

Supporting Information

Photochemical Regioselective C–H Arylation of imidazo[1, 2-*a*]pyridine derivatives using Chlorophyll as biocatalyst and Diazonium Salts

Ali Moazzam,¹ Sara Moghadam Farid,¹ Nima Khaleghi,¹ Naiemeh Alizadeh,¹ Mohammad Mahdavi*¹

¹*Endocrinology and Metabolism Research Center, Endocrinology and Metabolism Clinical Sciences Institute, Tehran University of Medical Sciences, Tehran, Iran*

momahdavi@sina.tums.ac.ir

Table of Contents

1. General remarks	S2
2. General experimental details	S2
2-1. Synthesis of imidazo[1, 2- <i>a</i>]pyridine derivatives	S2
2-2. General procedure for the preparation of aryl diazonium tetra fluoroborates	S3
2-3. General procedure for the extraction of spinach	S3
2-4. General procedure for the reaction of aryl diazonium salts and imidazo[1, 2- <i>a</i>] Pyridine derivatives	S3
3. Emission spectra of White LED lamp	S4
4. Radical trapping experiment	S5
5. Compounds characterization data	S6
6. Copies of ¹H NMR and ¹³C NMR spectra	S10

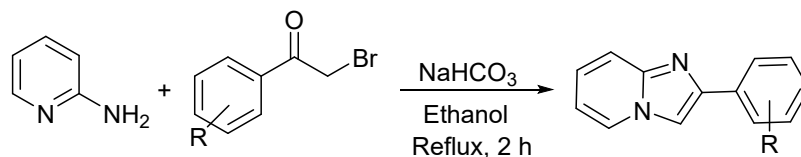
1. General remarks

All chemicals were purchased from Merck and Fluka companies. All yields refer to isolated products. ^1H NMR and ^{13}C NMR spectra were recorded on a Bruker, Rheinstetten, Germany NMR spectrometer (at 400 MHz) using tetramethylsilane (TMS) as internal standard. Melting points were determined in a capillary tube and are not corrected. The progress of the reaction was followed with TLC using silica gel SILG/UV 254 and 365 plates. All products are known compounds and their structures were deduced by ^1H and ^{13}C NMR spectroscopy.

2. General experimental details

2-1. Synthesis of imidazo[1,2-*a*]pyridine derivatives¹

A suspension of 2-aminopyridine (1.0 mmol), phenacylbromide (1 equiv.) and NaHCO_3 (2.5 equiv.) in ethanol (10 mL) was stirred at reflux condition for 2 h. The solution was evaporated and then 10 mL CH_2Cl_2 was added, the organic phase was washed with H_2O (3×10 mL), dried over anhydrous MgSO_4 and concentrated in vacuum to give imidazo[1,2-*a*]pyridine derivatives as light brown solids.



2-2. General procedure for the preparation of aryl diazonium tetra fluoroborates²

The appropriate aniline (10 mmol) was dissolved in a mixture of 4 mL of distilled water and 3.4 mL of 50% hydro fluoro boric acid. After cooling the reaction mixture to 0°C , using ice bath and the sodium nitrite (0.69 g in 1.5 mL) was added dropwise in 5 min interval of time. The resulting mixture was stirred for 40 min and the precipitate was collected by filtration and re-dissolved in minimum amount of acetone. Diethyl ether was added until precipitation of diazonium

¹ (a) S. A. Laufer, D. R. J. Hauser and A. J. Liedtke, *Synthesis* 2008, 253. (b) G. Kumar and G. R. N. Chinna, *J. Heterocycl. Chem.*, 2021, **58**, 250.

² P. Hanson, J. R. Jones, A. B. Taylor, P. H. Walton and A. W. Timms, *J. Chem. Soc. Perkin Trans. 2.*, 2002, **2**, 1135.

tetrafluoroborate, which is filtered, washed three times with diethyl ether and dried under vacuum.

2.3. General procedure for the extraction of spinach³

Fresh or frozen spinach (0.5 grams) was combined with 0.5 grams of anhydrous magnesium sulfate and 1.0 gram of sand. The mixture was ground in a mortar and pestle until a light green powder was obtained (5–10 minutes). The light green solid was transferred to a small test tube containing 2.0 mL of acetone. This heterogeneous mixture was agitated to ensure complete mixing of the acetone and the solid. This mixture was allowed to stand for 10 minutes and the green acetone solution was removed by pipette and transferred to a micro centrifuge tube. After centrifugation, the supernatant (green liquid) is poured in the plate for dry. After evaporate of solvent oil product is obtain.

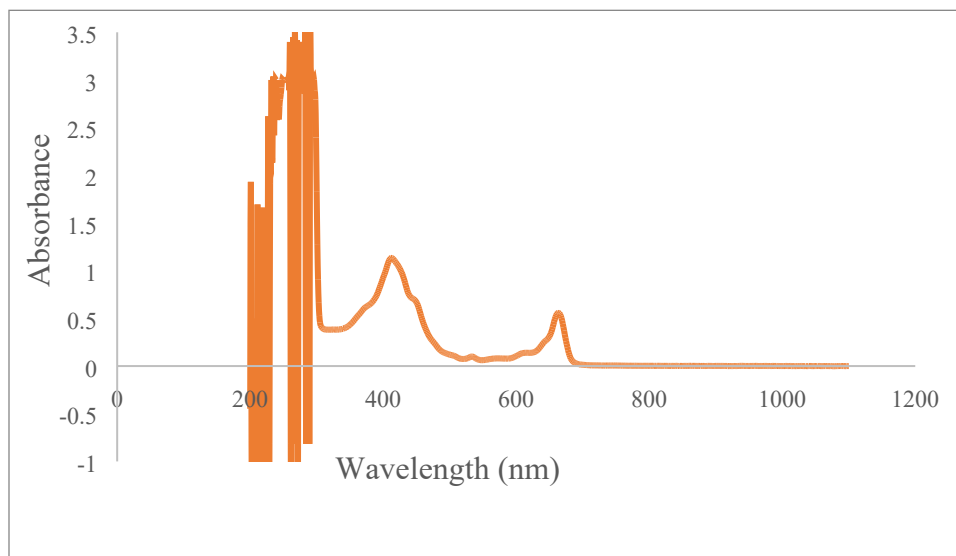


Figure 1. UV Visible Absorption Spectrum of mixture of chlorophyll in Acetone.

2.4. General procedure for the reaction of aryl diazonium salts and imidazo[1, 2-*a*]pyridine derivatives

In a 10 mL Pyrex tube with magnetic stirring bar the oil of chlorophyll (50 mg), aryl diazonium tetra fluoro borate (1 equiv.) and imidazo[1, 2-*a*]pyridine derivatives (3 equiv.) were dissolved in

³ H. T. Quach, R. L. Steeper and G. W. Griffin, *J. Chem. Educ.*, 2004, **81**, 385.

DMSO (0.4 mL) and the resulting mixture was stirred. The Pyrex tube was irradiated using 5 W white LED. After 16 h of irradiation the reaction mixture was transferred to separating funnel, diluted with diethyl ether and washed with 15 mL of water. The aqueous layer was washed three times with diethyl ether. The combined organic layers were dried over MgSO_4 , filtered and concentrated in vacuum. Purification of the crude product was achieved by flash column chromatography using n-hexane/ethyl acetate as eluent.



Figure 2. photocatalytic system

3.



Emission spectra of White LED

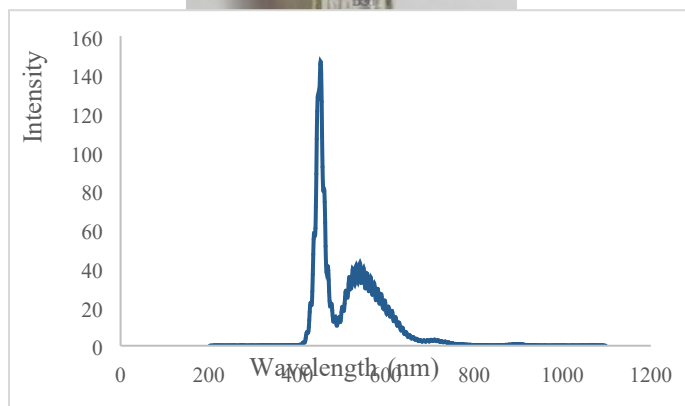
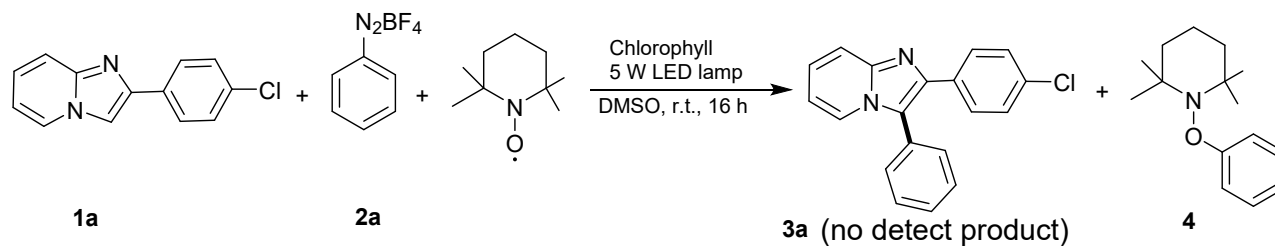


Figure 3. White LED and the emission spectrum of white LED

4. Radical trapping experiment



In a 10 mL the Pyrex tube with magnetic stirring bar the oil of chlorophyll (50 mg), aryl diazonium tetra fluoro borate (1 equiv.) and 2-(4-chlorophenyl)imidazo[1,2-a]pyridine (3 equiv.) were dissolved in DMSO (0.4 mL) and 2,2,6,6-tetramethylpiperidinyl-1-oxyl (TEMPO) (2.0 equiv.). Then the resulting mixture was irradiated using white LED for 16 h. While no desired product **3a** was found, the TEMPO-phenyl adduct **4** was detected.

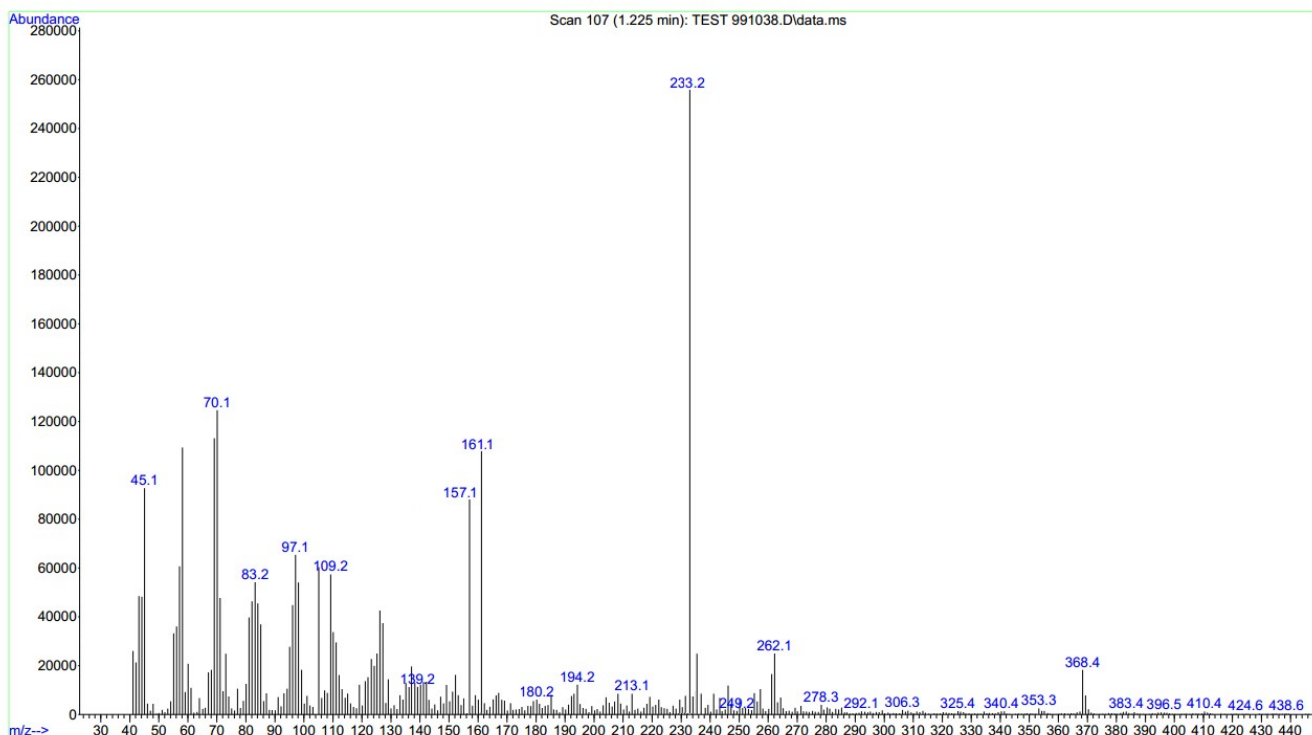


Figure 4. MS of TEMPO-Phenyl adduct

5. Compounds characterization data

5.1. 2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyridine (3a)⁴

White crystal, Yield 60% (18 mg); m.p. 138-140 °C; IR KBr: 3058, 2926, 1347, 1108, 871, 740 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.92 (d, *J* = 6.8 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.53 – 7.46 (m, 4H), 7.41 (d, *J* = 6.7 Hz, 2H), 7.25 – 7.17 (m, 3H), 6.73 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.8, 141.1, 133.5, 132.6, 130.7, 129.7, 129.5, 129.3, 129.2, 128.6, 125.2, 123.4, 121.3, 117.5, 112.6 ppm; MS: *m/z* (%) = 306 [M+2⁺, 37.5%], 304 [M⁺, 100%]; Anal. calcd. for C₁₉H₁₃ClN₂: C, 74.88; H, 4.30; N, 9.19. Found: C, 74.63; H, 4.49; N, 9.31.

5.2. 2-(4-chlorophenyl)-3-(*p*-tolyl)imidazo[1,2-*a*]pyridine (3b)⁵

White crystal, Yield 71% (22 mg); m.p.: 146-147 °C; IR KBr: 3061, 2932, 1362, 1088, 879, 745 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.67 (d, *J* = 7.6 Hz, 1H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.54 (d, *J* = 6.8 Hz, 1H), 7.46 – 7.40 (m, 2H), 7.35 (t, *J* = 6.9 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 7.22 – 7.18 (m, 3H), 6.71 (t, *J* = 6.8 Hz, 1H), 2.03 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.9, 141.0, 139.1, 133.3, 132.9, 131.8, 131.2, 129.9, 128.9, 128.6, 128.4, 127.1, 124.8, 123.5, 120.5, 117.5, 112.5, 19.4 ppm; MS: *m/z* (%) = 320 [M+2⁺, 37.5%], 318 [M⁺, 100%]; Anal. calcd. for C₂₀H₁₅ClN₂: C, 75.35; H, 4.74; N, 8.79. Found: C, 75.52; H, 4.53; N, 8.93.

5.3. 2-(4-chlorophenyl)-3-(4-methoxyphenyl)imidazo[1,2-*a*]pyridine (3c)⁵

White crystal, Yield 82% (27 mg); m.p. 115-117 °C; IR KBr: 3066, 2942, 1353, 1118, 873, 740 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.97 (d, *J* = 7.0 Hz, 1H), 7.66 – 7.61 (m, 3H), 7.43-7.37 (m, 4H), 7.33-7.19 (m, 1H), 7.16 (d, *J* = 7.6 Hz, 2H), 6.89 (t, *J* = 6.8 Hz, 1H), 3.86 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 160.2, 144.3, 140.1, 133.7, 132.5, 132.4, 129.3, 128.8, 125.7, 124.3, 121.3, 121.2, 117.3, 115.7, 113.1, 55.7 ppm; MS: *m/z* (%) = 336 [M+2⁺, 37.5%], 334 [M⁺, 100%]; Anal. calcd. for C₂₀H₁₅ClN₂O: C, 71.75; H, 4.52; N, 8.37. Found: C, 71.89; H, 4.77; N, 8.11.

5.4. 2-(4-chlorophenyl)-3-(3,4-dimethylphenyl)imidazo[1,2-*a*]pyridine (3d)

Yellow solid, Yield 76% (25 mg); m.p. 102-104 °C; IR KBr: 3056, 2969, 1341, 1071, 804, 736 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.90 (d, *J* = 6.9 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 2H), 7.50 (d, *J* = 6.9 Hz, 1H), 7.41 (d, *J* = 2.1 Hz, 1H), 7.36 (dd, *J* = 6.9, 2.1 Hz, 1H), 7.28 – 7.22 (m, 3H), 7.04-7.02 (m, 2H), 6.82 (t, *J* = 6.9 Hz, 1H), 2.30 (s, 3H), 2.27 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.6, 140.9, 137.6, 136.7, 135.4, 134.3, 132.2, 131.8, 131.1, 130.5, 129.3, 128.7, 127.5, 123.7, 119.1, 117.5, 112.4, 20.1, 19.9 ppm; MS: *m/z* (%) = 334 [M+2⁺, 37.5%], 332 [M⁺, 100%]; Anal. calcd. for C₂₁H₁₇ClN₂: C, 75.78; H, 5.15; N, 8.42. Found: C, 70.53; H, 5.39; N, 8.66.

⁴ M. Khoshneviszadeh, M. Soheilizad, M. Fardpour and M. Mahdavi, *Monatshefte fur Chemie.*, 2017, **148**, 1817.

⁵ R. Afshari, S. Emad Hooshmand, M. Atharnezhad and A. Shaabani, *Polyhedron.*, 2020, **175**, 114238.

5.5. 2-(4-chlorophenyl)-3-(4-fluorophenyl)imidazo[1,2-*a*]pyridine (3e)

White crystal; Yield: 64% (20 mg); m.p. 124-126 °C; IR KBr: 3050, 2962, 1384, 1220, 1086, 1013, 814, 749 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.86 (d, *J* = 7.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.56 (d, *J* = 7.4 Hz, 2H), 7.41 – 7.38 (m, 2H), 7.25 – 7.20 (m, 5H), 6.74 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 163.5 (¹*J*_{C-F}=239 Hz), 144.9, 141.5, 133.5, 132.7 (³*J*_{C-F}=9 Hz), 132.6, 129.3, 128.6, 125.6 (⁴*J*_{C-F}=2 Hz), 125.1, 123.2, 120.1, 117.7, 117.1 (²*J*_{C-F}=21 Hz), 112.7 ppm; ¹⁹F NMR (376 MHz, DMSO-*d*₆) δ -114.22; MS: *m/z* (%) = 324 [M+2⁺, 37.5%], 322 [M⁺, 100%]; Anal. calcd. for C₁₉H₁₂ClFN₂: C, 70.70; H, 3.75; N, 8.68. Found: C, 70.88; H, 3.54; N, 8.49.

5.6. 2-(4-chlorophenyl)-3-(4-nitrophenyl)imidazo[1,2-*a*]pyridine (3f)⁶

Orange solid, Yield 48% (16 mg); m.p. 158-160 °C. IR KBr: 3044, 2973, 1553, 1348, 1096, 810, 753 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆): δ 8.38 (d, *J* = 7.6 Hz, 2H), 8.01 (d, *J* = 7.4 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.31–7.23 (m, 3H), 6.78 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆): δ 147.7, 145.8, 143.3, 136.5, 134.3, 132.1, 131.1, 129.8, 128.9, 125.9, 124.9, 122.9, 118.9, 118.1, 113.6 ppm; MS: *m/z* (%) = 351 [M+2⁺, 37.5%], 349 [M⁺, 100%]; Anal. calcd. for C₁₉H₁₂ClN₃O₂: C, 65.24; H, 3.46; N, 12.01. Found: C, 65.63; H, 3.21; N, 11.86.

5.7. 2-(4-chlorophenyl)-3-(4-hydroxy)imidazo[1,2-*a*]pyridine (3g)

White solid, Yield 81% (26 mg); m.p. 147-149 °C. IR KBr: 3351, 2967, 1341, 1221, 761 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.73 (s, 1H), 7.95 (d, *J* = 7.4 Hz, 1H), 7.66 (d, *J* = 7.4 Hz, 2H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.39 (d, *J* = 7.7 Hz, 2H), 7.35 (d, *J* = 7.6 Hz, 2H), 7.29 (t, *J* = 6.8 Hz, 1H), 7.01 (d, *J* = 7.7 Hz, 2H), 6.91 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO) δ 158.47, 144.04, 139.82, 134.05, 132.80, 132.49, 131.98, 129.10, 125.44, 123.70, 122.03, 121.08, 117.57, 116.22, 113.85 ppm; MS: *m/z* (%) = 322 [M+2⁺, 36.8%], 320 [M⁺, 100%]; Anal. calcd. for C₁₉H₁₃ClN₂O: C, 71.14; H, 4.09; N, 8.73. Found: C, 71.37; H, 3.87; N, 8.95.

5.8. 2-(4-chlorophenyl)-7-methyl-3-phenylimidazo[1,2-*a*]pyridine (3h)

White solid, Yield 74% (23 mg); m.p. 127-129 °C. IR KBr: 2929, 1728, 1289, 1080, 699 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.84 (dd, *J* = 7.6, 1.8 Hz, 1H), 7.60 (d, *J* = 7.6 Hz, 2H), 7.55 – 7.49 (m, 3H), 7.44-7.42 (m, 3H), 7.25 (d, *J* = 7.7 Hz, 2H), 6.58 (dd, *J* = 7.4, 1.8 Hz, 1H), 2.42 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 145.29, 140.92, 135.93, 133.18, 132.89, 130.66, 129.77, 129.61, 129.22, 128.92, 128.44, 122.56, 120.69, 115.88, 115.06, 21.33 ppm; MS: *m/z* (%) = 320 [M+2⁺, 37.3%], 318 [M⁺, 100%]; Anal. calcd. for C₂₀H₁₅ClN₂: C, 75.35; H, 4.74; N, 8.79. Found: C, 75.17; H, 4.58; N, 8.66.

5.9. 6-chloro-2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyridine (3i)⁸

White solid, Yield 72% (20 mg); m.p. 187-189 °C. IR KBr: 2937, 1276, 1125, 731 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.98 (d, *J* = 1.8 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.60-7.58 (m, 4H), 7.45 (dd, *J* = 7.6, 1.8 Hz, 2H), 7.27 (d, *J* = 7.6 Hz, 3H), 7.21 (dd, *J* = 7.5, 1.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.21, 137.38, 136.48, 133.70, 132.22, 130.57, 129.88, 129.50, 129.22, 128.95, 128.57, 126.28, 121.17, 120.83, 117.94 ppm; MS: *m/z* (%) = 342 [M+4⁺, 11.2%], 340 [M+2⁺, 67.1%], 338 [M⁺, 100%]; Anal. calcd. for C₁₉H₁₂Cl₂N₂: C, 67.27; H, 3.57; N, 8.26. Found: C, 67.43; H, 3.84; N, 8.03.

⁶ H. Zali-Boeini, N. Norastehfar and H. Amiri Rudbari, *RSC Adv.*, 2016, 6, 81943.

5.10. 2-(4-chlorophenyl)-6-methyl-3-phenylimidazo[1,2-*a*]pyridine (3j)⁸

White solid, Yield 70% (22 mg); m.p. 148-150 °C. IR KBr: 2925, 1476, 1087, 700 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.70 (s, 1H), 7.58 – 7.52 (m, 5H), 7.51 (d, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.05 (d, *J* = 7.7 Hz, 1H), 2.25 (s, 3H); ¹³C NMR (100 MHz, cdcl₃) δ 143.93, 141.12, 136.18, 133.13, 132.90, 130.74, 129.85, 129.60, 129.12, 128.95, 128.42, 128.00, 122.08, 120.87, 116.83, 18.33 ppm; MS: *m/z* (%) = 320 [M+2⁺, 37.1%], 318 [M⁺, 100%]; Anal. calcd. for C₂₀H₁₅ClN₂: C, 75.35; H, 4.74; N, 8.79. Found: C, 75.61; H, 4.98; N, 9.03.

5.11. 2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyrimidine (3k)⁷

White crystal, Yield 68% (20 mg); m.p. 141-143 °C; IR KBr: 3035, 2929, 1326, 1048, 821, 729 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.59 (d, *J* = 4.0 Hz, 1H), 8.47 (d, *J* = 6.8 Hz, 1H), 7.62 – 7.52 (m, 7H), 7.38 (d, *J* = 7.6 Hz, 1H), 7.04 (t, *J* = 5.4 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 151.3, 147.7, 141.2, 133.0, 132.8, 131.0, 130.2, 129.9, 129.6, 128.9, 128.5, 119.9, 109.8 ppm; MS: *m/z* (%) = 307 [M+2⁺, 37.5%], 305 [M⁺, 100%]; Anal. calcd. for C₁₈H₁₂ClN₃: C, 70.71; H, 3.96; N, 13.74. Found: C, 70.95; H, 4.21; N, 13.58.

5.12. 2-(4-bromophenyl)-3-phenylimidazo[1,2-*a*]pyridine (3l)⁸

White crystal, Yield 58% (18 mg); m.p. 155-157 °C; IR KBr: 3044, 2936, 1349, 1057, 661 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.01 (d, *J* = 6.9 Hz, 1H), 7.67 (d, *J* = 7.6 Hz, 1H), 7.63 – 7.49 (m, 9H), 7.35-7.31 (m, 1H), 6.91 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.5, 140.5, 133.9, 131.7, 131.0, 130.2, 129.7, 129.7, 129.4, 125.9, 124.2, 121.4, 121.2, 117.4, 113.3 ppm; MS: *m/z* (%) = 350 [M+2⁺, 49.7%], 348 [M⁺, 50.3%]; Anal. calcd. for C₁₉H₁₃BrN₂: C, 65.35; H, 3.75; N, 8.02 Found: C, 65.69; H, 3.51; N, 8.22.

5.13. 3-phenyl-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (3m)⁸

White crystal; Yield: 74% (21 mg); m.p. 100-102 °C. IR KBr: 3060, 2948, 1365, 1189, cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.00 (d, *J* = 6.9 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.59 – 7.46 (m, 7H), 7.31-7.29 (m, 1H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.86 (t, *J* = 6.8, 1H), 2.26 (s, 3H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.4, 141.8, 137.1, 131.8, 131.0, 130.0, 129.9, 129.4, 129.3, 127.8, 125.4, 124.0, 120.7, 117.2, 113.0, 21.2 ppm; MS: *m/z* (%) = 284 [M⁺, 100%]; Anal. calcd. for C₂₀H₁₆N₂: C, 84.48; H, 5.67; N, 9.85 Found: C, 84.31; H, 5.89; N, 10.10.

5.14. 2-([1,1'-biphenyl]-4-yl)-3-phenylimidazo[1,2-*a*]pyridine (3n)

White crystal; Yield: 80% (27 mg); m.p. 148-150 °C. IR KBr: 3055, 2927, 13415, 1067, cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.01 (d, *J* = 6.9 Hz, 1H), 7.71 – 7.54 (m, 12H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.37 – 7.31 (m, 2H), 6.91 (t, *J* = 6.8 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.5, 141.2, 139.9, 139.4, 133.7, 131.2, 130.2, 129.8, 129.6, 129.3, 128.3, 127.9, 126.9, 126.9, 125.7, 124.1, 121.3, 117.3, 113.2 ppm; MS: *m/z* (%) = 346 [M⁺, 100%]; Anal. calcd. for C₂₅H₁₈N₂: C, 86.68; H, 5.24; N, 8.09 Found: C, 86.89; H, 5.43; N, 8.28.

⁷ H. P. L. Steenackers, D. S. Ermolov, B. Savaliya, A. De Weerd, D. De Coster, A. Shah, E. V. Van Der Eycken, D. E. De Vos, J. Vanderleyden and S. C. J. De Keersmaecker, *J. Med. Chem.*, 2011, **54**, 472.

⁸ R. Kumar, C. Ravi, D. Rawat and S. Adimurthy, *Eur. J. Org. Chem.*, 2018, **2018**, 1665.

5.15. 2,3-diphenylimidazo[1,2-*a*]pyridine (3o)⁴

White crystal; Yield: 56% (15 mg); m.p. 136-138 °C. IR KBr: 3069, 2932, 1355, 1196 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.02 (d, *J* = 6.9 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.64 – 7.42 (m, 7H), 7.38 – 7.18 (m, 4H), 6.90 (td, *J* = 6.8, 1.2 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.41, 141.63, 134.61, 131.15, 130.14, 129.82, 129.56, 128.75, 127.90, 125.72, 124.20, 121.17, 117.35, 113.22 ppm; MS: *m/z* (%) = 270 [*M*⁺, 100%]; Anal. calcd. for C₁₉H₁₄N₂: C, 84.42; H, 5.22; N, 10.36 Found: C, 84.68; H, 5.46; N, 10.65.

5.16. 2-(naphthalen-2-yl)-3-phenylimidazo[1,2-*a*]pyridine (3p)⁹

White crystal; Yield: 79% (22 mg); m.p. 127-128 °C. IR KBr: 3058, 2953, 1367, 1127 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.22 (s, 1H), 8.08 (d, *J* = 6.9 Hz, 1H), 7.86-7.84 (m, 1H), 7.80 – 7.77 (m, 2H), 7.71 (d, *J* = 6.9 Hz, 1H), 7.64 – 7.53 (m, 6H), 7.50 – 7.45 (m, 2H), 7.37-7.33 (m, 1H), 6.92 (td, *J* = 6.8, 1.2, Hz 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.6, 141.6, 133.3, 132.6, 132.2, 131.2, 130.1, 129.7, 129.6, 128.4, 128.0, 127.9, 126.8, 126.7, 126.5, 125.9, 125.8, 124.2, 121.6, 117.3, 113.2 ppm; MS: *m/z* (%) = 320 [*M*⁺, 100%]; Anal. calcd. for C₂₃H₁₆N₂: C, 86.22; H, 5.03; N, 8.74 Found: C, 86.49; H, 5.41; N, 8.66.

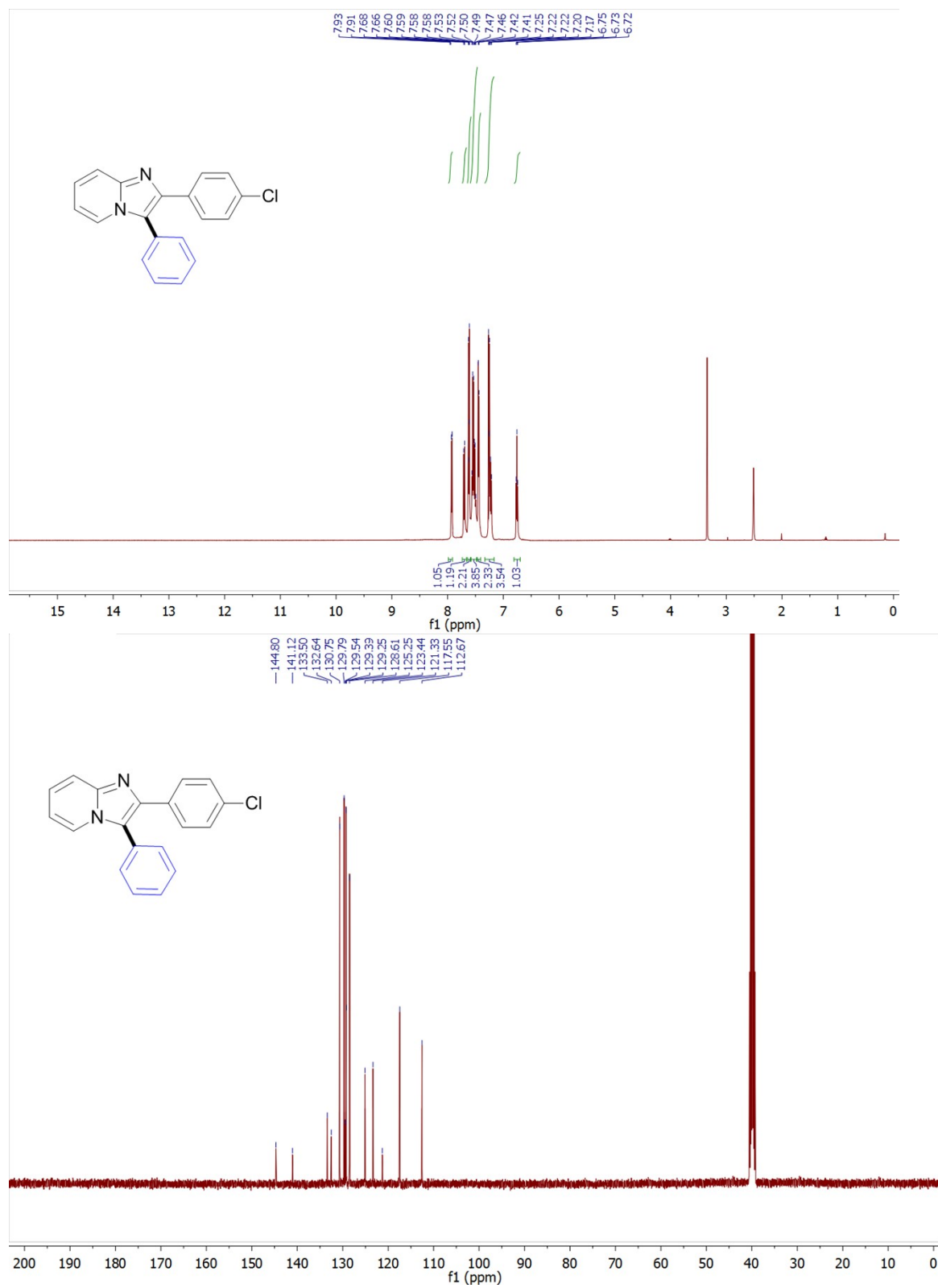
5.17. 3-(4-bromophenyl)-2-phenylimidazo[1,2-*a*]pyridine (3q)

White crystal; Yield: 54% (18 mg); m.p. 156-158 °C. IR KBr: 3046, 2922, 1346, 1067, 737, 695 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 7.91 (d, *J* = 6.9 Hz, 1H), 7.64 (d, *J* = 7.6 Hz, 1H), 7.52 – 7.47 (m, 5H), 7.42 – 7.37 (m, 4H), 7.20 -7.17 (m, 1H), 6.71 (td, *J* = 6.8, 1.2 Hz, 1H); ¹³C NMR (100 MHz, DMSO-*d*₆) δ 144.9, 141.3, 133.3, 131.5, 130.7, 130.2, 129.7, 129.6, 129.2, 124.9, 123.4, 121.5, 121.3, 117.6, 112.5 ppm; MS: *m/z* (%) = 350 [*M*⁺+2, 50%], 348 [*M*⁺, 50%]; Anal. calcd. for C₁₉H₁₃BrN₂: C, 65.35; H, 3.75; N, 8.02 Found: C, 65.60; H, 3.54; N, 7.82.

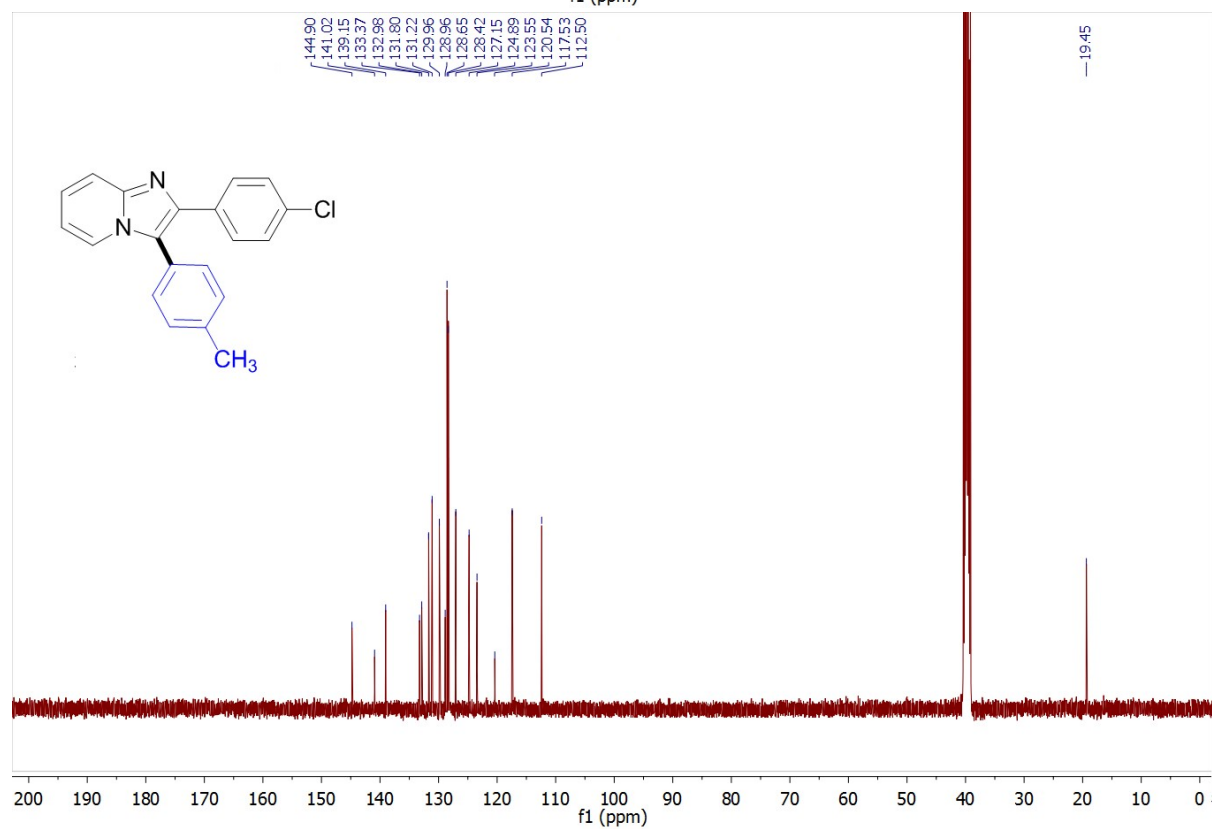
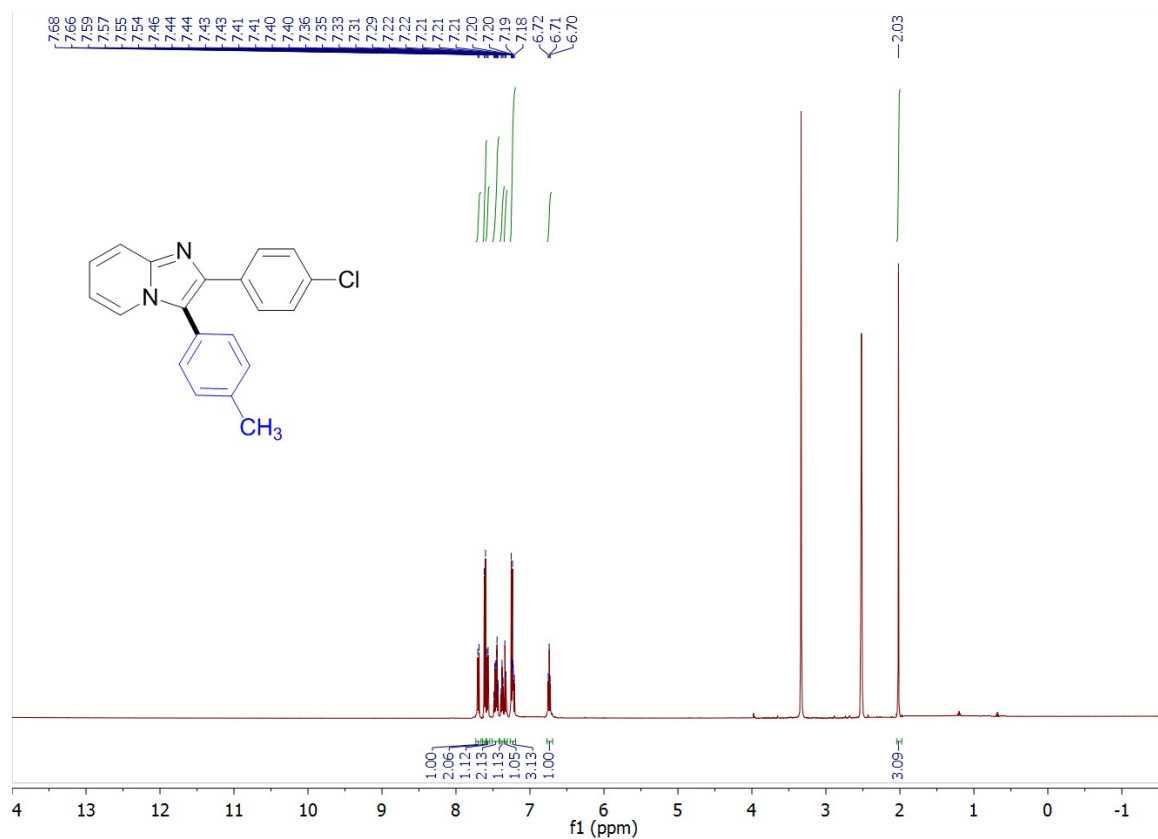
⁹ S. Jana, S. Samanta, A. K. Bagdi, V. Z. Shirinian and A. Hajra, *RSC Adv.*, (2018, 8, 12360.

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

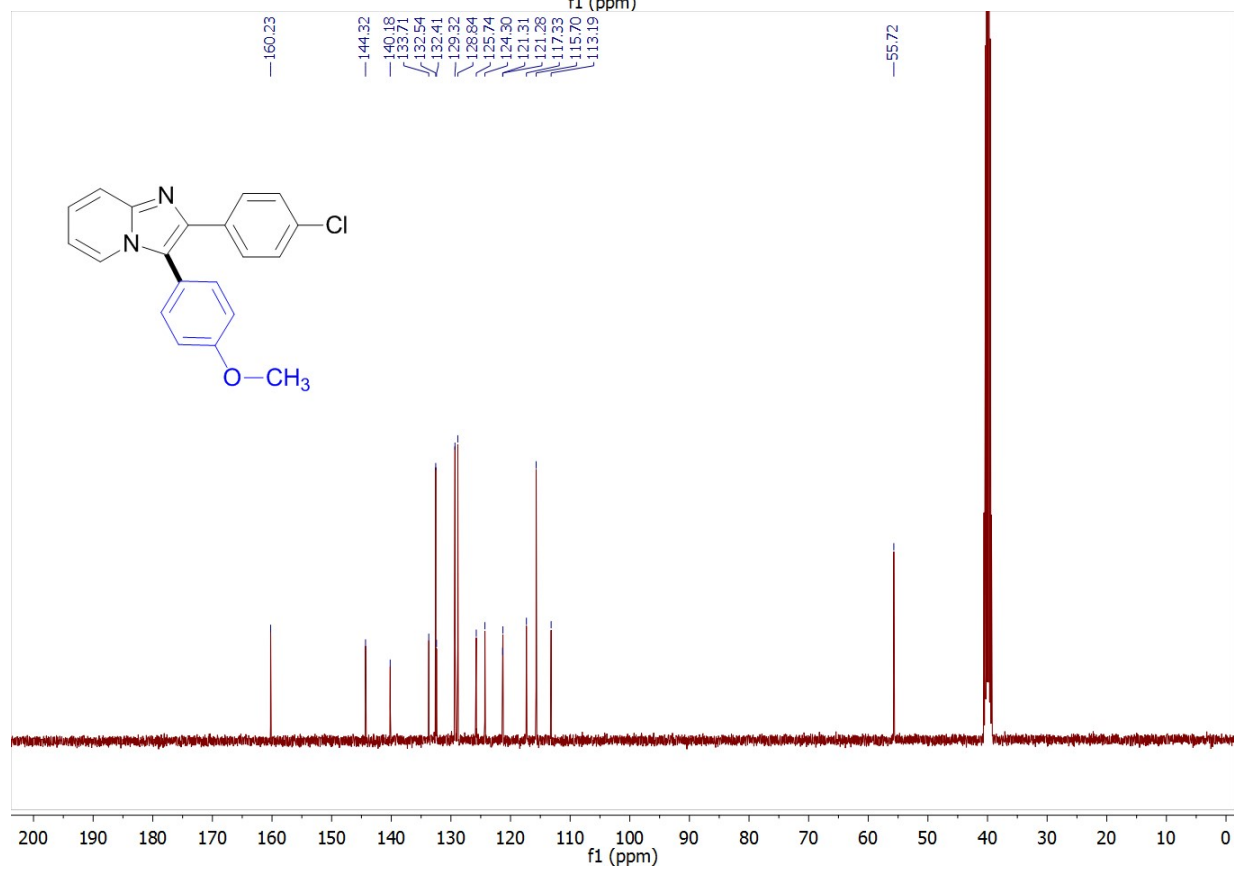
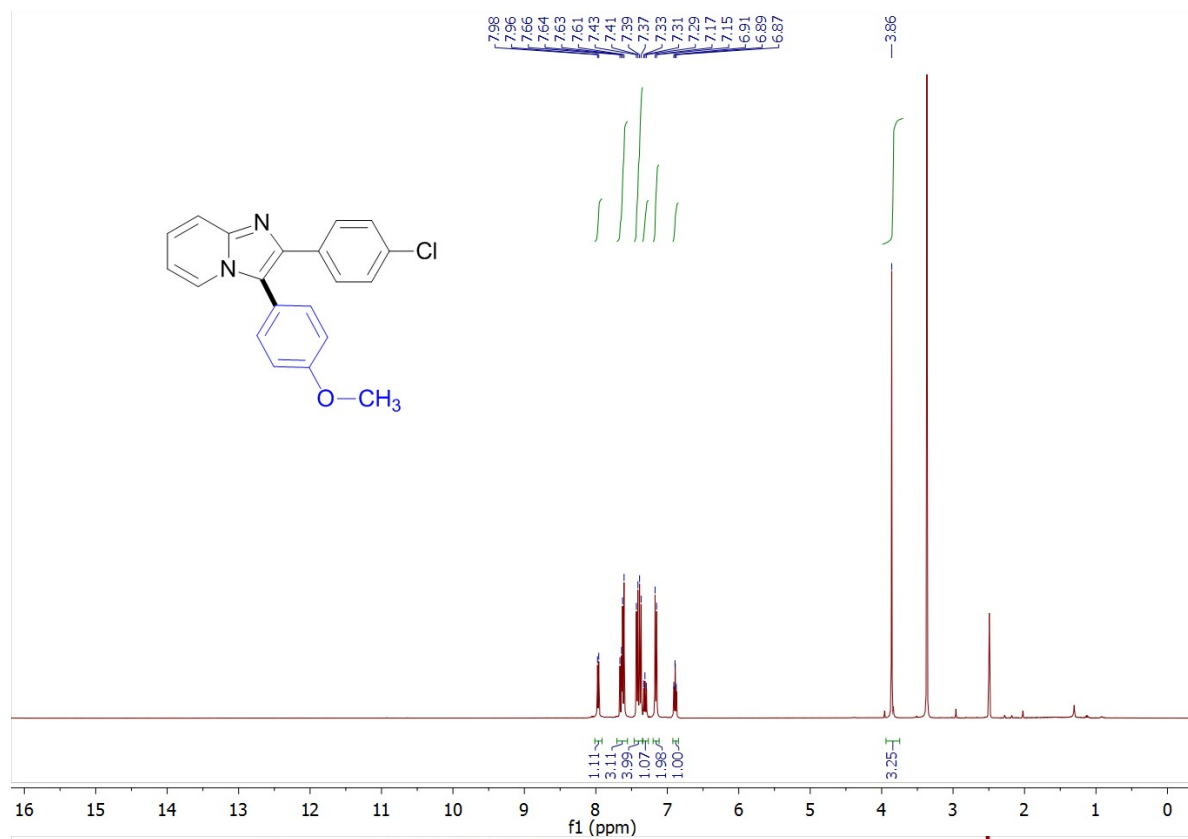
2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyridine (3a)



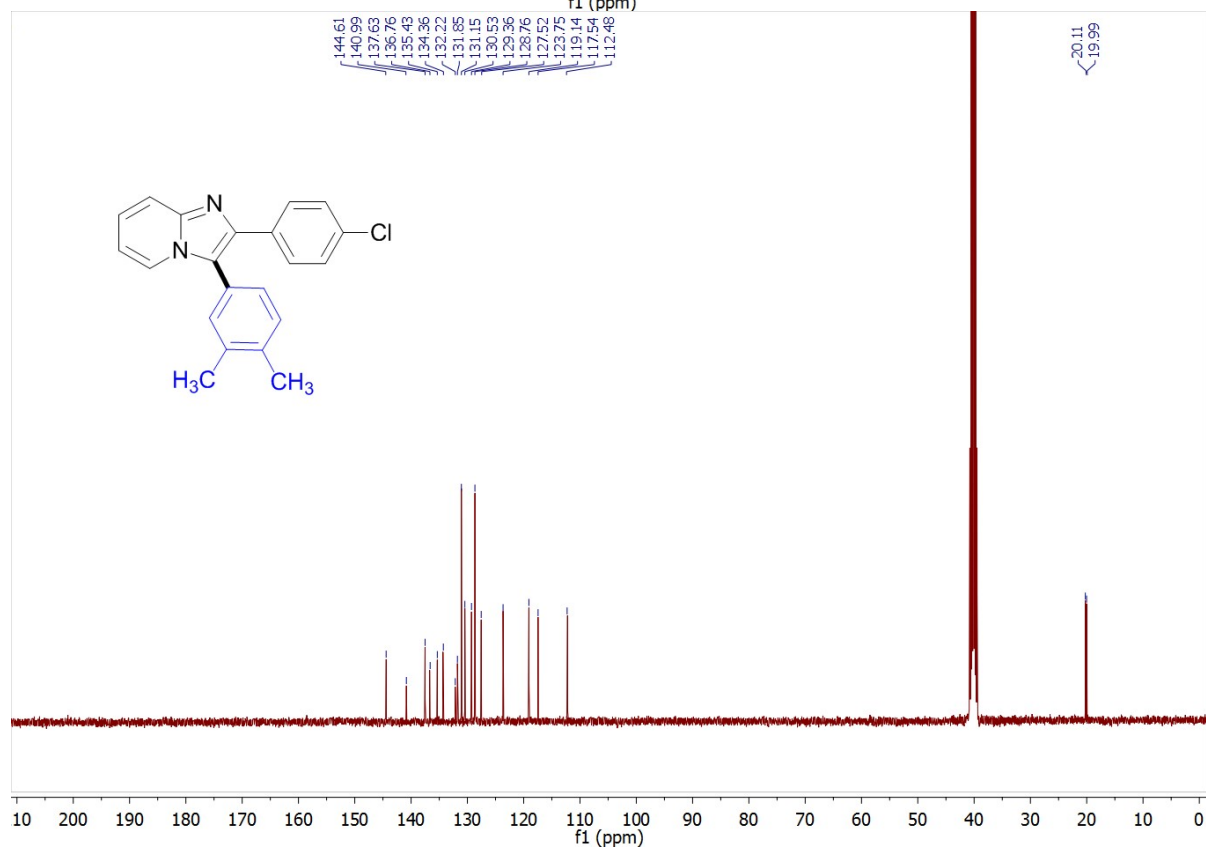
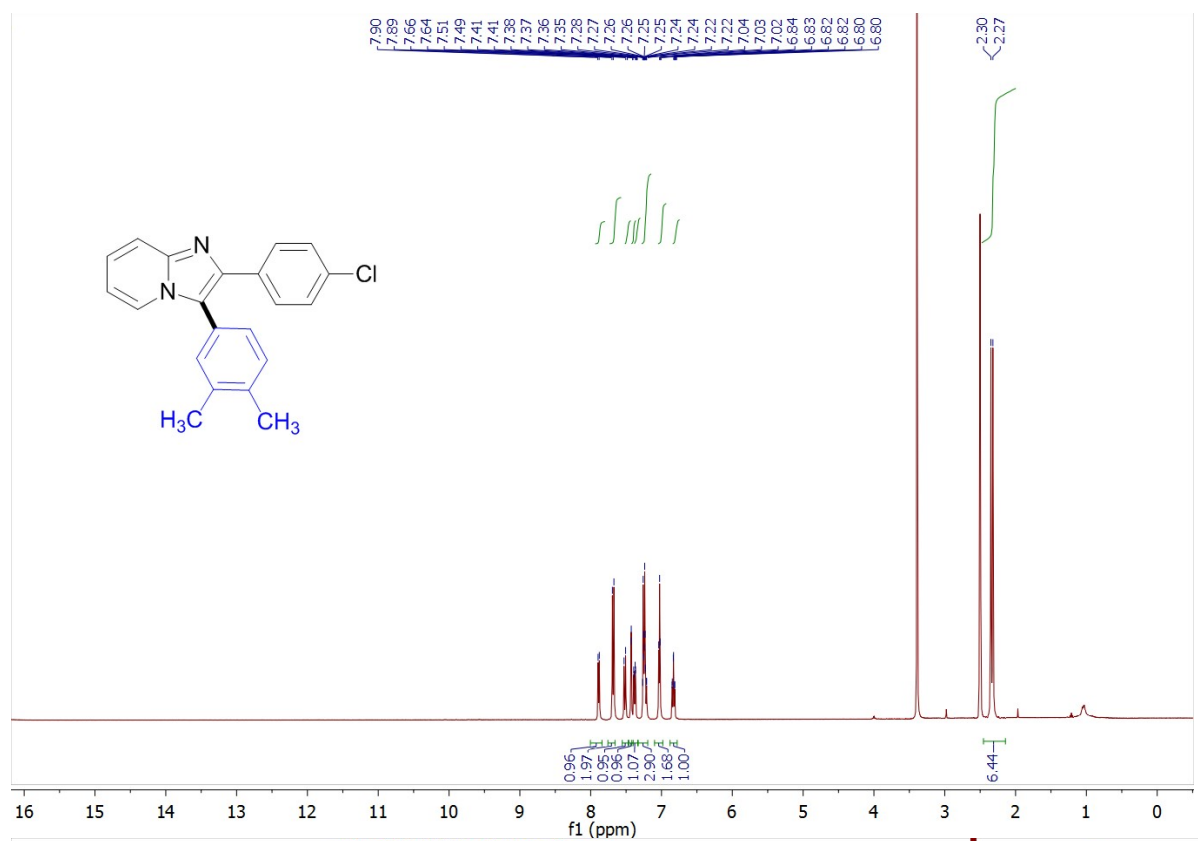
2-(4-chlorophenyl)-3-(*p*-tolyl)imidazo[1,2-*a*]pyridine (3b)



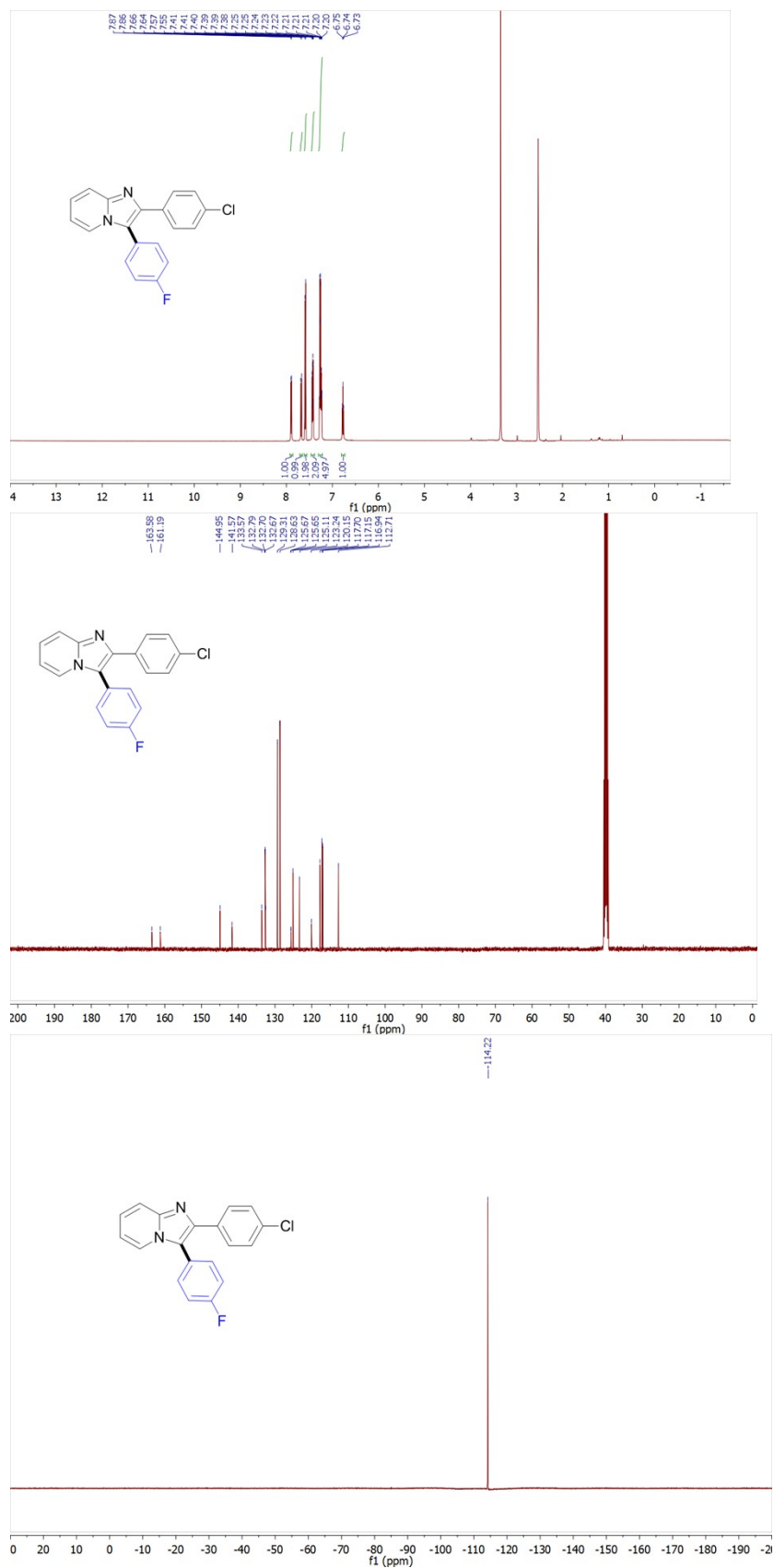
2-(4-chlorophenyl)-3-(4-methoxyphenyl)imidazo[1,2-a]pyridine (3c)



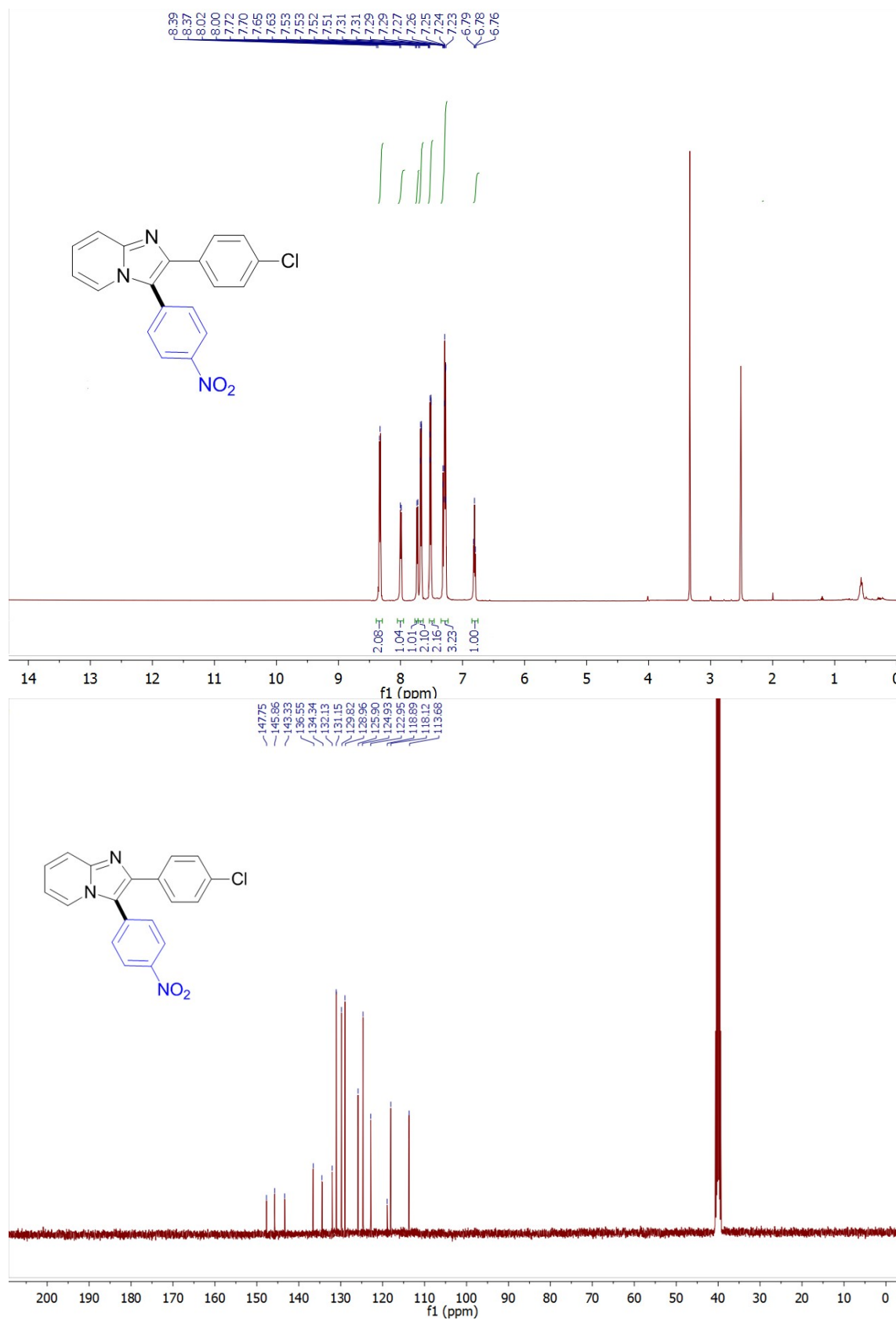
2-(4-chlorophenyl)-3-(3,4-dimethoxyphenyl)imidazo[1,2-a]pyridine (3d)



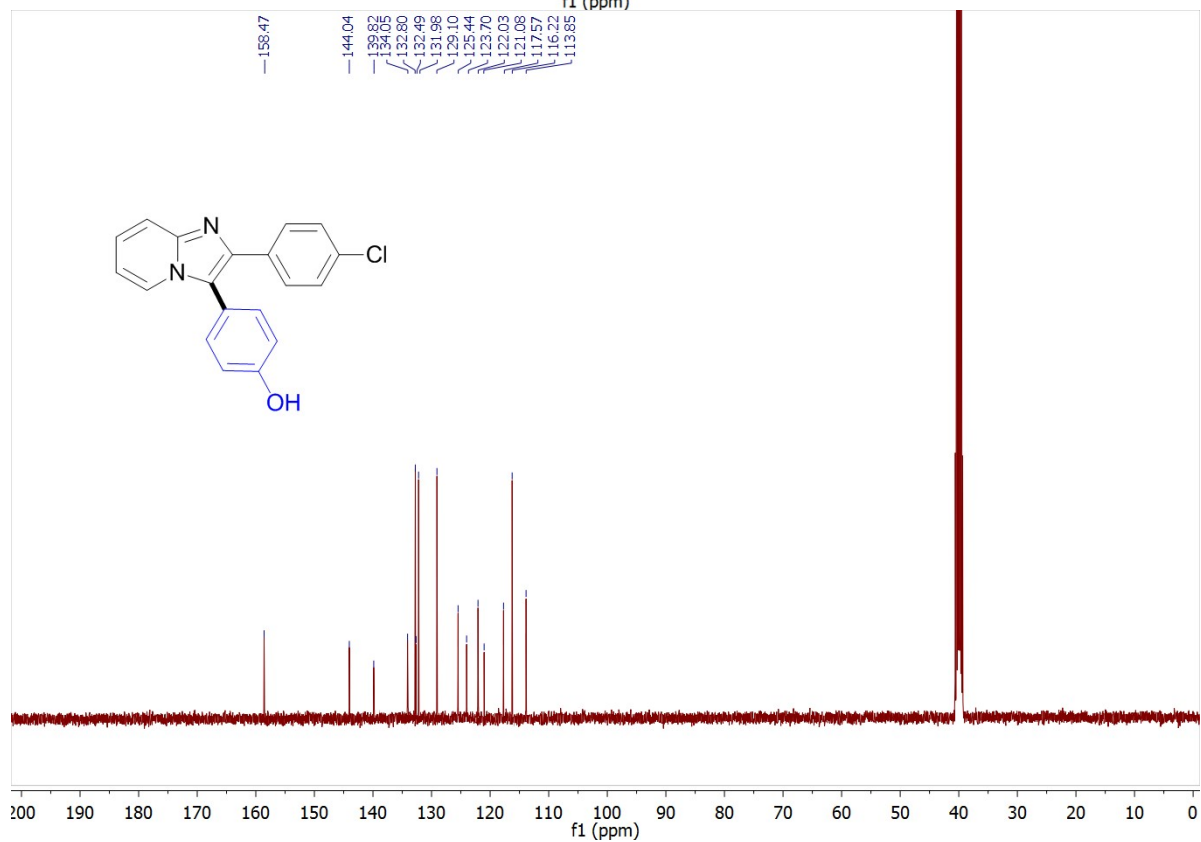
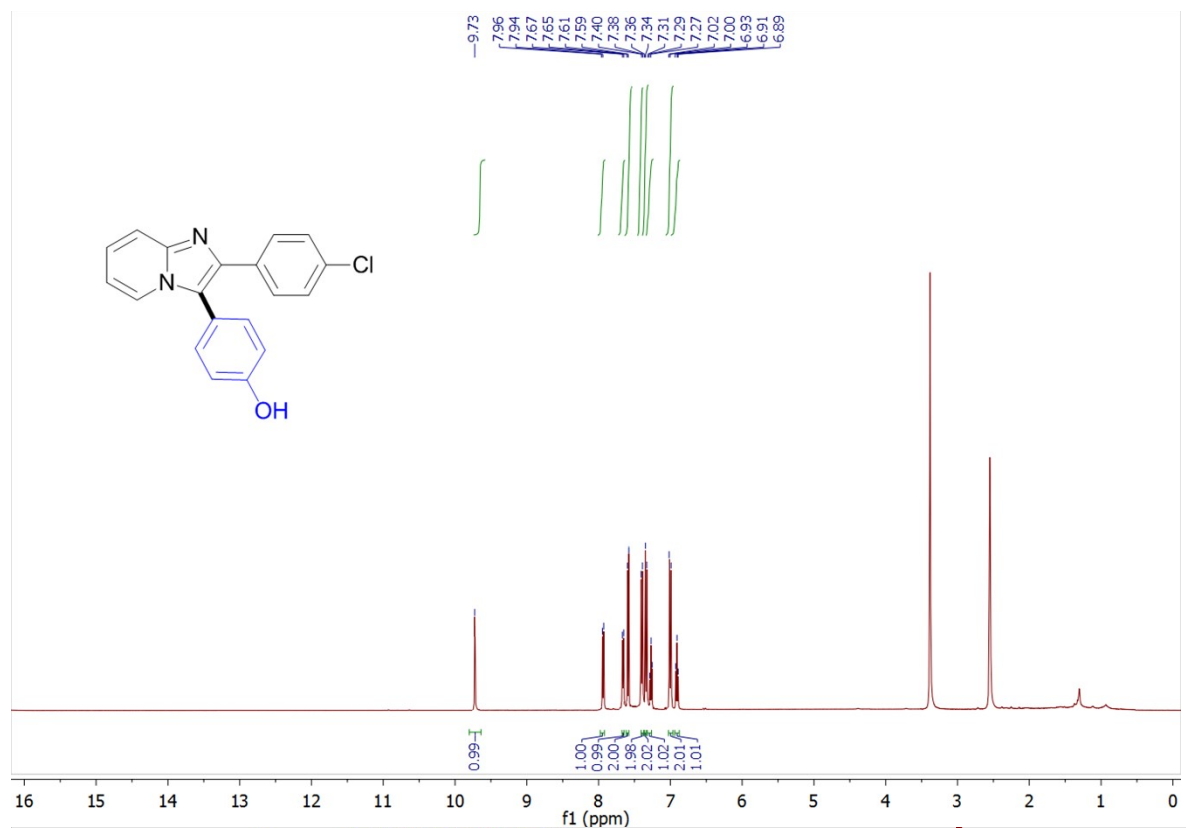
2-(4-chlorophenyl)-3-(4-fluorophenyl)imidazo[1,2-a]pyridine (3e)



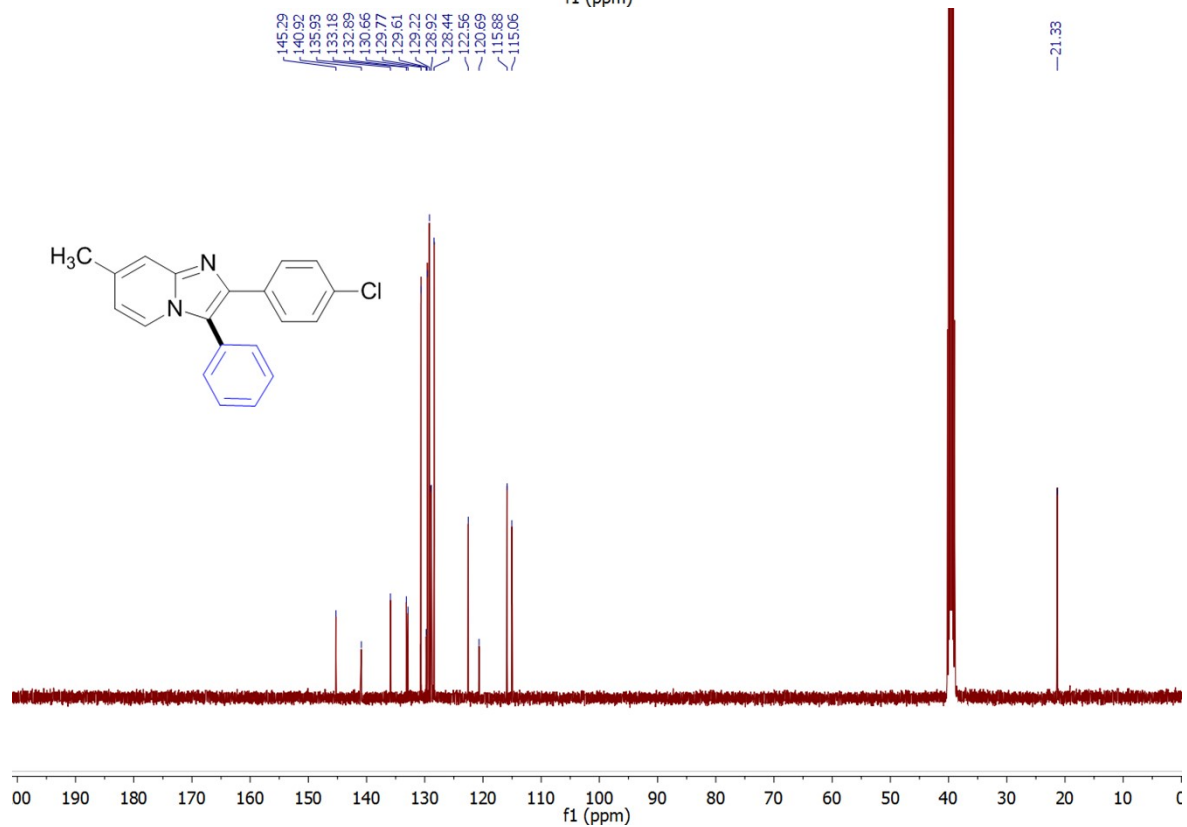
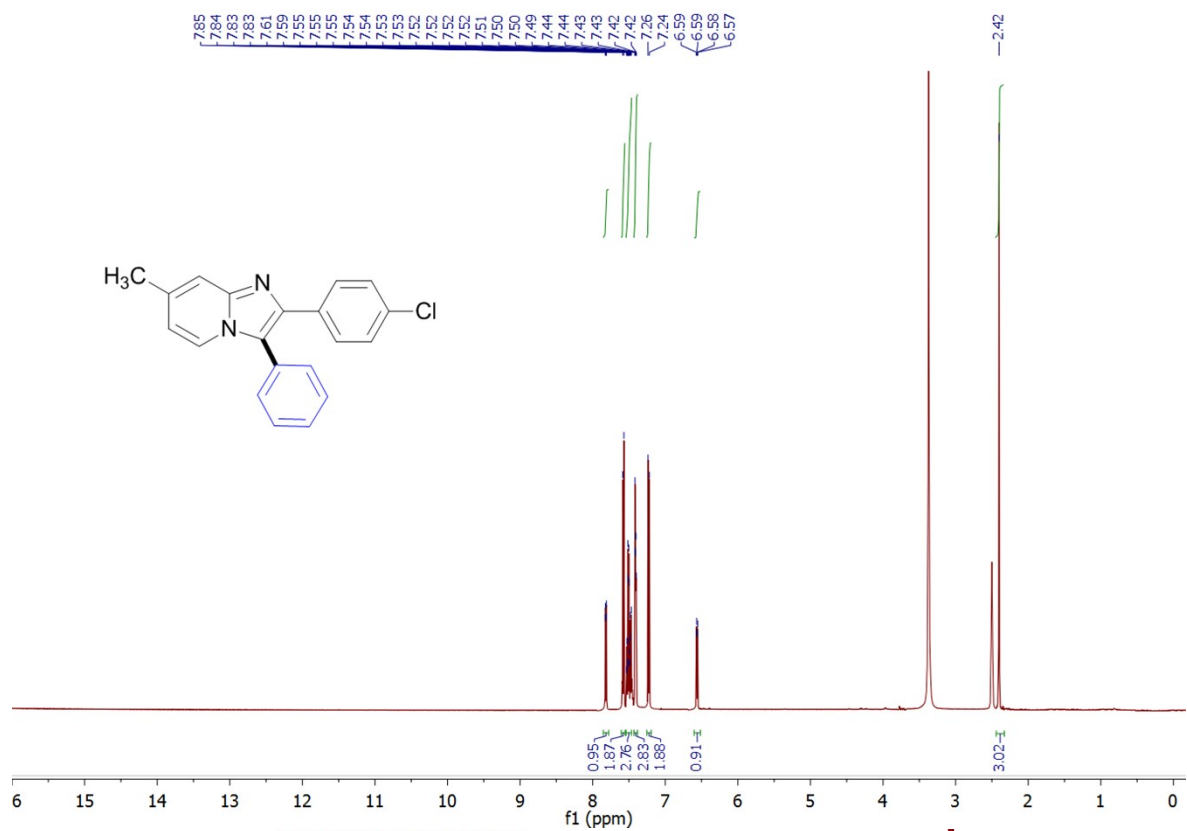
2-(4-chlorophenyl)-3-(4-nitrophenyl)imidazo[1,2-*a*]pyridine (3f)



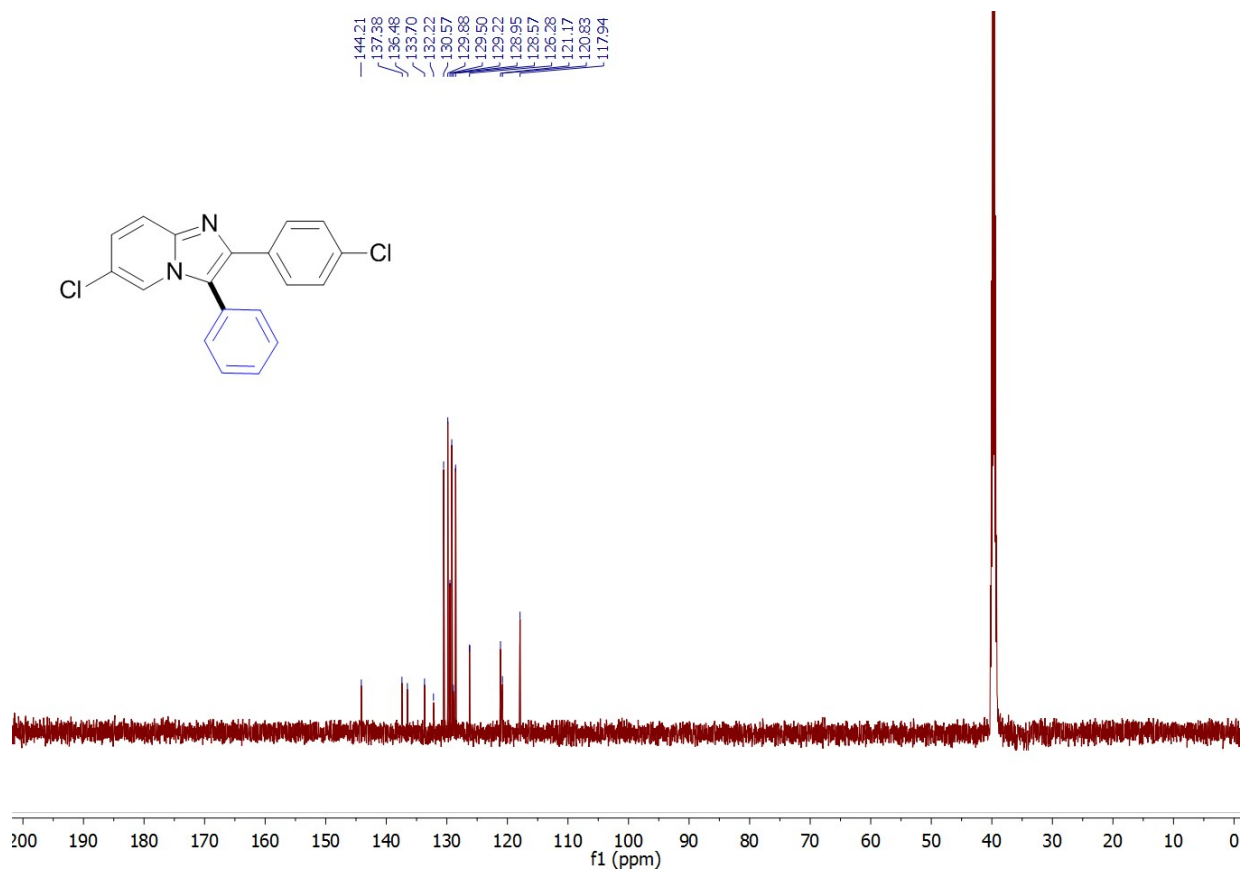
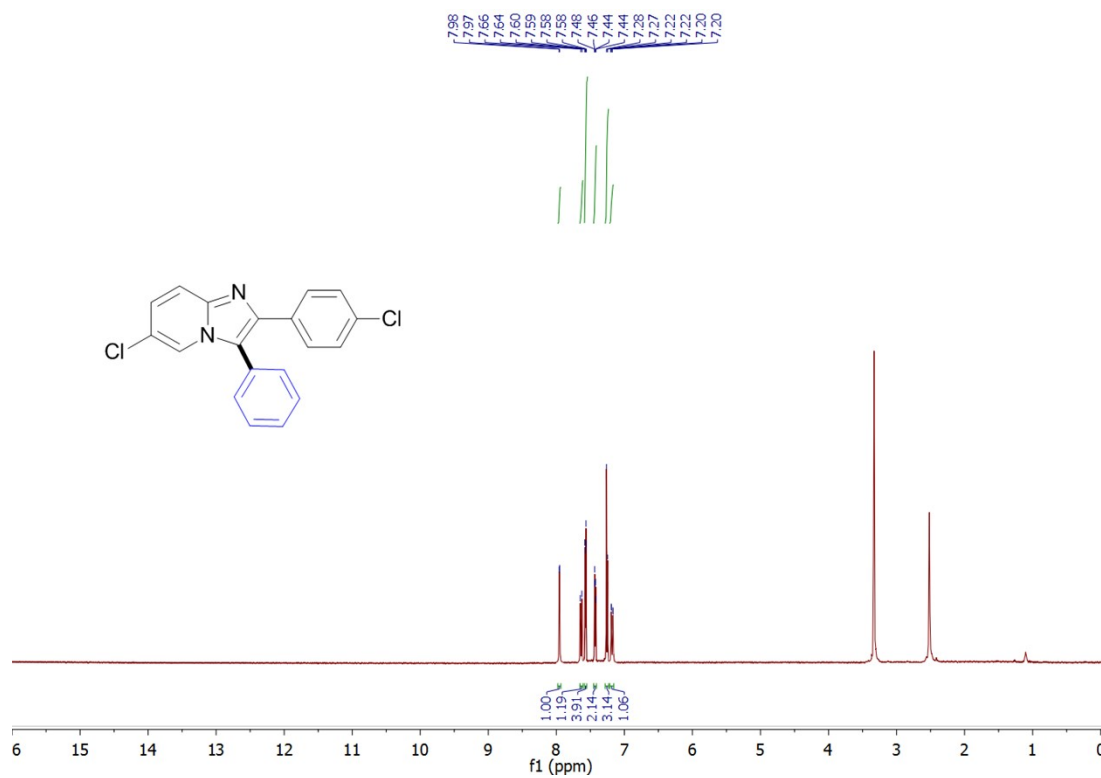
2-(4-chlorophenyl)-3-(4-hydroxy)imidazo[1,2-a]pyridine (3g)



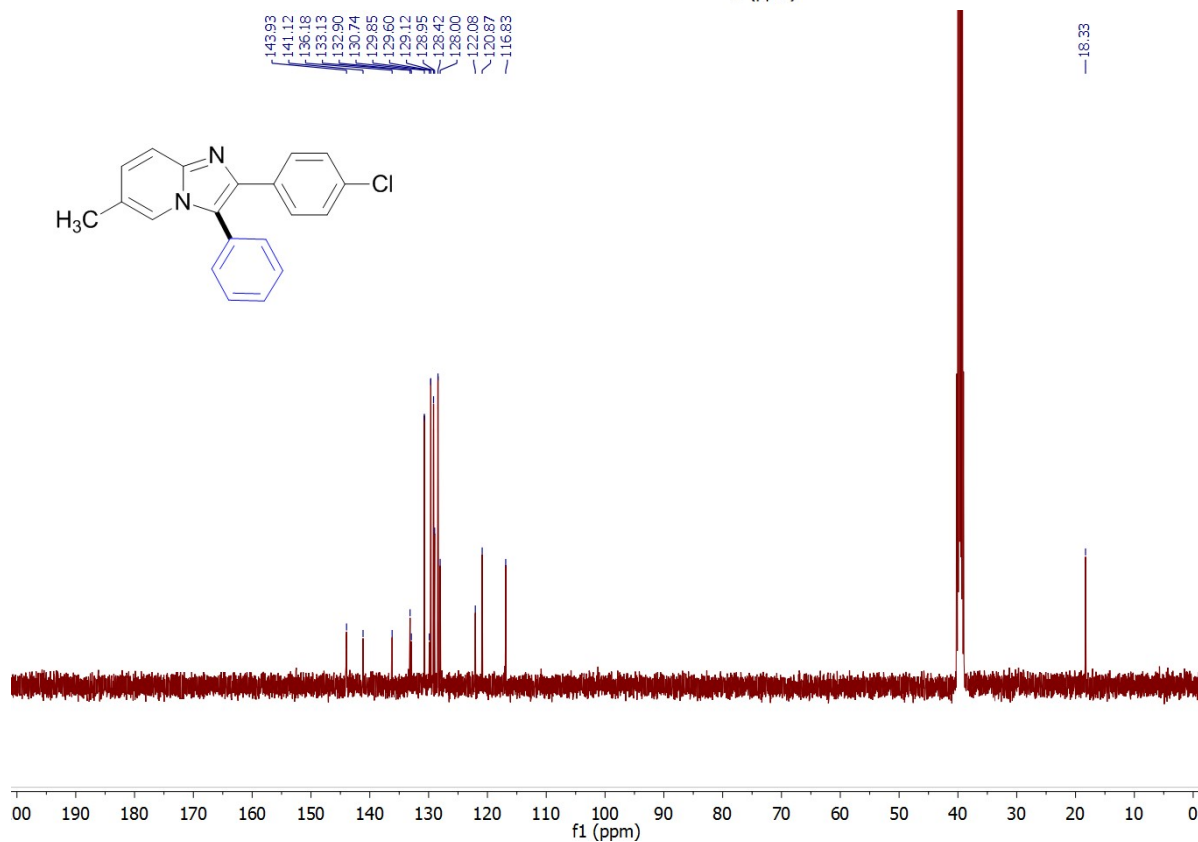
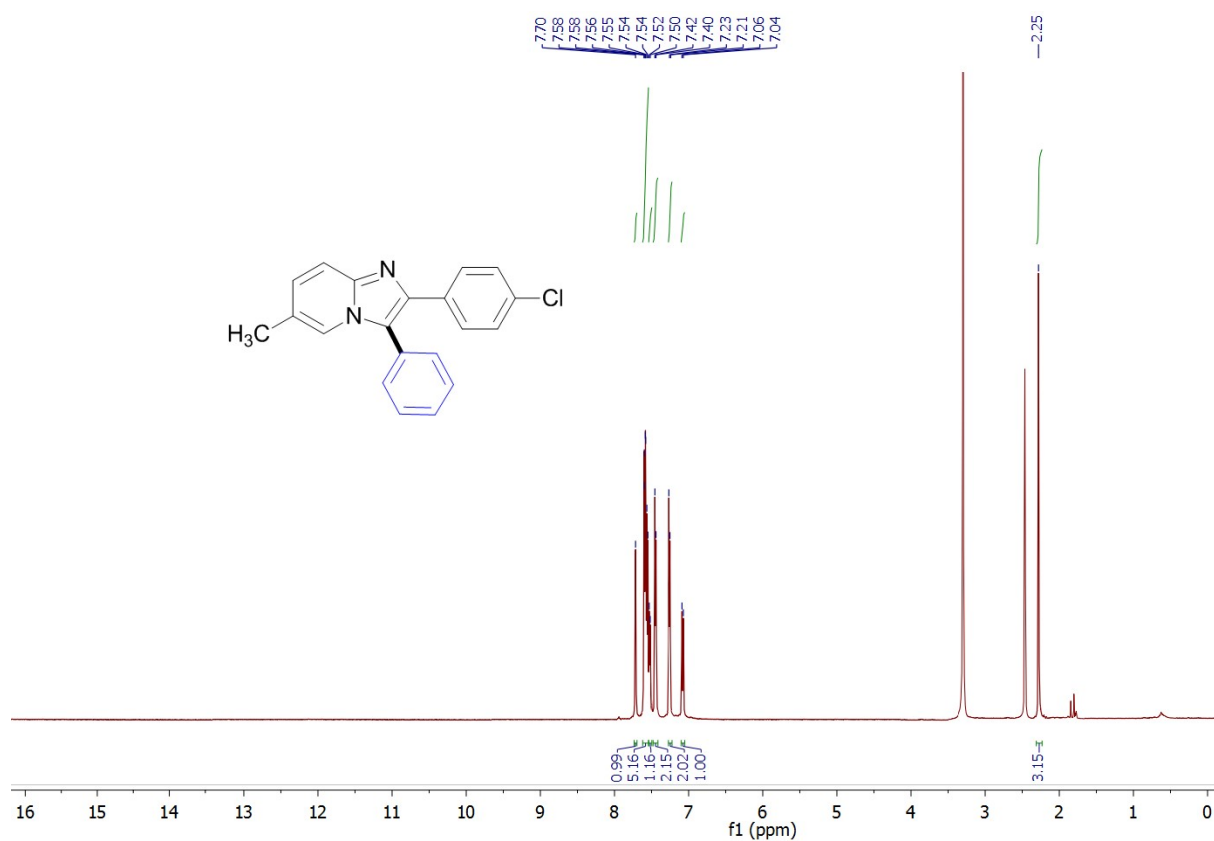
2-(4-chlorophenyl)-7-methyl-3-phenylimidazo[1,2-a]pyridine (3h)



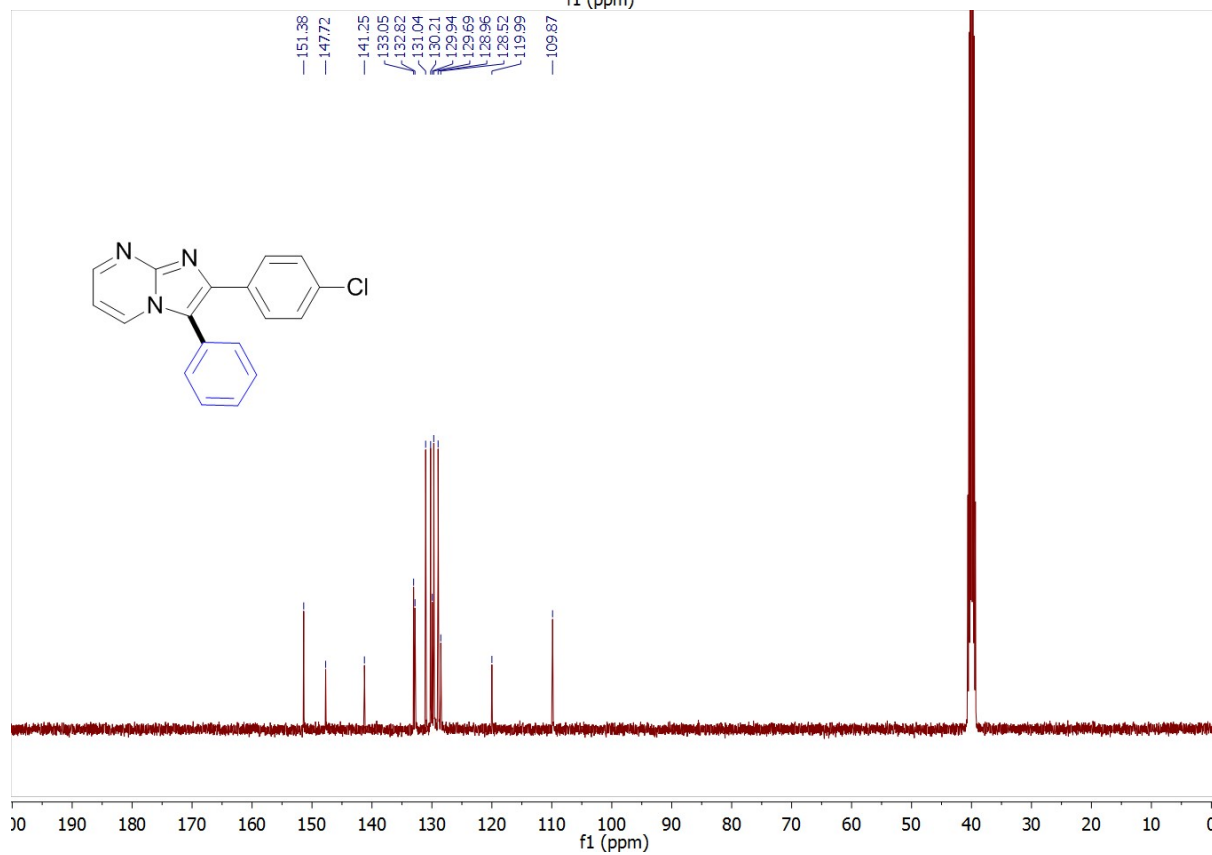
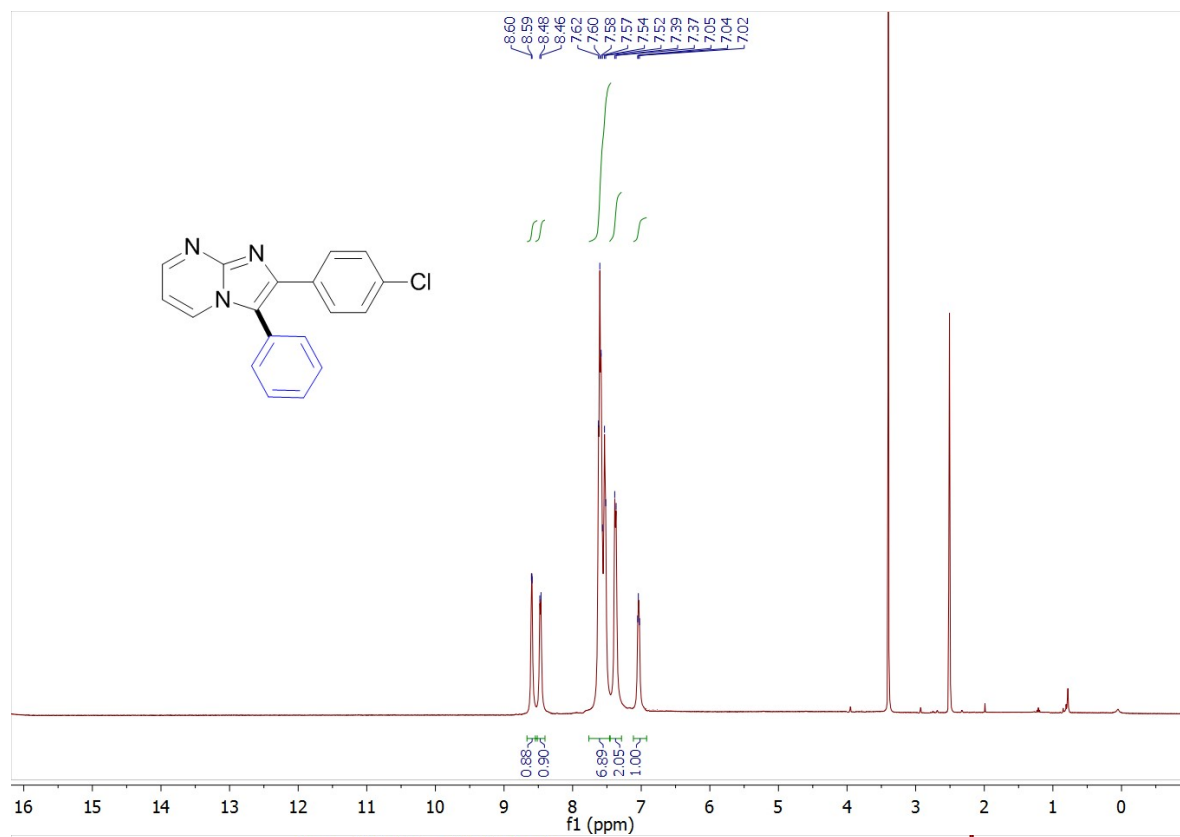
6-chloro-2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyridine (3i)



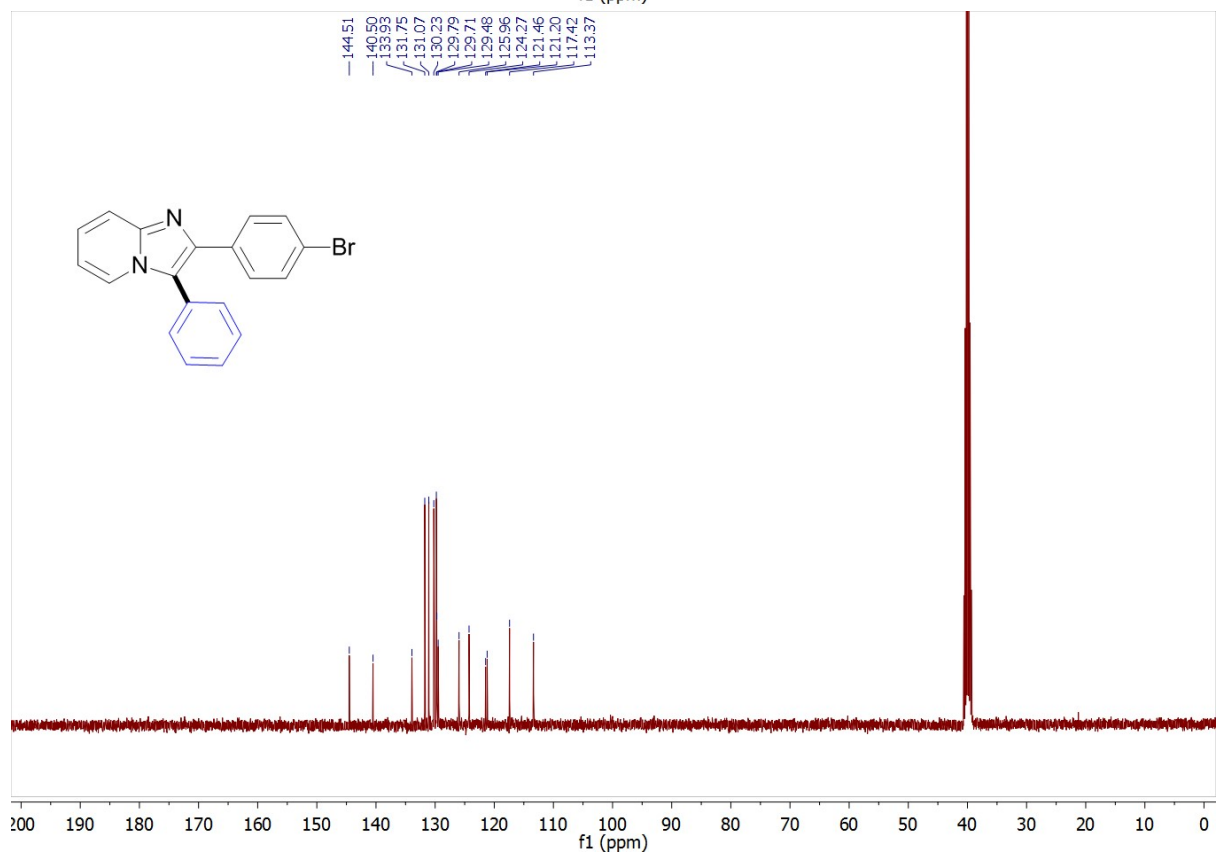
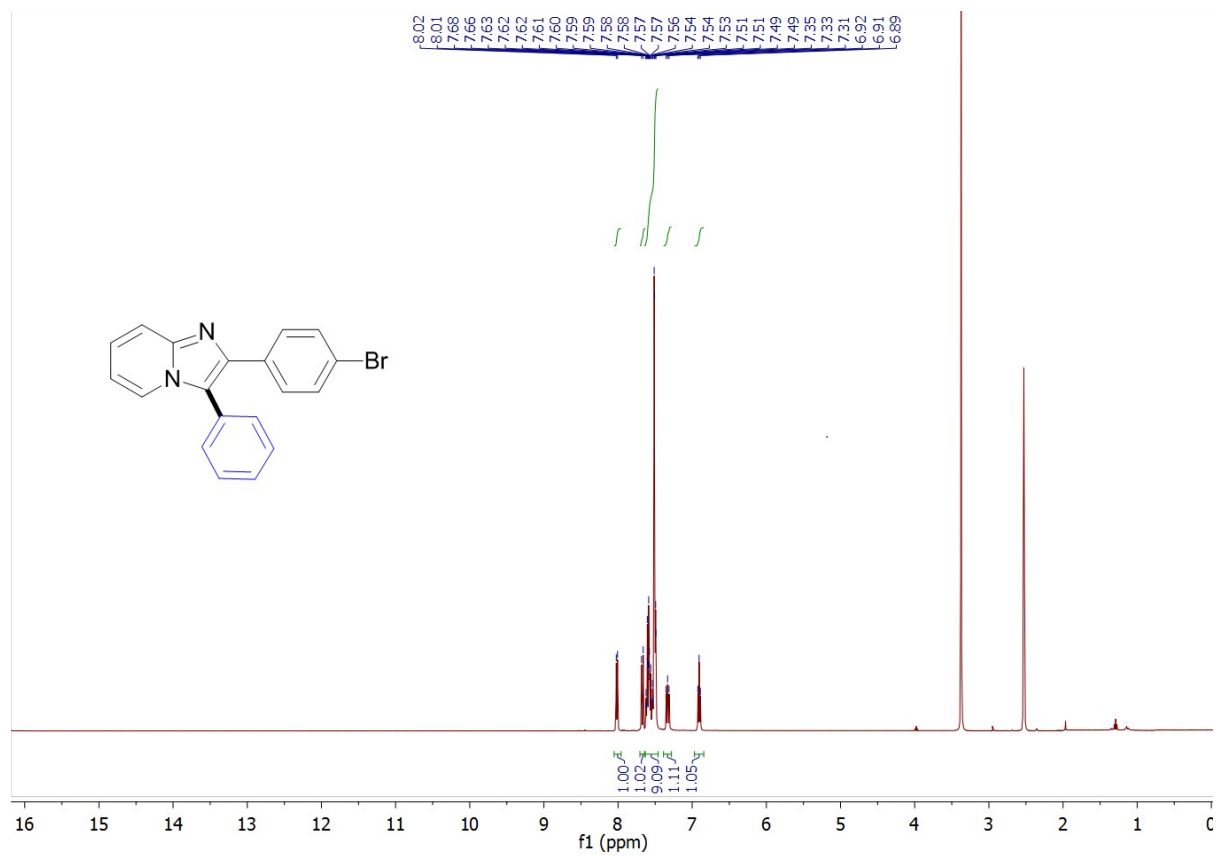
2-(4-chlorophenyl)-6-methyl-3-phenylimidazo[1,2-*a*]pyridine (3j)



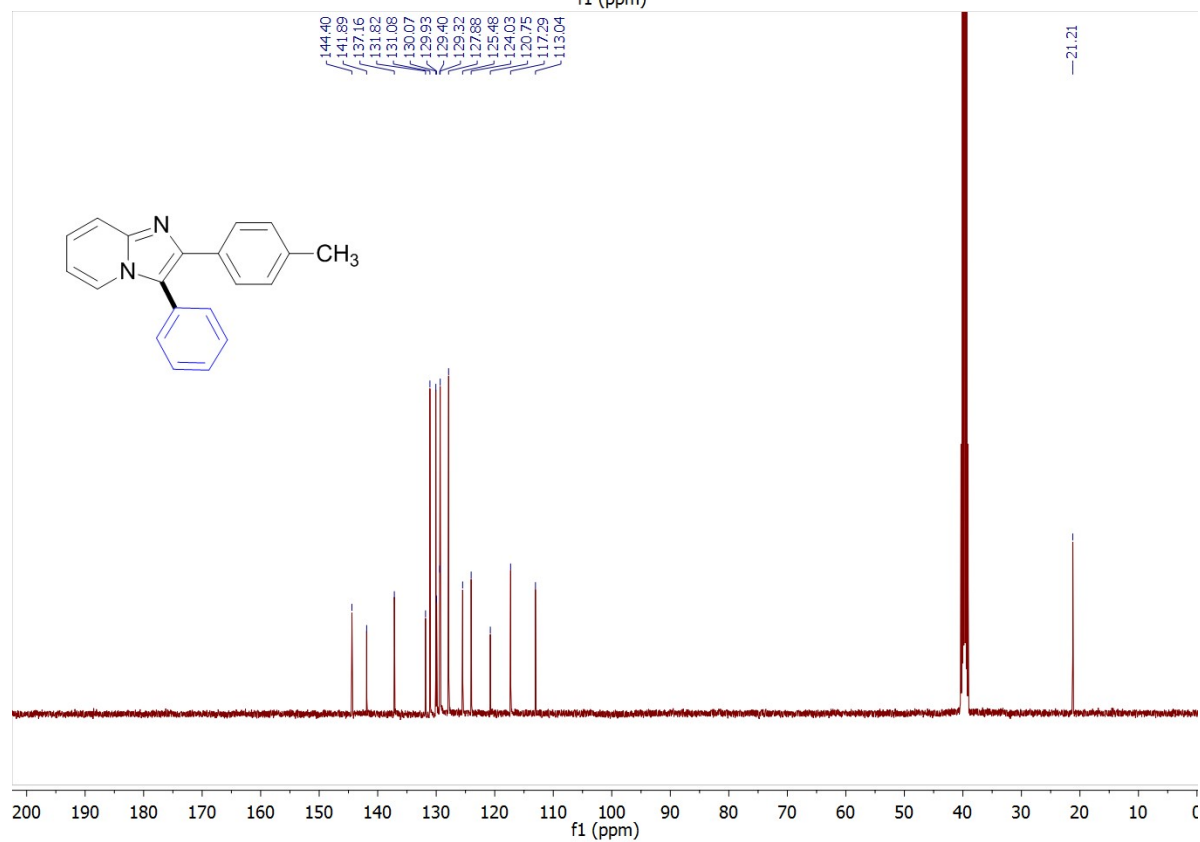
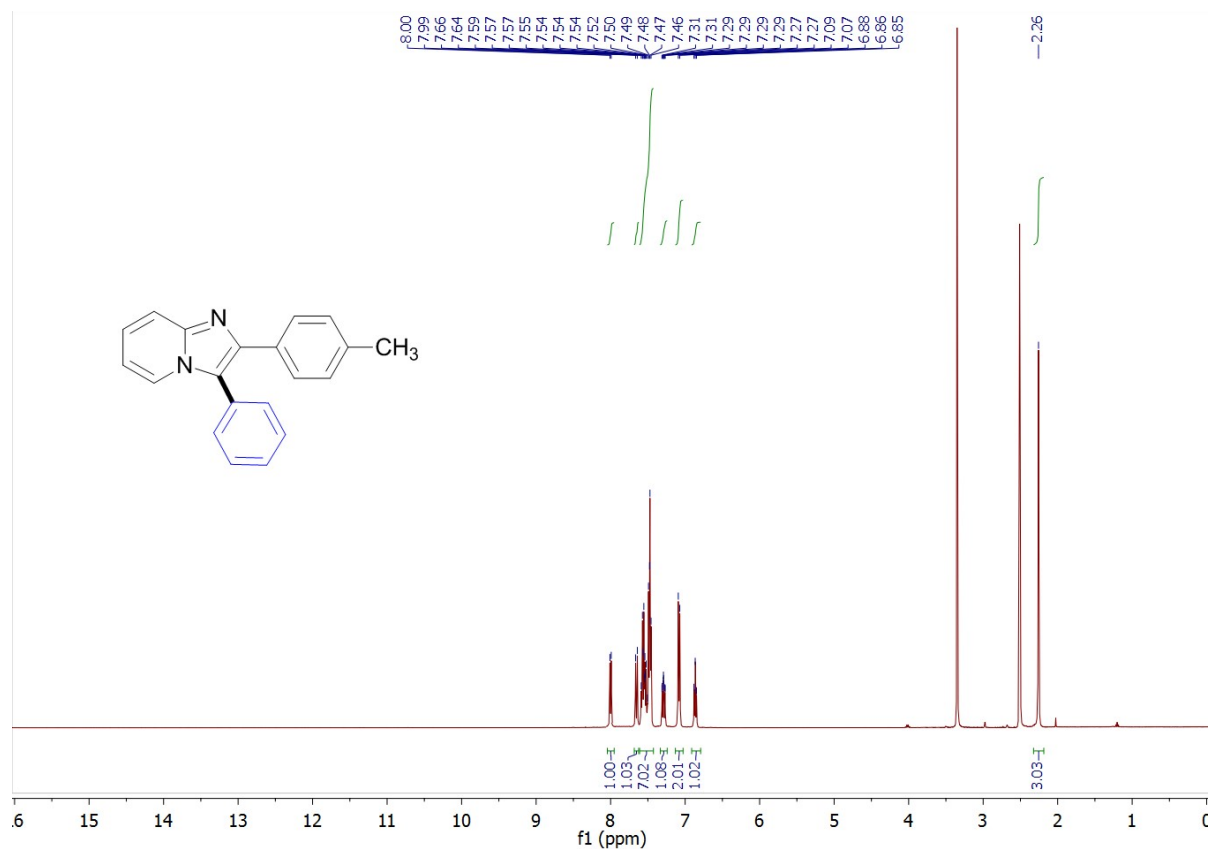
2-(4-chlorophenyl)-3-phenylimidazo[1,2-*a*]pyrimidine (3k)



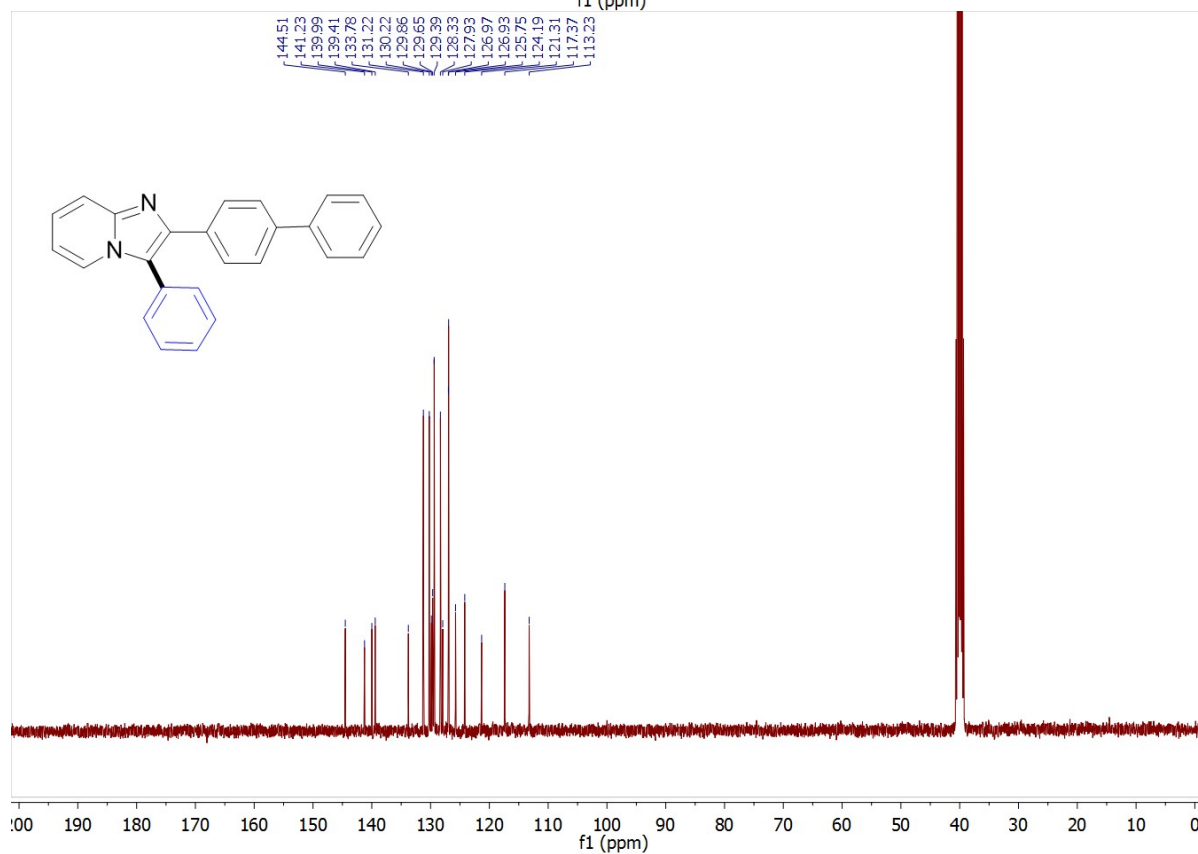
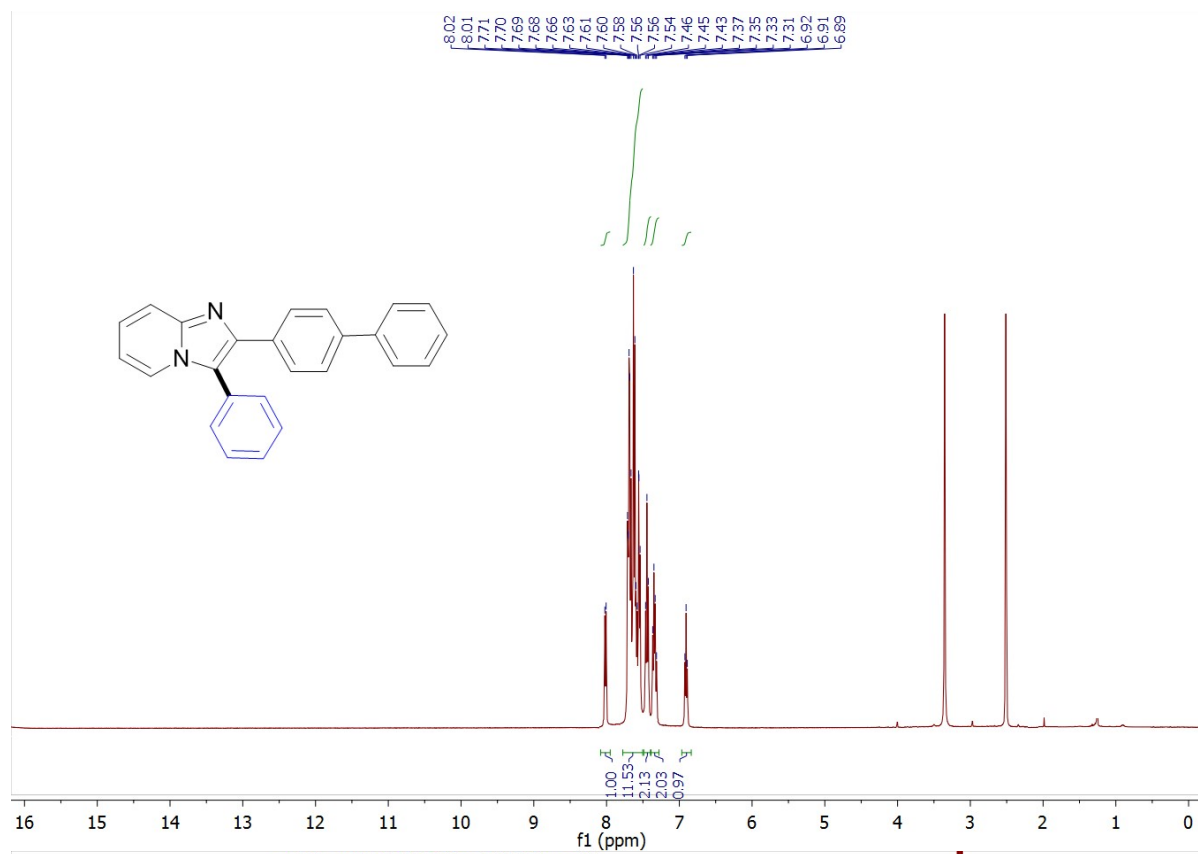
2-(4-bromophenyl)-3-phenylimidazo[1,2-a]pyridine (3l)



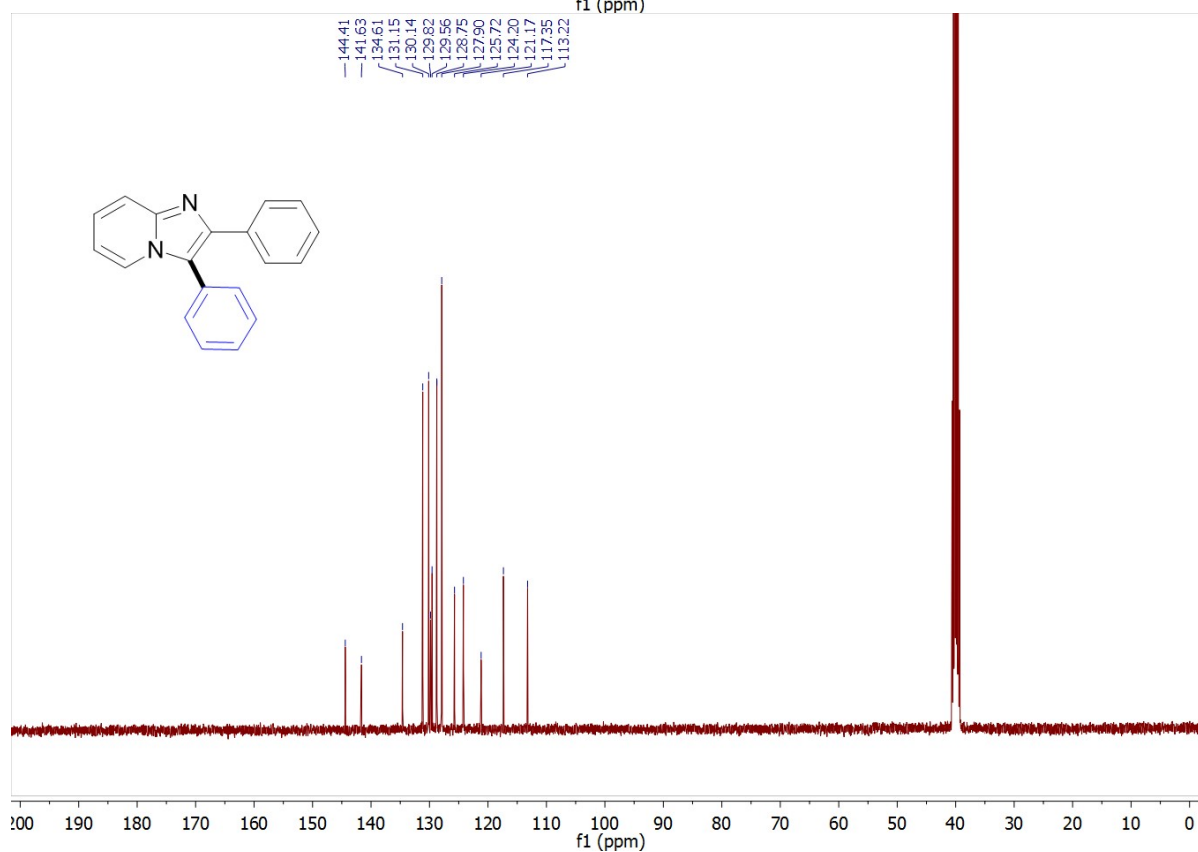
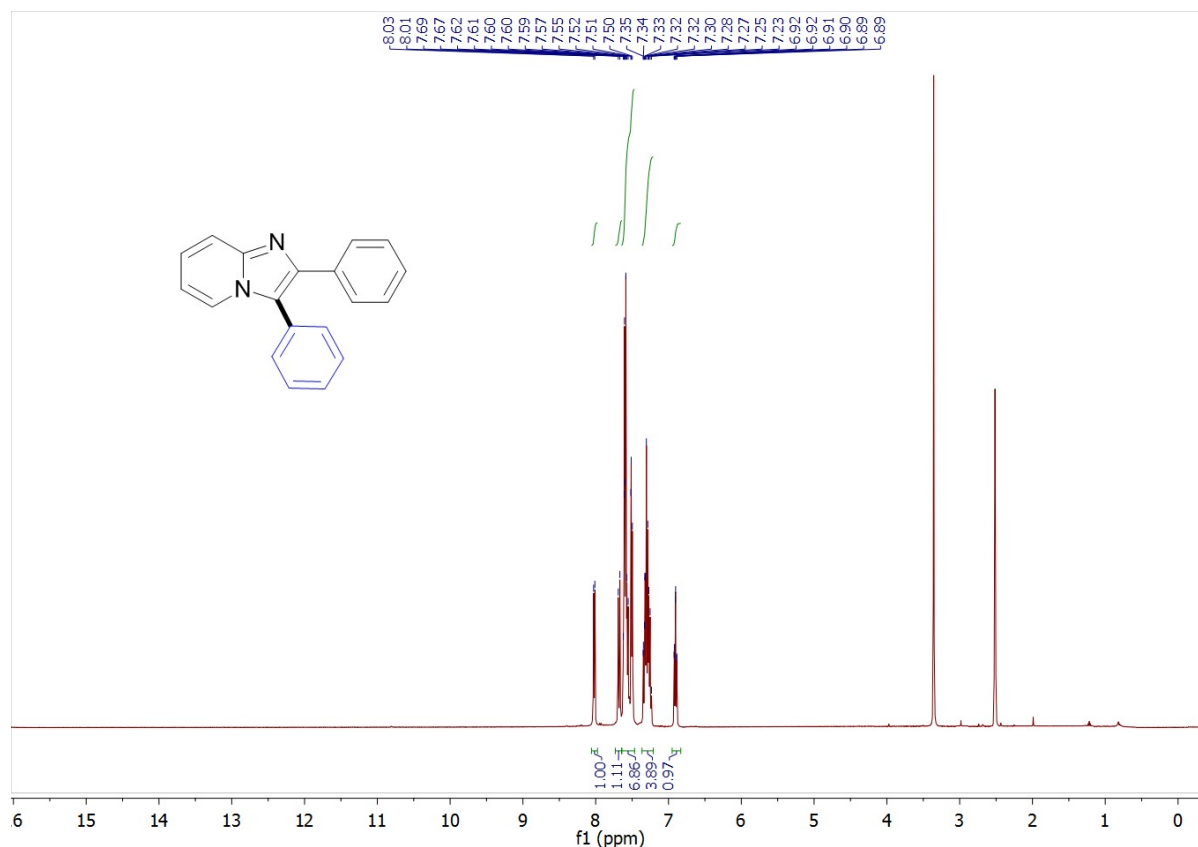
3-phenyl-2-(*p*-tolyl)imidazo[1,2-*a*]pyridine (3m)



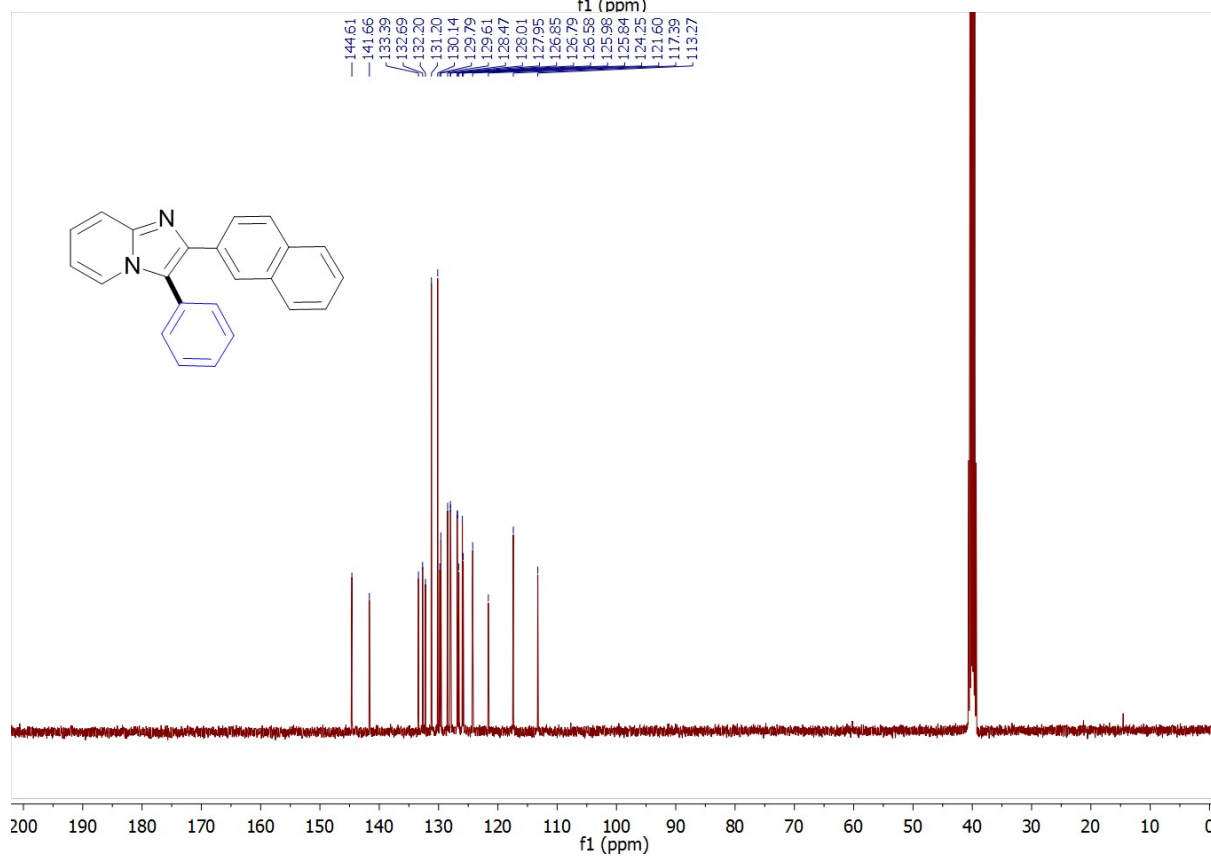
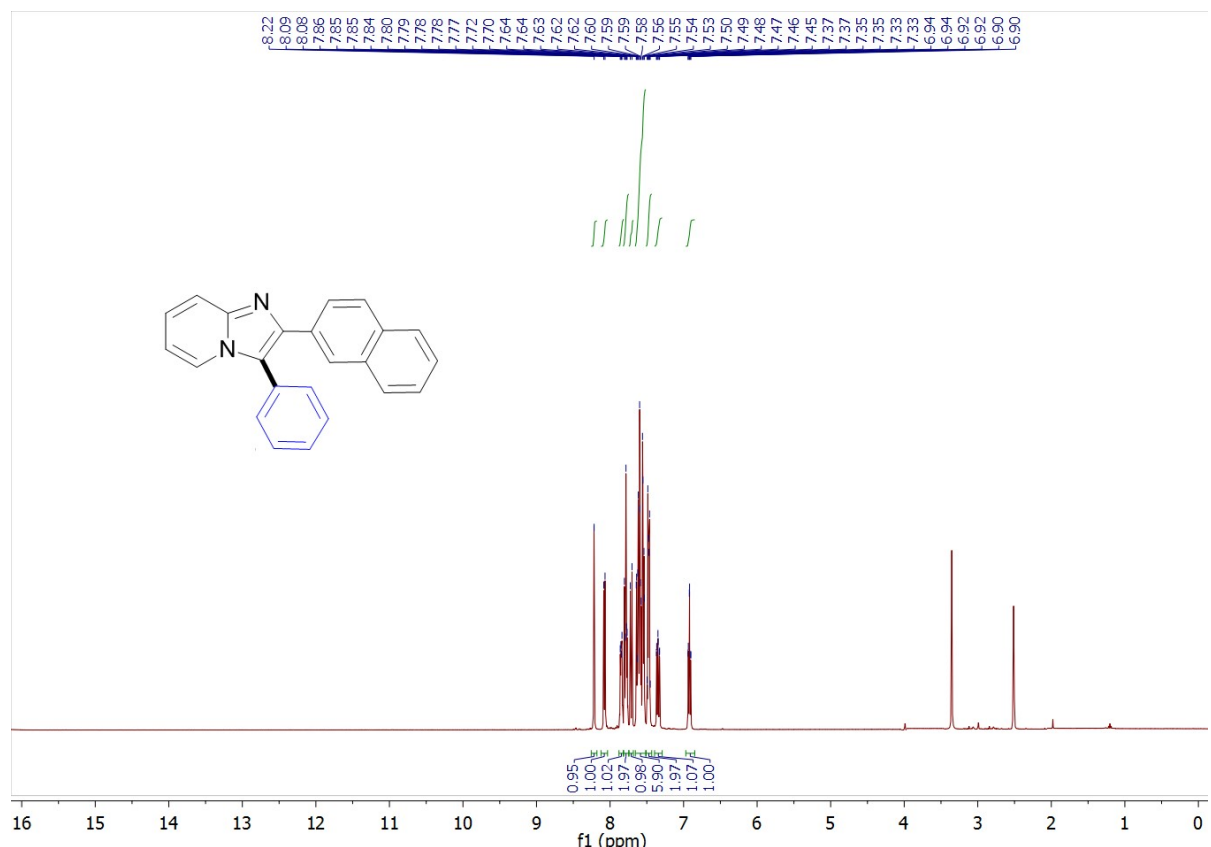
2-([1,1'-biphenyl]-4-yl)-3-phenylimidazo[1,2-a]pyridine (3n)



2,3-diphenylimidazo[1,2-*a*]pyridine (3o)



2-(naphthalen-2-yl)-3-phenylimidazo[1,2-a]pyridine (3p)



3-(4-bromophenyl)-2-phenylimidazo[1,2-a]pyridine (3q)

