0. MS (IE) m/z (relative intensity %) 346 (M+2, 9), 344 (M^+, 10), 272 (18), 220 (12), 192 (22), 110 (93), 78 (100), 69 (58). IR $\nu_{(C=O)}$ 1681.7 cm^{-1}

3.6. Ethyl 2-(3,4-dimethoxyphenyl)imidazo[1,2-a]pyridine-3-carboxylate (3fa)[4]

Yellow oil, (68%, 44.3 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.38 (d, *J* = 6.9 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.45-7.35 (m, 3H), 7.01 (t, *J* = 7.1 Hz, 1H), 6.93 (d, *J* = 8.2 Hz, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 3.93 (s, 6H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1, 153.4, 149.6, 148.2, 147, 128.4, 127.9, 127, 123.3, 117.3, 113.9, 113.4, 111.7, 110.2, 60.4, 55.9, 55.9, 14.2. MS (IE) m/z (relative intensity %) 326 (M^+, 91), 297 (19), 254 (14), 80 (51), 43 (100). IR $\nu_{(C=O)}$ 1683.9 cm^{-1}.

3.7. Ethyl 2-(thiophen-2-yl) imidazo[1,2-a]pyridine-3-carboxylate (3ga)

Pale yellow solid (76 %, 41.3 mg), mp 74-76 °C.^{1}H NMR (500 MHz, $CDCl_3$) δ 9.24 (d, *J* = 7.1 Hz, 1H), 7.99 (d, *J* = 3.8 Hz, 1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.41 (d, *J* = 5.0 Hz, 1H), 7.29 (t, *J* = 7.9 Hz, 1H), 7.08 (t, *J* = 4.3 Hz, 1H), 6.86 (t, *J* = 7.0 Hz, 1H), 4.41 (q, *J* = 7.2 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.7, 146.8, 146.6, 136.7, 129.8, 128.4, 128.1, 128.1, 127.3, 117, 113.9, 110.8, 60.8, 14.4. MS (IE) m/z (relative intensity %) 272 (M^+, 81), 244 (15), 200 (100), 155 (15), 78 (45). IR $\nu_{(C=O)}$ 1684.3 cm^{-1}. $C_{14}H_{12}N_2O_2S$ (272.32): calcd. C 61.75, H 4.44, N 10.29; found C 60.92, H 4.39, N 10.34.

3.8. Ethyl 8-methyl-2-(*p*-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ha)

Pale yellow solid (73 %, 43 mg), mp 91-93 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.28 (d, *J* = 7.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 7.9 Hz, 2H), 7.23 (d, *J* = 6.8 Hz, 1H), 6.94 (t, *J* = 7.0 Hz, 1H), 4.33 (q, *J* = 7.2 Hz, 2H), 2.70 (s, 3H), 2.44 (s, 3H), 1.26 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 153.3, 147.4, 138.3, 131.9, 130.2, 128.3, 127.4, 126.7, 126.1, 113.9, 112.2, 60.3, 21.4, 17.1, 14.1. MS (IE) m/z (relative intensity %) 294 (M^+, 78), 265 (24), 249 (16), 222 (100), 91 (14). IR $\nu_{(C=O)}$ 1675.5 cm^{-1}. $C_{18}H_{18}N_2O_2$ (294.35): calcd. C 73.45, H 6.16, N 9.52; found C 73.21, H 6.19, N 9.47.

3.9. Ethyl 2-(4-fluorophenyl)-8-methylimidazo[1,2-a]pyridine-3-carboxylate (3ia)

White solid (78%, 46.5 mg), mp 107-109 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.29 (d, *J* = 7.0 Hz, 1H), 7.77 (t, *J* = 6.4 Hz, 2H), 7.25 (d, *J* = 7.0 Hz, 1H), 7.14 (t, *J* = 9.0 Hz, 2H), 6.97 (t, *J* = 7.0 Hz, 1H), 4.32 (q, *J* = 7.0 Hz, 2H), 2.70 (s, 3H), 1.24 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1 (d, *J* = 247.7 Hz), 161.1, 152.1, 147.3, 132.1 (d, *J* = 8.5 Hz), 130.9 (d, *J* = 3.4 Hz), 127.5, 126.9, 126.1, 114.5 (d, *J* = 21.6 Hz), 114.2, 112.3, 60.4, 17.1, 14. MS (IE) m/z (relative intensity %) 298 (M^+, 72), 269 (13), 253 (25), 226 (100), 107 (10), 92 (12). IR $\nu_{(C=O)}$ 1675.6 cm^{-1}. $C_{17}H_{15}FN_2O_2$ (298.32): calcd. C 68.45, H 5.07, N 9.39; found C 68.81, H 5.13, N 9.31.

3.10. Ethyl 7-methyl-2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ja)

Pale yellow solid (77 %, 45.2 mg), mp 83-85 °C. ^{1}H NMR (500 MHz, CD_3OD) δ 9.27 (d, *J* = 7.1 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.46 (s, 1H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.04 (dd, *J* = 7.1, 1.8 Hz, 1H), 4.27 (q, *J* = 7.1 Hz, 2H), 2.48 (s, 3H), 2.41 (s, 3H), 1.20 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 160.9, 152.8, 147.1, 140.8, 138.7, 131, 129.8, 127.9, 127.3, 116.8, 114.6, 111.5, 60.2, 20, 19.9, 13. MS (IE) m/z (relative intensity %) 294 (M^+, 90), 265 (27), 222 (100), 206 (17), 110 (15), 91 (18), 69 (30). IR $\nu_{(C=O)}$ 1683.9 cm^{-1}. $C_{18}H_{18}N_2O_2$ (294.35): calcd. C 73.45, H 6.16, N 9.52; found C 73.77, H 6.20, N 9.56.

3.11. Ethyl 6-methyl-2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ka)[5]

White solid (71 %, 41.7 mg), mp 85-87 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.25 (s, 1H), 7.71–7.64 (m, 3H), 7.32–7.28 (m, 1H), 7.25 (d, *J* = 8.1 Hz, 2H), 4.33 (q, *J* = 7.1 Hz, 2H), 2.44 (s, 6H), 1.27 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 153.4, 146.1, 138.5, 131.5, 130.9, 130.1, 128.3, 126.2, 123.9, 116.6, 111.5, 60.4, 21.4, 18.5, 14.1. MS (IE) m/z (relative intensity %) 294 (M^+, 92), 279 (25), 249 (50), 222 (100), 119 (21), 84 (22). IR $\nu_{(C=O)}$ 1680.3 cm^{-1}

3.12. Ethyl 2-(4-methoxyphenyl)-7-methyl imidazo[1,2-a] pyridine-3-carboxylate (3la)

Yellow solid (64 %, 39.6 mg), mp 79-81 °C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.26 (d, *J* = 7.1 Hz, 1H), 7.75 (d, *J* = 8.6 Hz, 2H), 7.47 (s, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.84 (dd, *J* = 7.2, 1.8 Hz, 1H), 4.32 (q, *J* = 7.2 Hz, 2H), 3.87 (s, 3H), 2.46 (s, 3H), 1.27 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3, 160.1, 153.5, 147.7, 139.2, 131.6, 127.6, 127.4, 127.0, 116.4, 116.0, 113.0, 60.3, 55.3, 21.4, 14.2. MS (IE) m/z (relative intensity %) 310 (M^+, 100), 281 (28), 223 (73), 135 (72), 77 (27).

IR $\nu_{(C=O)}$ 1677.2 cm^{-1}. $C_{18}H_{18}N_2O_3$ (310.35): calcd. C 69.66, H 5.85, N 9.03; found C 69.43, H 5.88, N 9.09.

3.13. Ethyl 7-chloro-2-(3-methoxyphenyl)imidazo[1,2-a]pyridine-3-carboxylate (3ma)

Off-white solid (82%, 54.1 mg), mp 87-89 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.53 (s, 1H), 7.70 (d, *J* = 9.4 Hz, 1H), 7.43 (dt, *J* = 9.5, 1.6 Hz, 1H), 7.39-7.30 (m, 3H), 7.03-6.98 (m, 1H), 4.35 (q, *J* = 7.2 Hz, 2H), 3.89 (s, 3H), 1.26 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9, 159, 153.7, 145.3, 135.2, 129.2, 128.6, 126.3, 122.8, 122.4, 117.7, 115.5, 114.9, 112.5, 60.8, 55.4, 14. MS (IE) m/z (relative intensity %) 332 (M+2, 35), 330 (M^+, 100), 303 (12), 301 (33), 287

(14), 285 (23), 259 (40), 257 (83), 228 (47), 179 (17), 112 (23), 76 (19). IR $\nu_{(C=O)}$ 1674.3 cm^{-1} $C_{17}H_{15}ClN_2O_3$ (330.77): calcd. C 61.73, H 4.57, N 8.47; found C 61.27, H 4.61, N 8.42.

3.14. Ethyl 7-chloro-2-(4-chlorophenyl)imidazo[1,2-a]pyridine-3-carboxylate (3na)[6]

White solid (87%, 58.1 mg), mp 127-129 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.53 (s, 1H), 7.74 (d, *J* = 7.9 Hz, 2H), 7.69 (d, *J* = 9.1 Hz, 1H), 7.44 (d, *J* = 7.6 Hz, 3H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.29 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 152.7, 145.4, 135, 132.5, 131.5, 129.4, 127.9, 126.4, 122.6, 117.7, 112.4, 60.9, 14.1. MS (IE) m/z (relative intensity %) 338 (M+4, 6), 336 (M+2, 31), 334 (M^+, 47), 307 (9), 305 (14), 291 (9), 289 (14), 266 (11), 264 (66), 262 (100), 226 (18), 191 (10), 112 (17), 76 (10). IR $\nu_{(C=O)}$ 1680.2 cm^{-1}.

3.15. Methyl 2-(*p*-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ab)

Yellow solid (91 %, 48.4 mg), mp 123-125 °C.^{1}H NMR (500 MHz, CD_3OD) δ 9.28 (d, *J* = 7.1 Hz, 1H), 7.60 (d, *J* = 9.0 Hz, 1H), 7.53-7.46 (m, 3H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.06 (t, *J* = 7.1 Hz, 1H), 3.72 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (125 MHz, CD_3OD) δ 161.1, 152.7, 146.7, 138.7, 130.8, 129.7, 128.8, 128.1, 128, 116.0, 114.4, 111.5, 50.3, 20. MS (IE) m/z (relative intensity %) 266 (M^+, 100), 251 (56), 235 (28), 208 (75), 192 (16), 78 (17).IR $\nu_{(C=O)}$ 1685.3 cm^{-1}. $C_{16}H_{14}N_2O_2$ (266.29): calcd. C 72.16, H 5.30, N 10.52; found C 27.39, H 5.34, N 10.58.

3.16. Propyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ac)

Yellow oil (83 %, 48.8 mg).^{1}H NMR (500 MHz, $CDCl_3$) δ 9.40 (d, *J* = 7.3 Hz, 1H), 7.74 (d, *J* = 8.9 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.23 (d, *J* = 7.7 Hz, 2H), 7.02 (t, *J* = 6.9 Hz, 1H), 4.20 (t, *J* = 6.6 Hz, 2H), 2.40 (s, 3H), 1.60 (h, *J* = 7.5 Hz, 2H), 0.79 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 153.5, 146.9, 138.6, 131.3, 130, 128.3, 128.3, 128.1, 117.2, 114.1, 111.9, 66.2, 21.8, 21.4, 10.4. MS (IE) m/z (relative intensity %) 294 (M^+, 40), 251 (11), 208 (100), 110 (47), 78 (14). IR $\nu_{(C=O)}$ 1683.2 cm^{-1}. $C_{18}H_{18}N_2O_2$ (294.35): calcd. C 73.45, H 6.16, N 9.52; found C 73.26, H 6.13, N 9.45.

3.17. Phenethyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ad)

Pale yellow solid (87 %, 62 mg), mp 87-89 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.33 (d, *J* = 7.0 Hz, 1H), 7.74 (d, *J* = 9.0 Hz, 1H), 7.68 (d, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.30-7.20 (m, 5H), 7.06 (d, *J* = 6.7 Hz, 2H), 6.98 (t, *J* = 7.0 Hz, 1H), 4.53 (t, *J* = 6.9 Hz, 2H), 2.96 (t, *J* = 6.9 Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.1, 154, 147.2, 138.7, 137.8, 131.6, 130.2, 128.9, 128.5, 128.4, 127.9, 126.5, 117.4, 114, 111.7, 65.1, 34.9, 21.5. MS (IE) m/z (relative intensity %) 356 (M^+, 88), 252 (54), 235 (33), 208 (100), 104 (20), 78 (17). IR $\nu_{(C=O)}$ 1678.2 cm^{-1}. $C_{23}H_{20}N_2O_2$ (356.42): calcd. C 77.51, H 5.66, N 7.86; found C 77.84, H 5.71, N 7.81.

3.18. Isopentyl 2-(*p*-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ae)

Pale yellow solid (76%, 49 mg), mp. 77-79 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.41 (d, *J* = 7.0 Hz, 1H), 7.71 (d, *J* = 8.9 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 2H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.00 (t, *J* = 7.0 Hz, 1H), 4.27 (t, *J* = 6.5 Hz, 2H), 2.41 (s, 3H), 1.50–1.36 (m, 3H), 0.82 (d, *J* = 6.4 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 153.9, 147.1, 138.4, 131.7, 130, 128.3, 128.3, 127.8, 117.4, 113.9, 111.9, 62.9, 37.1, 24.7, 22.3, 21.4. MS (IE) m/z (relative intensity %) 322 (M^+, 83), 252 (40), 235 (27), 208 (100), 192 (23), 119 (38), 91 (20), 78 (22). IR $\nu_{(C=O)}$ 1674.4 cm^{-1}. $C_{20}H_{22}N_2O_2$ (322.40): calcd. C 74.51, H 6.88, N 8.69; found C 74.79, H 6.84, N 8.65.

3.19. 3-cyclohexylpropyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3af)

Colorless oil (83%, 62.4 mg).^{1}H NMR (500 MHz, $CDCl_3$) δ 9.43 (d, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.41 (dd, *J* = 8.9, 6.9 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 2H), 7.01 (t, *J* = 6.9 Hz, 1H), 4.23 (t, *J* = 6.4 Hz, 2H), 2.42 (s, 3H), 1.70-1.56 (m, 8H), 1.22-1.08 (m, 4H), 1.06-0.99 (m, 2H), 0.84-0.77 (m, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.4, 153.8, 147.1, 138.4, 131.7, 130, 128.3, 127.8, 117.4, 113.9, 111.9, 65, 37.3, 33.6, 33.2, 26.6, 26.3, 25.9, 21.4. MS (IE) m/z (relative intensity %) 376 (M^+, 31), 252 (22), 208 (100), 80 (29). IR $\nu_{(C=O)}$ 1681.2 cm^{-1}. $C_{24}H_{28}N_2O_2$ (376.49): calcd. C 76.56, H 7.50, N 7.44; found C 76.87, H 7.57, N 7.52.

3.20. Isopropyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ag)

Yellow oil (69%, 40.5 mg). ^{1}H NMR (500 MHz, CD_3OD) δ 9.38 (d, *J* = 7.0 Hz, 1H), 7.64 (d, *J* = 9.0 Hz, 1H), 7.57 – 7.49 (m, 3H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.12 (t, *J* = 6.9 Hz, 1H), 5.16 (hept, *J* = 6.4 Hz, 1H), 2.40 (s, 3H), 1.17 (d, *J* = 6.3 Hz, 6H). ^{13}C NMR (125 MHz, CD_3OD) δ 158.8, 151.1, 145, 137.1, 129.5, 128.4, 127.2, 126.5, 126.3, 114.5, 112.8, 110.5, 66.8, 19.1, 19.1, 18.5. MS (IE) m/z (relative intensity %) 294 (M^+, 81), 252 (28), 235 (30), 208 (100), 43 (9.2). IR $\nu_{(C=O)}$ 1679.4 cm^{-1}. $C_{18}H_{18}N_2O_2$ (294.35): calcd. C 73.45, H 6.16, N 9.52; found C 73.68, H 5.21, N 9.55.

3.21. Cyclopentyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ah)

Pale yellow solid (71 %, 45.4 mg), mp 90-92 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.44 (d, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 9.0 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 2H), 7.42 (t, *J* = 7.9 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 2H), 7.02 (t, *J* = 6.9 Hz, 1H), 5.41 (tt, *J* = 5.7, 2.7 Hz, 1H), 2.43 (s, 3H), 1.88–1.79 (m, 2H), 1.73–1.65 (m, 2H), 1.57–1.48 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 161, 153.7, 147, 138.4, 131.8, 130, 128.3, 128.2, 127.7, 117.4, 113.9, 112.2, 77.6, 32.6, 23.5, 21.4. MS (IE) m/z (relative intensity %) 320 (M^+, 86), 252 (71), 235 (22), 208 (100), 192 (28), 78 (20). IR $\nu_{(C=O)}$ 1676.7 cm^{-1}. $C_{20}H_{20}N_2O_2$ (320.39): calcd. C 74.98, H 6.29, N 8.74; found C 74.63, H 6.22, N 8.82.

3.22. Cyclohexyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ai)[7]

White solid (65 %, 43.4 mg), mp 105-107 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.42 (d, *J* = 7.0 Hz, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 7.66 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.7 Hz, 2H), 7.01 (t, *J* = 6.9 Hz, 1H), 5.02 (tt, *J* = 8.7, 3.9 Hz, 1H), 2.42 (s, 3H), 1.89–1.83 (m, 2H), 1.62–1.51 (m, 2H), 1.44–1.28 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8, 153.7, 147, 138.4, 131.7, 130.1, 128.4, 128.3, 127.7, 117.4, 113.9, 112.2, 73.2, 31.5, 25.3, 23.5, 21.4. MS (IE) m/z (relative intensity %) 334 (M^+, 83), 252 (98), 208 (100), 115 (55), 78 (43). IR $\nu_{(C=O)}$ 1673.8 cm^{-1}

3.23. Pentan-2-yl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3aj)

Yellow oil (60 %, 38.6 mg). ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.43 (d, *J* = 7.0 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.65 (d, *J* = 7.8 Hz, 2H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.7 Hz, 2H), 7.02 (t, *J* = 6.8 Hz, 1H), 5.14 (q, *J* = 6.3 Hz, 1H), 2.43 (s, 3H), 1.55 – 1.48 (m, 1H), 1.46 – 1.38 (m, 1H), 1.25 (d, *J* = 6.3 Hz, 3H), 1.23 – 1.14 (m, 2H), 0.84 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9, 153.8, 147, 138.3, 131.7, 130.1, 128.3, 128.1, 127.7, 117.4, 113.8, 112.2, 71.4, 38, 21.4, 19.9, 18.5, 13.9. MS (IE) m/z (relative intensity %) 322 (M^+, 93), 308 (35), 252 (98), 235(36), 208 (100), 192 (43), 78 (30). IR $\nu_{(C=O)}$ 1677.9 cm^{-1}. $C_{20}H_{22}N_2O_2$ (322.40): calcd. C 74.51, H 6.88, N 8.69; found C 74.28, H 6.95, N 8.62.

3.24. *tert*-butyl 2-(p-tolyl)imidazo[1,2-a]pyridine-3-carboxylate (3ak)

Yellow solid (57 %, 35.1 mg), mp 83-85 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.35 (d, *J* = 7.0 Hz, 1H), 7.66 (d, *J* = 8.9 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.32 (dd, *J* = 8.8, 7.0 Hz, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 6.92 (t, *J* = 7.1 Hz, 1H), 2.37 (s, 3H), 1.43 (s, 9 H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.6, 153.2, 146.7, 138.2, 131.9, 130.1, 128.2, 127.4, 117.3, 113.6, 112.9, 81.8, 28.3, 21.4. MS (IE) m/z (relative intensity %) 308 (M^+, 18), 252 (49), 208 (100), 192 (20), 119 (22), 57 (35). IR $\nu_{(C=O)}$ 1679 cm^{-1}. $C_{19}H_{20}N_2O_2$ (308.37): calcd. C 74.00, H 6.54, N 9.08; found C 74.29, H 6.59, N 9.14.

4. References

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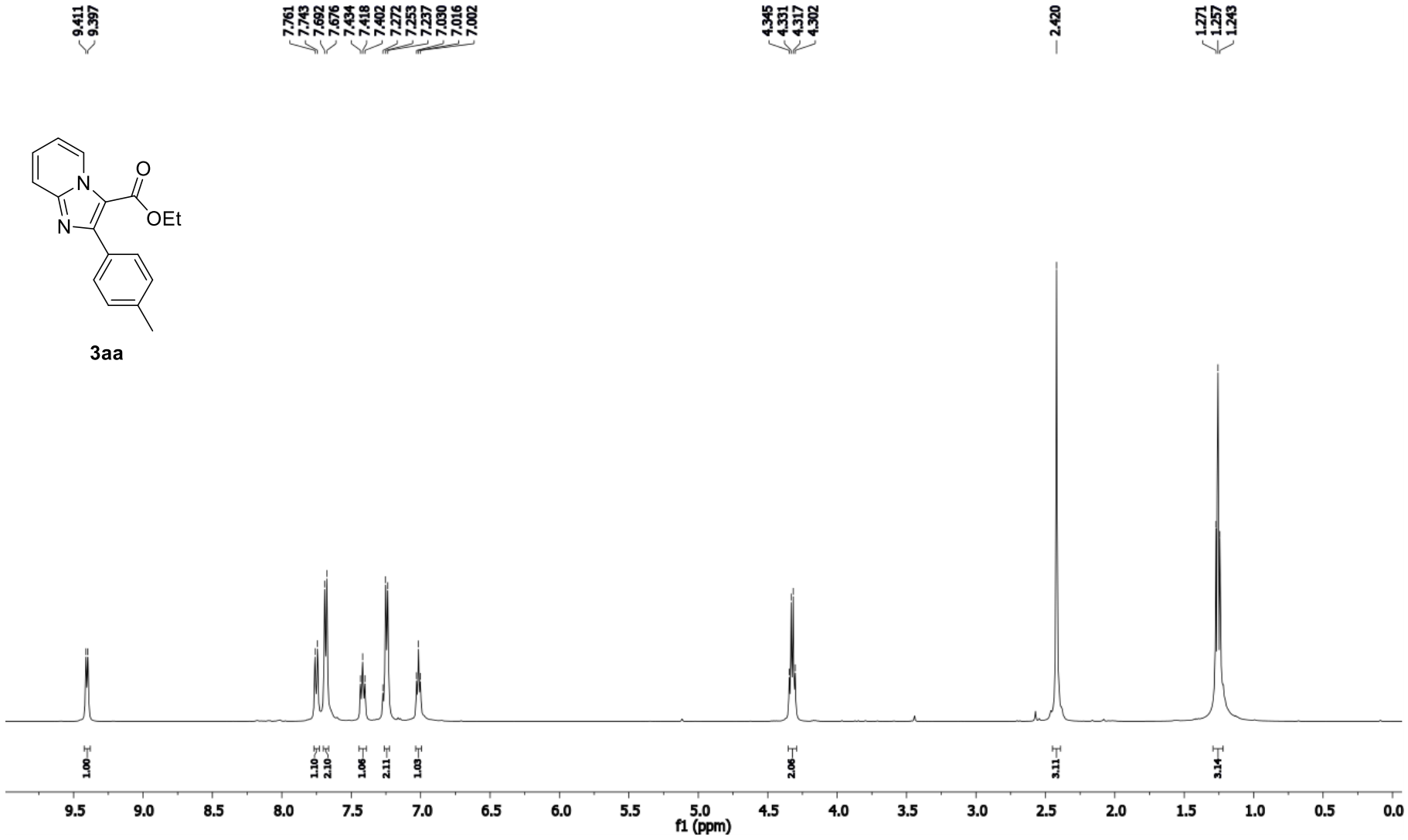
5. Copies of ^{1}H and ^{13}C NMR spectra



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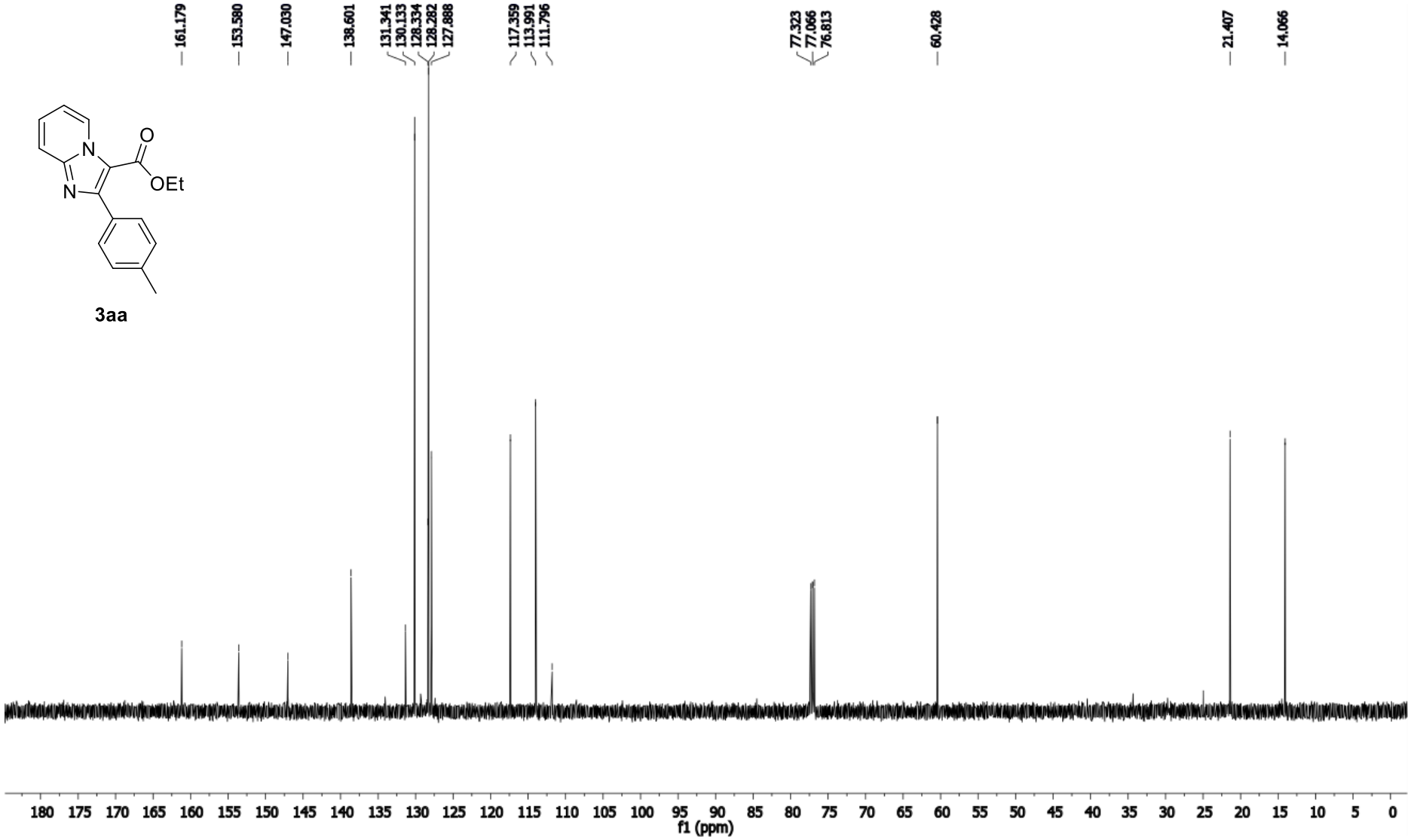
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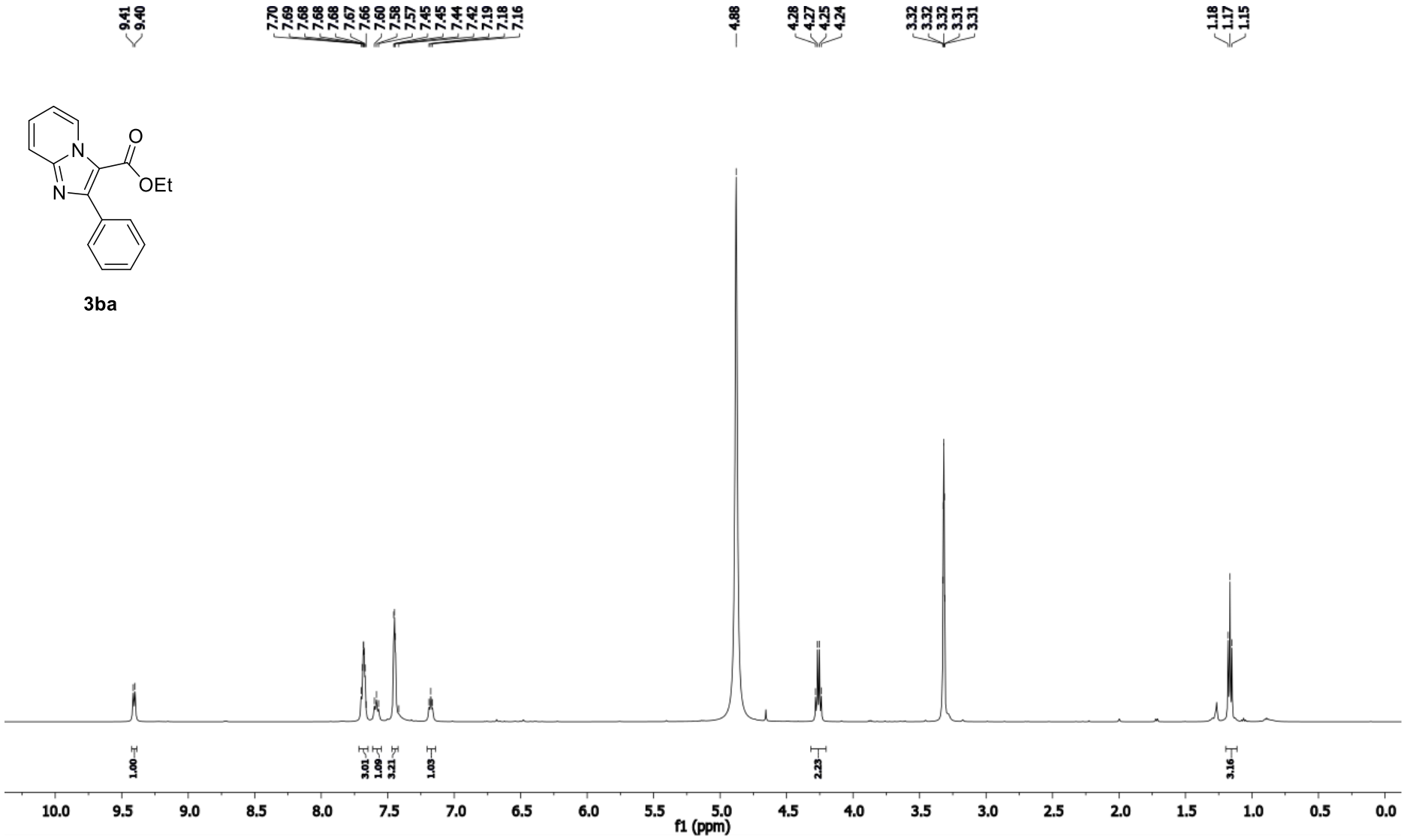
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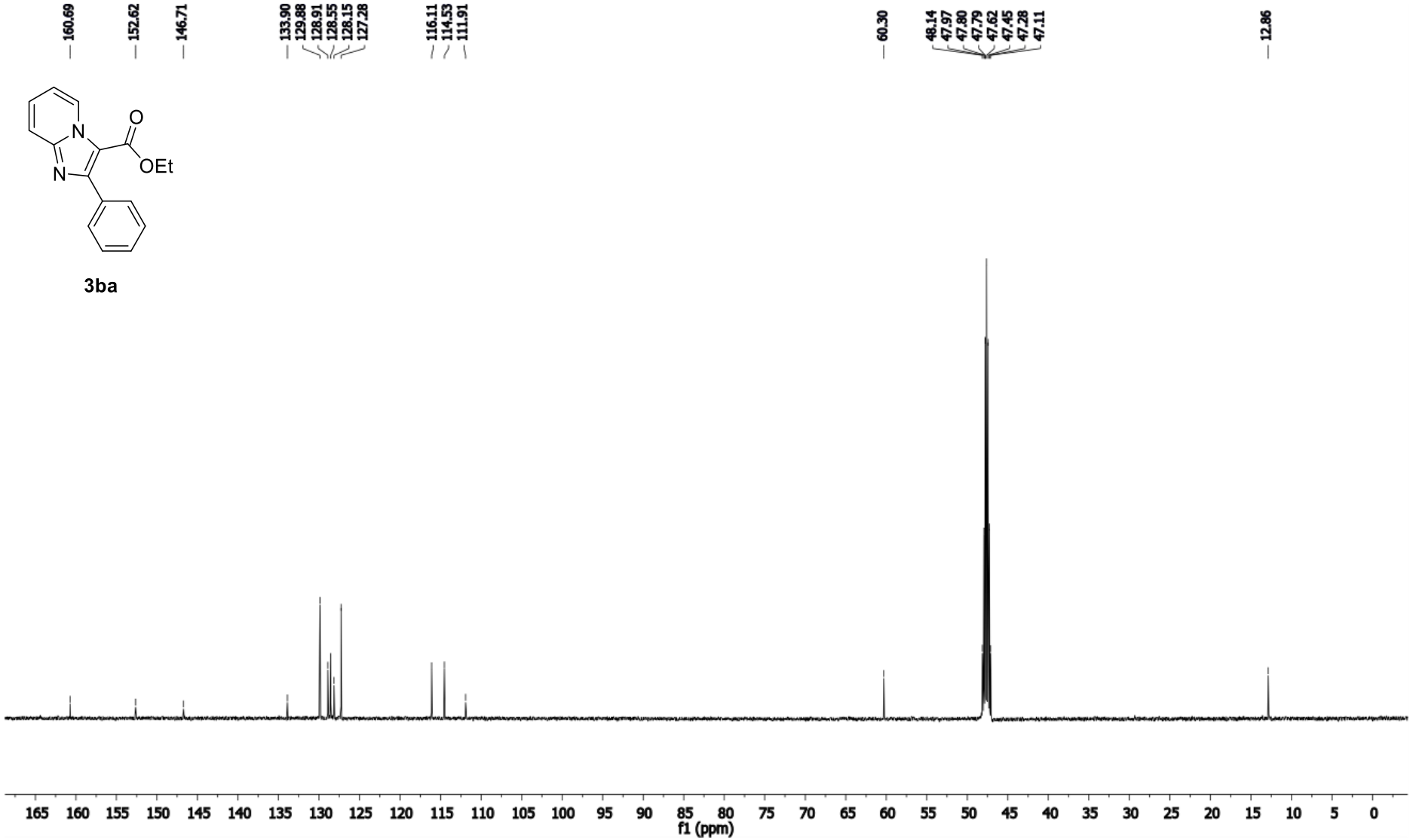
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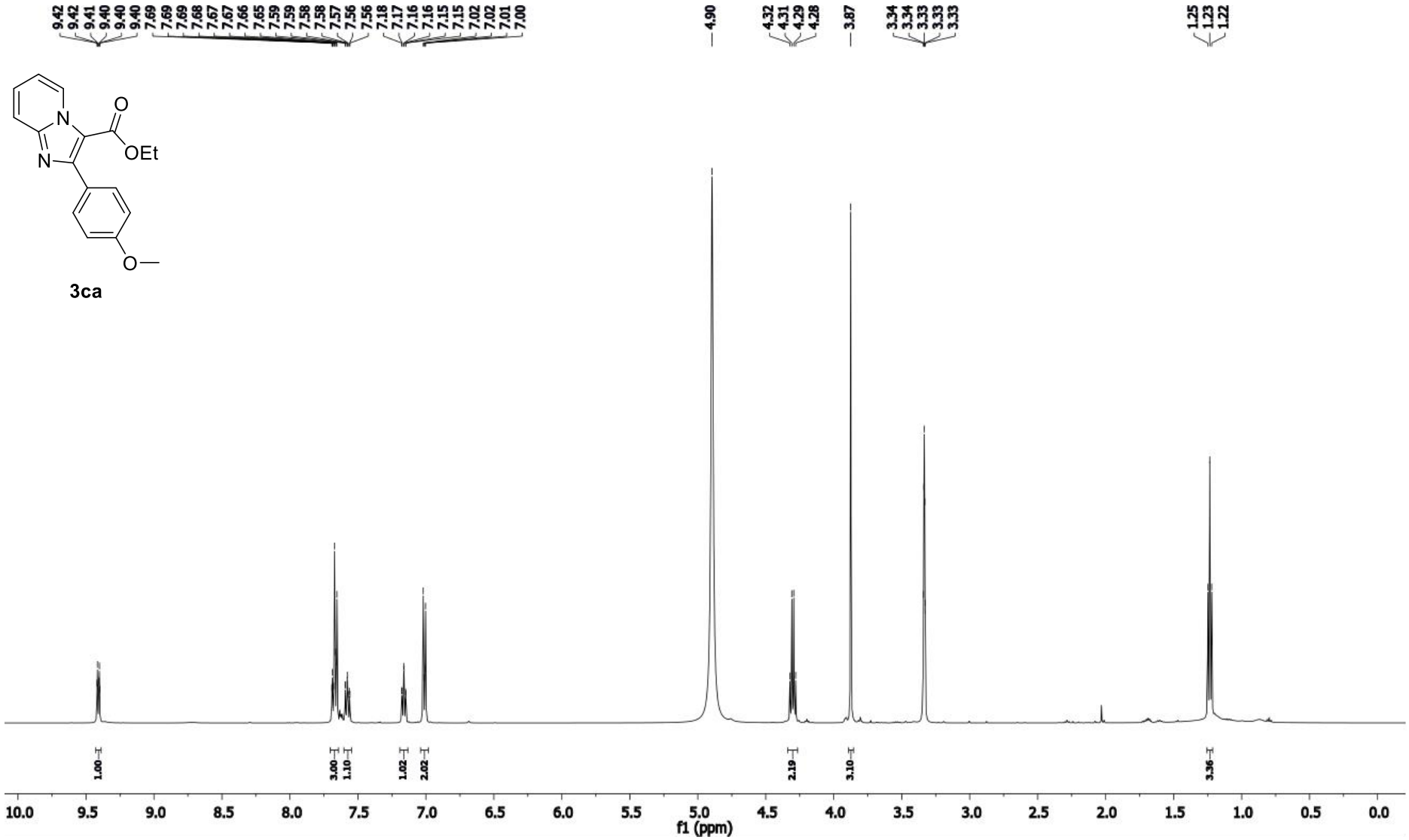
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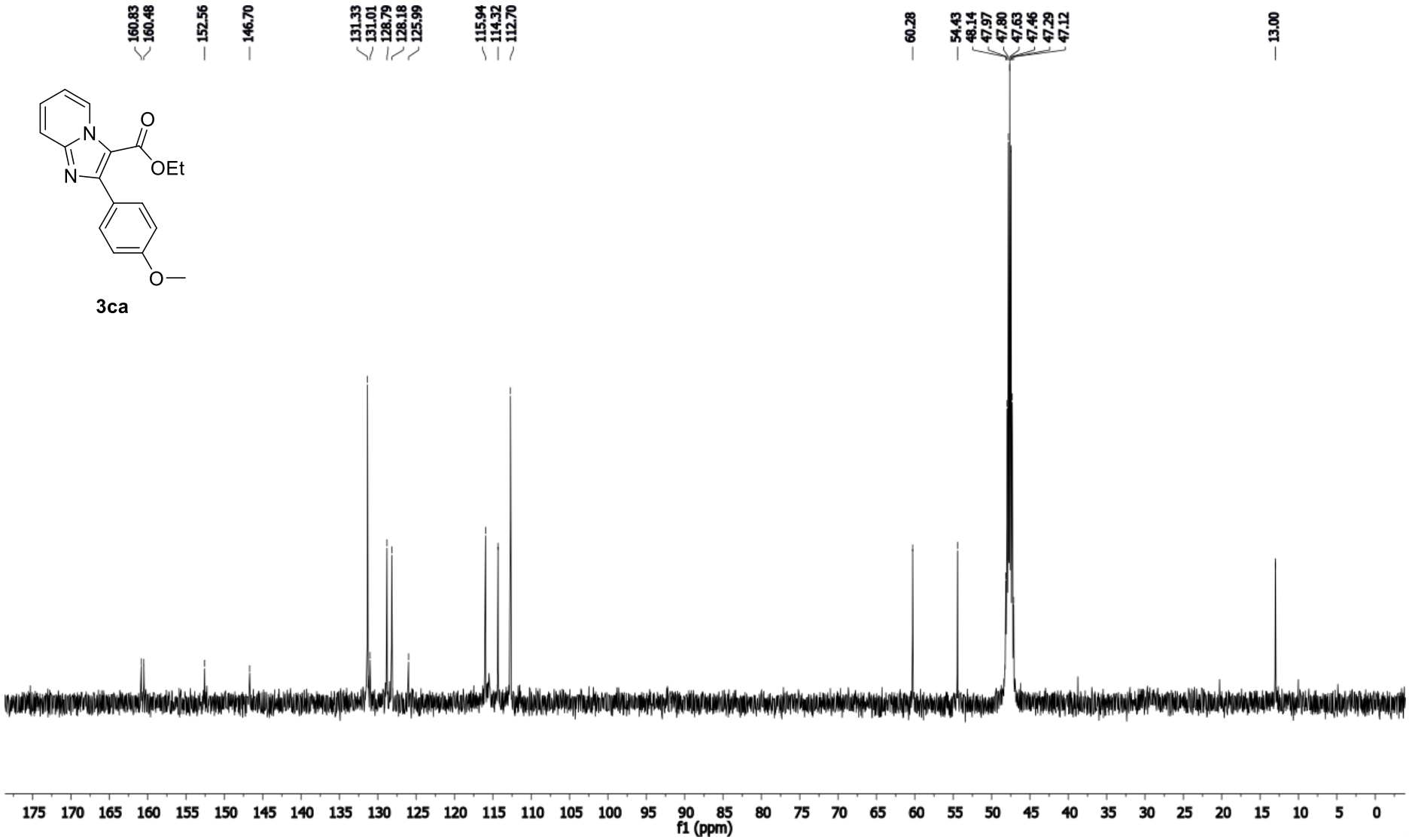
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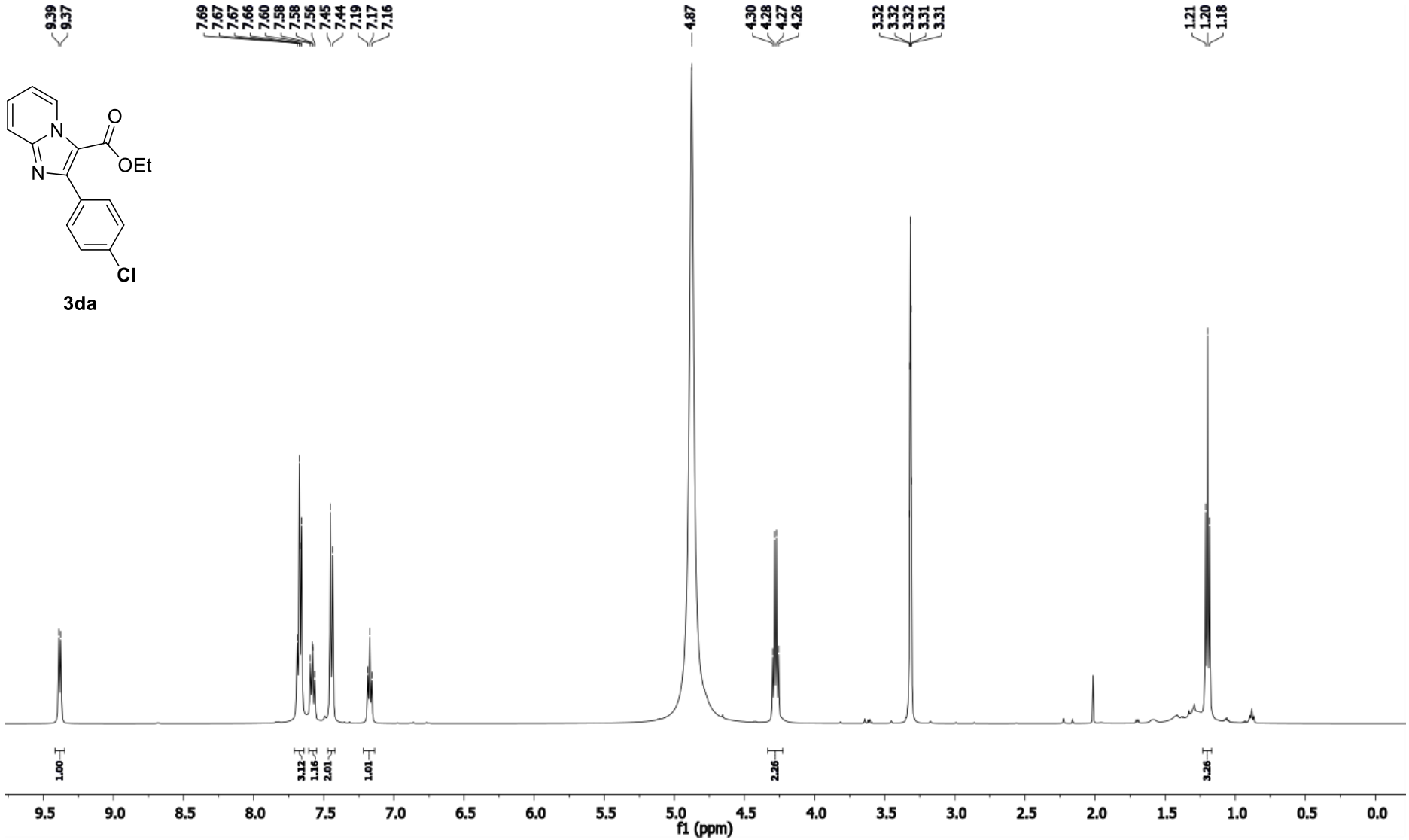
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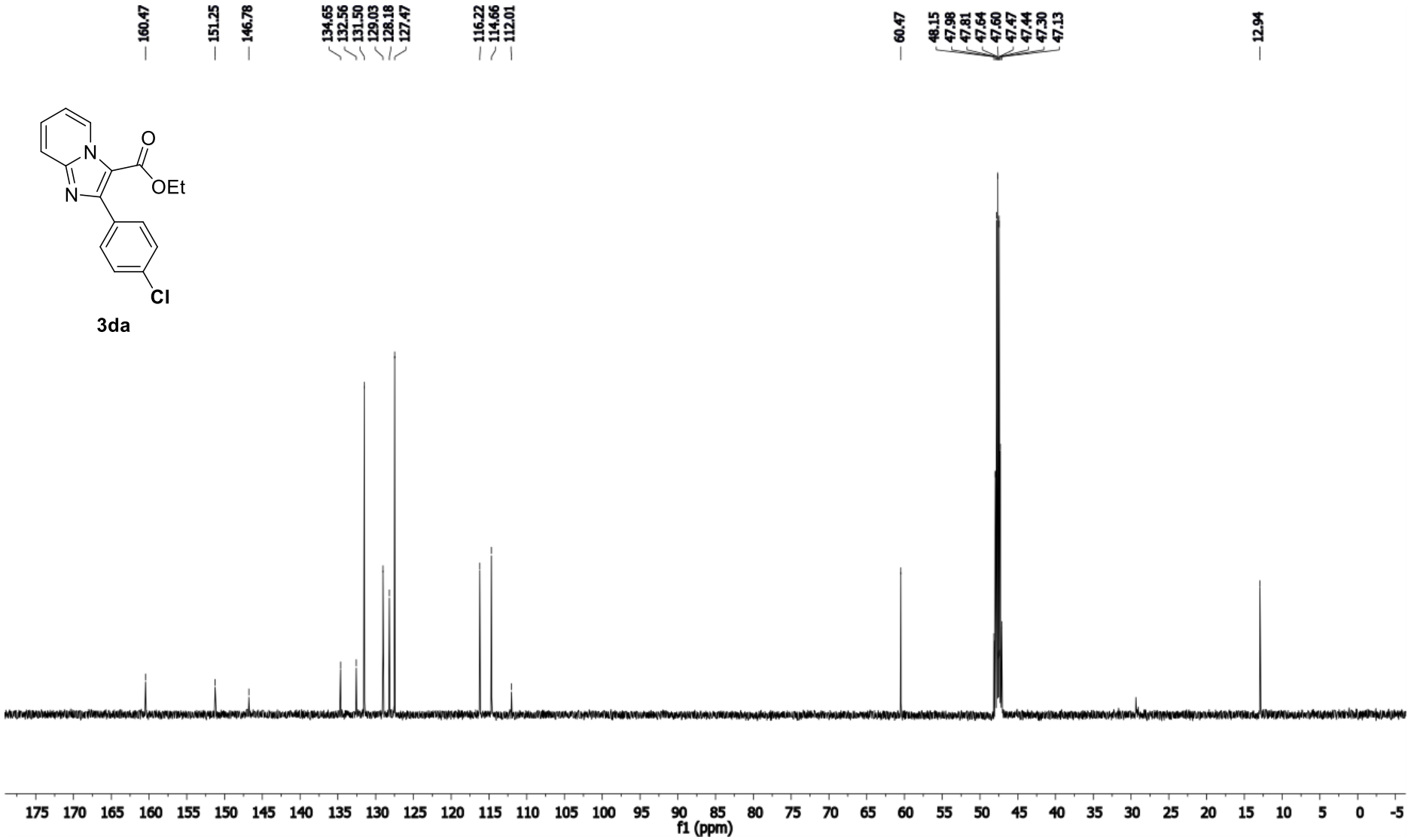
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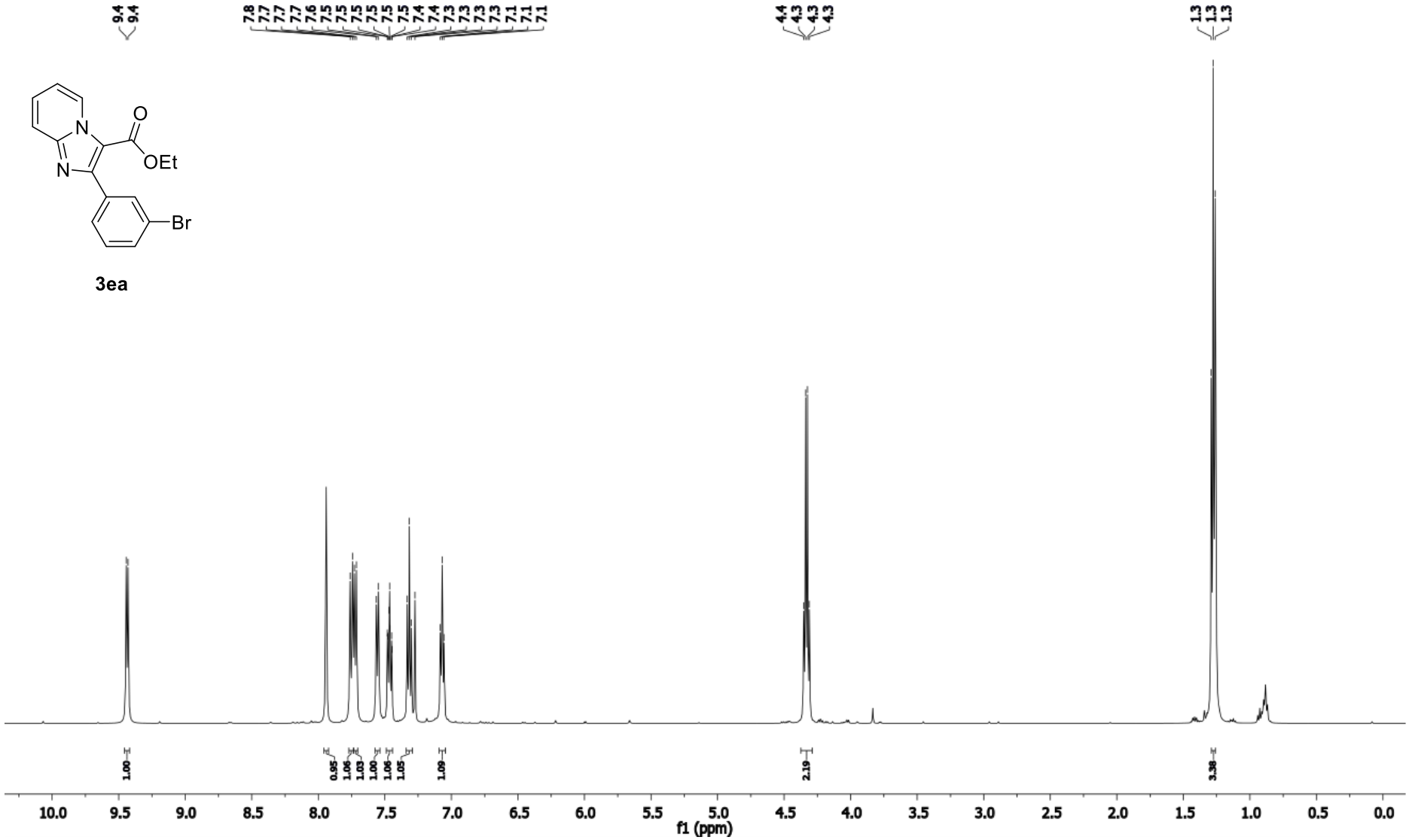
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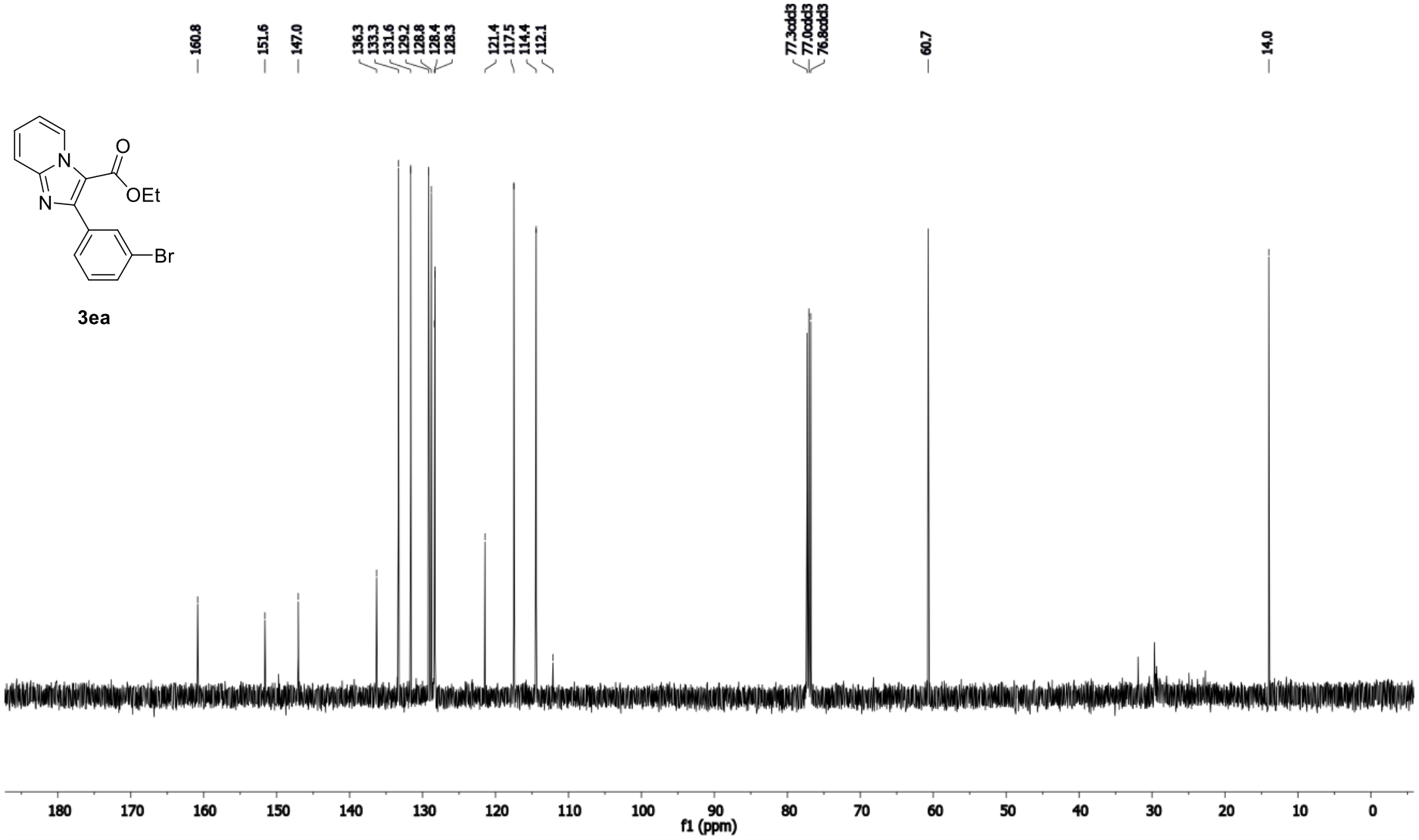
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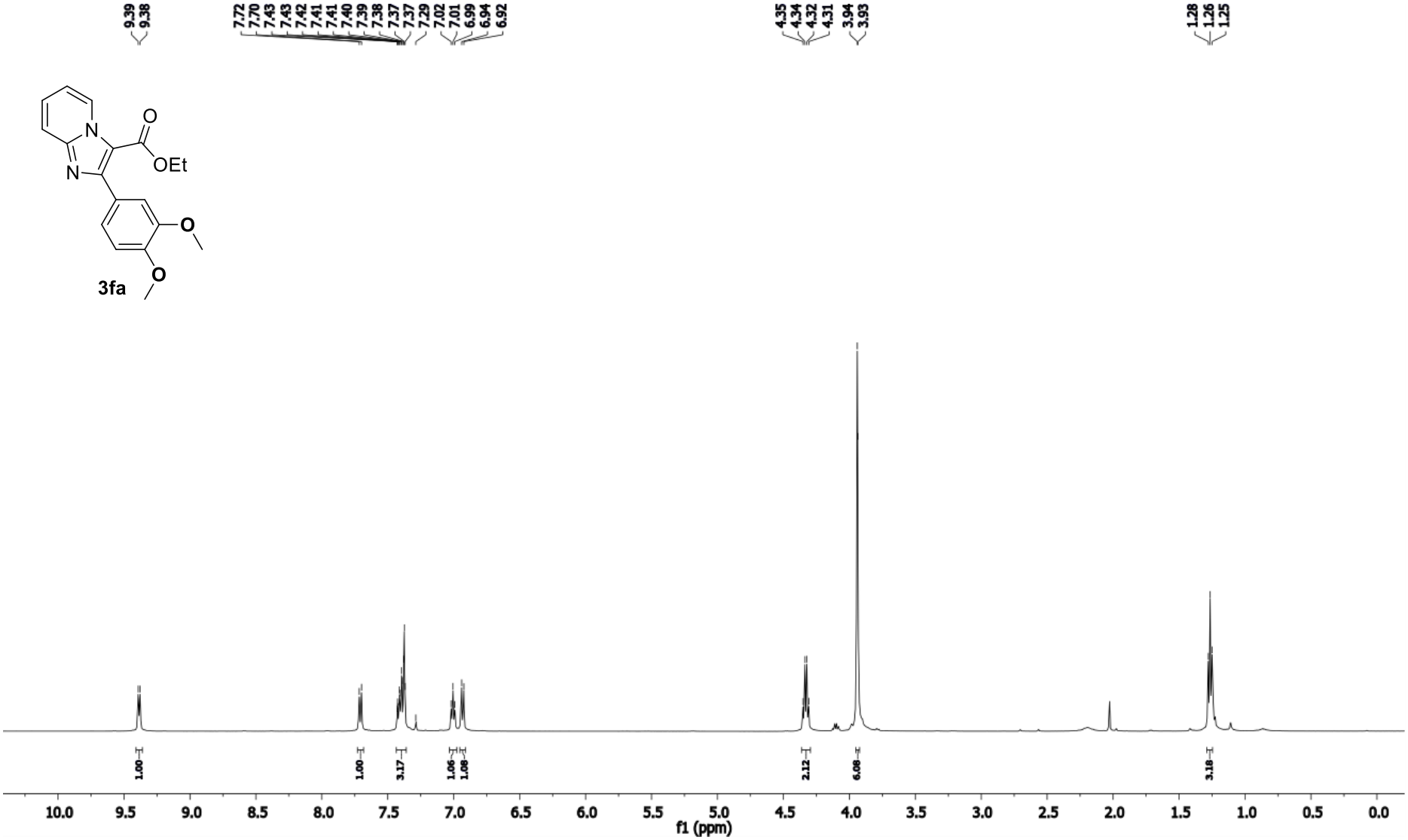
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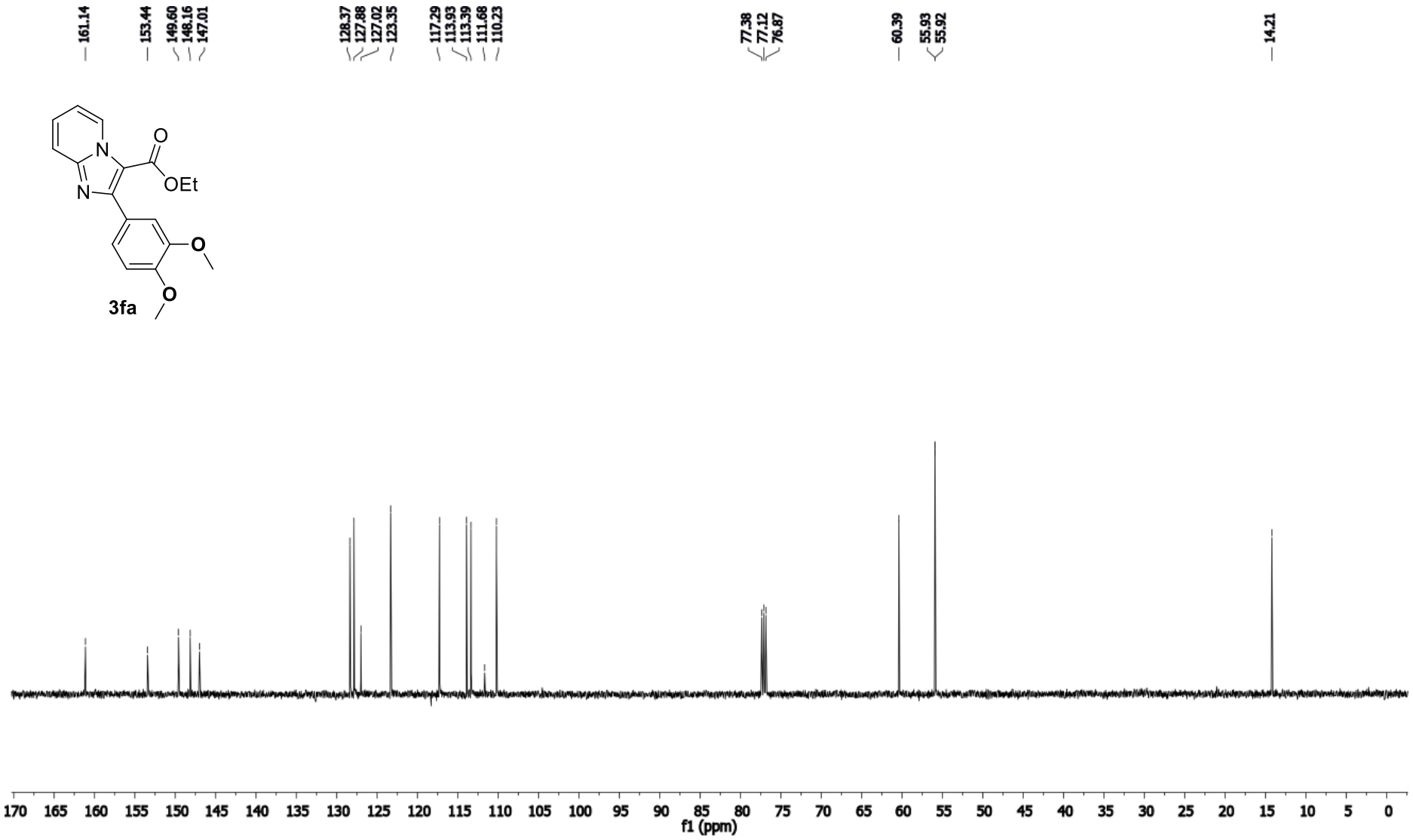
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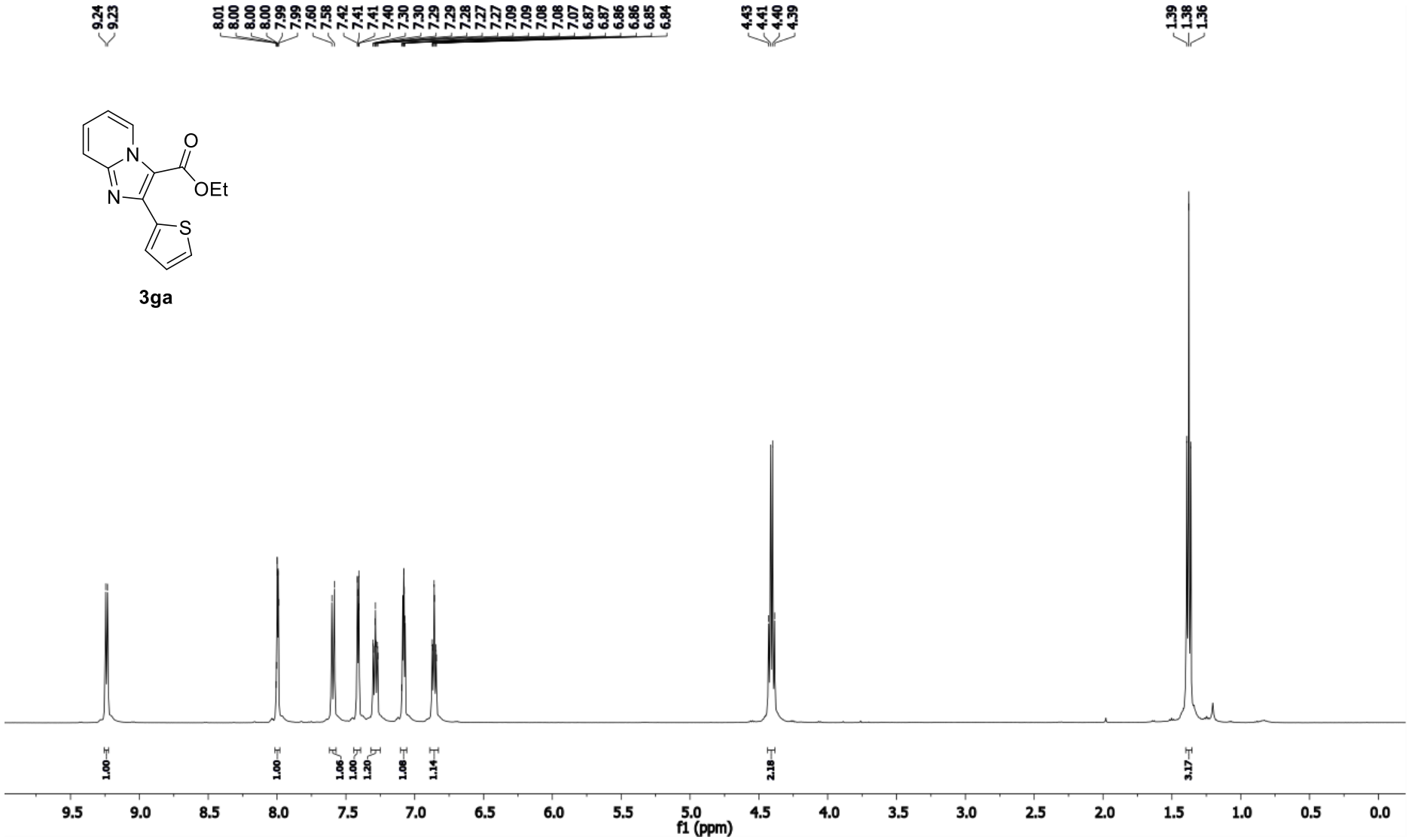
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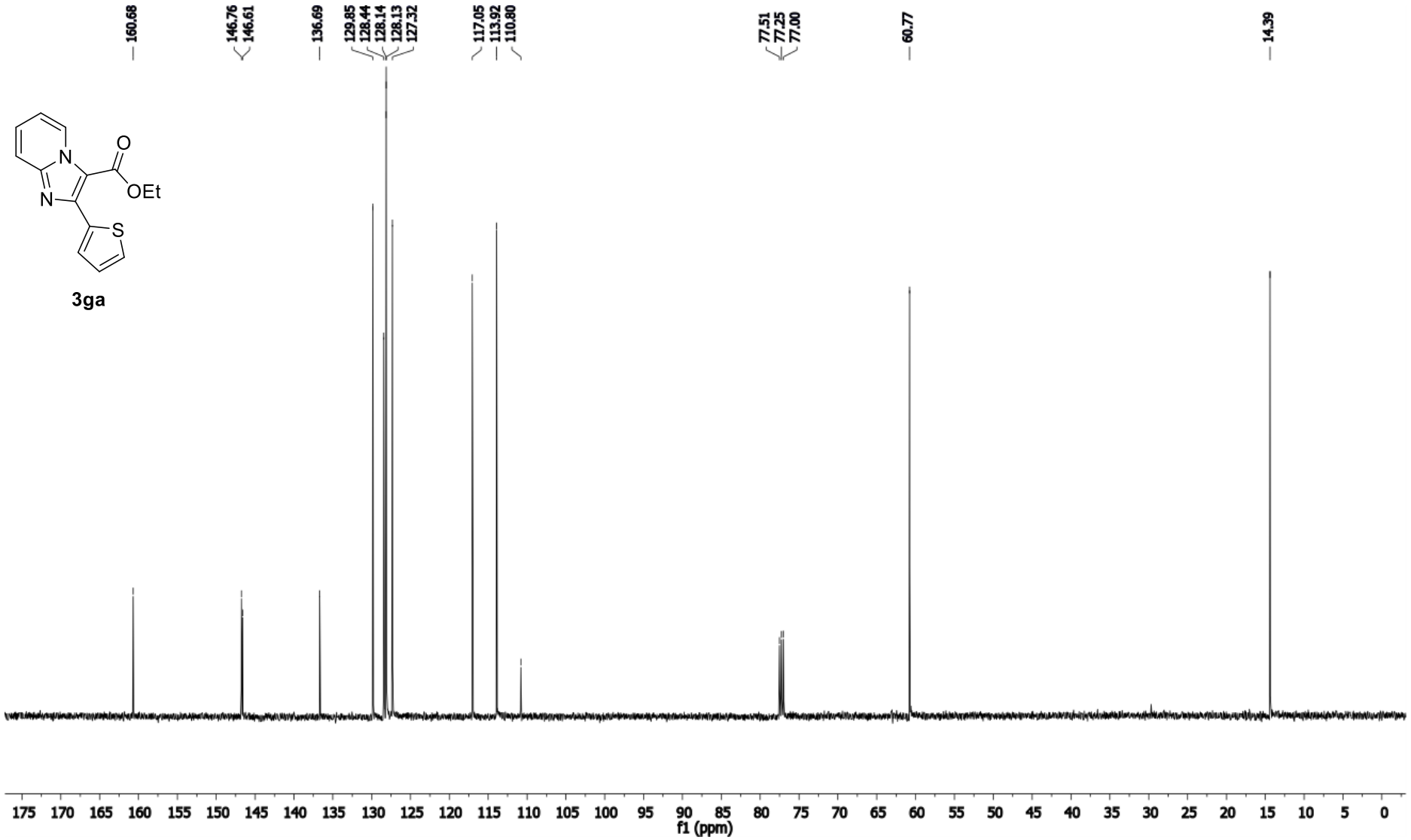
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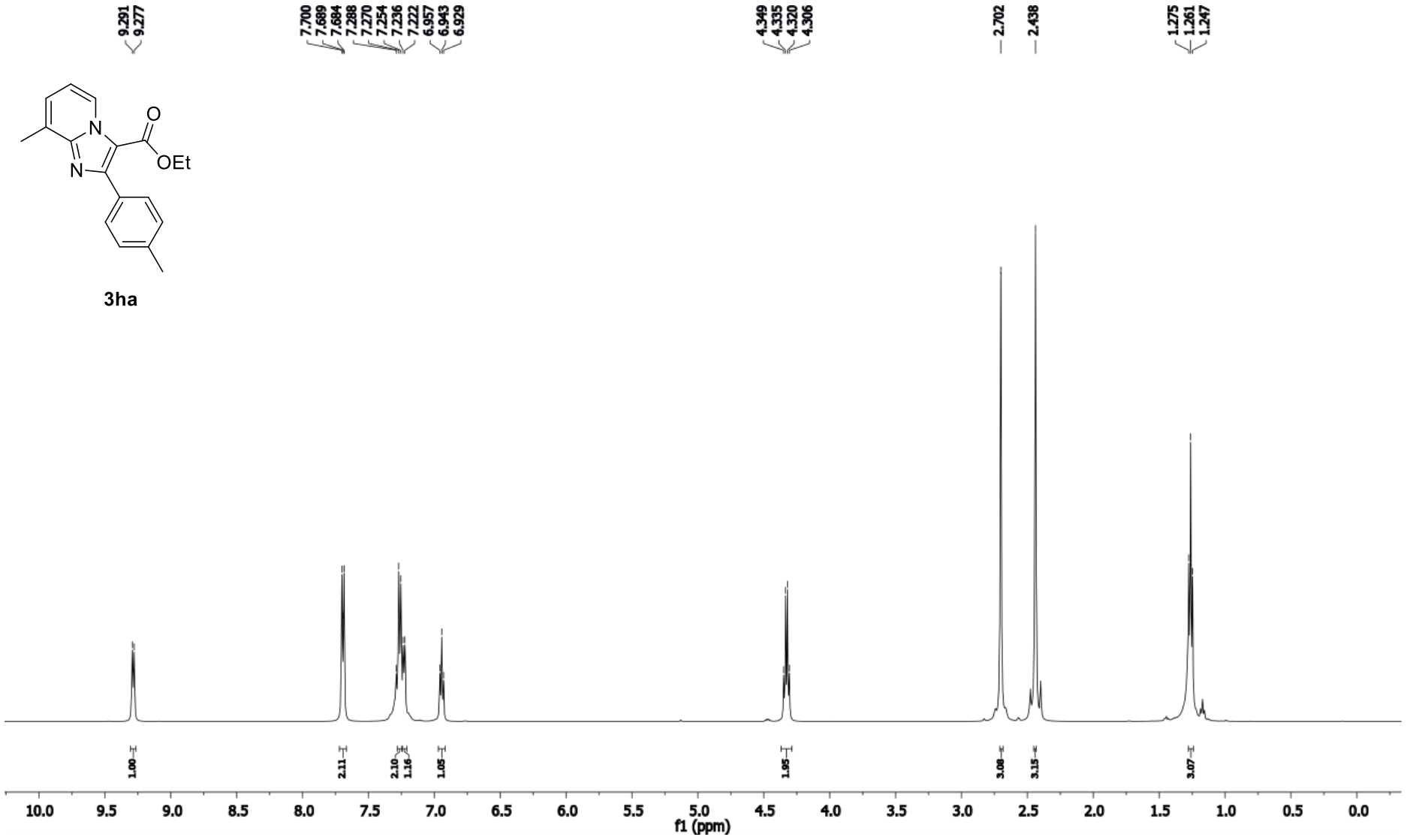
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OEt
N
N
3ha
1.00
2.11
2.10
1.16
1.05
1.95
3.08
3.15
3.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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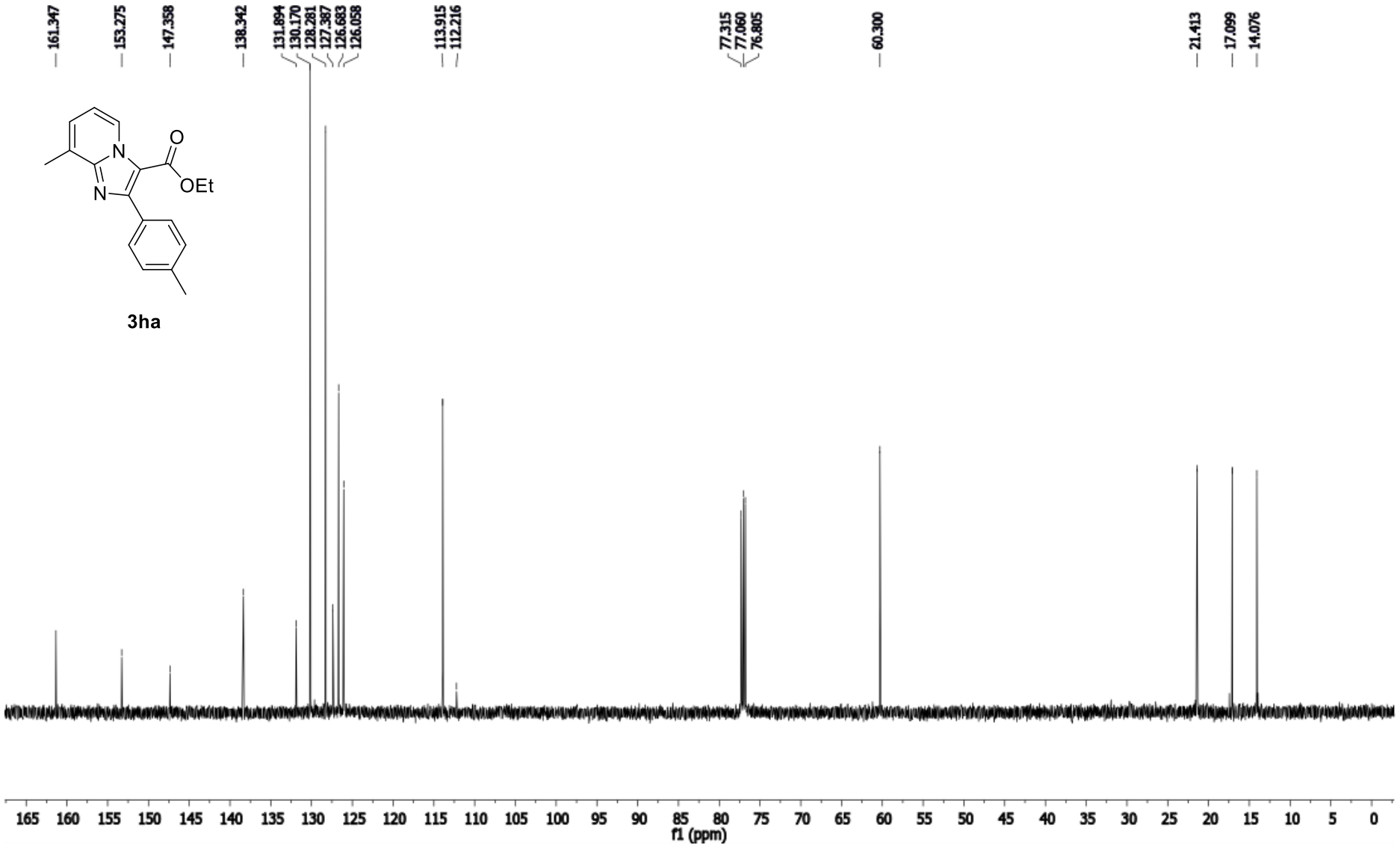
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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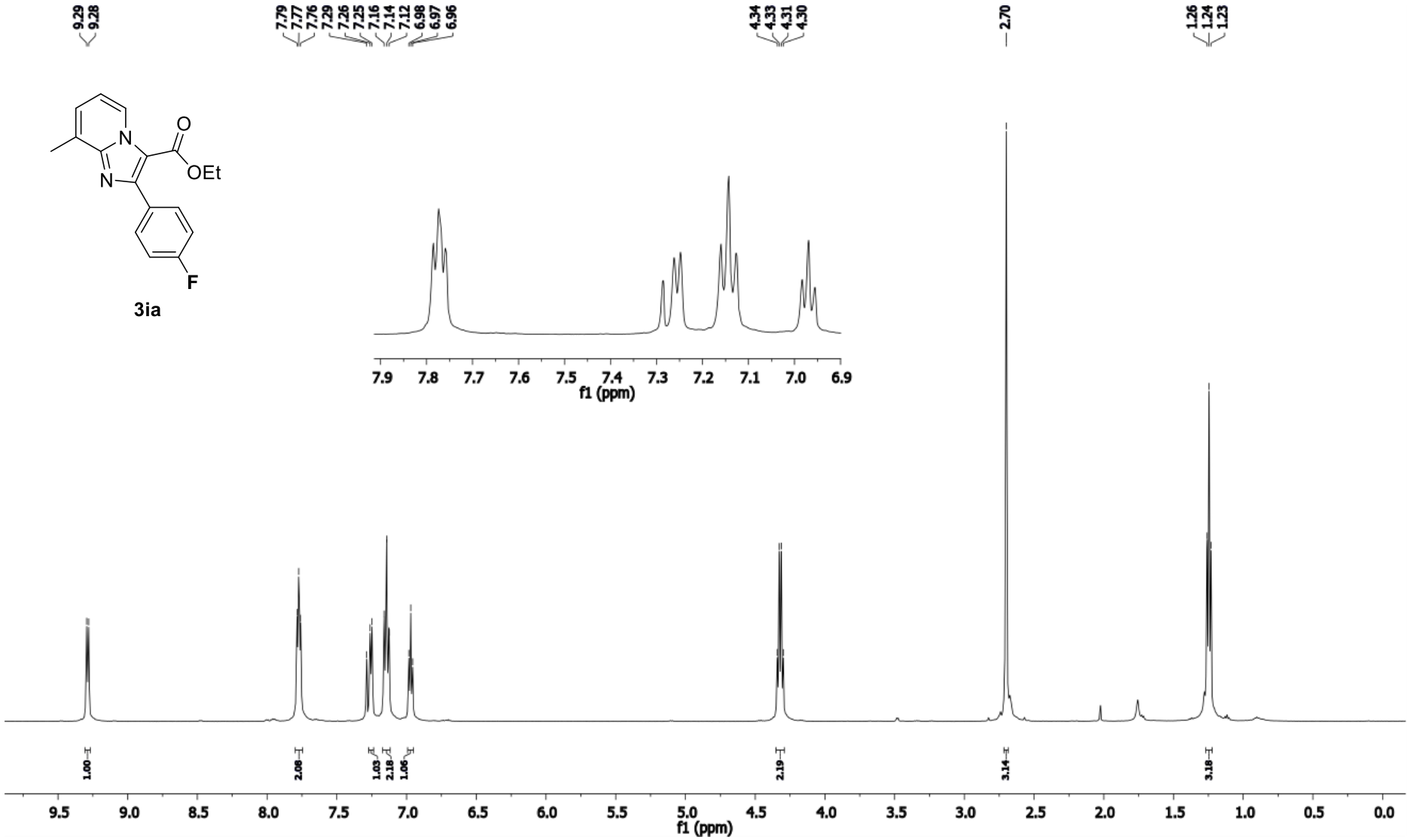
113.915
112.216
77.315
77.060
76.805
60.300
21.413
17.099
14.076
O
OEt
N
N
3ha
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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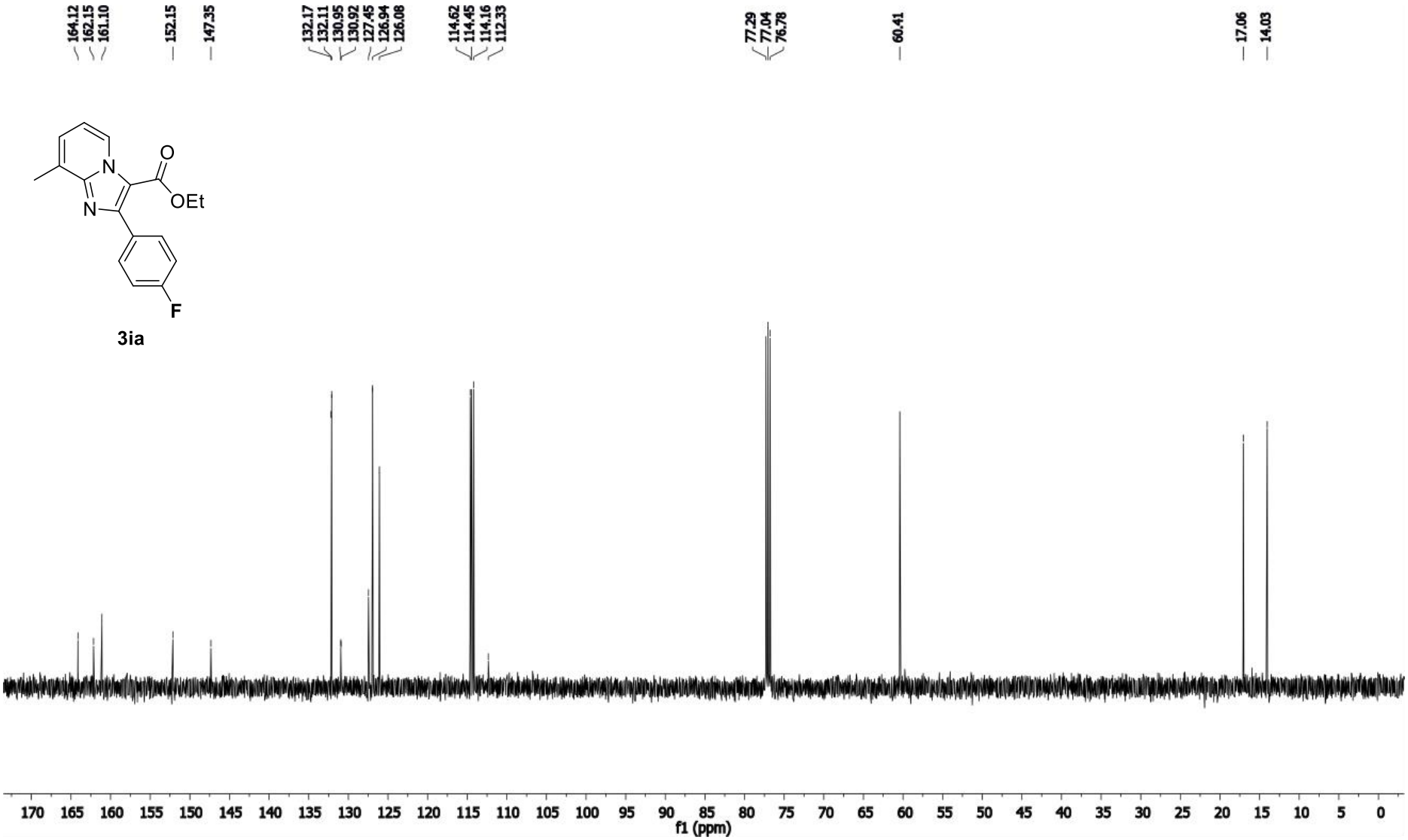
7.14
7.12
6.98
6.97
6.96
4.34
4.33
4.31
4.30
2.70
1.26
1.24
1.23
O
OEt
N
N
F
3ia
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9
f1 (ppm)
1.00
2.08
1.03
2.18
1.06
2.19
3.14
3.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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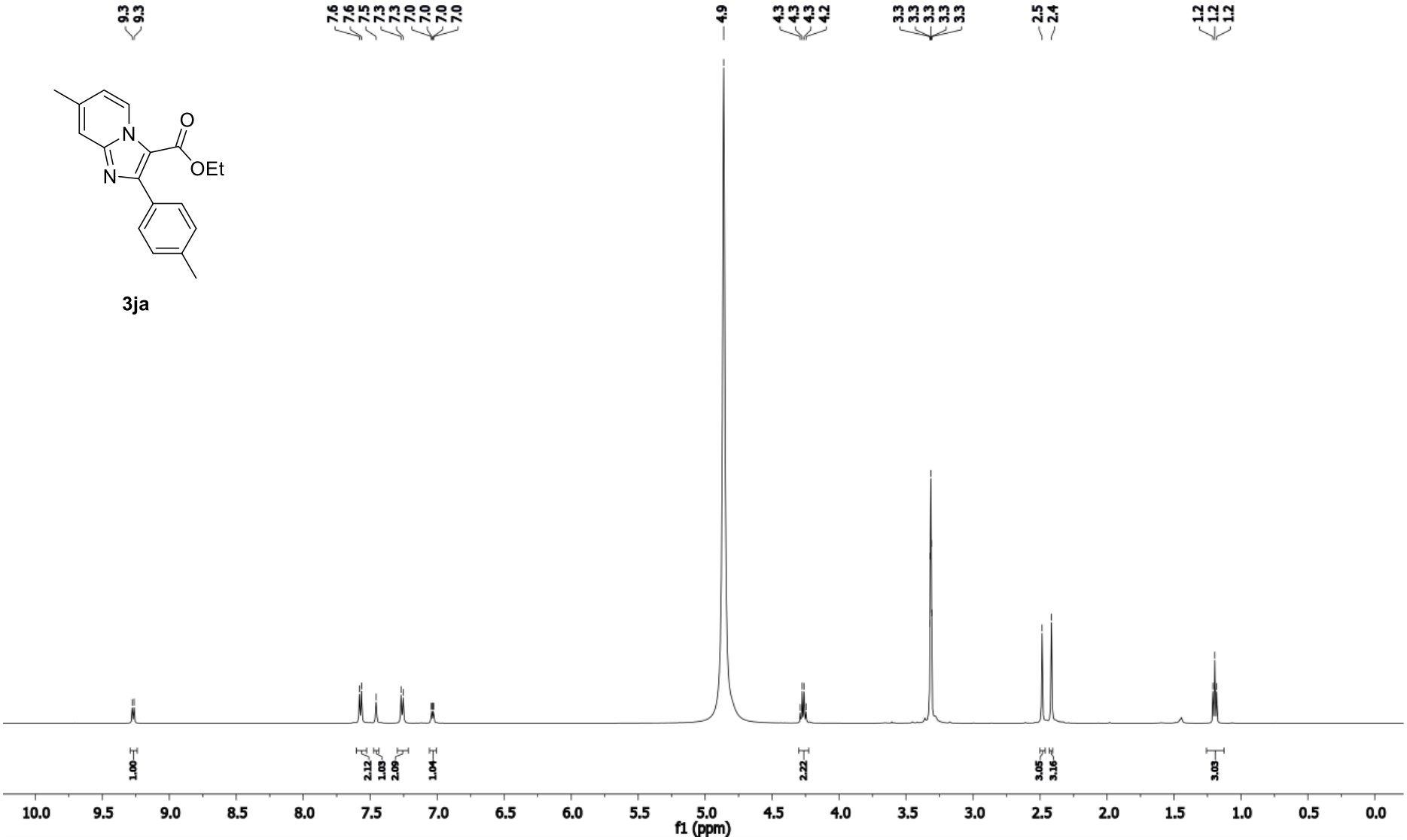
132.11
130.95
130.92
127.45
126.94
126.08
114.62
114.45
114.16
112.33
77.29
77.04
76.78
60.41
17.06
14.03
O
OEt
N
N
F
3ia
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.0
7.0
4.9
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4.3
4.3
4.2
3.3
3.3
3.3
3.3
3.3
2.5
2.4
1.2
1.2
1.2
O
OEt
N
N
1.00
2.12
1.03
2.09
1.04
2.22
3.05
3.16
3.03
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
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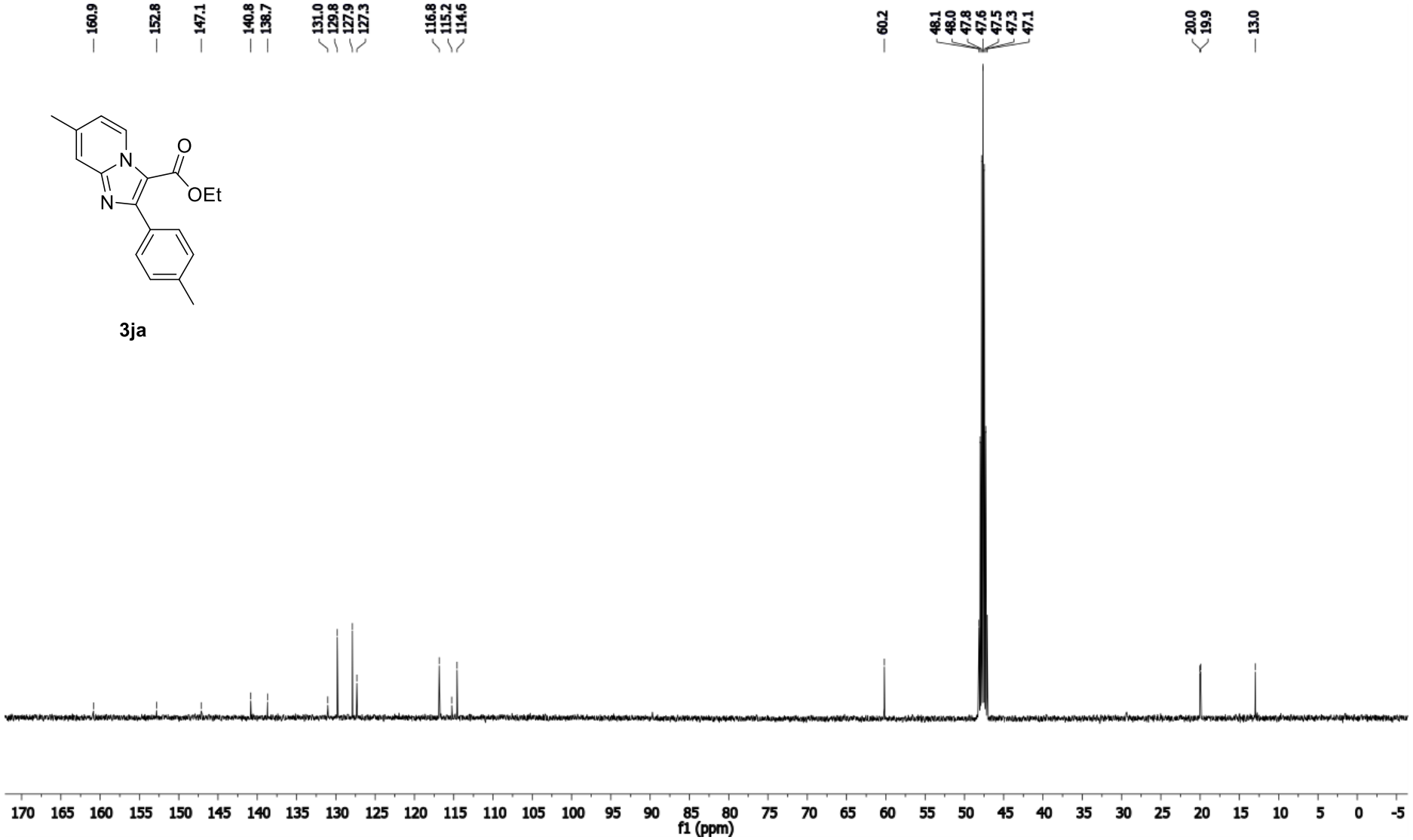
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ja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152.8
147.1
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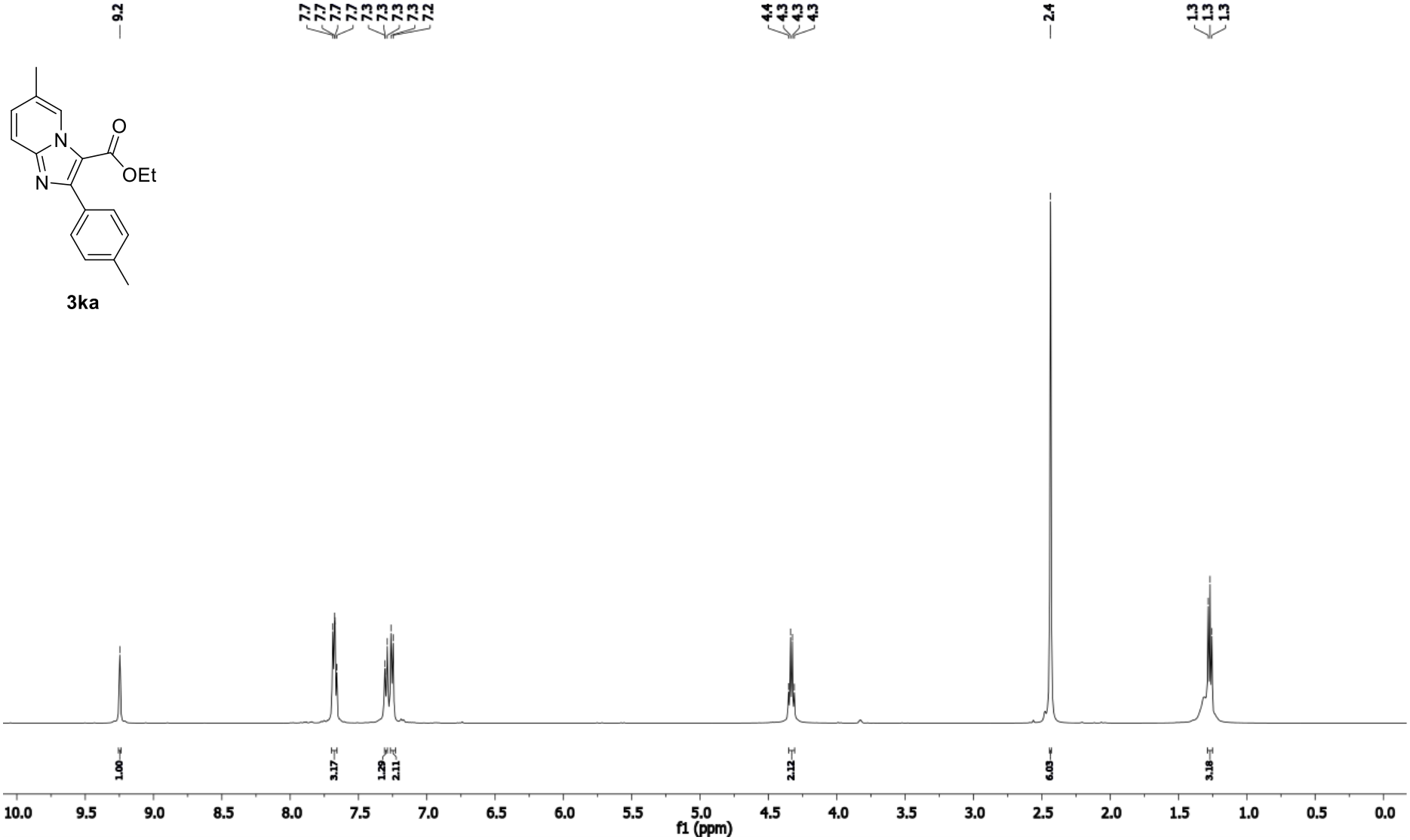
129.8
127.9
127.3
116.8
115.2
114.6
60.2
48.1
48.0
47.8
47.6
47.5
47.3
47.1
20.0
19.9
13.0
O
N
N
OEt
3ja
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5
f1 (ppm)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7.7
7.7
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7.3
7.3
7.3
7.3
7.2
4.4
4.3
4.3
4.3
2.4
1.3
1.3
1.3
O
N
N
OEt
3ka
1.00
3.17
1.29
2.11
2.12
6.03
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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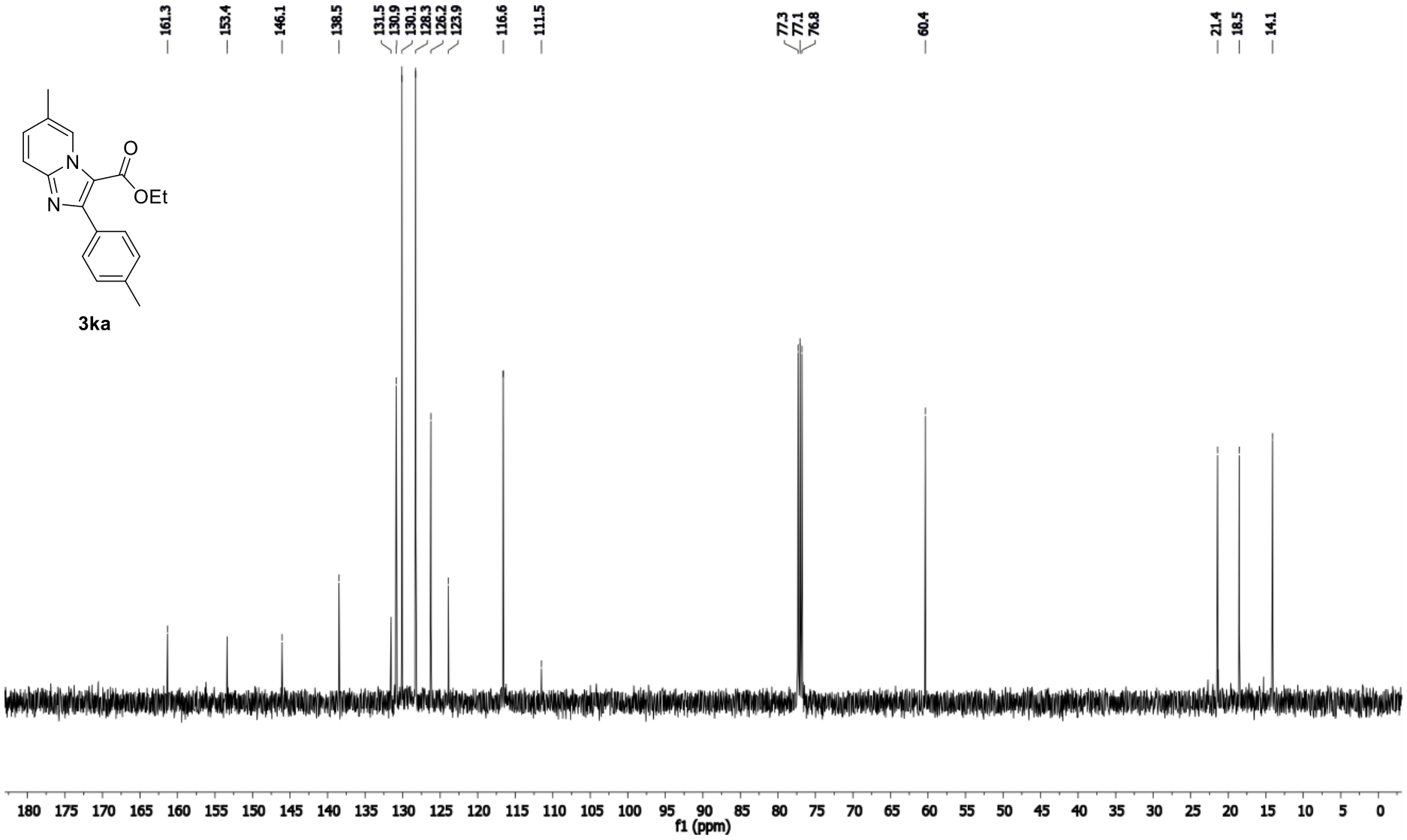
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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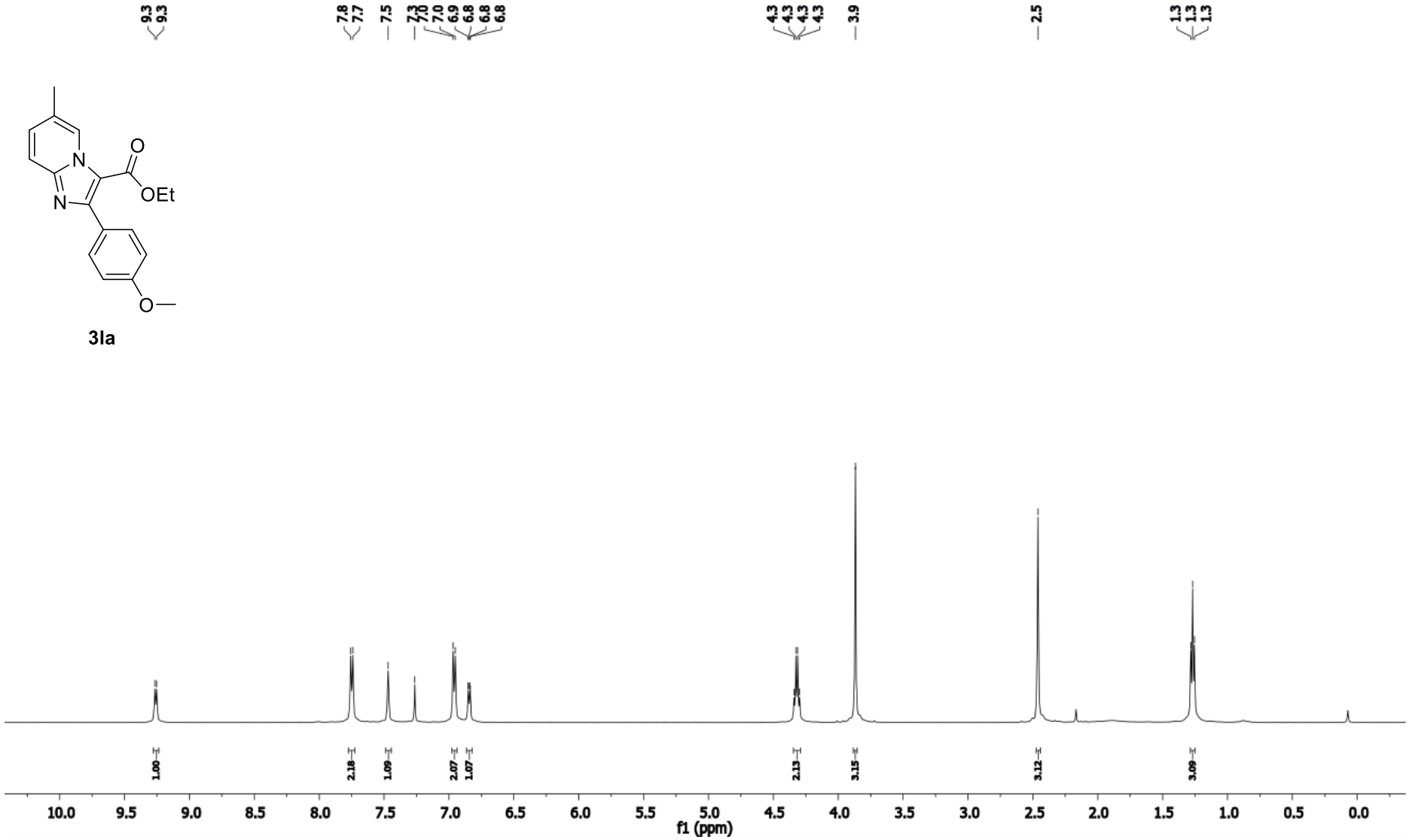
153.4
146.1
138.5
131.5
130.9
130.1
128.3
126.2
123.9
116.6
111.5
77.3
77.1
76.8
60.4
21.4
18.5
14.1
O
OEt
N
N
3ka
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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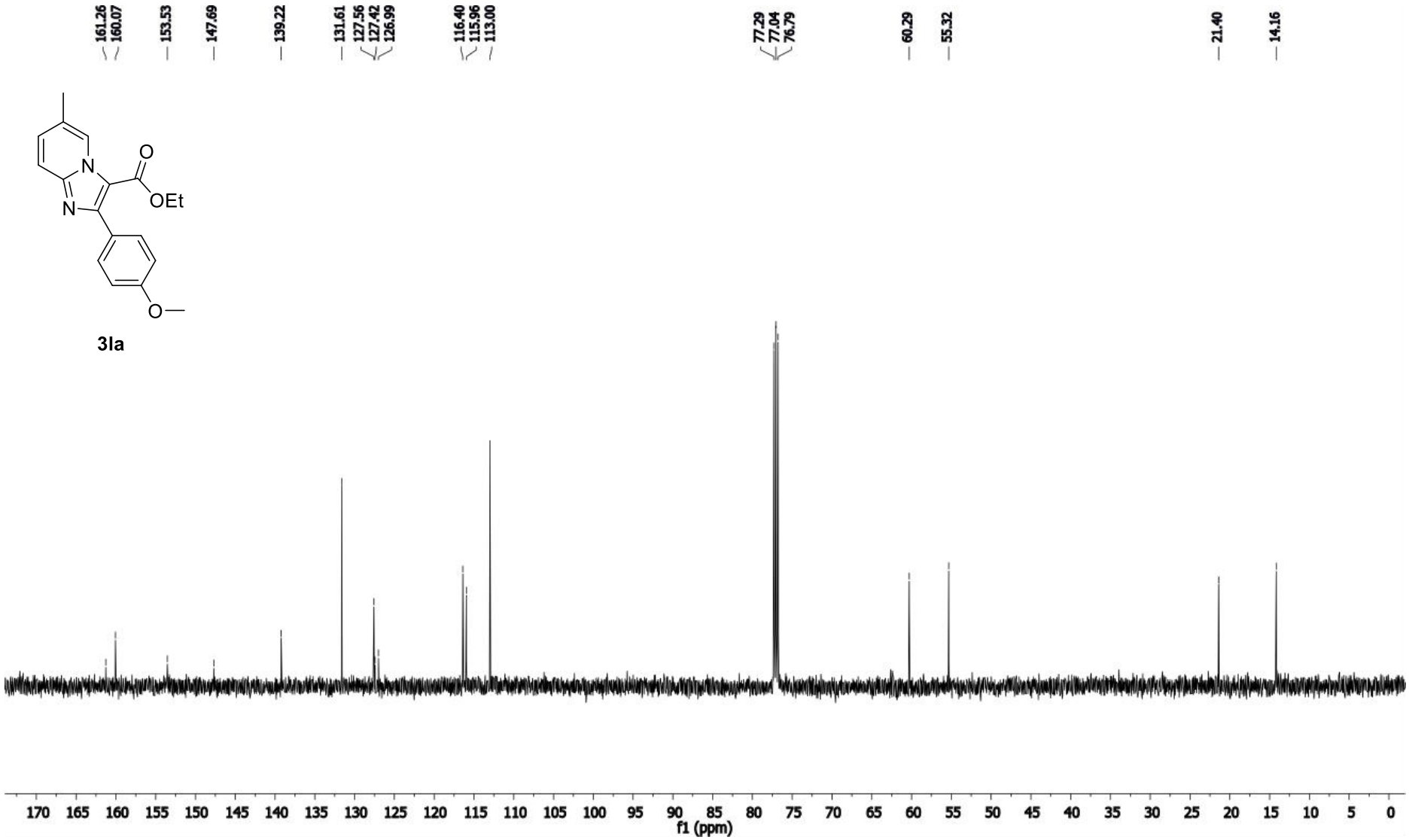
7.8
7.7
7.5
7.3
7.0
7.0
6.9
6.8
6.8
6.8
4.3
4.3
4.3
4.3
3.9
2.5
1.3
1.3
1.3
O
N
N
OEt
O
1.00
2.18
1.09
2.07
1.07
2.13
3.15
3.12
3.09
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3la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160.07
153.53
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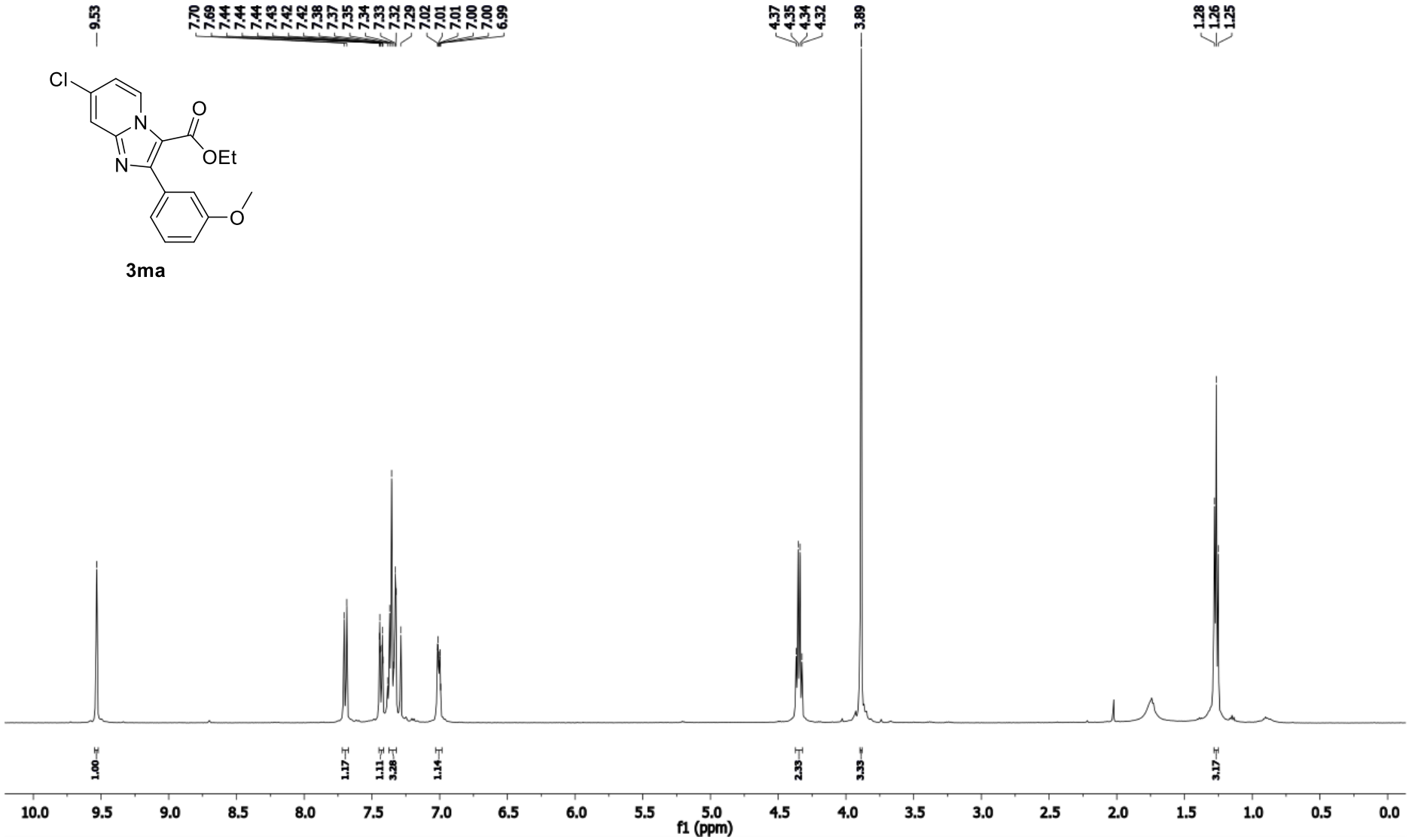
139.22
131.61
127.56
127.42
126.99
116.40
115.96
113.00
77.29
77.04
76.79
60.29
55.32
21.40
14.16
O
N
N
OEt
O
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

3la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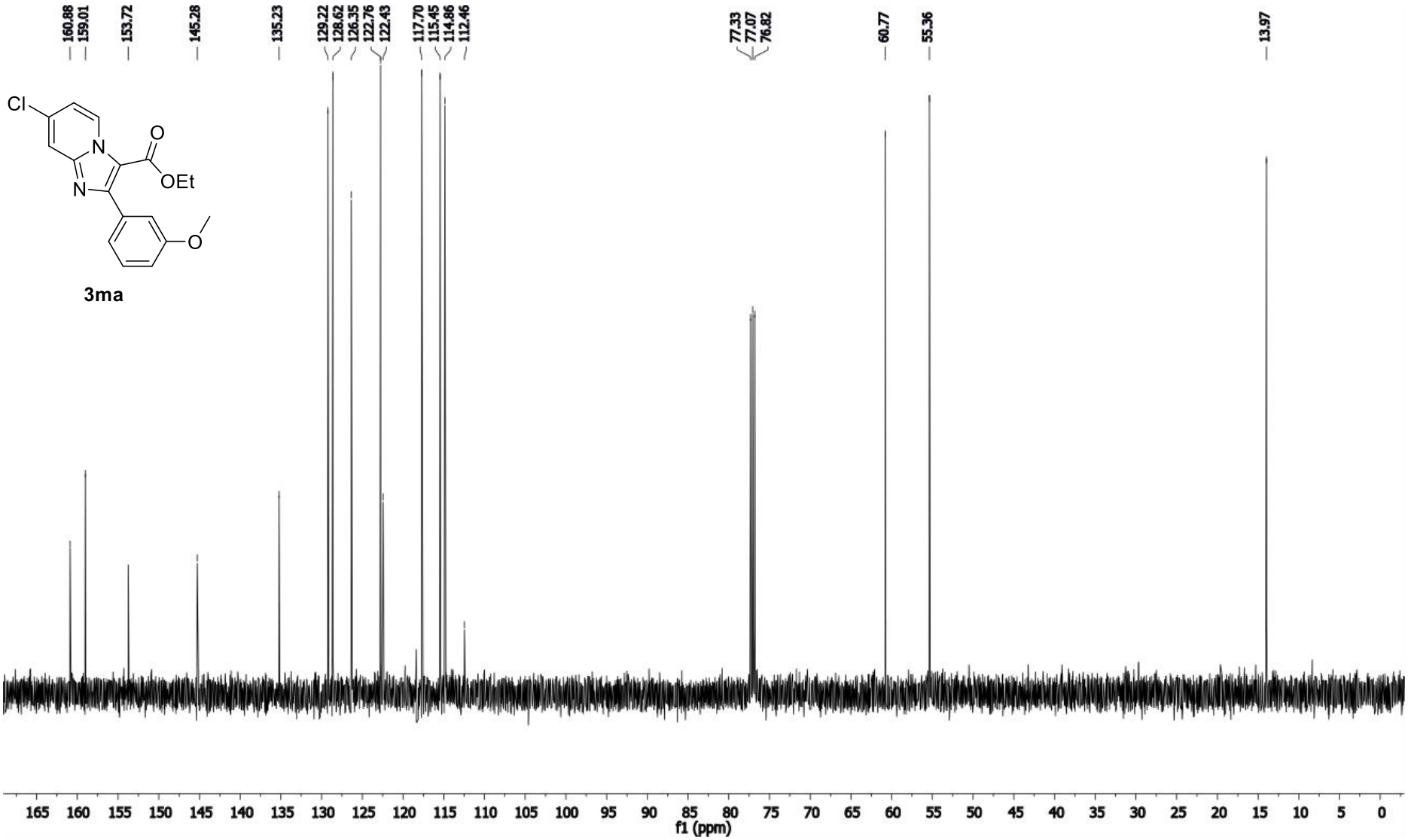
7.44
7.43
7.42
7.42
7.38
7.37
7.35
7.34
7.33
7.32
7.29
7.02
7.01
7.01
7.00
7.00
6.99
4.37
4.35
4.34
4.32
3.89
1.28
1.26
1.25
Cl
N
N
O
OEt
O
3ma
1.00
1.17
1.11
3.28
1.14
2.33
3.33
3.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.22
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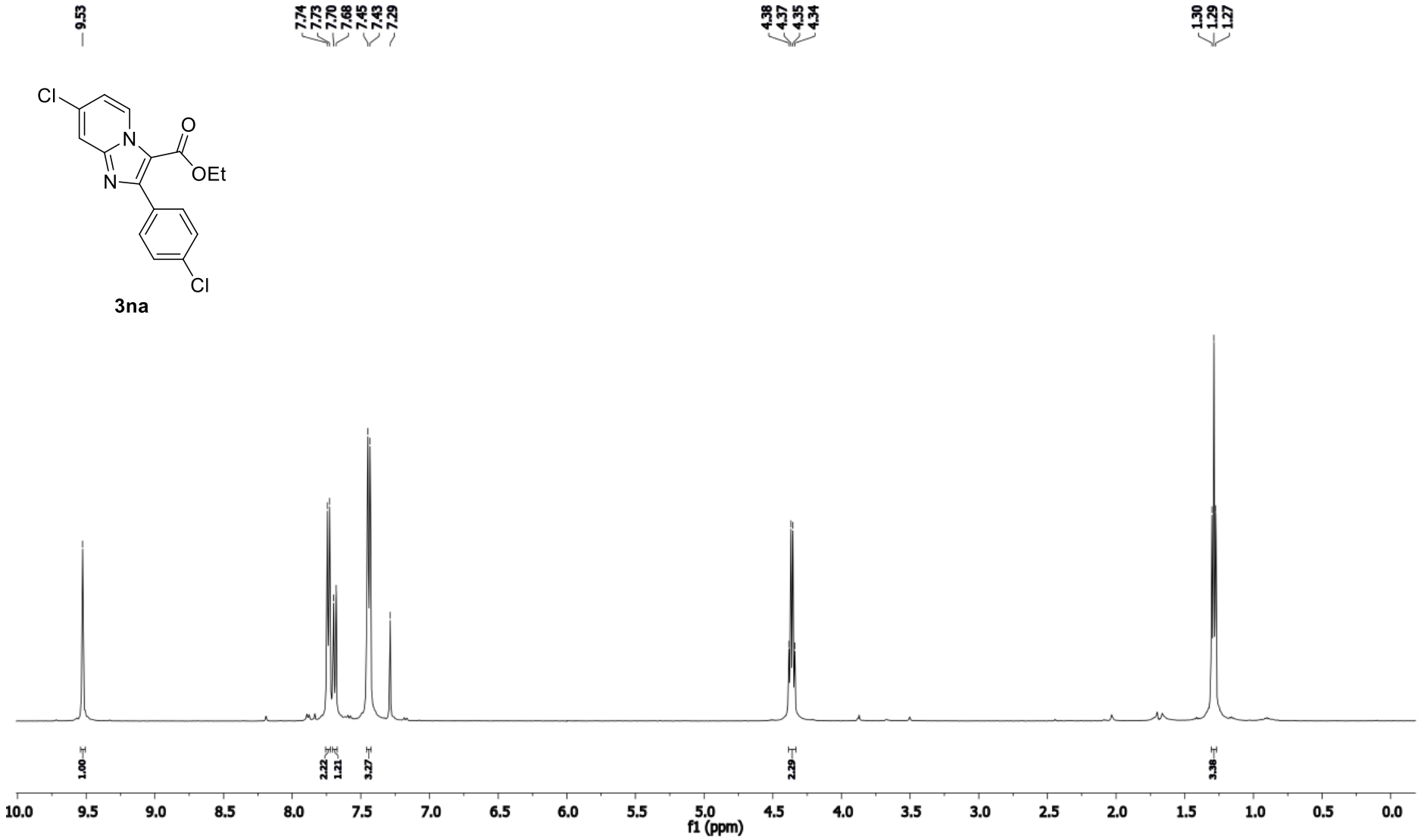
126.35
122.76
122.43
117.70
115.45
114.86
112.46
77.33
77.07
76.82
60.77
55.36
13.97
Cl
N
N
O
OEt
O
3ma
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.70
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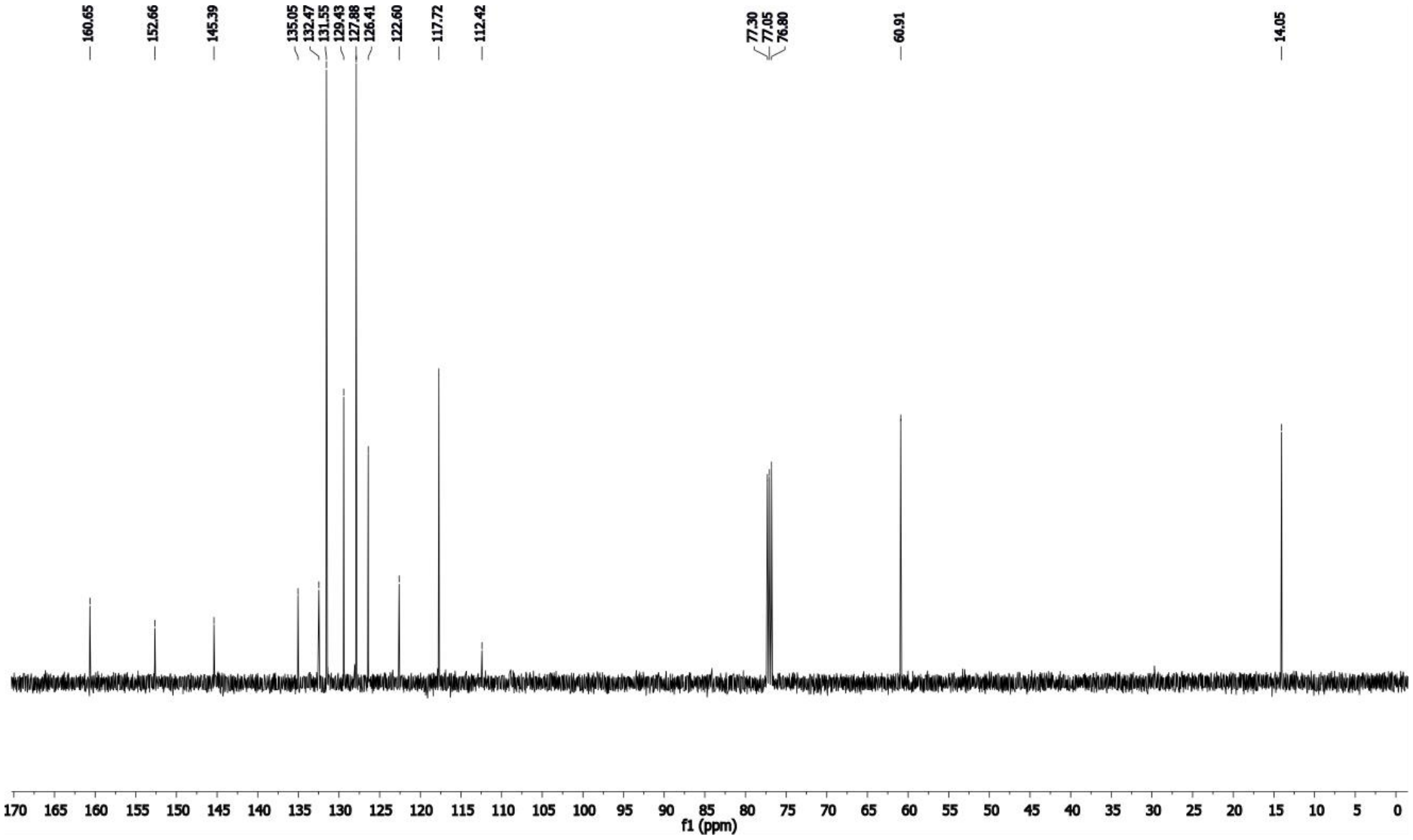
7.45
7.43
7.29
4.38
4.37
4.35
4.34
1.30
1.29
1.27
Cl
O
N
N
OEt
Cl
3na
1.00
2.22
1.21
3.27
2.29
3.38
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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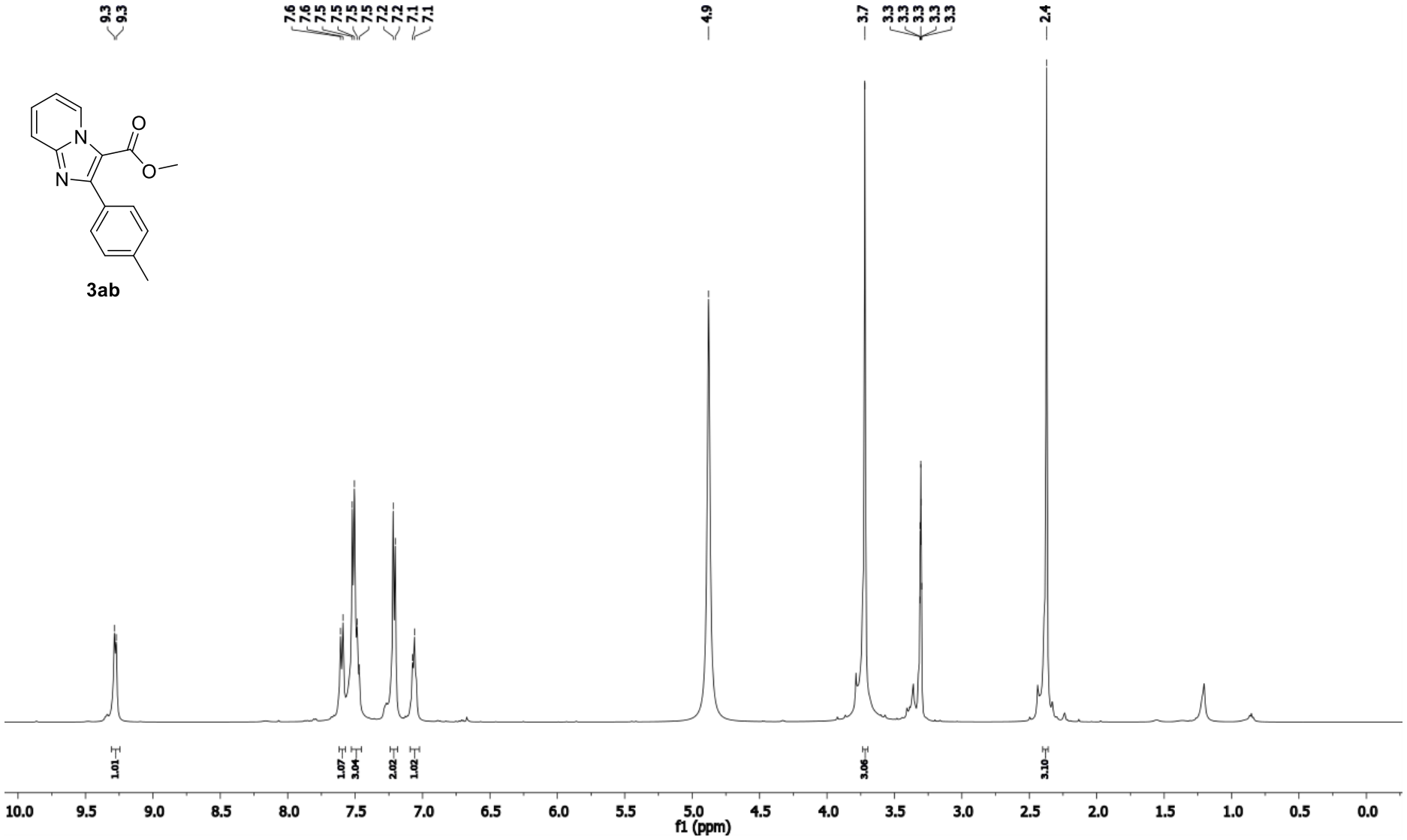
152.66
145.39
135.05
132.47
131.55
129.43
127.88
126.41
122.60
117.72
112.42
77.30
77.05
76.80
60.91
14.05
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.6
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7.5
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7.5
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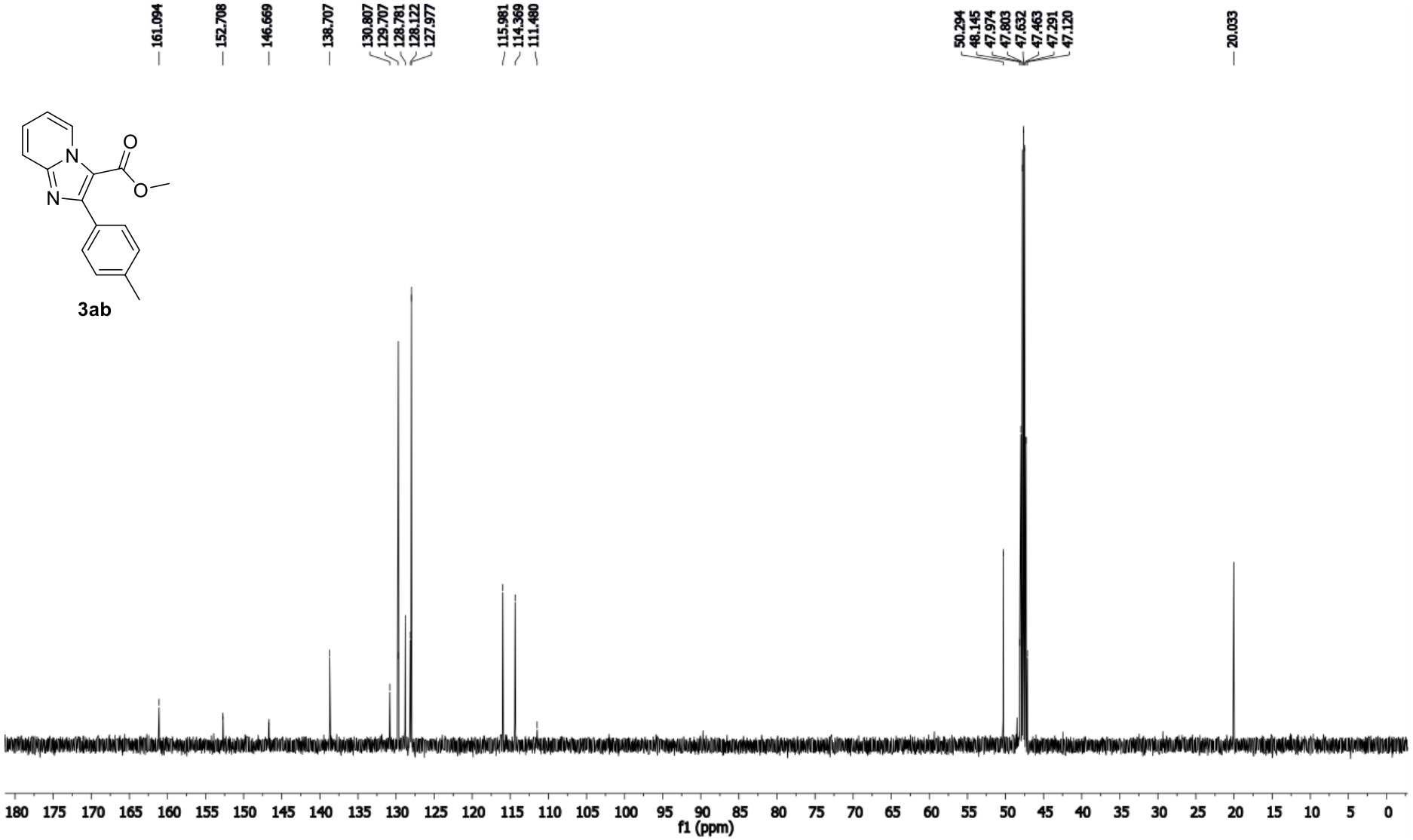
7.2
7.1
7.1
4.9
3.7
3.3
3.3
3.3
3.3
3.3
2.4
O
N
N
O
3ab
1.01
1.07
3.04
2.02
1.02
3.06
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.122
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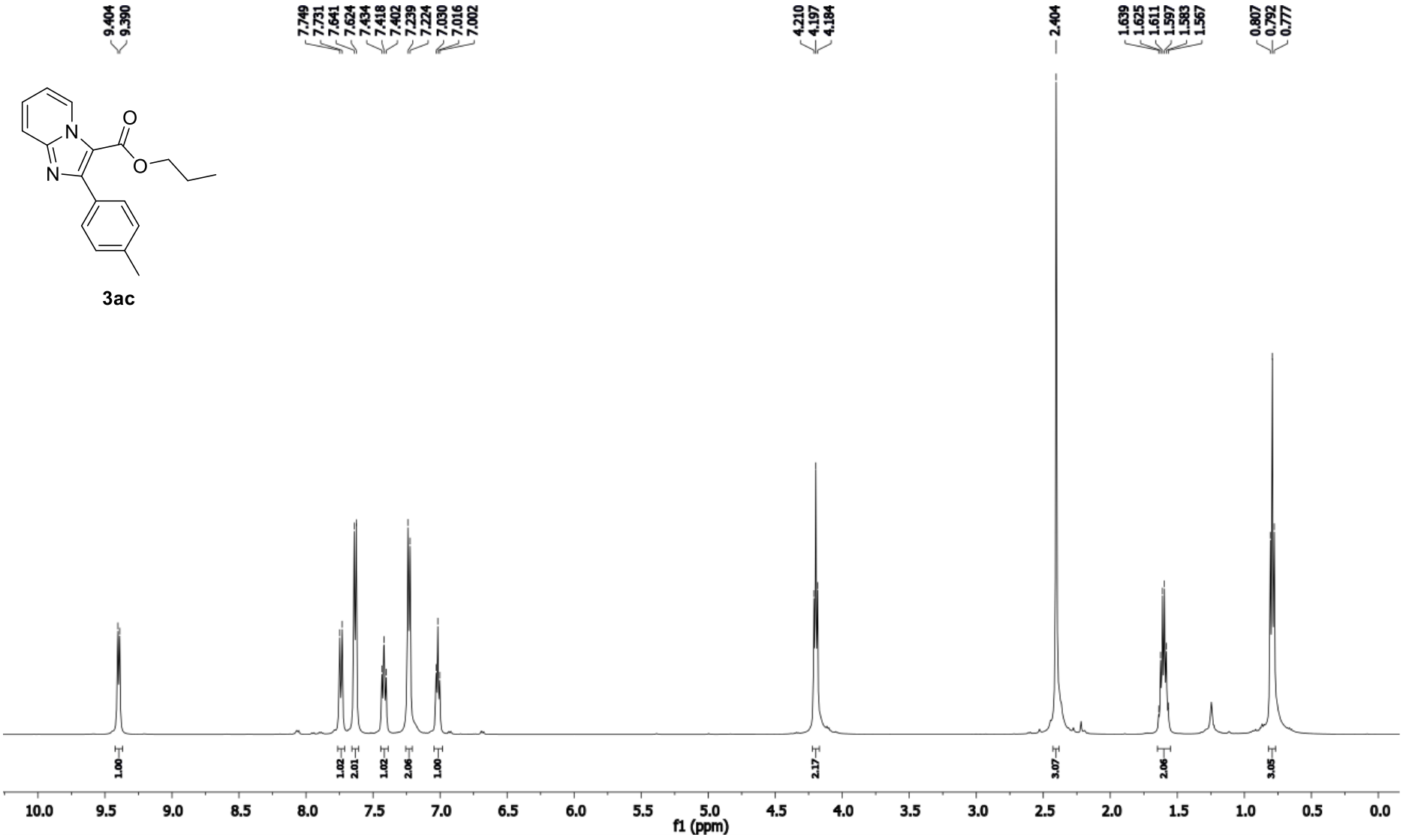
114.369
111.480
50.294
48.145
47.974
47.803
47.632
47.463
47.291
47.120
20.033
O
O
N
N
3ab
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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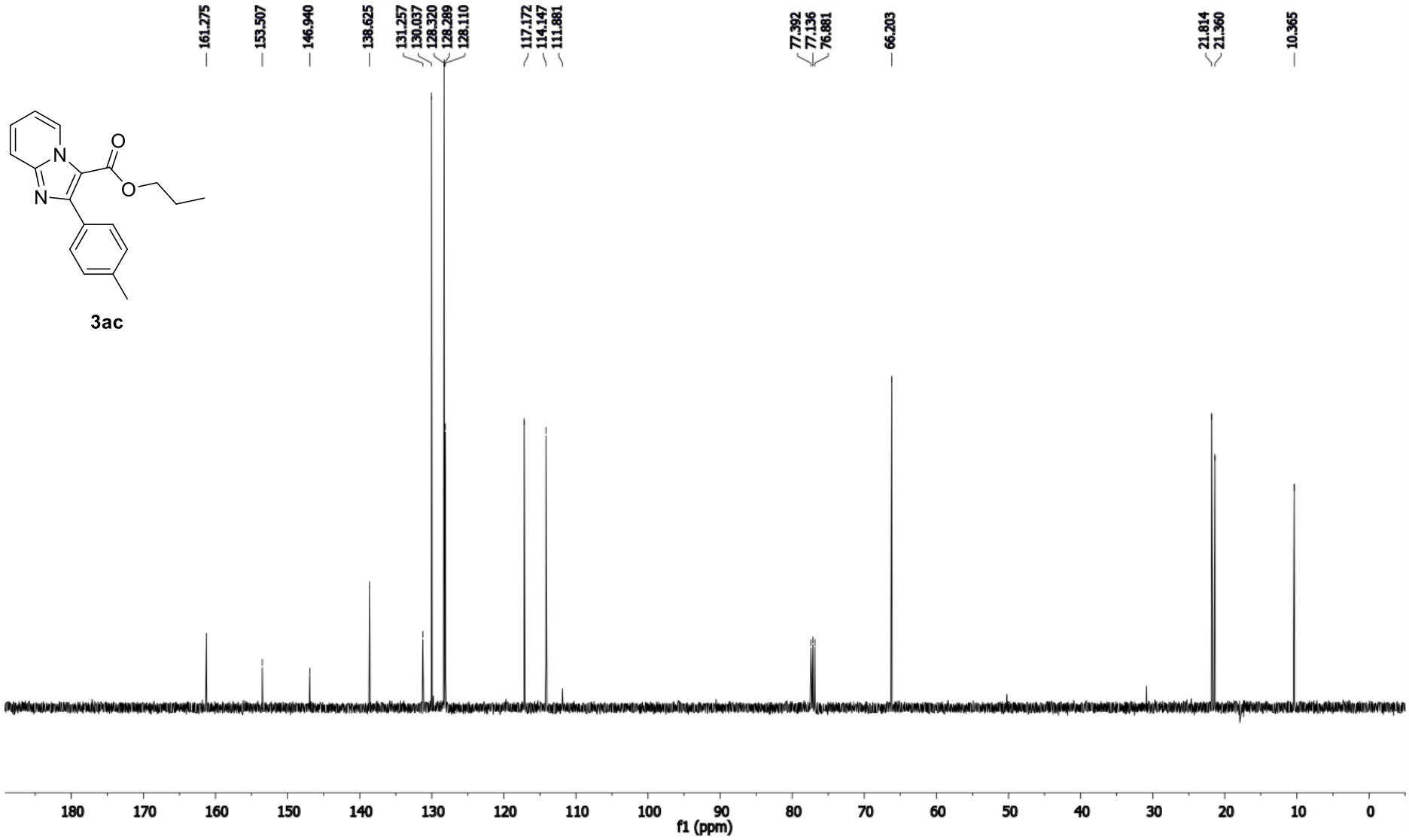
7.418
7.402
7.239
7.224
7.030
7.016
7.002
4.210
4.197
4.184
2.404
1.639
1.625
1.611
1.597
1.583
1.567
0.807
0.792
0.777
3ac
1.00
1.02
2.01
1.02
2.06
1.00
2.17
3.07
2.06
3.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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130.037
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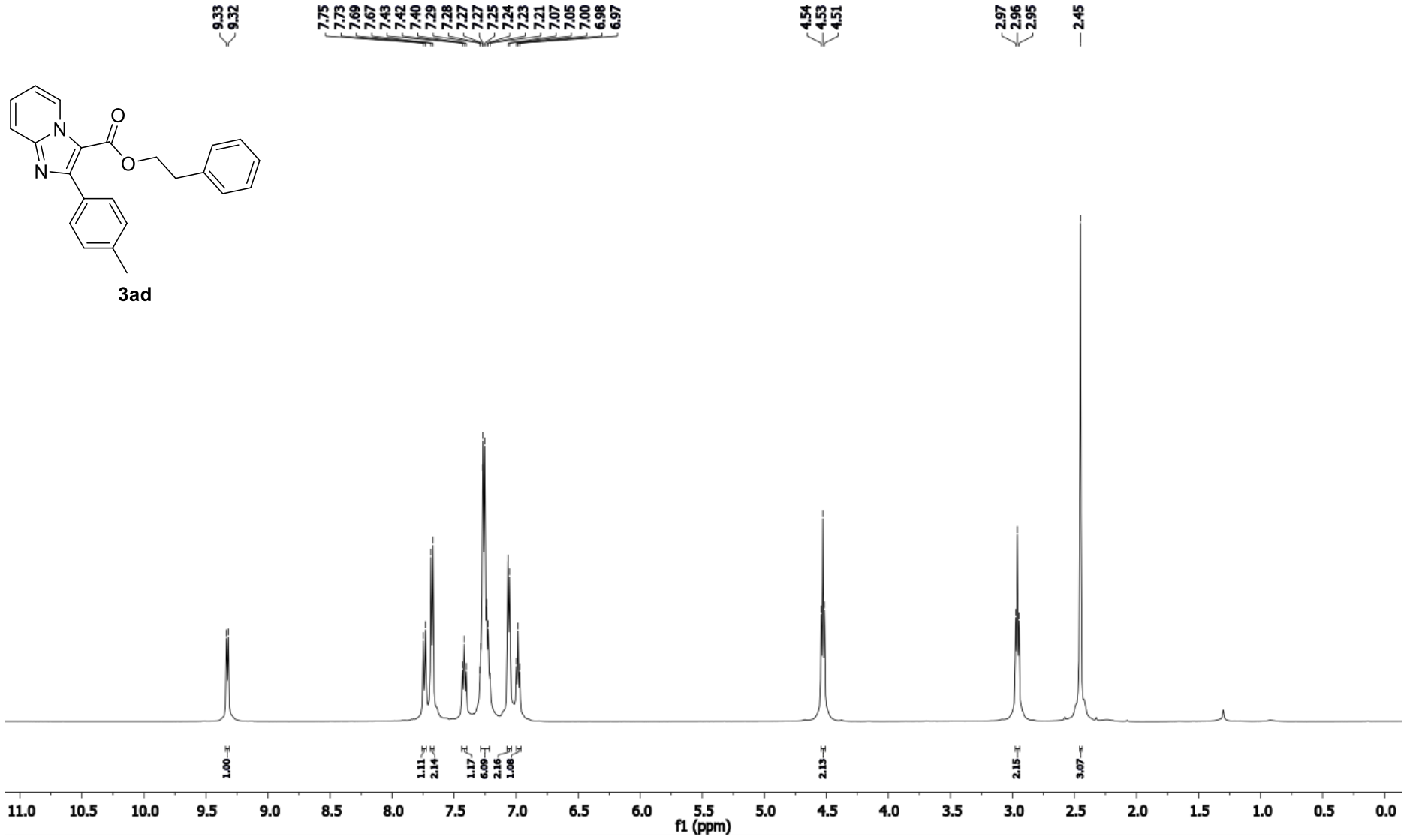
128.289
128.110
117.172
114.147
111.881
77.392
77.136
76.881
66.203
21.814
21.360
10.365
O
N
N
O
3ac
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.42
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7.28
7.27
7.27
7.25
7.24
7.23
7.21
7.07
7.05
7.00
6.98
6.97
4.54
4.53
4.51
2.97
2.96
2.95
2.45
O
N
N
O
3ad
1.00
1.11
2.14
1.17
6.09
2.16
1.08
2.13
2.15
3.07
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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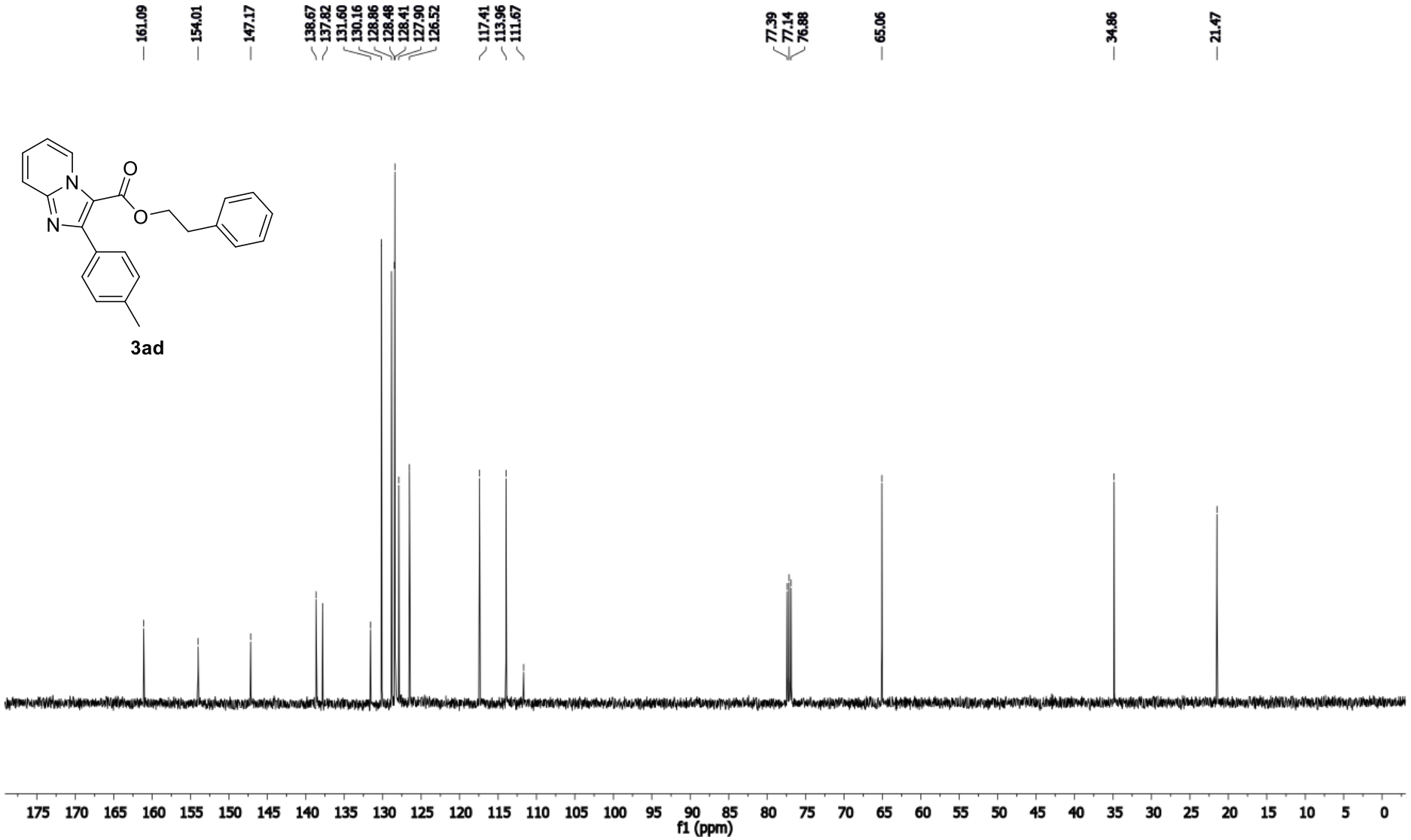
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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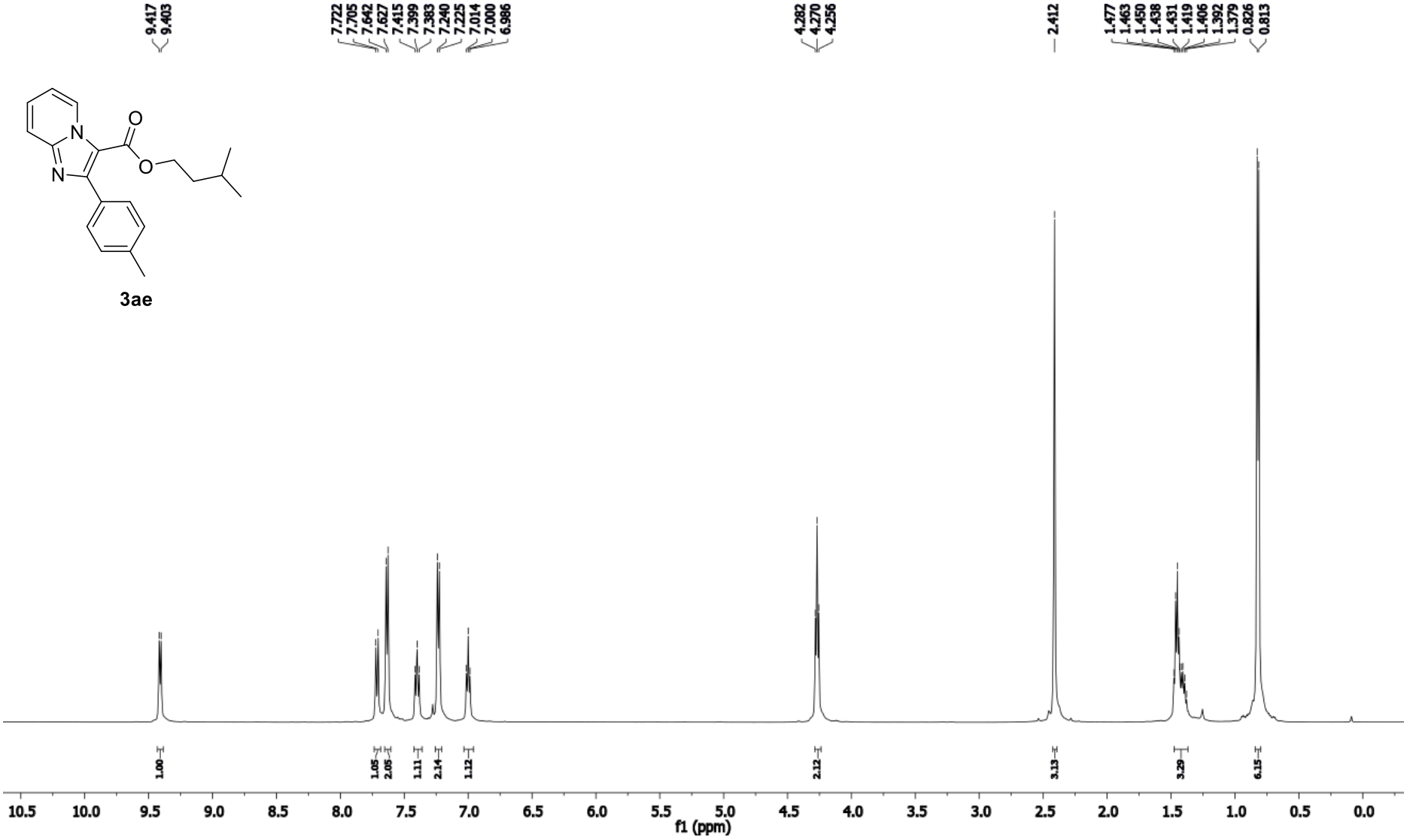
128.41
127.90
126.52
117.41
113.96
111.67
77.39
77.14
76.88
65.06
34.86
21.47
O
N
N
O
3ad
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.240
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7.014
7.000
6.986
4.282
4.270
4.256
2.412
1.477
1.463
1.450
1.438
1.431
1.419
1.406
1.392
1.379
0.826
0.813
O
N
N
O
1.00
1.05
2.05
1.11
2.14
1.12
2.12
3.13
3.29
6.15
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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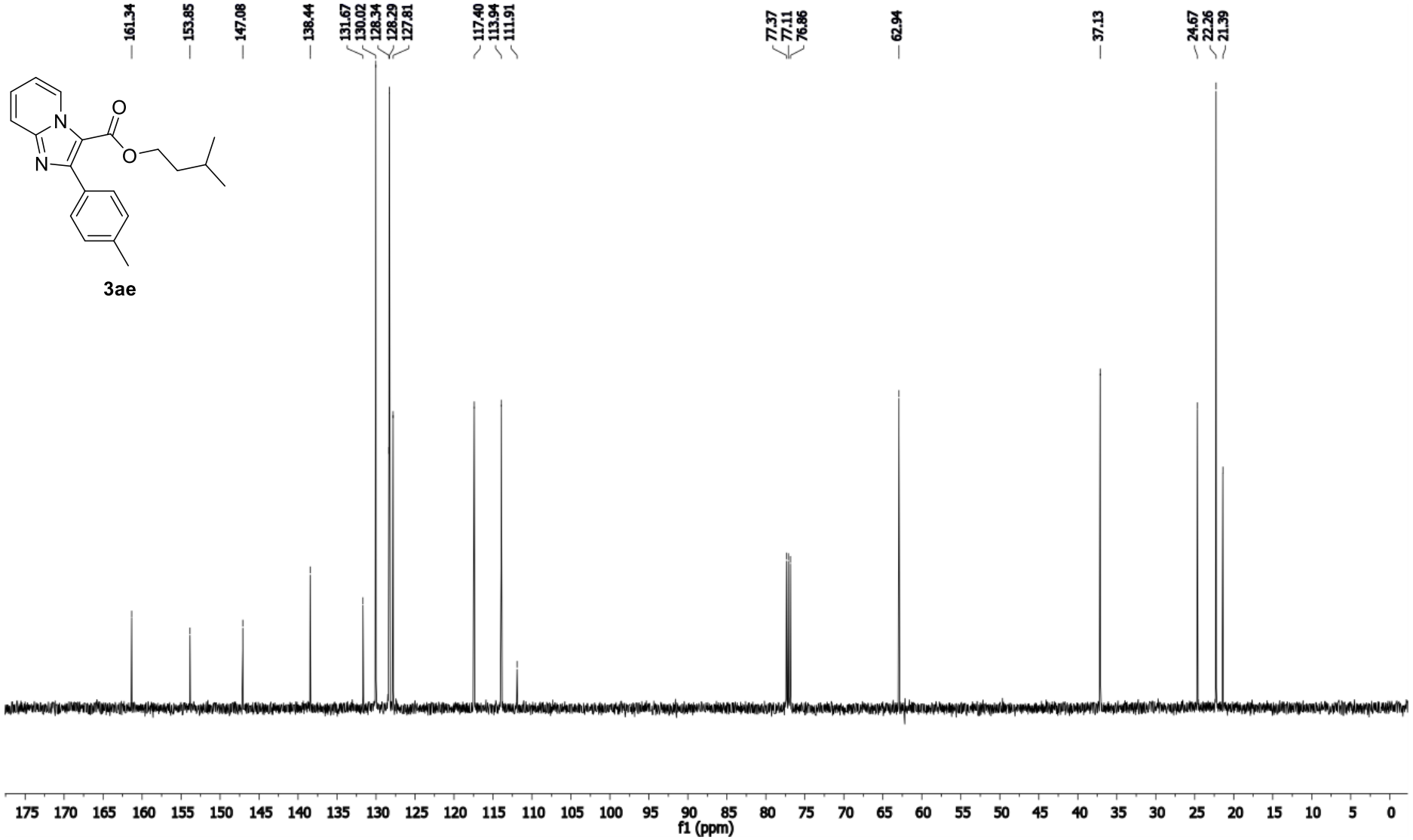
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ae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128.29
127.81
117.40
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111.91
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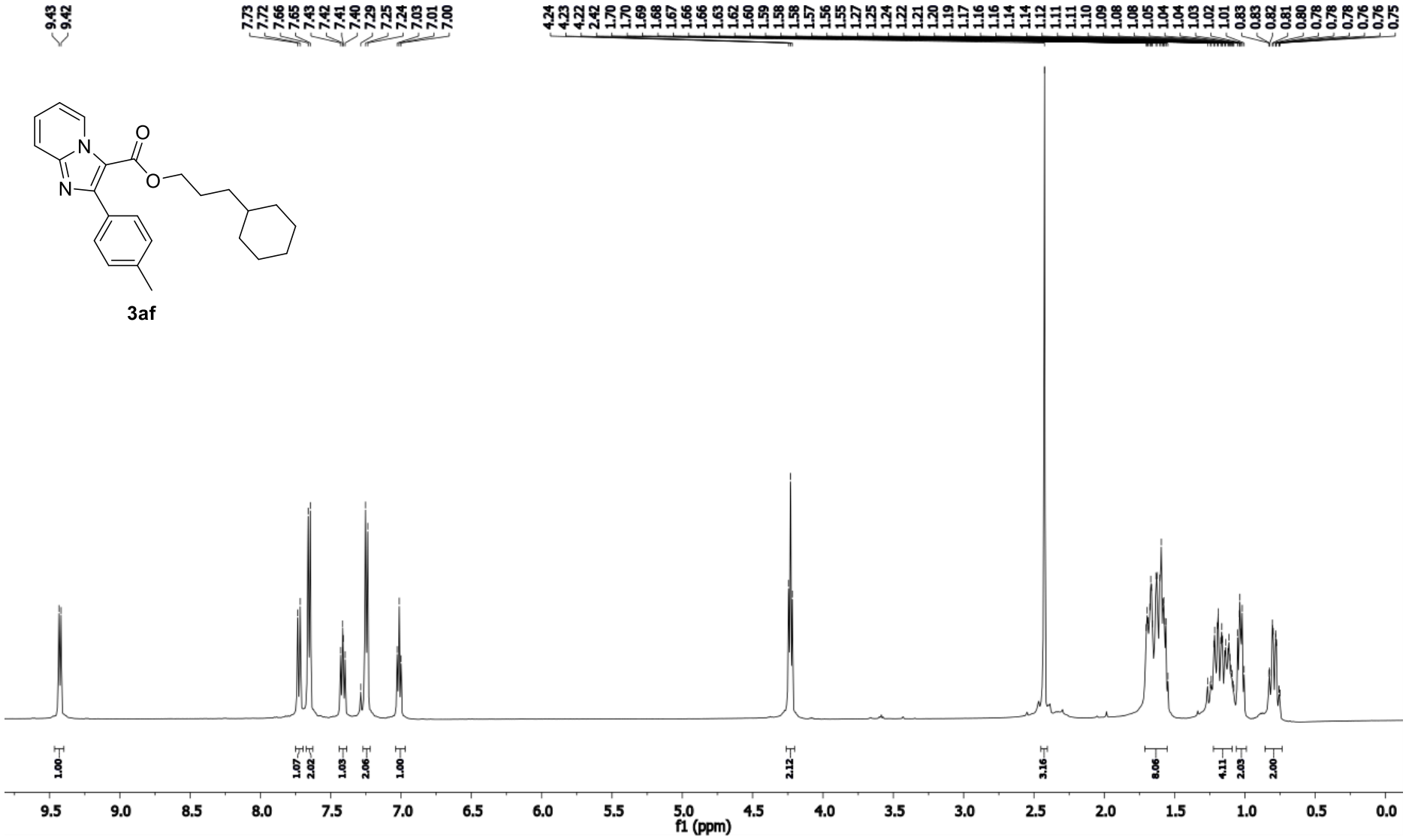
77.11
76.86
62.94
37.13
24.67
22.26
21.39
N
N
O
O
3ae
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.40
7.29
7.25
7.24
7.03
7.01
7.00
4.24
4.23
4.22
2.42
1.70
1.70
1.69
1.68
1.67
1.66
1.66
1.63
1.62
1.60
1.59
1.58
1.58
1.57
1.56
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1.27
1.25
1.24
1.22
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1.20
1.19
1.17
1.16
1.16
1.14
1.14
1.12
1.11
1.11
1.10
1.09
1.08
1.08
1.05
1.04
1.04
1.03
1.02
1.01
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0.83
0.82
0.81
0.80
0.78
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0.78
0.76
0.76
0.75
O
N
N
O
3af
1.00
1.07
2.02
1.03
2.06
1.00
2.12
3.16
8.06
4.11
2.03
2.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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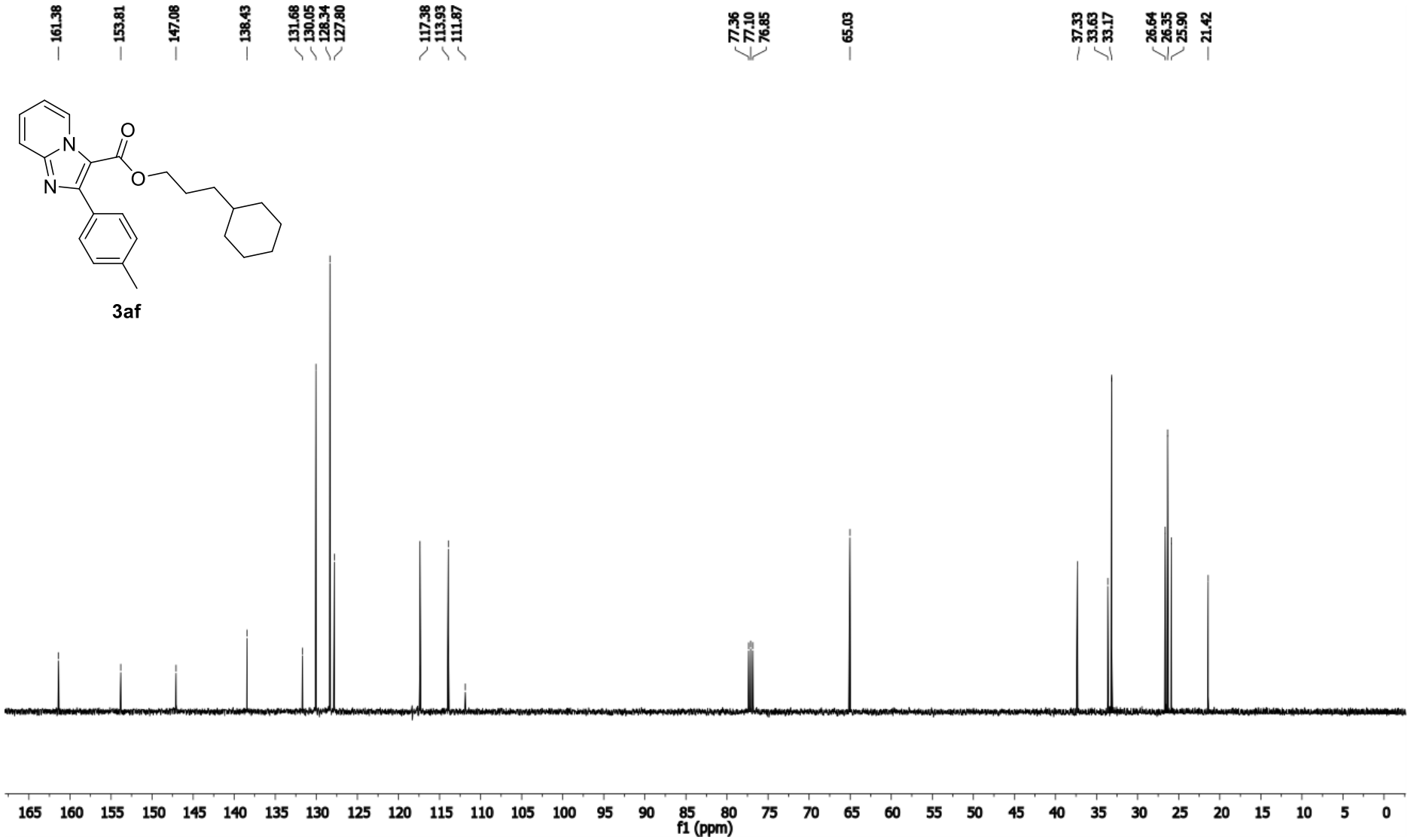
0.0
f1 (ppm)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127.80
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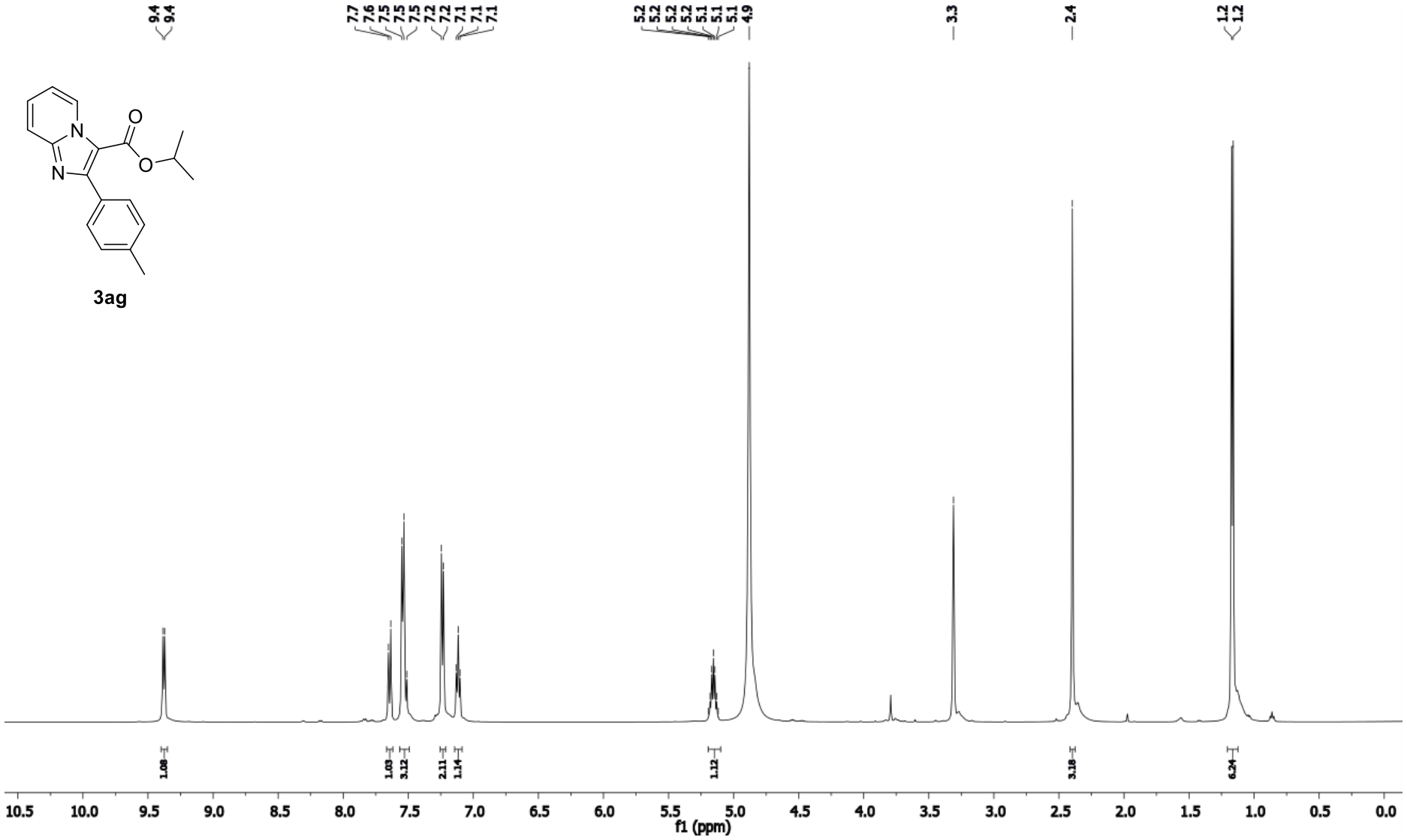
113.93
111.87
77.36
77.10
76.85
65.03
37.33
33.63
33.17
26.64
26.35
25.90
21.42
N
N
O
O
3af
165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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9.4
7.7
7.6
7.5
7.5
7.5
7.2
7.2
7.1
7.1
7.1
5.2
5.2
5.2
5.2
5.1
5.1
5.1
4.9
3.3
2.4
1.2
1.2
N
N
O
O
1.08
1.03
3.12
2.11
1.14
1.12
3.18
6.24
10.5
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
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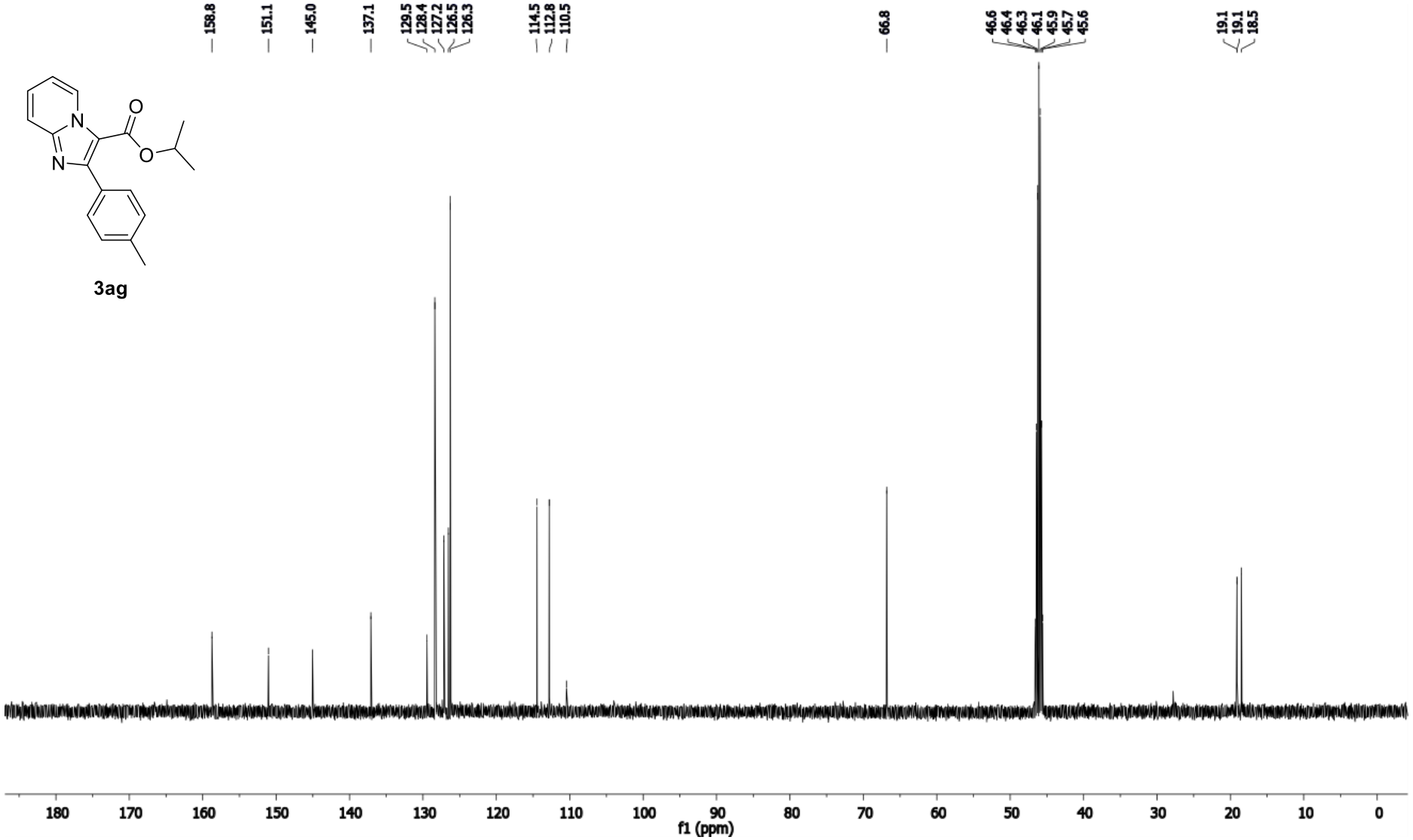
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ag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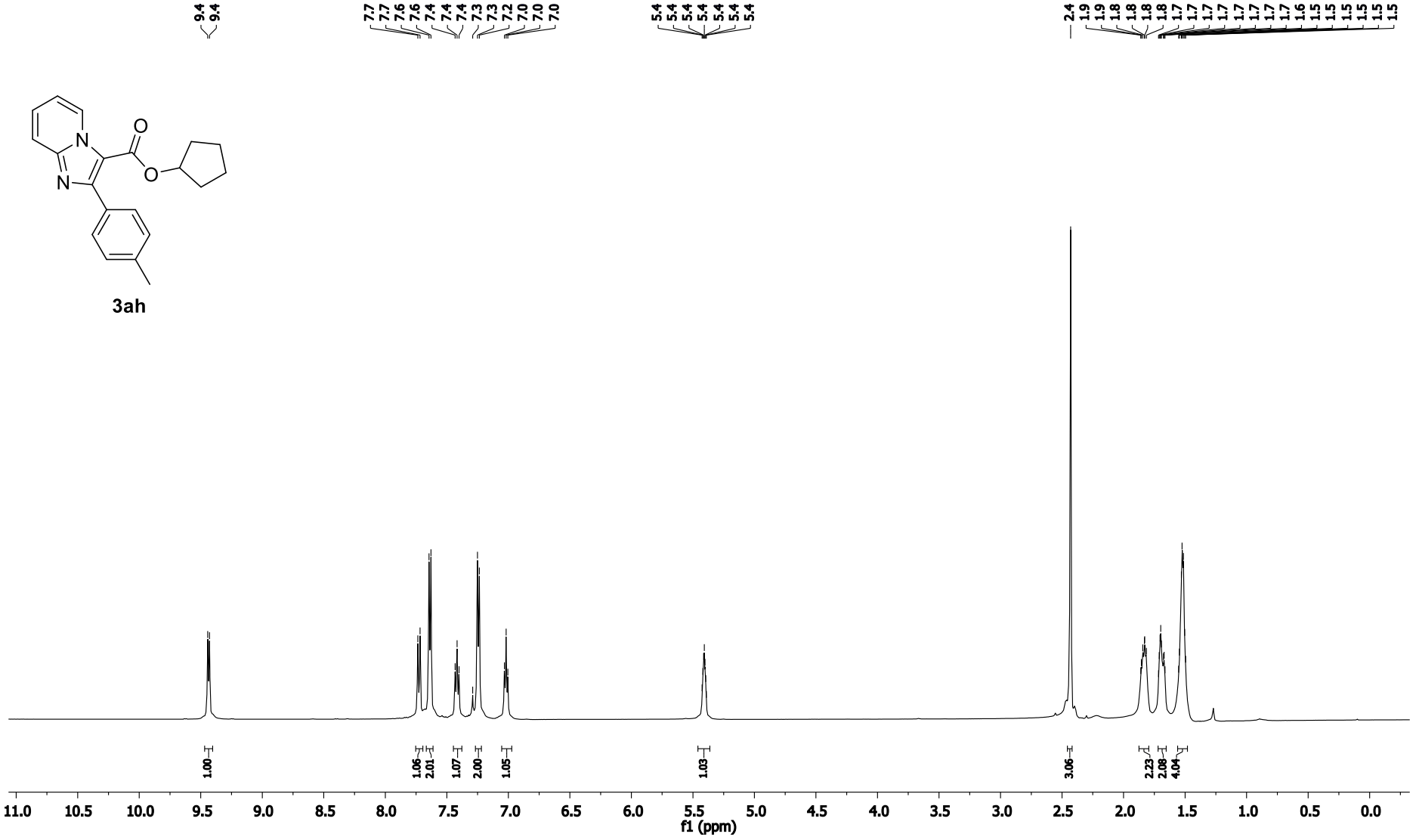
137.1
129.5
128.4
127.2
126.5
126.3
114.5
112.8
110.5
66.8
46.6
46.4
46.3
46.1
45.9
45.7
45.6
19.1
19.1
18.5
O
N
N
O
3ag
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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9.4
7.7
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7.6
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7.4
7.4
7.4
7.3
7.3
7.2
7.0
7.0
7.0
5.4
5.4
5.4
5.4
5.4
5.4
2.4
1.9
1.9
1.8
1.8
1.8
1.7
1.7
1.7
1.7
1.7
1.7
1.6
1.5
1.5
1.5
1.5
1.5
1.5
O
N
N
O
3ah
1.00
1.06
2.01
1.07
2.00
1.05
1.03
3.06
2.23
2.08
4.04
11.0
10.5
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
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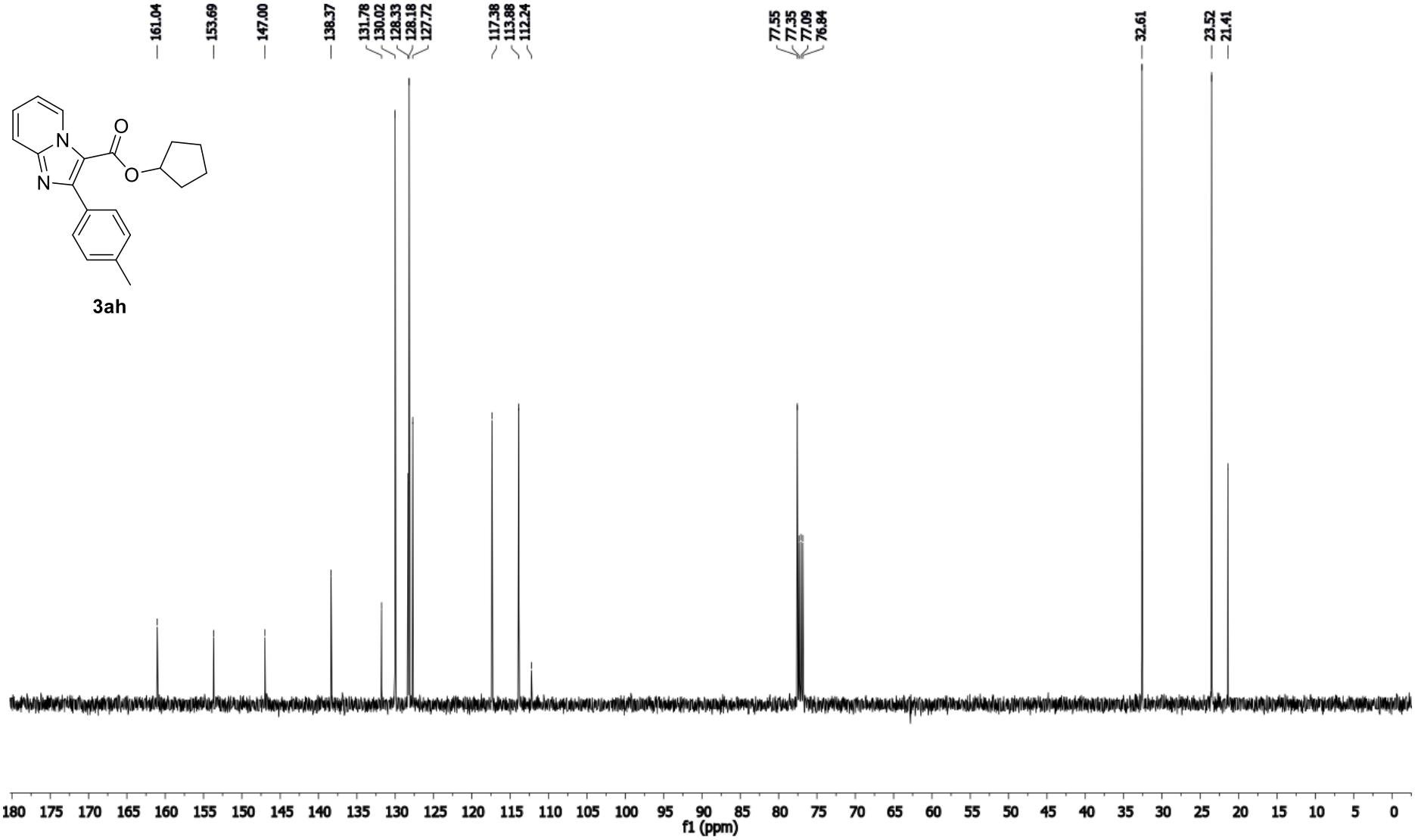
0.0
f1 (ppm)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130.02
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128.18
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117.38
113.88
112.24
77.55
77.35
77.09
76.84
32.61
23.52
21.41
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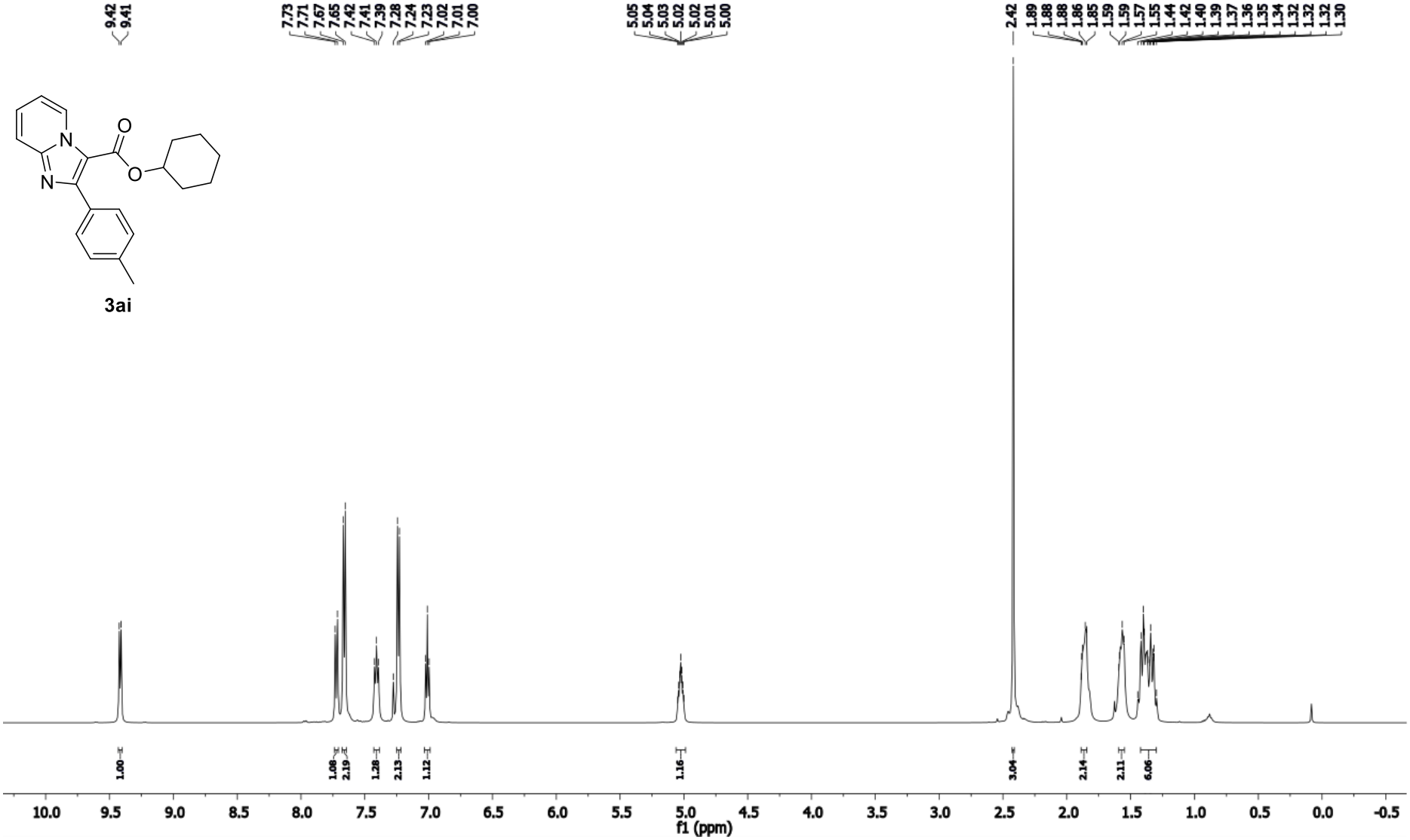
N
N
O
3ah
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.65
7.42
7.41
7.39
7.28
7.24
7.23
7.02
7.01
7.00
5.05
5.04
5.03
5.02
5.02
5.01
5.00
2.42
1.89
1.88
1.88
1.86
1.85
1.59
1.59
1.57
1.55
1.44
1.42
1.40
1.39
1.37
1.36
1.35
1.34
1.32
1.32
1.32
1.30
N
N
O
O
3ai
1.00
1.08
2.19
1.28
2.13
1.12
1.16
3.04
2.14
2.11
6.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
2.0
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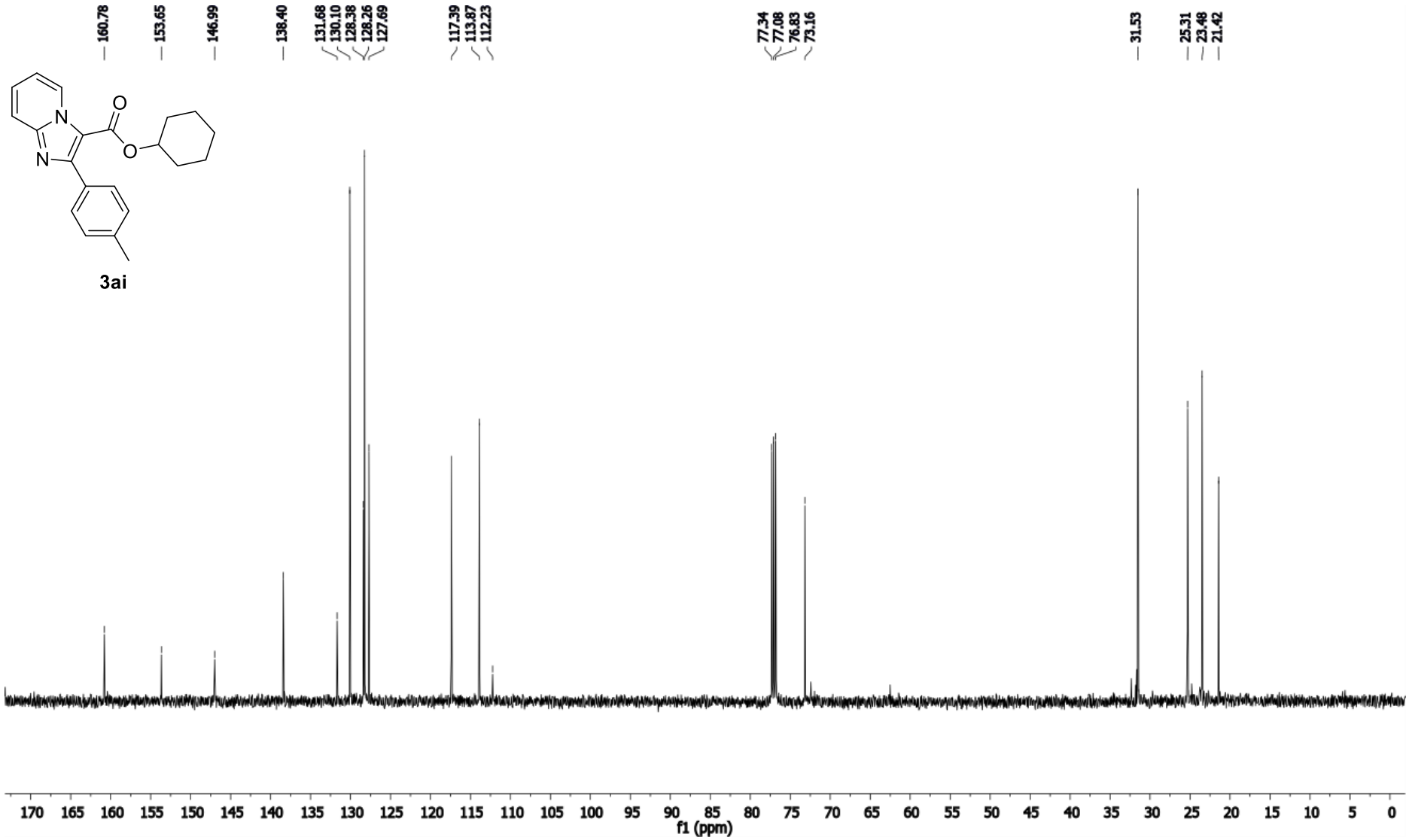
1.0
0.5
0.0
-0.5
f1 (ppm)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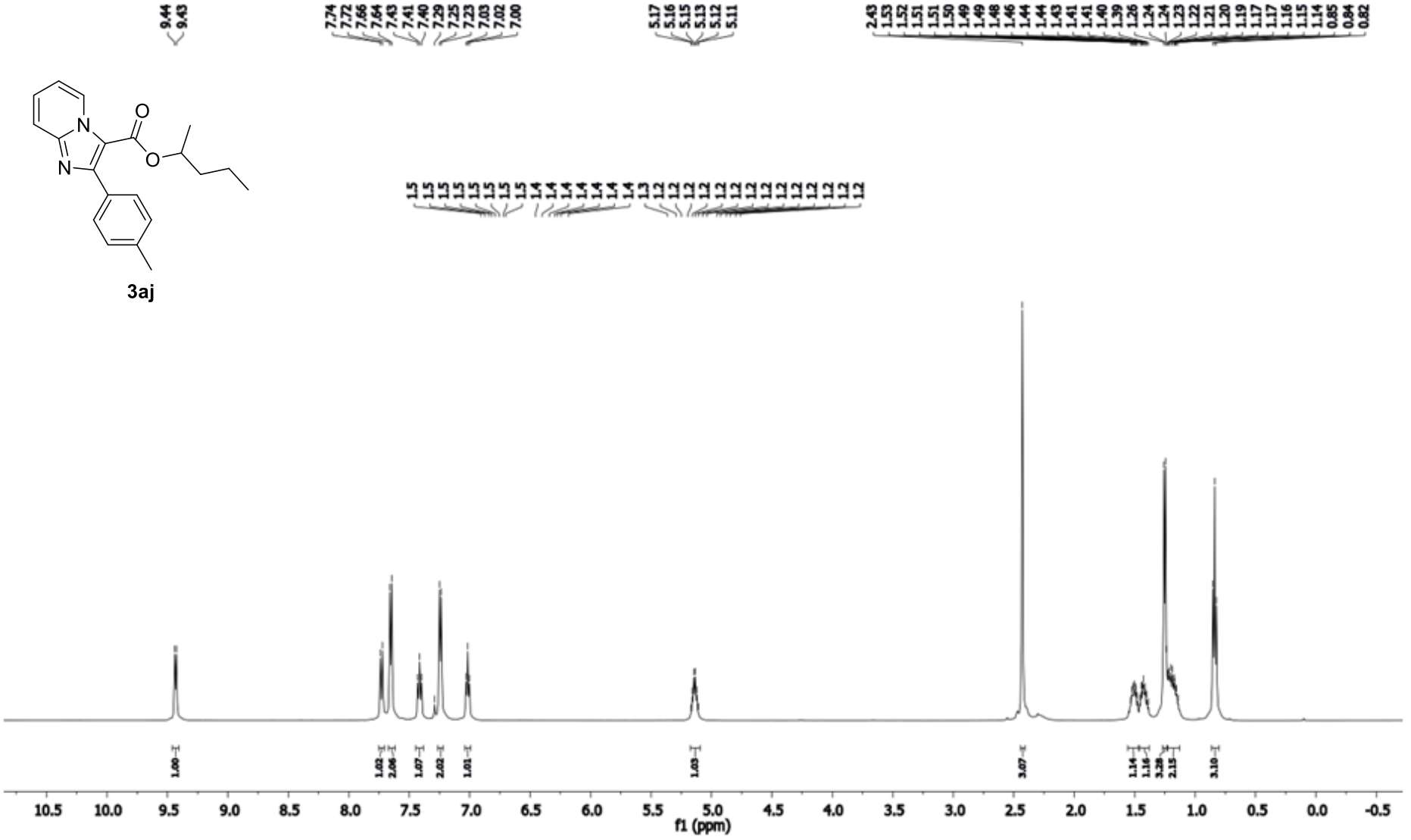
128.26
127.69
117.39
113.87
112.23
77.34
77.08
76.83
73.16
31.53
25.31
23.48
21.42
O
N
N
O
3ai
170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.74
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7.64
7.43
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7.40
7.29
7.25
7.23
7.03
7.02
7.00
5.17
5.16
5.15
5.13
5.12
5.11
2.43
1.53
1.52
1.51
1.51
1.50
1.49
1.49
1.48
1.46
1.44
1.44
1.43
1.41
1.41
1.40
1.39
1.26
1.24
1.24
1.23
1.22
1.21
1.20
1.19
1.17
1.17
1.16
1.15
1.14
0.85
0.84
0.82
O
N
N
O
3aj
1.00
1.03
2.06
1.07
2.02
1.01
1.03
3.07
1.14
1.16
3.28
2.15
3.10
10.5
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
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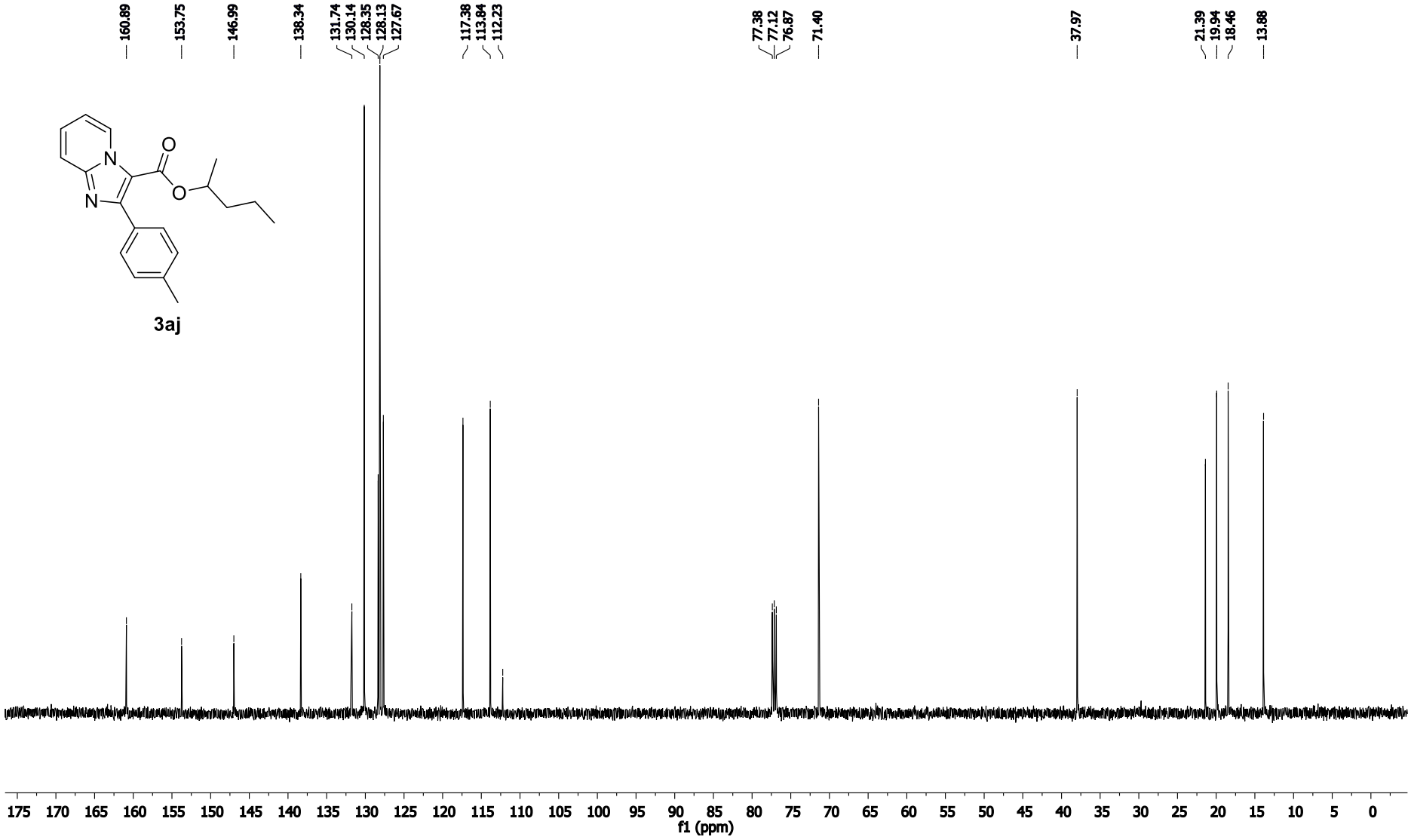
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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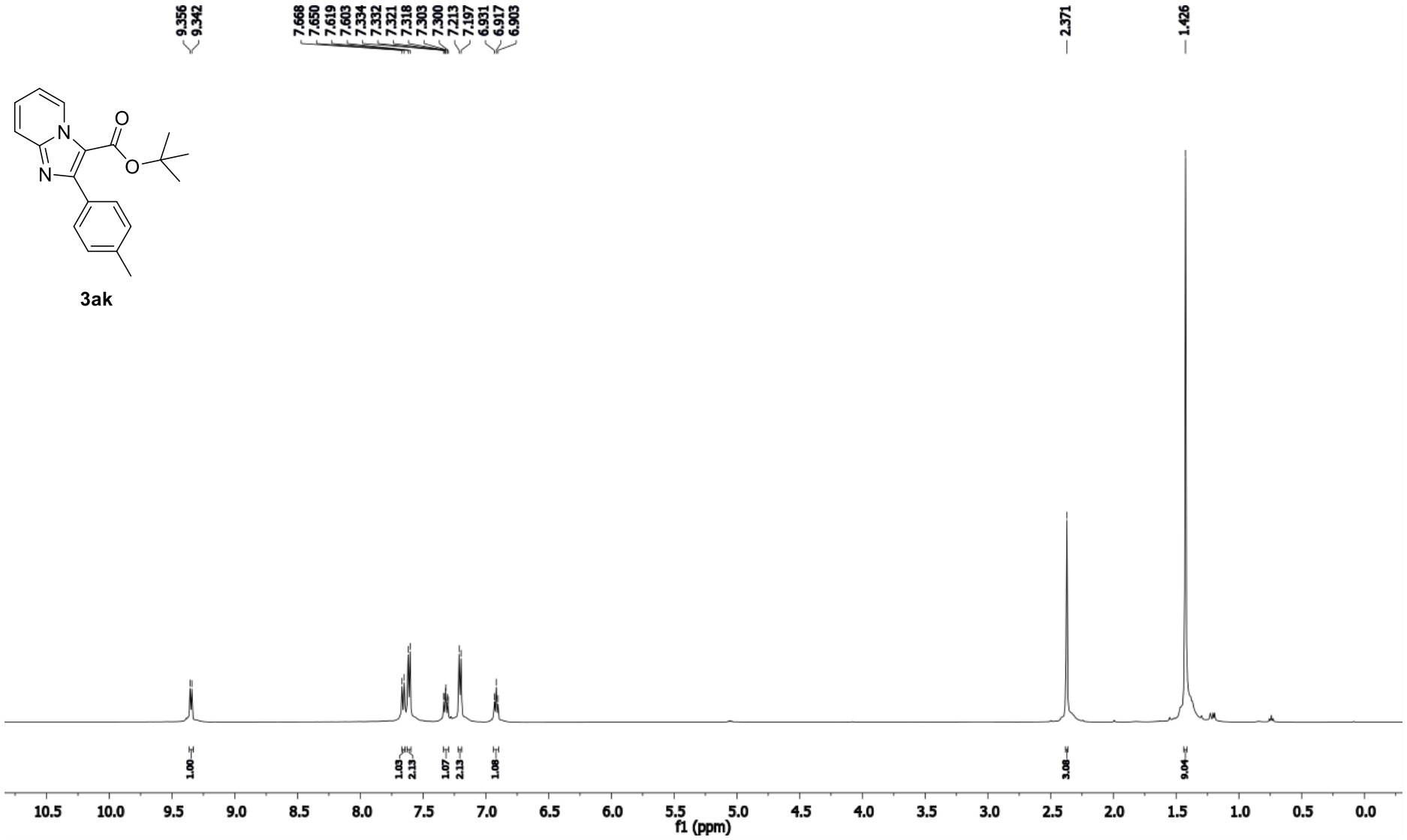
130.14
128.35
128.13
127.67
117.38
113.84
112.23
77.38
77.12
76.87
71.40
37.97
21.39
19.94
18.46
13.88
O
N
N
O
3aj
175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)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7.603
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7.332
7.321
7.318
7.303
7.300
7.213
7.197
6.931
6.917
6.903
2.371
1.426
O
N
N
O
1.00
1.03
2.13
1.07
2.13
1.08
3.08
9.04
10.5
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
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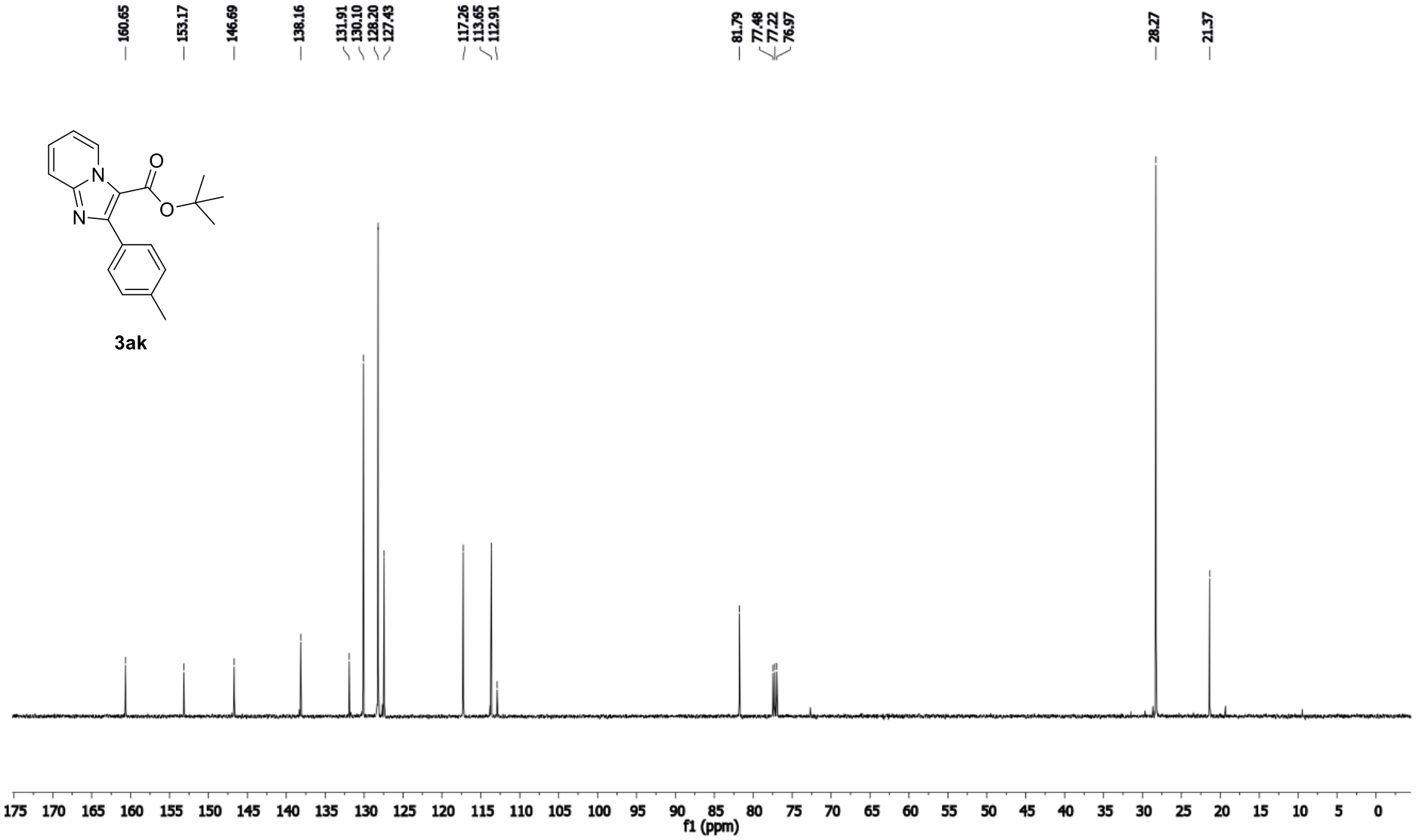
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

3ak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138.16
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130.10
128.20
127.43
117.26
113.65
112.91
81.79
77.48
77.22
76.97
28.27
21.37
3ak
f1 (ppm)