

Supporting Information

Direct synthesis of 2-substituted benzimidazoles via dehydrogenative coupling of aromatic-diamine and primary alcohol catalyzed by Co Complex

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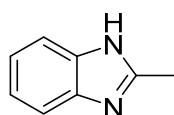
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General Information

All starting materials were purchased from TCI; the reagents were obtained from J&K Chemical Company and used without further purification unless specified. The dehydrogenative coupling reactions were monitored by thin layer chromatography (TLC), and the products were purified by column chromatography on silica gel (300 ~ 400 mesh). ¹H NMR and ¹³C NMR spectra were recorded on a Bruker Ultrashield™ 400 spectrometer operating at 400 MHz and 100 MHz in DMSO-*d*₆ or Chloroform. Chemical shifts were reported in ppm with tetramethylsilane (TMS) as internal standard. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, m = multiple. Coupling constants (*J*) are reported in Hertz (Hz). Melting points were recorded on a WRR melting point apparatus. Elemental analyses of C, H, N were performed on a Elementar Vario MICRO cube.

Characterization of the data

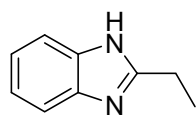
2-methyl-1*H*-benzo[*d*]imidazole^[1]



White solid, m.p.: 174-175°C, ¹H NMR (400 MHz, CDCl₃) δ = 7.55 (dd, *J* = 5.9, 3.2, 2H), 7.24-7.19 (m, 2H), 2.64 (s, 3H) (**Figure S1**). Anal. calcd for: C₈H₈N₂: C

72.70, H 6.10, N 21.20. Found: C 72.73, H 6.13, N 21.23.

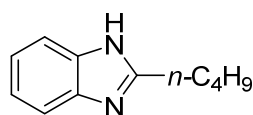
2-ethyl-1H-benzo[d]imidazole^[1]



White solid, m.p.: 168-170°C, ¹H NMR (400 MHz, CDCl₃) δ = 8.10 (s, 1H), 7.38 – 7.65 (m, 4H), 3.56 (dt, *J* = 14.7, 7.1 Hz, 2H), 2.47 (s, 6H) (**Figure S2**). ¹³C NMR (101 MHz, CDCl₃) δ = 157.3, 140.0, 126.6, 113.2, 113.1, 19.1, 12.7

(**Figure S3**). Anal.calcd for: C₉H₁₀N₂: C 73.94, H 6.89, N 19.16. Found: C, 73.97; H, 6.90; N, 19.18.

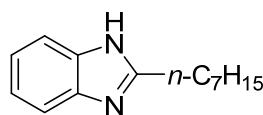
2-butyl-1H-benzo[d]imidazole^[2]



White solid, m.p.: 162-176°C, ¹H NMR (400 MHz, CDCl₃) δ = 7.68 – 7.59 (m, 1H), 7.21 – 7.06 (m, 4H), 2.79 – 2.67 (m, 2H), 1.80 (dt, *J* = 15.5, 7.7 Hz, 2H), 1.17 – 1.61 (m, 2H), 1.42 – 1.32 (m, 2H) (**Figure S4**). ¹³C NMR (101 MHz, CDCl₃) δ = 152.3, 132.3, 132.1, 127.6, 114.0, 29.0, 28.2,

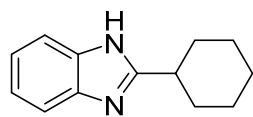
20.0, 13.6 (**Figure S5**). Anal.calcd for: C₁₁H₁₄N₂: C 75.82, H 8.10, N 16.08. Found: C 75.85, H 8.12, N 16.10.

Figure S4 2-hexyl-1H-benzo[d]imidazole^[1]



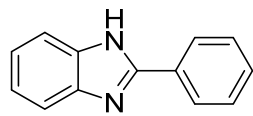
White solid, m.p.: 176-178°C, ¹H NMR (400 MHz, CDCl₃) δ = 7.63 (dd, *J* = 5.9, 3.1 Hz, 1H), 7.23 – 7.08 (m, 4H), 3.97 (t, *J* = 7.5 Hz, 2H), 2.78 – 2.73 (m, 2H), 1.80 (dt, *J* = 15.4, 7.7 Hz, 2H), 1.73-1.63 (m, 2H), 1.26 (dd, *J* = 7.0, 3.5 Hz, 4H), 0.89 (t, *J* = 7.3 Hz, 3H) (**Figure S6**). ¹³C NMR (101 MHz, CDCl₃) δ = 157.3, 138.0, 137.9, 121.8, 115.0, 31.2, 29.2, 29.1, 28.8, 25.0, 22.8, 14.1 (**Figure S7**). Anal.calcd for: C₁₄H₂₀N₂: C 77.73, H 9.32, N 12.95. Found: C 77.76, H 9.35, N 12.98.

2-cyclohexyl-1H-benzo[d]imidazole^[2]



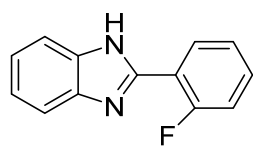
White solid, m.p.: 284-286°C, ¹H NMR (400 MHz, CDCl₃) δ = 12.11 (s, 1H), 7.60 (dd, *J* = 5.9, 3.2 Hz, 2H), 7.22-7.17 (m, 2H), 2.79 (tt, *J* = 10.8, 3.5 Hz, 1H), 2.00 (d, *J* = 8.3, 2H), 1.77 (d, *J* = 11.7, 2H), 1.72-1.51 (m, 3H), 1.46 – 1.15 (m, 3H) (**Figure S8**). ¹³C NMR (101 MHz, DMSO) δ = 157.4, 138.4, 137.1, 123.2, 122.9, 118.3, 114.7, 33.8, 29.9, 26.2, 26.0 (**Figure S9**). Anal.calcd for: C₁₃H₁₆N₂: C 77.96, H 8.05, N 13.99 Found: C 78.01, H 8.08, N 14.03.

2-phenyl-1H-benzo[d]imidazole^[2]



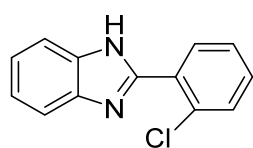
Creamy-white solid, m.p.: 292-294°C. ¹H NMR (400 MHz, DMSO) δ = 12.88 (s, 1H), 8.24 – 8.14 (m, 2H), 7.64 – 7.47 (m, 5H), 7.27 – 7.15 (m, 2H) (**Figure S10**). Anal.calcd for: C₁₃H₁₀N₂: C 80.39, H 5.19, N 14.42 Found: C 80.43, H 5.22, N 14.44.

2-(2-fluorophenyl)-1H-benzo[d]imidazole^[4]



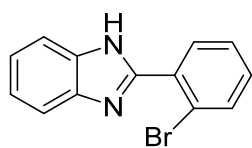
White solid, m.p.: 180-183°C. ¹H NMR (400 MHz, DMSO) δ = 12.59 (s, 1H), 8.25 (t, *J* = 7.6, 1H), 7.60 (dd, *J* = 23.0, 15.8, 3H), 7.49 – 7.36 (m, 2H), 7.25 (s, 2H) (**Figure S11**). Anal.calcd for: C₁₃H₉FN₂: C 73.57, H 4.27, F 8.95, N 13.20. Found: C 73.59, H 4.29, F 8.97.

2-(2-chlorophenyl)-1H-benzo[d]imidazole^[4]



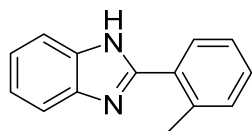
White solid, m.p.: 229-232°C. ¹H NMR (400 MHz, DMSO) δ = 12.72 (s, 1H), 7.93 (s, 1H), 7.62 (d, 5H), 7.27 (s, 2H) (**Figure S12**). Anal.calcd for: C₁₃H₉ClN₂: C 68.28, H 3.97, Cl 15.50, N 12.25. Found: C 68.31, H 4.00, Cl 15.53, N 12.28.

2-(2-bromophenyl)-1H-benzo[d]imidazole^[5]



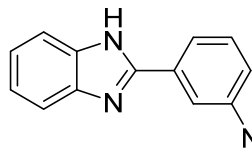
White solid, m.p.: 210-212°C. ¹H NMR (400 MHz, DMSO) δ = 12.74 (s, 1H), 7.85 – 7.74 (m, 2H), 7.60 (d, J = 17.5, 2H), 7.55 (d, J = 7.6, 1H), 7.49 – 7.44 (m, 1H), 7.24 (dd, J = 6.0, 3.1, 2H) (**Figure S13**). Anal.calcd for: C₁₃H₉BrN₂: C, 57.17; H, 3.32; Br, 29.25; N, 10.26. Found: C 57.19, H 3.34, N 10.28, Br 29.27.

2-(o-tolyl)-1H-benzo[d]imidazole^[3]



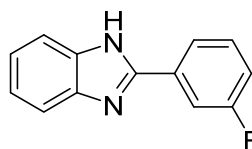
White solid, m.p.: 215-218°C. ¹H NMR (400 MHz, DMSO) δ = 12.62 (s, 1H), 7.73 (dd, J = 24.3, 6.6, 2H), 7.54 (d, J = 6.8, 1H), 7.40 (s, 3H), 7.28 – 7.17 (m, 2H), 2.63 (s, 3H) (**Figure S14**). Anal.calcd for: C₁₄H₁₂N₂: C 80.74, H 5.81, N 13.45. Found: C 80.76, H 5.83, N 13.47.

2-(3-nitrophenyl)-1H-benzo[d]imidazole^[5]



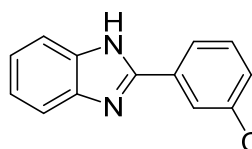
White solid, m.p.: 234-239°C. ¹H NMR (400 MHz, DMSO) δ = 9.03 (s, 1H), 8.61 (d, J = 7.8, 1H), 8.37 (d, J = 8.1, 1H), 7.89 (t, J = 8.0, 1H), 7.70 (dd, J = 6.0, 3.1, 2H), 7.33 (dd, J = 6.0, 3.1, 2H) (**Figure S15**). Anal.calcd for: C₁₃H₉N₃O₂: C 65.27, H 3.79, N 17.56, O 13.38. Found: C 65.29, H 3.81, N 17.58.

2-(3-fluorophenyl)-1H-benzo[d]imidazole^[6]



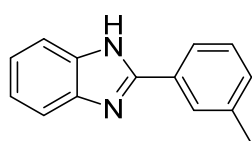
White solid, m.p.: 252-255°C. ¹H NMR (400 MHz, DMSO) δ = 13.03 (s, 1H), 8.05 (d, J = 7.8, 2H), 7.98 (d, J = 10.2, 0H), 7.62 (dd, J = 13.9, 7.4, 3H), 7.35 (t, J = 8.2, 3H), 7.24 (dd, J = 5.8, 3.0, 1H) (**Figure S16**). Anal.calcd for: C₁₃H₉FN₂: C 73.57, H 4.27, F 8.95, N 13.20. Found: C 73.58, H 4.28, F 8.96, N 13.21.

2-(3-chlorophenyl)-1H-benzo[d]imidazole^[6]



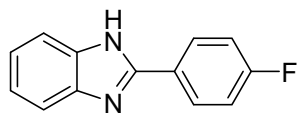
White solid, m.p.: 231-235°C. ¹H NMR (400 MHz, DMSO) δ = 13.00 (s, 1H), 8.14 (d, J = 7.2, 2H), 7.78 (d, J = 7.3, 2H), 7.62 (d, J = 47.5, 2H), 7.24 (s, 2H) (**Figure S17**). Anal.calcd for: C₁₃H₉ClN₂: C 68.28, H 3.97, Cl 15.50, N 12.25. Found: C 68.30, H 3.99, Cl 15.52, N 12.27.

2-(m-tolyl)-1H-benzo[d]imidazole^[7]



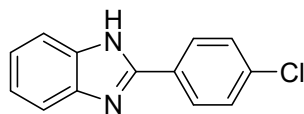
White solid, m.p.: 234-237°C. ¹H NMR (400 MHz, DMSO) δ = 12.85 (s, 1H), 8.06 – 7.94 (m, 2H), 7.59 (s, 2H), 7.44 (t, J = 7.6, 1H), 7.31 (d, J = 7.5, 1H), 7.20 (dd, J = 5.8, 2.9, 2H), 2.42 (s, 3H) (**Figure S18**). Anal.calcd for: C₁₄H₁₂N₂: C 80.74, H 5.81, N 13.45. Found: C 80.76, H 5.83, N 13.47.

2-(4-fluorophenyl)-1H-benzo[d]imidazole^[8]



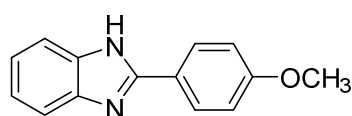
Yellow solid, m.p.: 241-242 °C. ¹H NMR (400 MHz, DMSO) δ = 8.25 (dd, J = 8.7, 5.4, 2H), 7.74 (dd, J = 5.9, 3.0, 2H), 7.52 (t, J = 8.7, 2H), 7.43 – 7.36 (m, 2H) (**Figure S19**). Anal.calcd for: C₁₃H₉FN₂: C 73.57, H 4.27, F 8.95, N 13.20. Found: C 73.59, H 4.29, F 8.97, N 13.22.

2-(4-chlorophenyl)-1H-benzo[d]imidazole^[8]



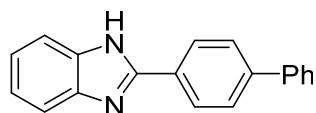
White crystal, m.p.: 288-290°C. ¹H NMR (400 MHz, DMSO) δ = 12.99 (s, 1H), 8.21 (d, J = 8.5, 2H), 7.73 – 7.51 (m, 4H), 7.24 (d, J = 6.7, 2H) (**Figure S20**). Anal.calcd for: C₁₃H₉ClN₂: C 68.28, H 3.97, Cl 15.50, N 12.25. Found: C 68.30, H 3.99, Cl 15.52, N 12.27.

2-(4-methoxyphenyl)-1H-benzo[d]imidazole^[9]



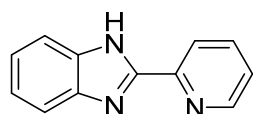
White crystal, m.p.: 222-225°C. ¹H NMR (400 MHz, DMSO) δ = 12.75 (s, 1H), 8.14 (d, J = 8.0, 2H), 7.58 (d, J = 52.4, 2H), 7.26 – 7.02 (m, 4H), 3.85 (s, 3H) (**Figure S21**). Anal.calcd for: C₁₄H₁₂N₂O: C 74.98, H 5.39, N 12.49. Found: C 74.99, H 5.40, N 12.50.

2-([1,1'-biphenyl]-4-yl)-1H-benzo[d]imidazole^[10]



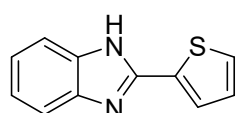
Brown solid, m.p.: 276-277°C. ¹H NMR (400 MHz, DMSO) δ = 12.99 (s, 1H), 8.31 (d, J = 8.2, 2H), 7.89 (d, J = 8.2, 2H), 7.78 (d, J = 7.3, 2H), 7.71 (d, J = 5.4, 1H), 7.58 (d, J = 5.7, 1H), 7.51 (t, J = 7.4, 3H), 7.45 – 7.38 (m, 1H), 7.24 (s, 2H) (**Figure S22**). Anal.calcd for: C₁₉H₁₄N₂: C 84.42, H 5.22, N 10.36. Found: C 84.44, H 5.24, N 10.38.

2-(pyridin-2-yl)-1H-benzo[d]imidazole^[4]



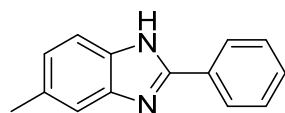
White crystal, m.p.: 218-220°C. ¹H NMR (400 MHz, DMSO) δ = 13.09 (s, 1H), 8.74 (d, J = 4.2, 1H), 8.34 (d, J = 7.9, 1H), 8.01 (td, J = 7.7, 1.7, 1H), 7.72 (d, J = 7.6, 1H), 7.58 – 7.49 (m, 2H), 7.29 – 7.18 (m, 2H) (**Figure S23**). Anal.calcd for: C₁₂H₉N₃: C 73.83, H 4.65, N 21.52. Found: C 73.85, H 4.67, N 21.54.

2-(thiophen-2-yl)-1H-benzo[d]imidazole^[10]



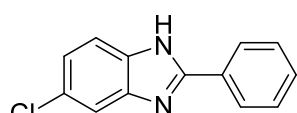
White crystal, m.p.: 341-343°C. ¹H NMR (400 MHz, DMSO) δ 12.82 (s, 1H), 7.88 – 7.78 (m, 1H), 7.70 (d, J = 4.9 Hz, 1H), 7.55 (s, 2H), 7.28 – 7.12 (m, 3H) (**Figure S24**). Anal.calcd for: C₁₁H₈N₂S: C 65.98, H 4.03, N 13.99, S 16.01. Found: C 65.99, H 4.04, N 14.00, S 16.02.

5-methyl-2-phenyl-1H-benzo[d]imidazole^[11]



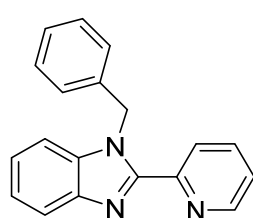
White crystal, m.p.: 243-245°C. ¹H NMR (400 MHz, CDCl₃) δ = 8.06 (dd, J = 6.5, 3.0, 2H), 7.52 (d, J = 7.8, 1H), 7.46 – 7.35 (m, 4H), 7.08 (d, J = 8.2, 1H), 2.45 (s, 3H) (**Figure S25**). Anal.calcd for: C₁₄H₁₂N₂: C 80.74, H 5.81, N 13.45. Found: C 80.76, H 5.83, N 13.48.

5-chloro-2-phenyl-1H-benzo[d]imidazole^[12]



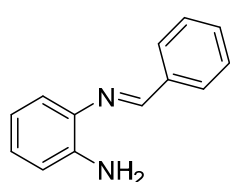
Light yellow crystal, m.p.: 214-216°C. ¹H NMR (400 MHz, DMSO) δ = 13.13 (s, 1H), 8.20 (dd, J = 5.2, 1.5, 2H), 7.77 – 7.50 (m, 5H), 7.25 (s, 1H) (**Figure S26**). Anal.calcd for: C₁₃H₉ClN₂: C 68.28, H 3.97, Cl 15.50, N 12.25. Found: C 68.29, H 3.98, Cl 15.51, N 12.26.

1-benzyl-2-phenyl-1H-benzo[d]imidazole^[8]



White solid, m.p.: 116-118°C. ¹H NMR (400 MHz, CDCl₃) δ = 8.55 (d, J = 4.7 Hz, 1H), 8.42 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 7.9 Hz, 1H), 7.74 (td, J = 7.9, 1.7 Hz, 1H), 7.28 (dd, J = 12.1, 7.8 Hz, 2H), 7.17 (dt, J = 20.8, 7.7 Hz, 7H), 6.14 (s, 2H) (**Figure S27**). Anal.calcd for: C₁₉H₁₅N₃: C 79.98, H 5.30, N 14.73. Found: C 79.99, H 5.31, N 14.74.

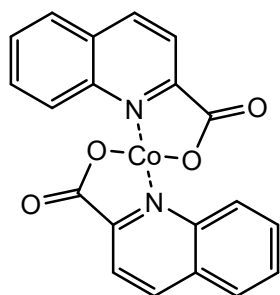
2-(benzylideneamino) aniline^[12]



White solid, m.p.: 63-64°C. ¹H NMR (400 MHz, DMSO) δ = 8.30 (d, J = 1.2 Hz, 1H), 7.63 – 7.48 (m, 5H), 7.13 (td, J = 7.5, 2.0 Hz, 1H), 7.04 (dd, J = 7.4, 2.0 Hz, 1H), 6.66 – 6.54 (m, 2H), 5.60 (s, 2H) (**Figure S28**). Anal.calcd for: C₁₃H₁₂N₂: C 79.56, H 6.16, N 14.27. Found: C 79.58, H 6.18,

N 14.29.

Complex: Co (C₁₀H₁₀NO₂)₂ · 2C₂H₅OH



Pale pink crystal. ¹H NMR (400 MHz, DMSO-*d*₆) δ=8.50 (d, *J*= 7.6Hz, 1H), 8.32 (dd, *J*=7.4,1.5Hz, 1H), 8.19 (td, *J*=7.4, 1.4Hz, 2H), 8.01 (qd, *J*=7.7,1.5,1H), 7.72 (td, *J*=7.5,1.5Hz, 1H) (**Figure S29**). ¹³C NMR (100 MHz, DMSO-*d*₆) δ 170.22, 148.01, 146.50, 134.82, 130.50, 128.35, 128.23, 127.90, 125.68, 122.27 (**Figure S30**). FTIR (KBr, C=O, cm⁻¹): 1613, 1401, 1383, 1350. Anal.calcd for: C₂₀H₁₂CoN₂O₄ C 59.57, H 3.00, N 6.95. Found: C 59.52, H 3.12, N 6.97. UV-vis spectra absorption peak: 274.60nm. HRMS: C₂₀H₁₂CoN₂O₄ for [M+H]:

403.0129. Found:403.0121. m.p.:241-243°C.

NMR spectra

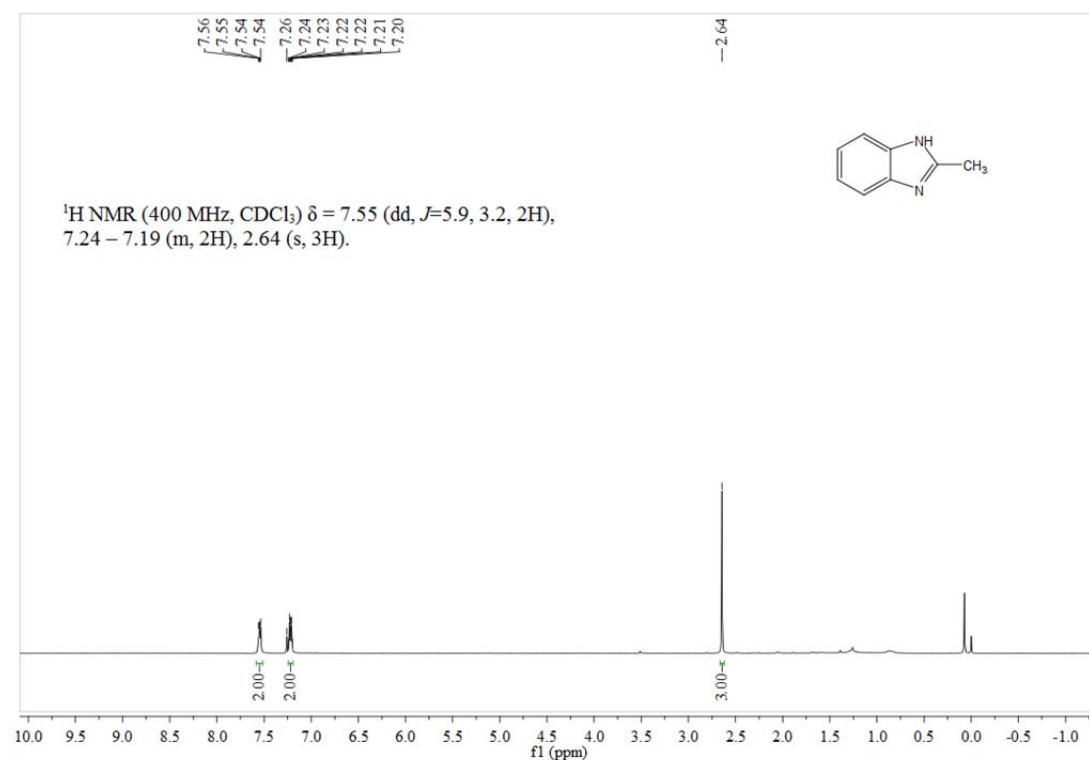


Figure S1 ¹H NMR spectrum of 2-methyl-1*H*-benzo[d]imidazole

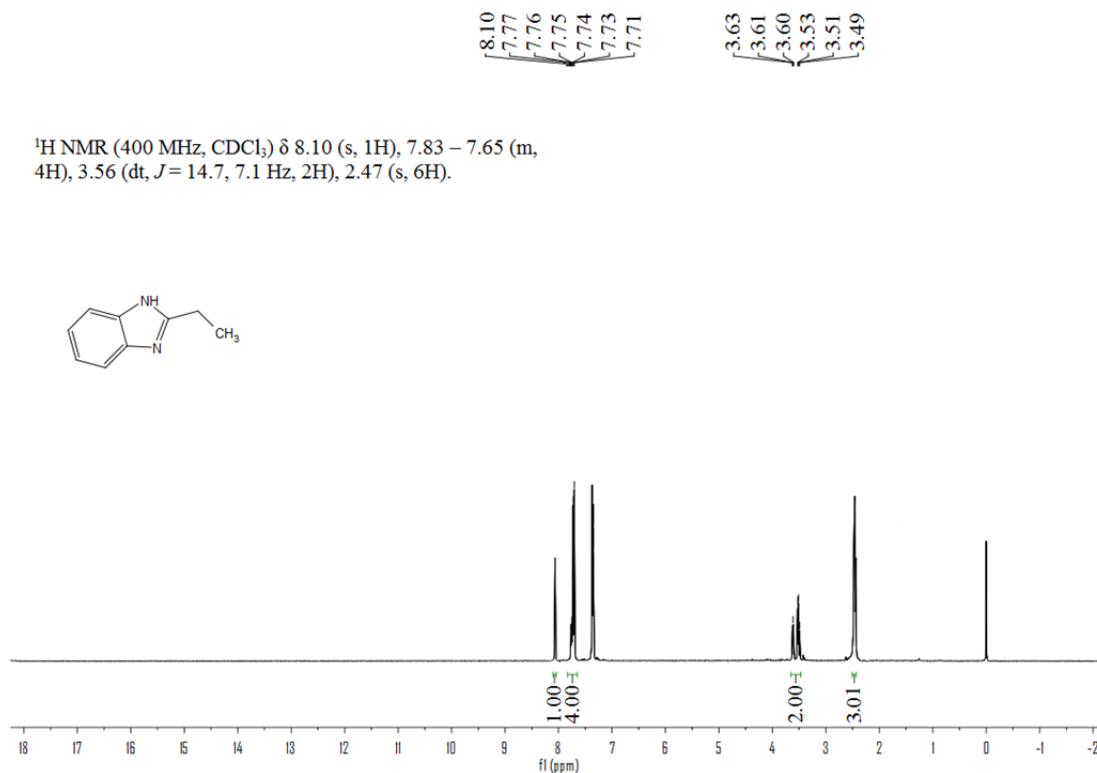


Figure S2 ¹H NMR spectrum of 2-ethyl-1*H*-benzo[d]imidazole

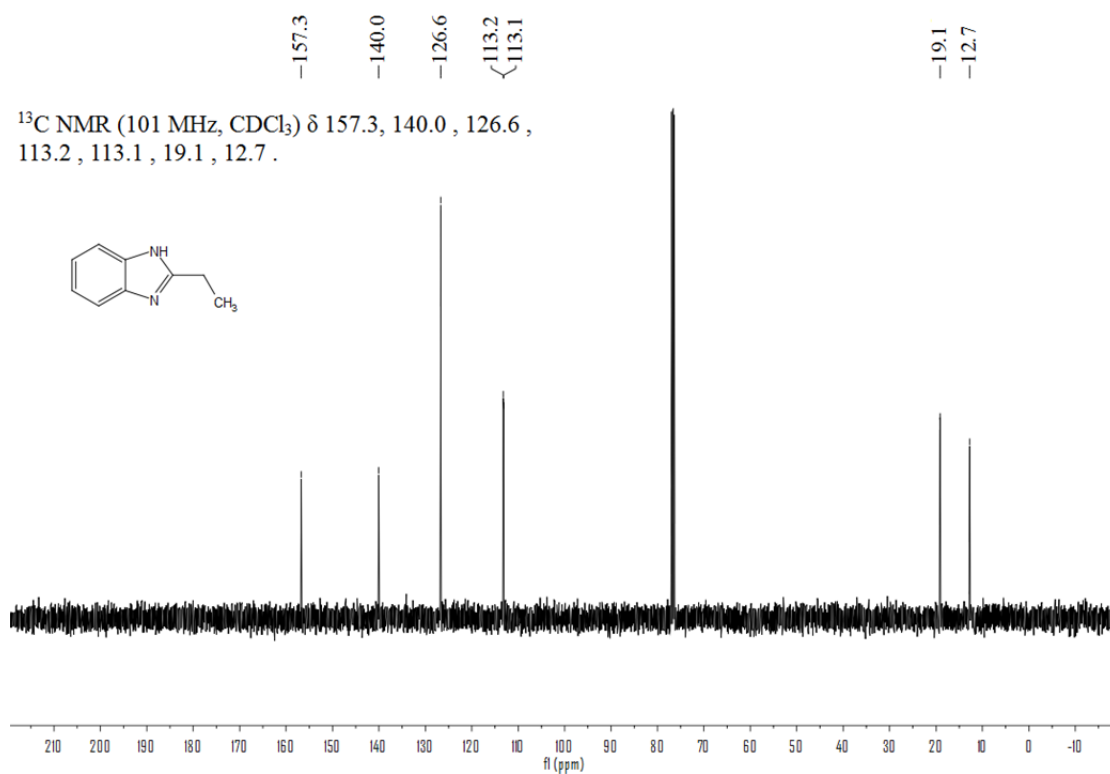


Figure S3 ^{13}C NMR spectrum of 2-ethyl-1*H*-benzo[*d*]imidazole

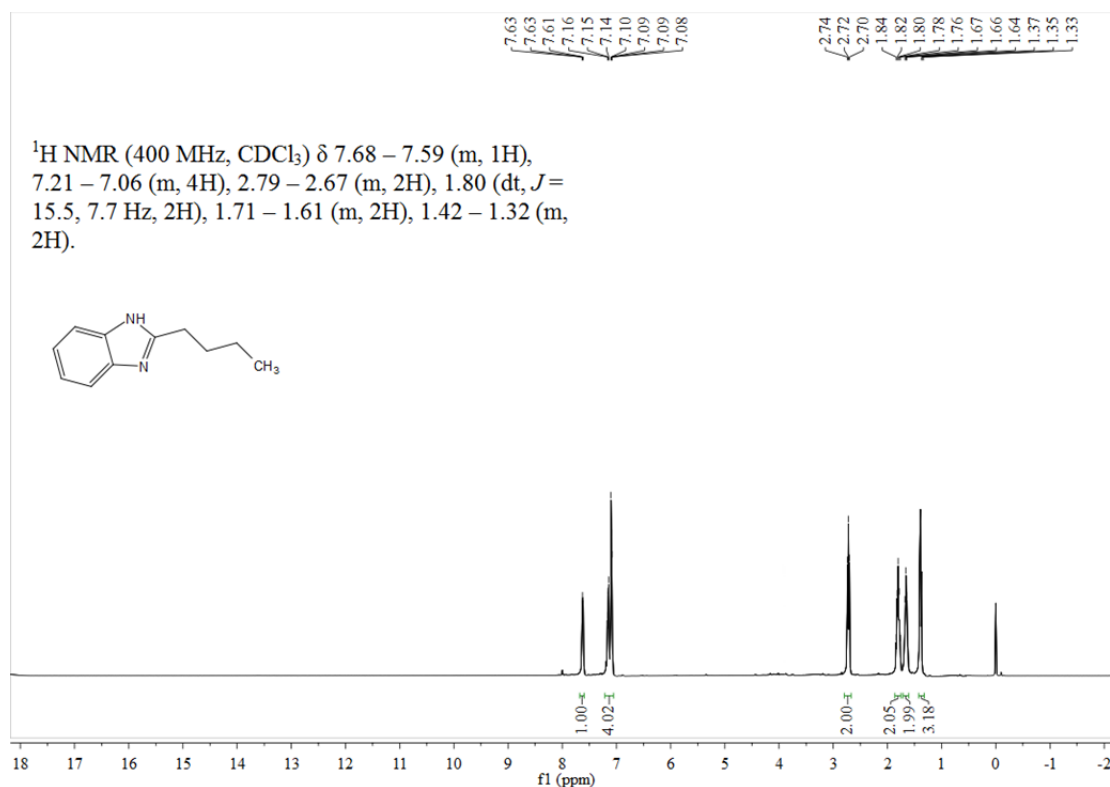


Figure S4 ^1H NMR spectrum of 2-butyl-1*H*-benzo[*d*]imidazole

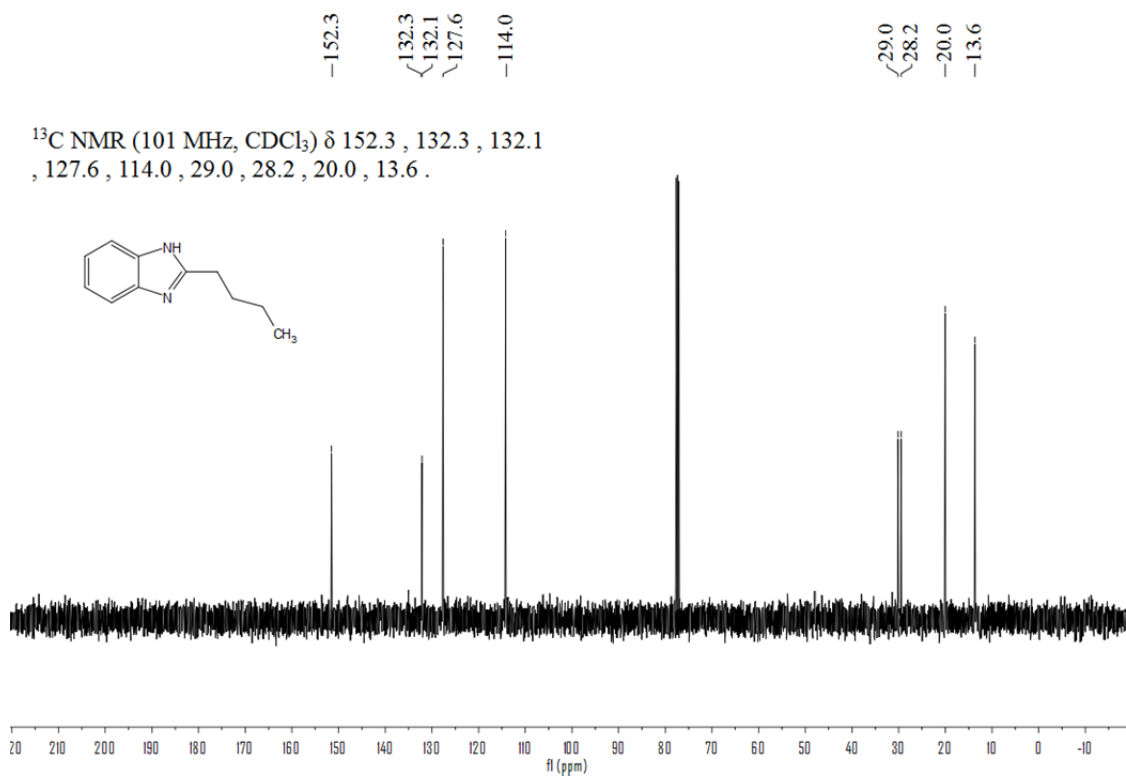


Figure S5 ^{13}C NMR spectrum of 2-butyl-1H-benzo[d]imidazole

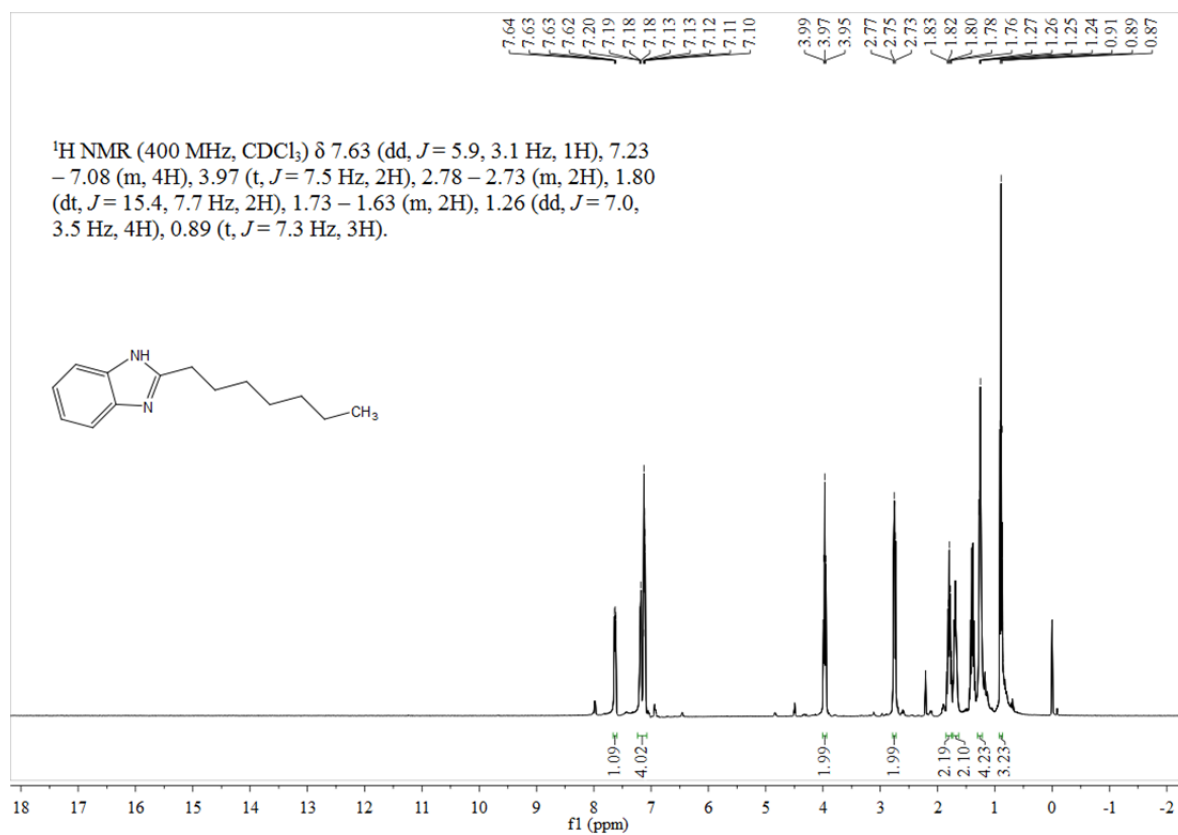


Figure S6 ^1H NMR spectrum of 2-hexyl-1H-benzo[d]imidazole

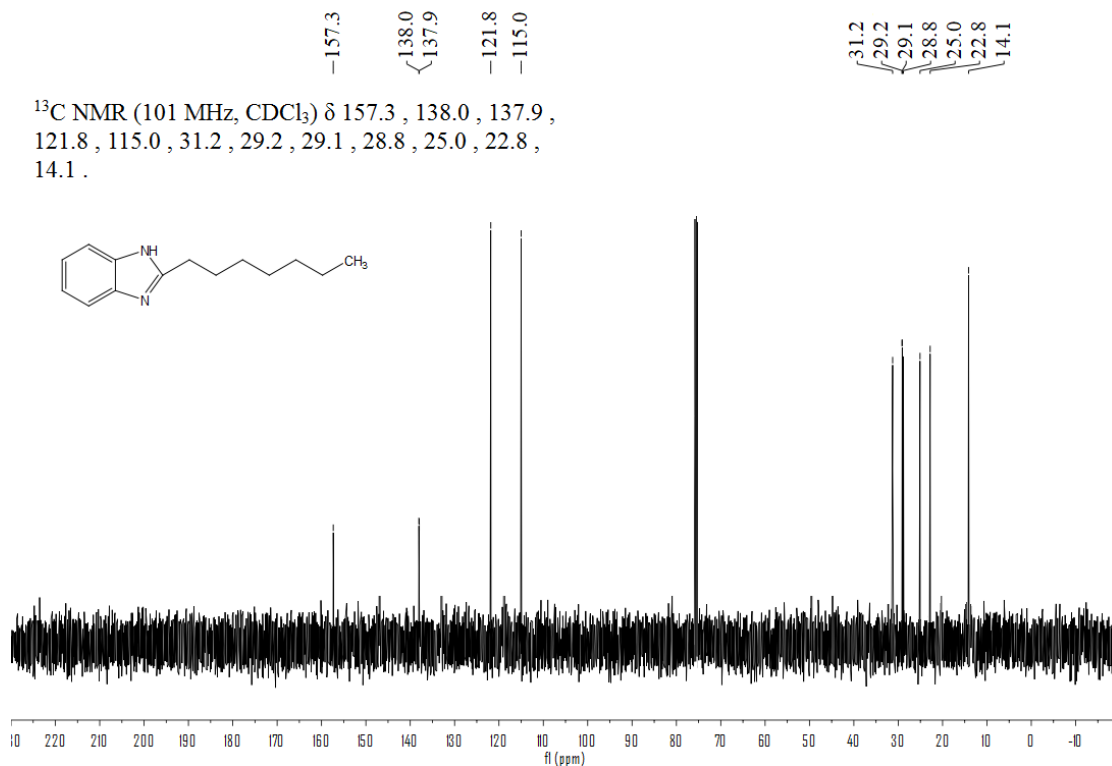


Figure S7 ^{13}C NMR spectrum of 2-hexyl-1H-benzo[d]imidazole

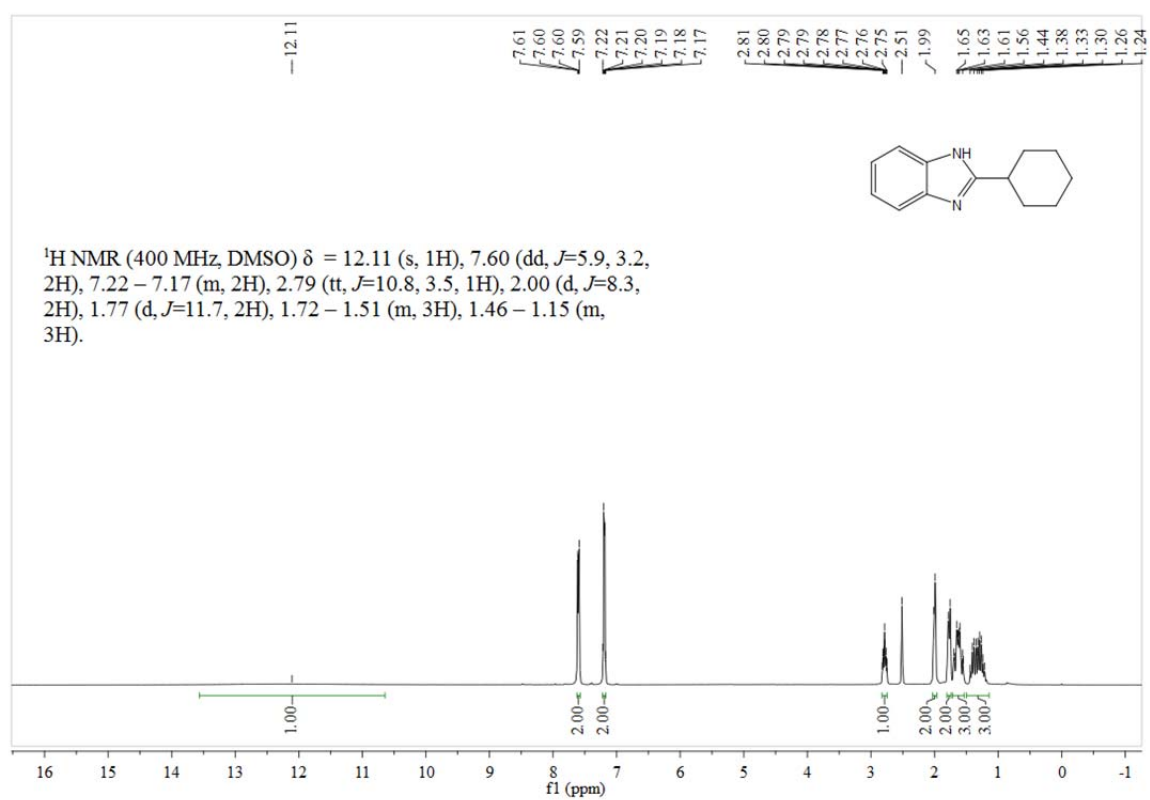


Figure S8 ^1H NMR spectrum of 2-cyclohexyl-1H-benzo[d]imidazole

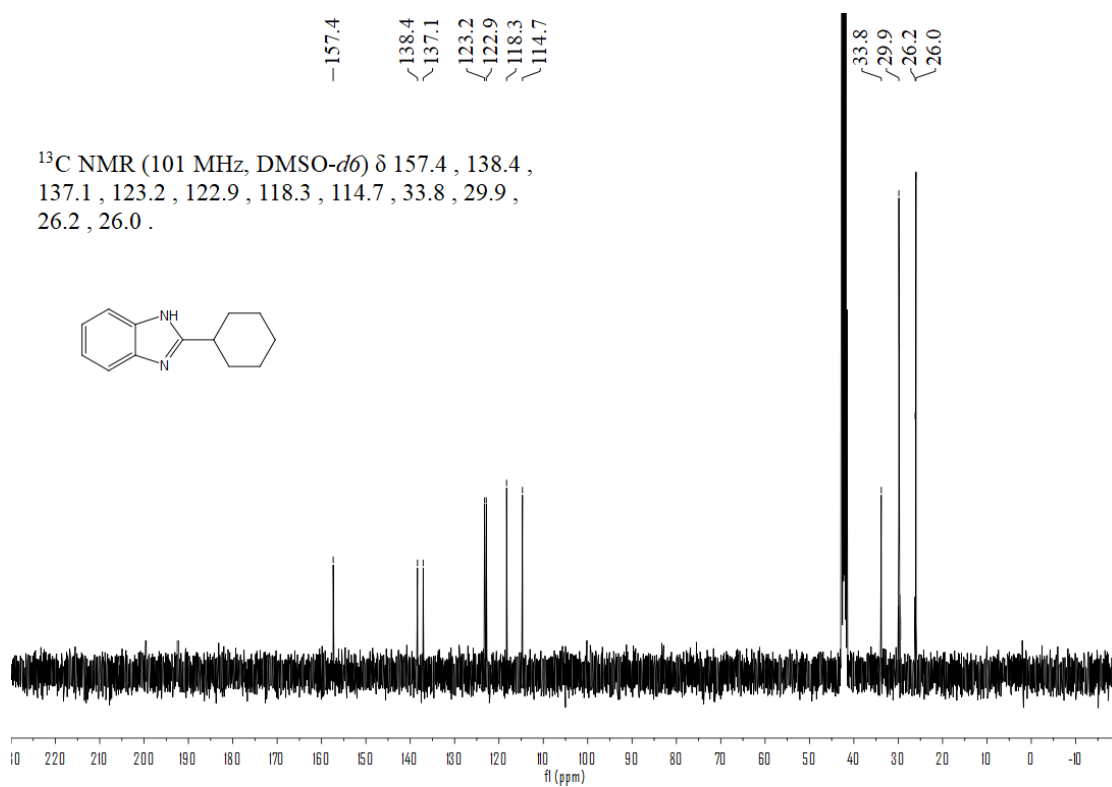


Figure S9 ^{13}C NMR spectrum of 2-cyclohexyl-1H-benzo[d]imidazole

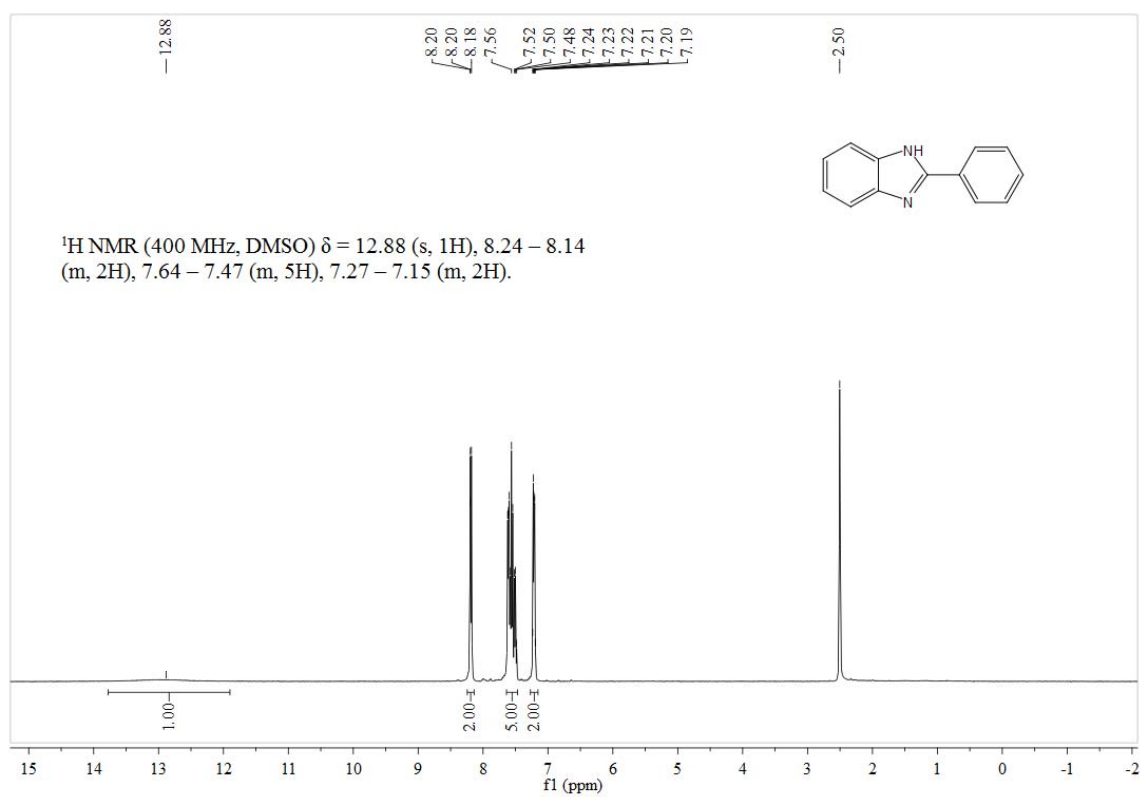


Figure S10 ^1H NMR spectrum of 2-phenyl-1H-benzo[d]imidazole

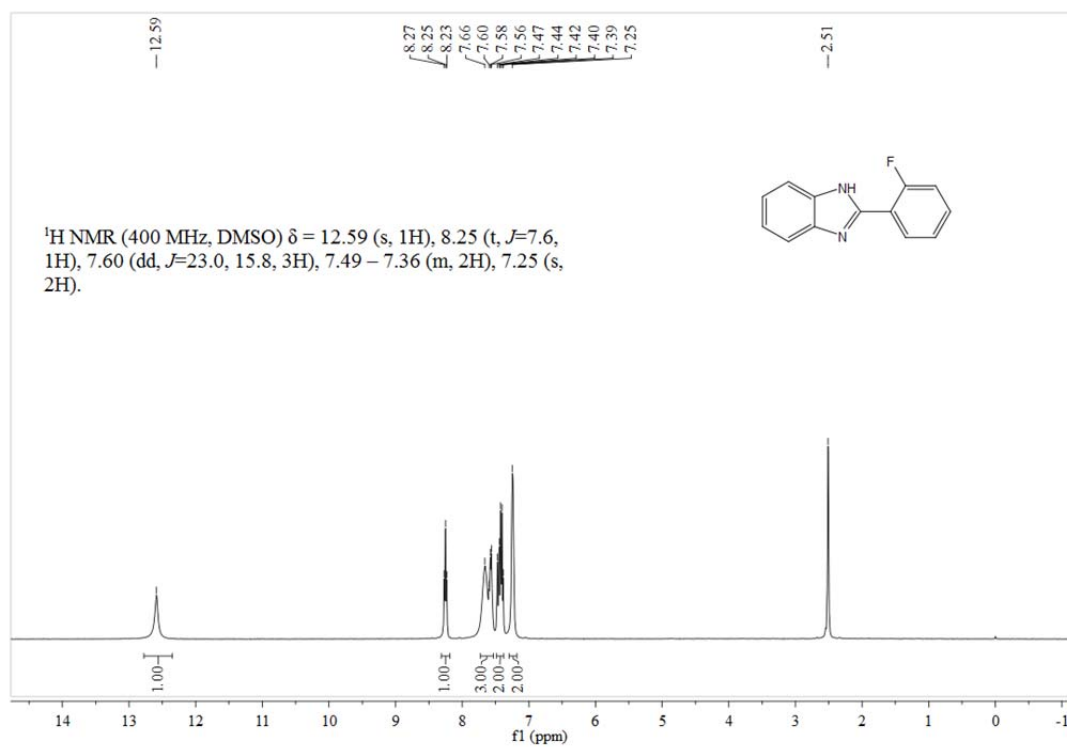


Figure S11 ¹H NMR spectrum of 2-(2-fluorophenyl)-1H-benzo[d]imidazole

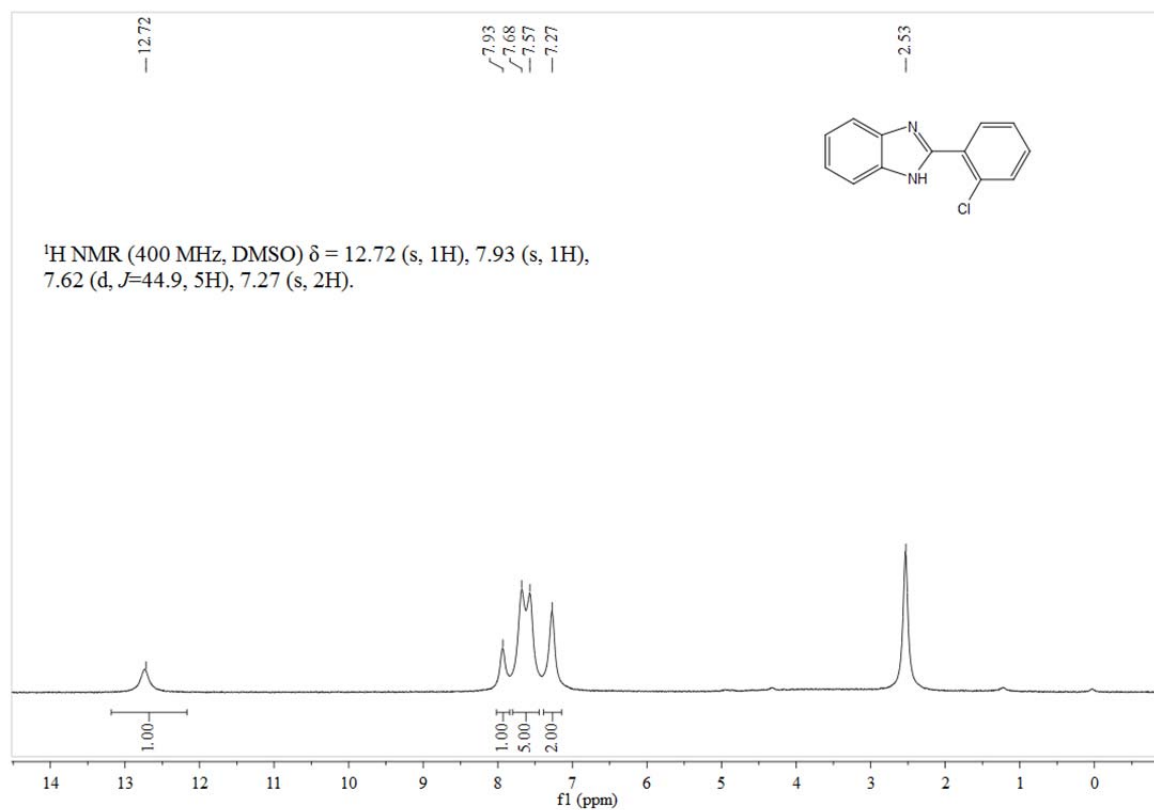


Figure S12 ¹H NMR spectrum of 2-(2-chlorophenyl)-1H-benzo[d]imidazole

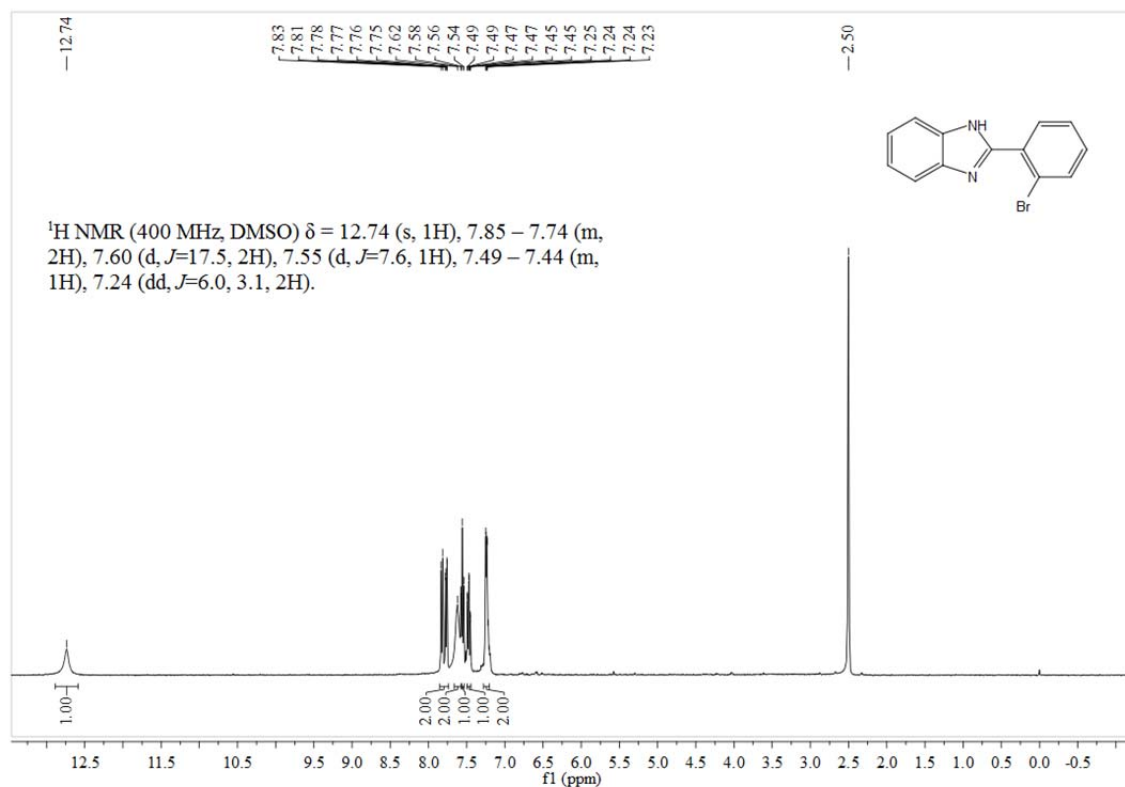


Figure S13 ¹H NMR spectrum of 2-(2-bromophenyl)-1H-benzo[d]imidazole

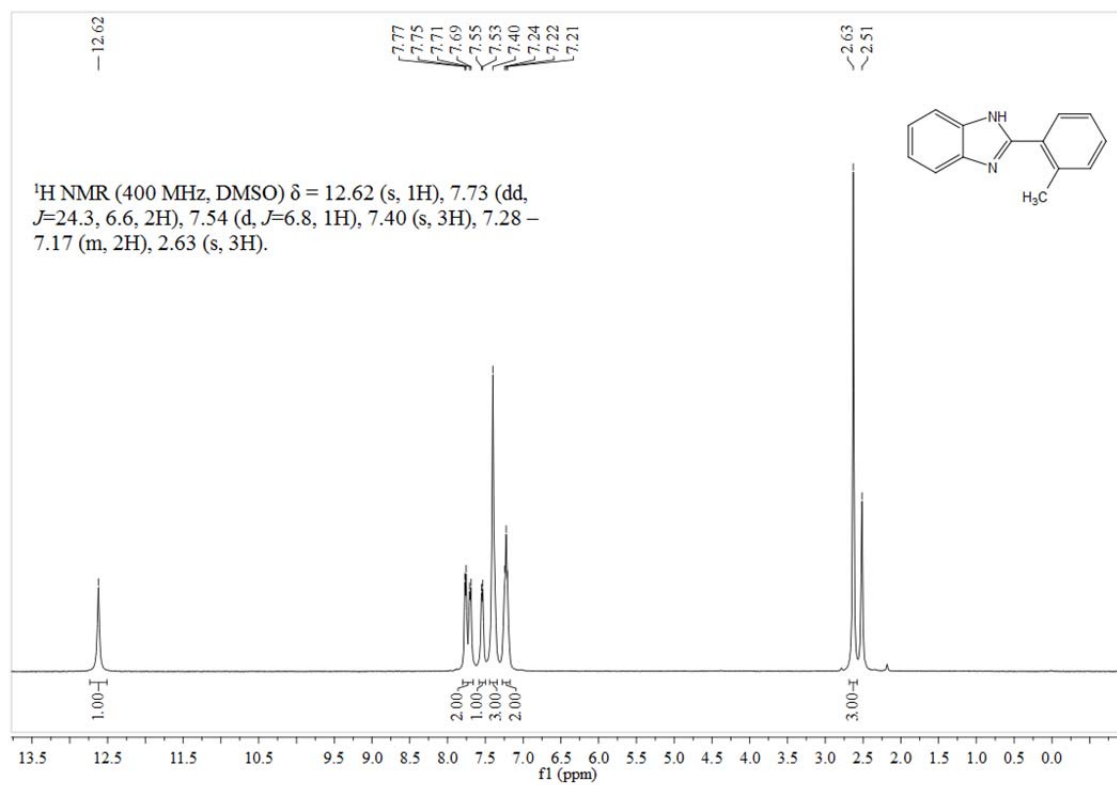


Figure S14 ¹H NMR spectrum of 2-(o-tolyl)-1H-benzo[d]imidazole

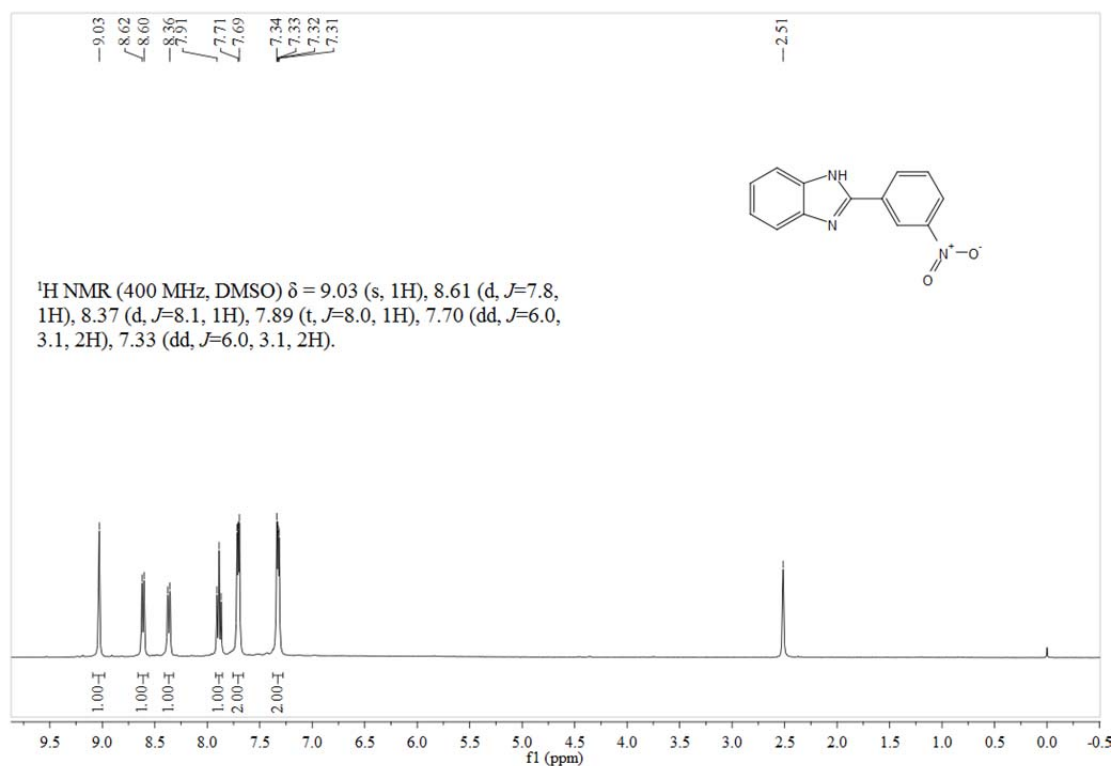


Figure S15 ¹H NMR spectrum of 2-(3-nitrophenyl)-1*H*-benzo[*d*]imidazole

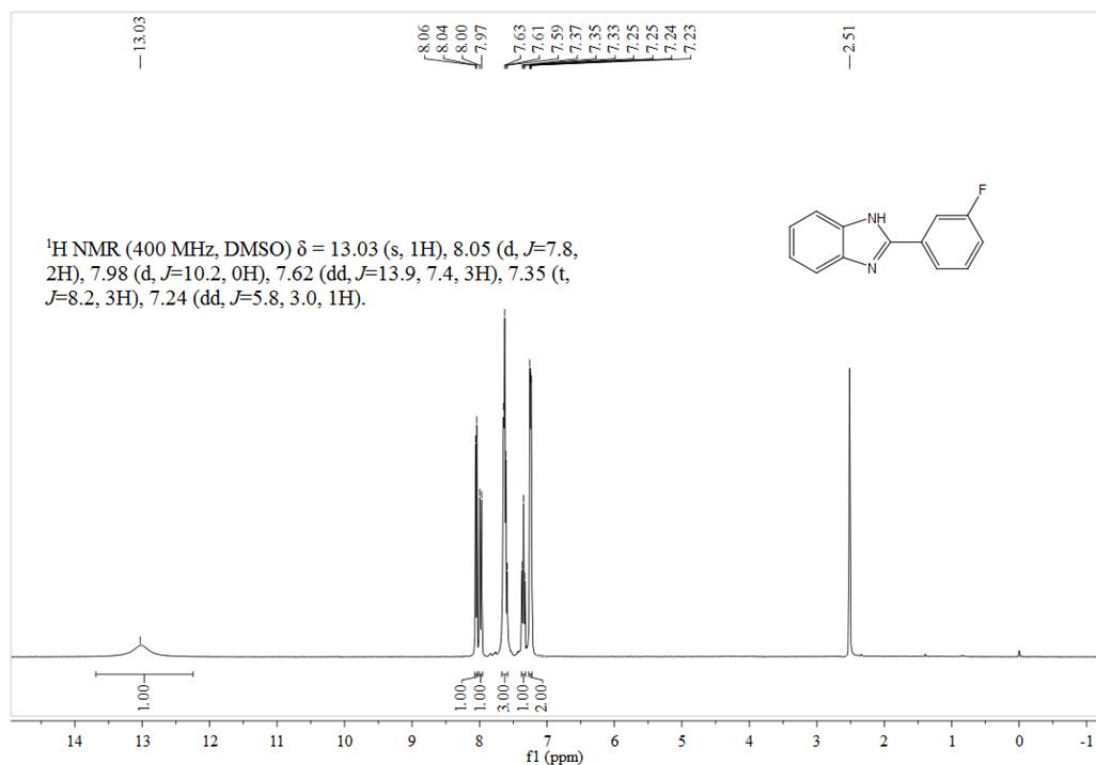


Figure S16 ¹H NMR spectrum of 2-(3-fluorophenyl)-1*H*-benzo[*d*]imidazole

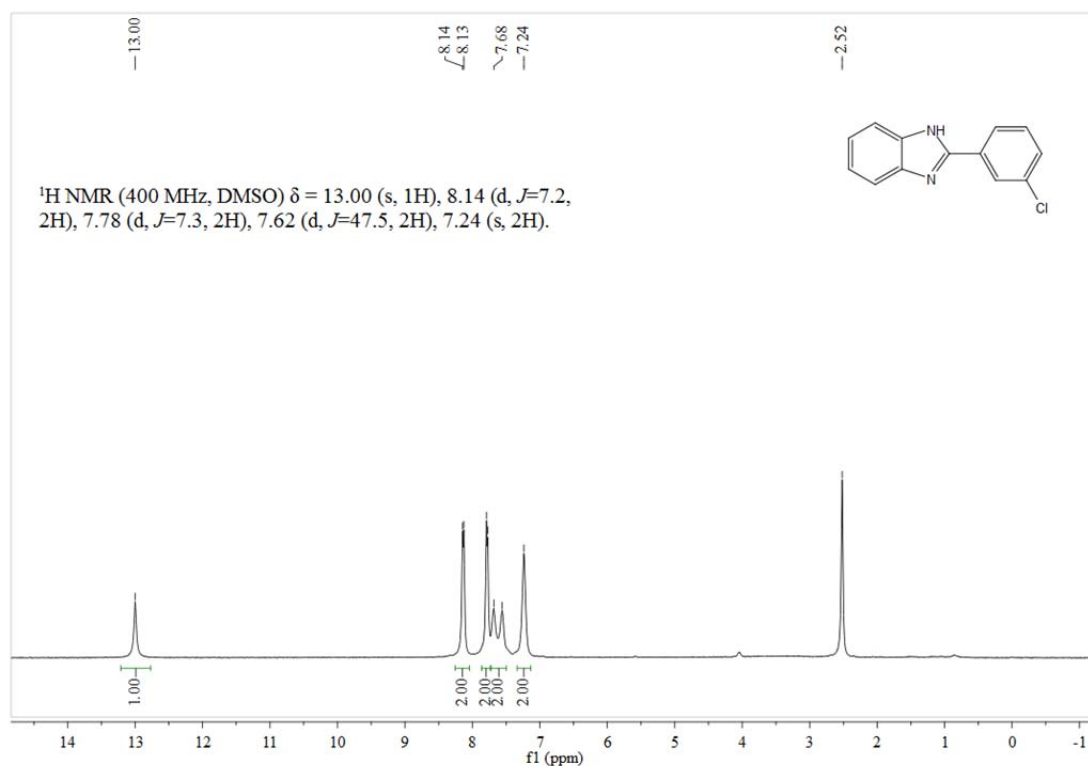


Figure S17 ¹H NMR spectrum of 2-(3-chlorophenyl)-1H-benzo[d]imidazole

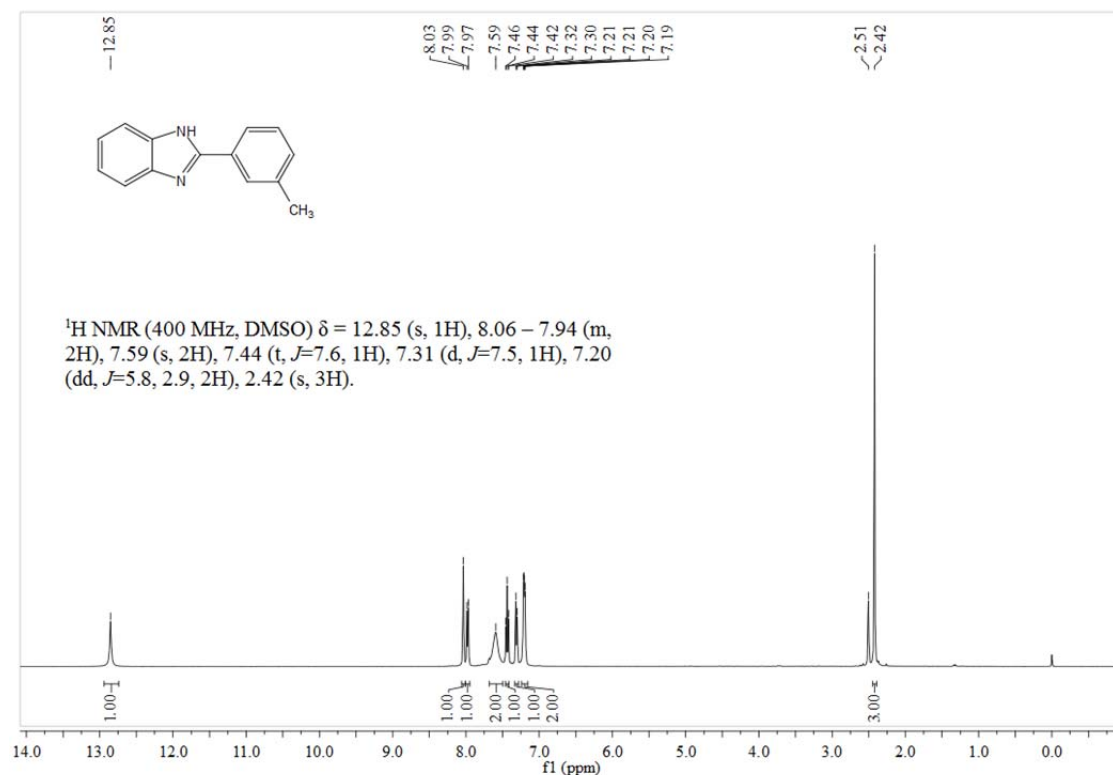


Figure S18 ¹H NMR spectrum of 2-(m-tolyl)-1H-benzo[d]imidazole

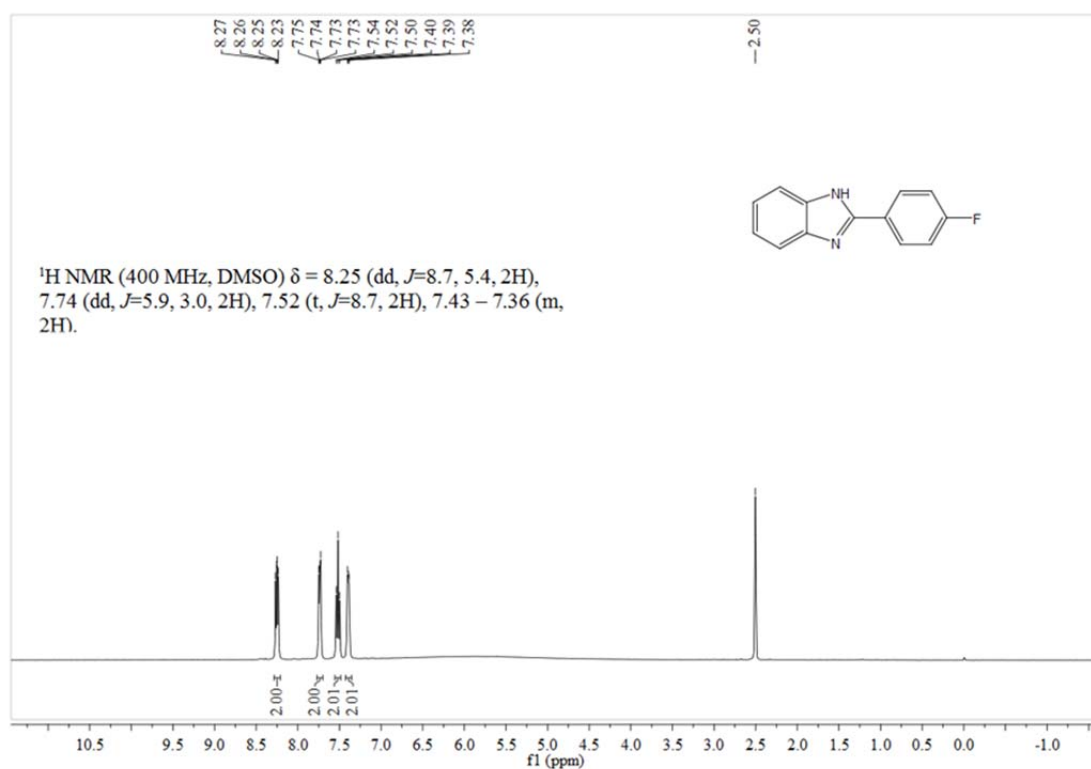


Figure S19 ¹H NMR spectrum of 2-(4-fluorophenyl)-1*H*-benzo[*d*]imidazole

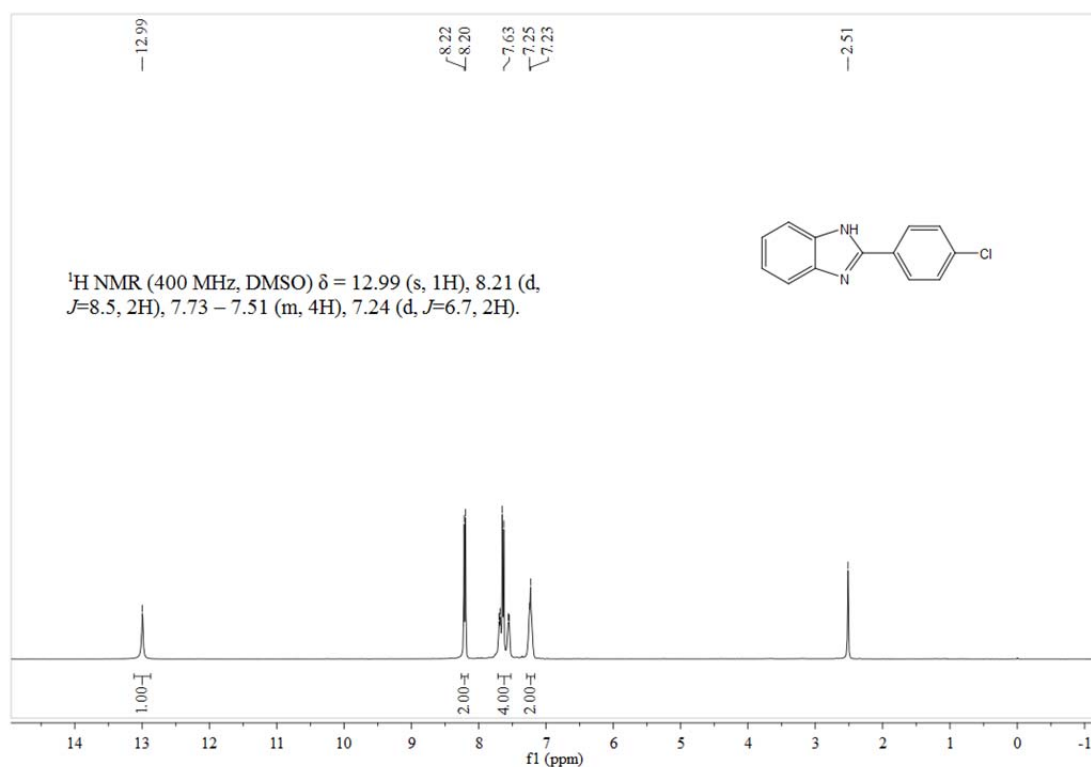


Figure S20 ¹H NMR spectrum of 2-(4-chlorophenyl)-1*H*-benzo[*d*]imidazole

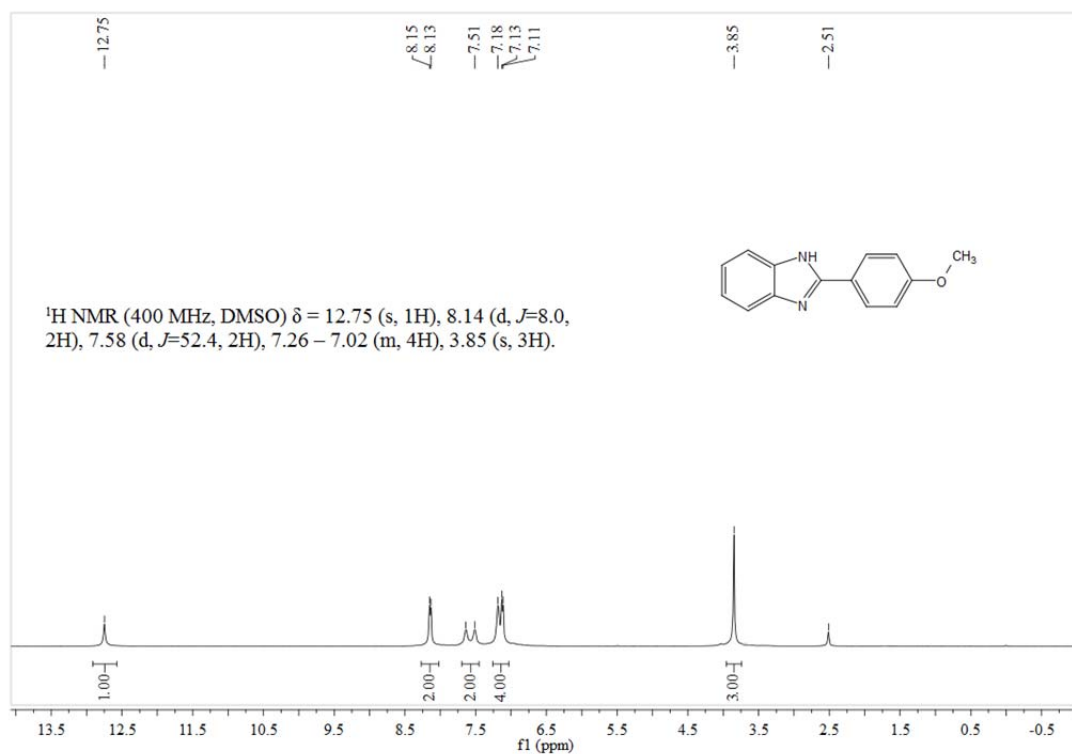


Figure S21 ¹H NMR spectrum of 2-(4-methoxyphenyl)-1*H*-benzo[*d*]imidazole

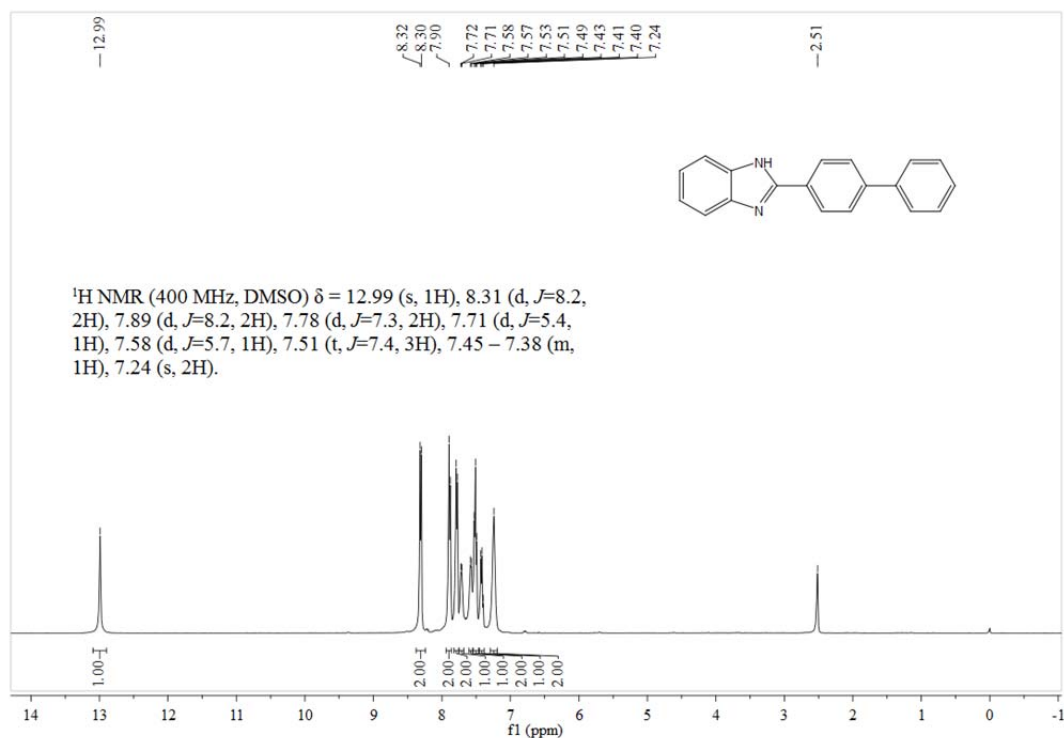


Figure S22 ¹H NMR spectrum of 2-([1,1'-biphenyl]-4-yl)-1*H*-benzo[*d*]imidazole

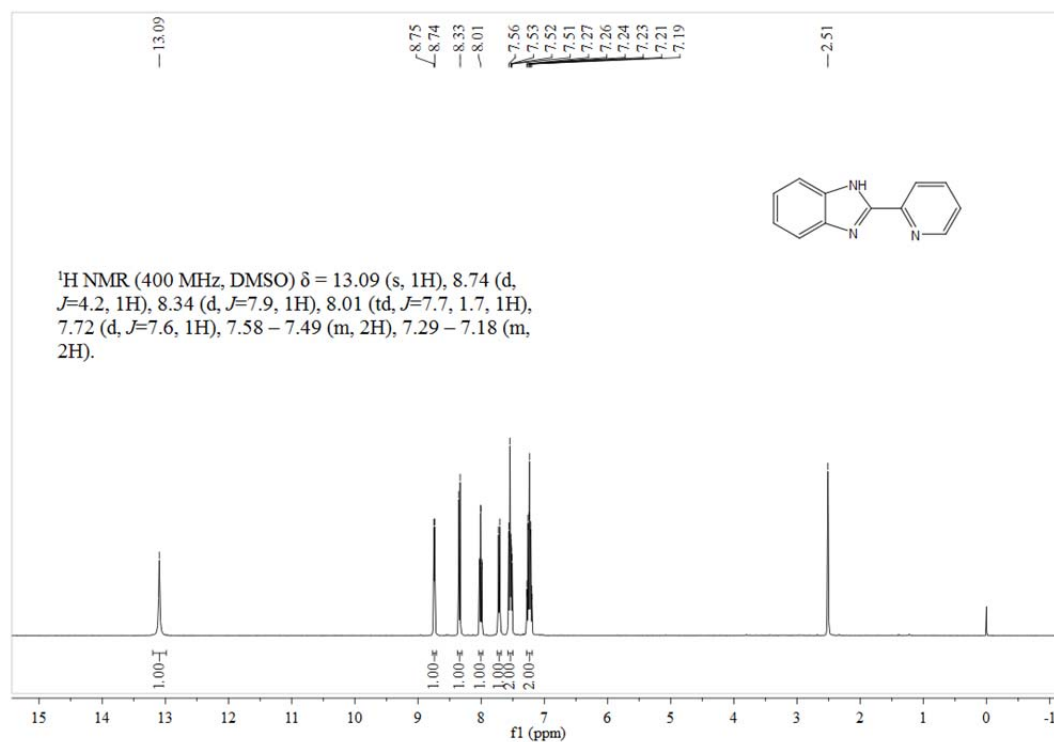


Figure S23 ¹H NMR spectrum of 2-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole

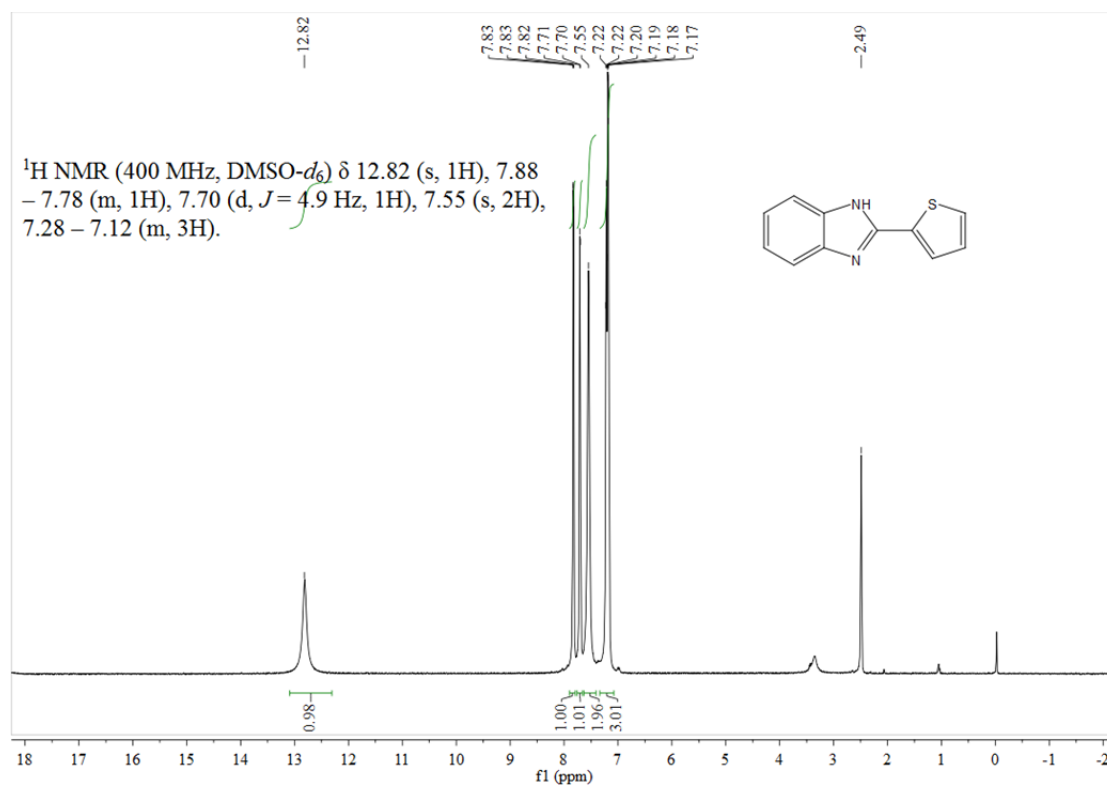


Figure S24 ¹H NMR spectrum of 2-(thiophen-2-yl)-1*H*-benzo[*d*]imidazole

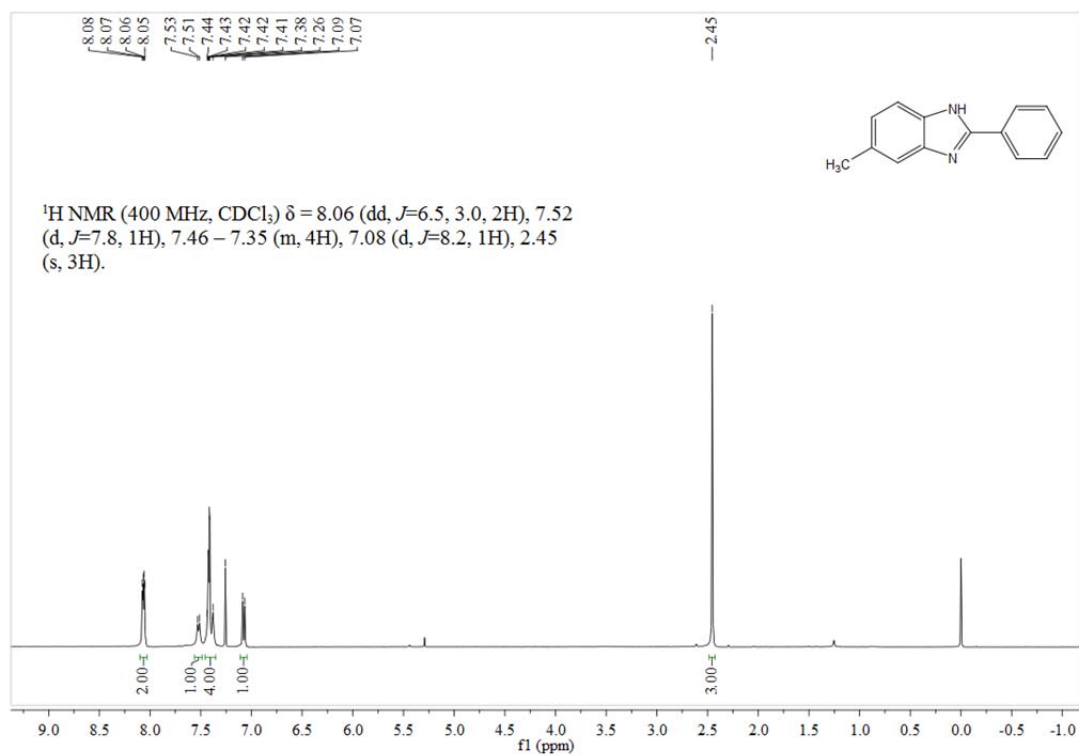


Figure S25 ¹H NMR spectrum of 5-methyl-2-phenyl-1*H*-benzo[*d*]imidazole

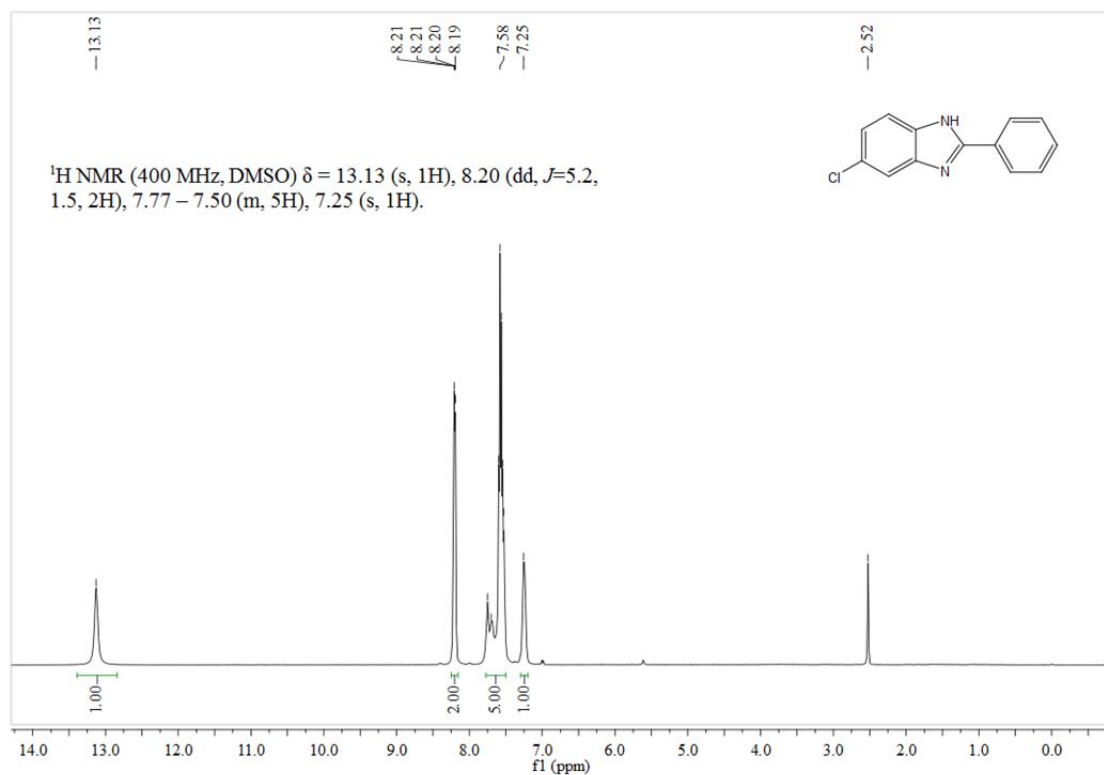


Figure S26 ¹H NMR spectrum of 5-chloro-2-phenyl-1*H*-benzo[*d*]imidazole

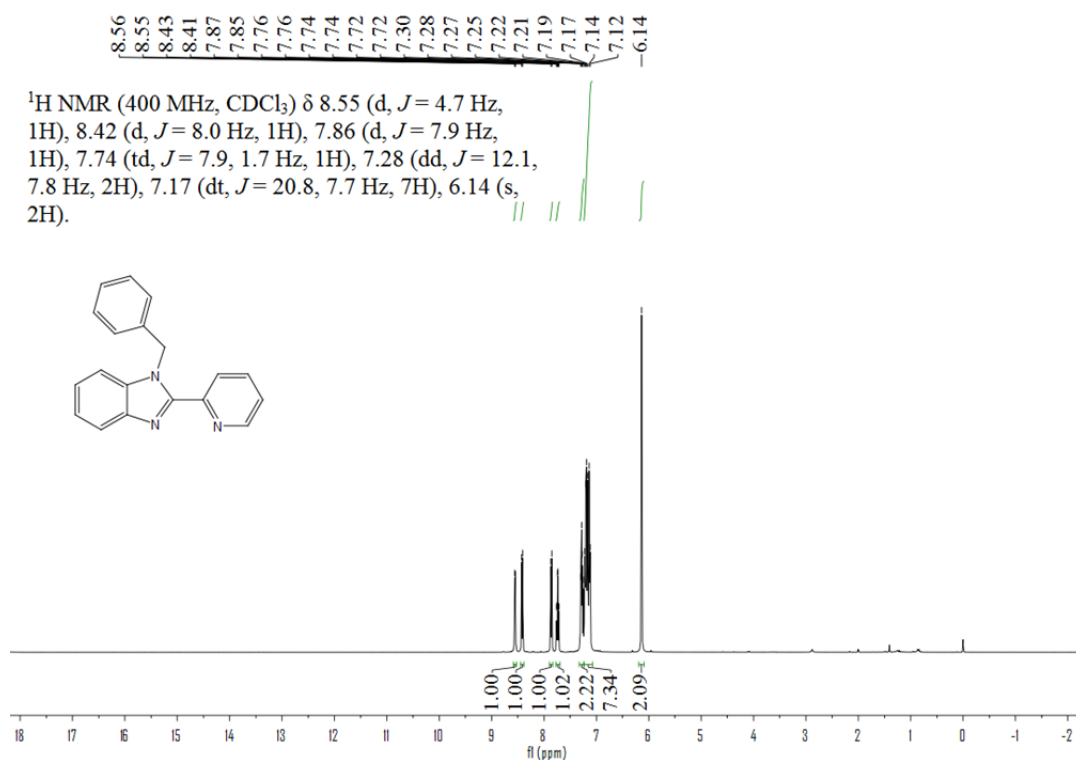


Figure S27 ¹H NMR spectrum of 1-benzyl-2-phenyl-1*H*-benzo[*d*]imidazole

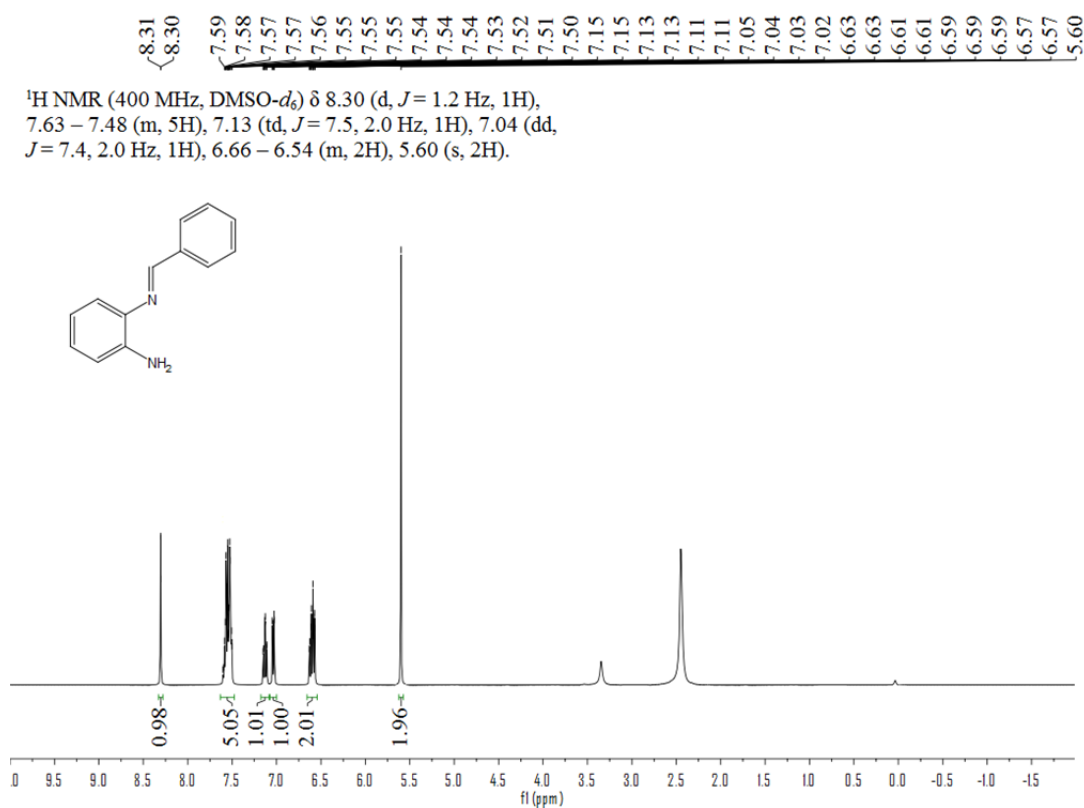


Figure S28 ¹H NMR spectrum of 2-(benzylideneamino) aniline

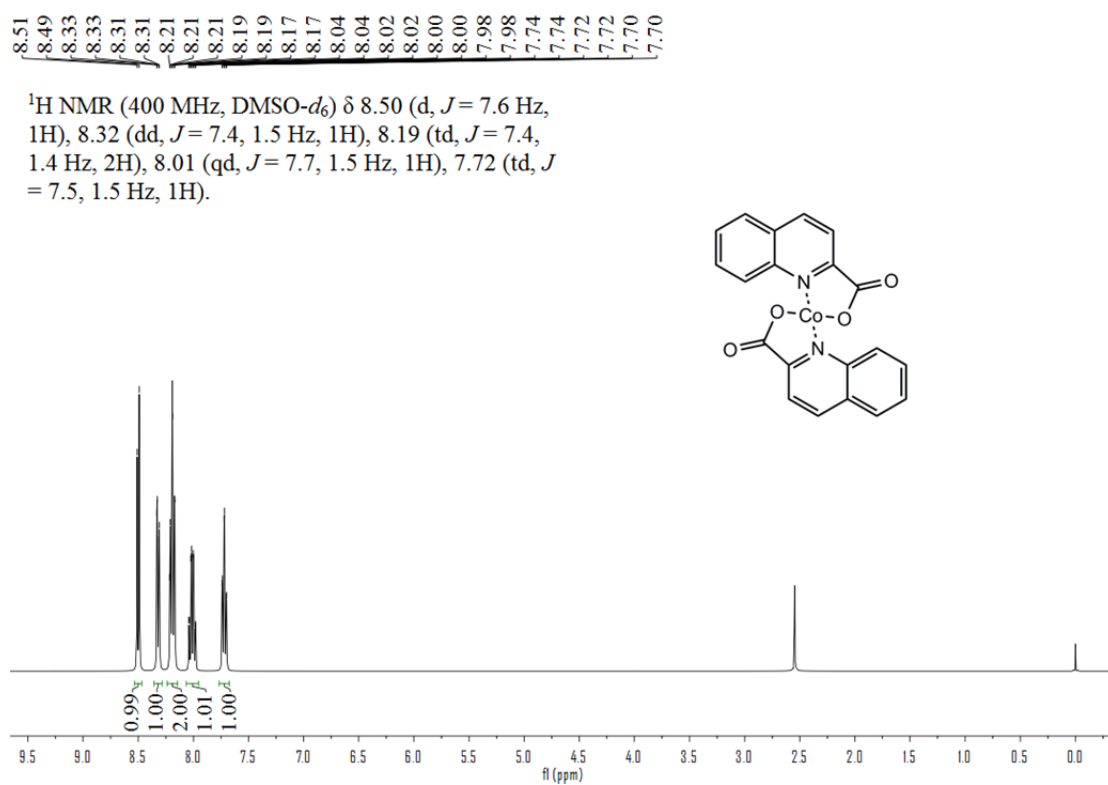


Figure S29 ¹H NMR spectrum of Complex

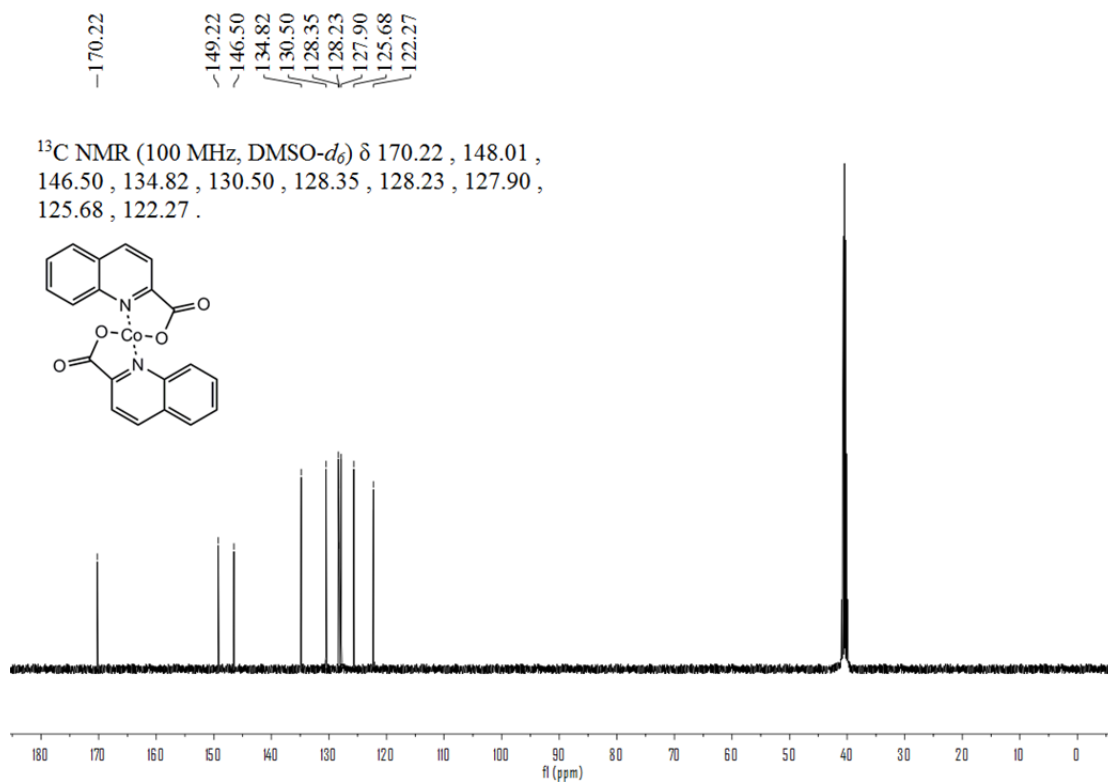


Figure S30 ¹³C NMR spectrum of Complex

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Table S1 The optimized intermediates and transition states and their Cartesian coordinates

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2.40228200	-0.52242500				
C		4.33812300			
1.13995000	0.06991400				
H		5.51831300			
-0.52852100	0.81390300				
H		7.72705000			
0.55017000	0.30861900				
H		7.82891500			
2.76769000	-0.79476800				
H		5.59217100			
3.11221700	-2.09931900				
H		3.38908400			
0.69301300	0.36325900				
N		3.20001000			

	TS2		-4.64120400	-1.41218500	
C		2.32990200	C		4.19703200
2.66454000	-1.20636500		-4.74385500	-0.05369200	
C		3.09367400	C		-0.29890900
1.59044700	-1.94760800		2.73843300	1.31169200	
O		2.83877700	C		-1.09901800
0.39600500	-1.49347200		3.67348900	1.93469400	
Co		1.82196500	C		-0.96254300
0.31068500	0.08723100		5.05461400	1.66249400	
N		1.48958100	C		-0.02756000
2.22921400	-0.26404800		5.48164400	0.74938200	
N		2.52874900	H		3.70001400
-1.48292900	0.67808100		-4.67812200	2.60046800	
C		2.33766700	H		2.53962700
-1.63350800	1.99118700		-2.75929500	3.79231200	
C		1.60638900	H		1.85045700
-0.50714200	2.68753900		6.01917100	-1.12331700	
O		1.28784300	H		3.21352100
0.46093400	1.88000200		4.24986400	-2.32982300	
O		1.36590100	H		3.07922200
-0.57392000	3.88531000		-1.52633000	-1.93572200	
O		3.83007400	H		4.11136600
1.87934000	-2.87979000		-3.39213200	-3.16008200	
C		3.14894400	H		4.85249500
-2.51048500	-0.01495900		-5.44797500	-1.96435000	
C		3.57943900	H		4.51875900
-3.69467600	0.67474600		-5.62906900	0.48774500	
C		3.37009100	H		-0.38772000
-3.78764600	2.07192400		1.68903900	1.54669700	
C		2.74748000	H		-1.84544500
-2.75946200	2.72929800		3.33848300	2.64803500	
C		0.68452400	H		-1.59928400
3.15143700	0.37685600		5.77168700	2.17121700	
C		0.80581100	H		0.08466100
4.54999000	0.07752800		6.53712800	0.51794400	
C		1.74747200	C		-4.78437600
4.96119000	-0.89729500		-2.45724400	-0.48363600	
C		2.49553400	C		-5.30090700
4.01771300	-1.55267800		-1.23600500	-0.03808000	
C		3.35636800	C		-6.61829600
-2.43217400	-1.41616200		-0.89124600	-0.37562600	
C		3.95611700	C		-7.40267200
-3.47538300	-2.08872800		-1.75035900	-1.14183200	
C		4.38048300	C		-5.57054800

-3.31969300	-1.25207200		-3.63890300	-2.18242600	
H		-3.76083800	O		-5.00704100
-2.72371500	-0.24001700		-0.33765400	2.18776400	
H		-7.02499800	H		-2.77967600
0.05545400	-0.02925600		-1.04874100	1.74536300	
H		-8.42016200	H		-4.63673700
-1.47007900	-1.39889800		0.74113300	0.50696100	
H		-5.15681100	H		-5.33416300
-4.26375300	-1.59487100		-1.23506800	2.34034600	
C		0.23666700			
-0.52990600	-0.84813300				
C		-0.15534700			
0.24683000	-2.04089900				
C		-1.39257500			
0.73036500	-2.21374800				
C		-2.51448600			
0.57739700	-1.21717700				
C		-2.11233900			
-0.28610000	-0.03224300				
C		-0.85633000			
-0.80888300	0.07507900				
H		0.79548100			
-1.42674700	-1.12722400				
H		0.59749900			
0.39886900	-2.80779200				
H		-1.64513600			
1.28000500	-3.11948900				
H		-3.35606300			
0.07358700	-1.71951300				
H		-0.65638800			
-1.48133400	0.90651400				
N		-3.07544900			
-0.55755200	0.91336900				
N		-3.06271200			
1.87632900	-0.75126400				
H		-2.31682700			
2.40764100	-0.30540600				
H		-3.35793400			
2.41726800	-1.56214400				
C		-4.50746000			
-0.28680700	0.85763800				
C		-6.87940800			
-2.96958700	-1.58193500				
H		-7.48852900			

	IMC		-4.31072000	-1.34882600	
C		2.47415200	C		4.17455100
2.84269200	-0.21475200		-4.78148200	-0.26575300	
C		3.50982700	C		-0.77725300
1.94123300	-0.84940000		2.42199300	1.46272400	
O		3.20288300	C		-1.78417800
0.65250000	-0.73774800		3.22939100	1.97992500	
Co		1.68592900	C		-1.68091900
0.22837600	0.32893700		4.65153400	1.95495900	
N		1.41235800	C		-0.55714200
2.22493800	0.34707000		5.24866800	1.40333800	
N		2.19260100	H		2.63781300
-1.71762200	0.64822800		-5.42054600	1.87804200	
C		1.49390500	H		1.02399600
-2.21566200	1.69172200		-3.82315200	3.03017400	
C		0.50386100	H		1.73818700
-1.27316300	2.33919200		6.13603100	0.25895800	
O		0.45572200	H		3.53646300
-0.09166400	1.73302900		4.63184400	-0.73335900	
O		-0.16851200	H		3.80247600
-1.62496600	3.33376700		-1.05145800	-1.40275600	
O		4.51622400	H		5.33387400
2.41455900	-1.42400700		-2.58447500	-2.60306200	
C		3.10110100	H		5.59267300
-2.55546100	-0.01017100		-4.96422800	-1.87455200	
C		3.26465700	H		4.28504500
-3.92531000	0.42587900		-5.80853200	0.07500900	
C		2.51200500	H		-0.83322700
-4.39393700	1.54256700		1.34433100	1.53430800	
C		1.63133000	H		-2.66015500
-3.53800200	2.17897300		2.76247400	2.42197800	
C		0.38939000	H		-2.48009700
3.00935500	0.88782600		5.25906400	2.37112100	
C		0.49563000	H		-0.45818300
4.45204500	0.85727700		6.33164300	1.37718300	
C		1.65090500	C		-5.34696000
5.05232700	0.27629100		-2.39573500	0.11670800	
C		2.63844400	C		-5.47344200
4.24784400	-0.26340200		-1.20973100	-0.65040600	
C		3.87428100	C		-6.76786800
-2.09305400	-1.11664000		-0.73643700	-0.97633200	
C		4.74813900	C		-7.91267000
-2.95643900	-1.76650900		-1.43274300	-0.55157300	
C		4.90165800	C		-6.48986300

-3.08814300	0.54146300		-3.15061800	0.54008800	
H		-4.34855500	H		-4.48961800
-2.74211900	0.36591500		0.47723100	-1.64237400	
H		-6.87162300			
0.17653500	-1.56095100				
H		-8.90206200			
-1.06138800	-0.80796800				
H		-6.38602700			
-3.99505300	1.13262000				
C		0.57984100			
-0.25695600	-1.35921500				
C		0.54720500			
0.87113500	-2.31455700				
C		-0.61741900			
1.43679800	-2.71682600				
C		-1.98965400			
1.02169800	-2.21050700				
C		-1.92577900			
-0.20944100	-1.30097400				
C		-0.72651500			
-0.77916700	-0.95507800				
H		1.31600500			
-1.02223900	-1.61322600				
H		1.49373300			
1.21534900	-2.72250400				
H		-0.60880400			
2.25059400	-3.44346100				
H		-2.61104700			
0.75540300	-3.08369700				
H		-0.77480100			
-1.68948000	-0.36467100				
N		-3.08303700			
-0.87767000	-0.85644000				
N		-2.71036400			
2.14429300	-1.53641500				
H		-2.29229200			
2.40849300	-0.64531600				
H		-2.85292000			
2.95167500	-2.14232300				
C		-4.29458500			
-0.45987600	-1.11026100				
C		-7.77685700			
-2.61100600	0.20835900				
H		-8.66103500			

	TS3		-3.53828100	-1.43456000	
C		2.95332600	C		4.89259500
2.58990300	1.47214700		-4.23429800	-1.32512100	
C		4.06625700	C		-0.01623700
1.58796800	1.65522700		2.80716100	-0.62238100	
O		3.87649700	C		-1.00109600
0.49366600	0.95637600		3.72374800	-0.92353100	
Co		2.24746000	C		-1.03790500
0.35037300	0.09692700		4.98818600	-0.29257800	
N		1.97939100	C		-0.07348300
2.20952300	0.63501100		5.32173800	0.63031800	
N		2.54579100	H		2.41596400
-1.47551800	-0.46380800		-5.32604200	-1.10712900	
C		1.38158200	H		0.30904700
-2.16393600	-0.45665200		-4.00513900	-0.65428600	
C		0.18067800	H		1.97598400
-1.31845200	-0.26848400		5.71199100	2.36255800	
O		0.43469100	H		3.82793100
-0.04217500	-0.15932000		4.03042500	2.78317600	
O		-0.95672100	H		4.95791500
-1.81821600	-0.25379200		-0.39340700	-0.72744900	
O		5.02422200	H		7.02467900
1.83279800	2.36920100		-1.59401200	-1.32499900	
C		3.70898100	H		6.99859300
-2.15042800	-0.77213300		-4.05990600	-1.68313500	
C		3.68571500	H		4.86162200
-3.56749300	-1.00564300		-5.30807600	-1.49265300	
C		2.44164300	H		-0.00478600
-4.25349400	-0.93386100		1.83185800	-1.08714600	
C		1.29130100	H		-1.76190700
-3.54704700	-0.68016600		3.46450000	-1.65392800	
C		0.98121500	H		-1.82412100
3.11675900	0.33439800		5.69503200	-0.54219300	
C		0.96028400	H		-0.07991700
4.40809200	0.96026100		6.29375500	1.11698100	
C		1.98873600	C		-3.64462100
4.73909600	1.87757400		-2.75390500	1.47984600	
C		2.99421600	C		-4.64548700
3.83630800	2.11844400		-1.77280900	1.25244100	
C		4.93653600	C		-5.80488800
-1.45844800	-0.90820300		-1.77916200	2.07034700	
C		6.09187100	C		-5.95831400
-2.14271000	-1.23017200		-2.72570900	3.06893200	
C		6.07877200	C		-3.82122700

-3.69927000	2.48726000	-1.08550200	-0.42720200
H		-2.74171900	
-2.77094400	0.88143500		
H		-6.57796200	
-1.02548200	1.93694600		
H		-6.84975300	
-2.71064600	3.69009000		
H		-3.04948800	
-4.44690700	2.64838600		
C		-3.46102500	
1.72032300	-3.46560100		
C		-4.78396900	
2.15098100	-3.28161500		
C		-5.57650900	
1.65202900	-2.24281900		
C		-4.99305900	
0.70910100	-1.40038400		
C		-3.66408400	
0.27529500	-1.58212200		
C		-2.87611700	
0.77371400	-2.61828500		
H		-2.88025200	
2.12295500	-4.29027100		
H		-5.20635800	
2.88330600	-3.96312300		
H		-6.60123300	
1.98304700	-2.10469800		
H		-1.85878300	
0.42614100	-2.76247200		
N		-3.40210600	
-0.66384000	-0.59851000		
N		-5.46885400	
0.01751900	-0.29430500		
H		-6.42860900	
-0.00157500	0.01340000		
C		-4.49721000	
-0.83225800	0.18758100		
C		-4.96690600	
-3.69688000	3.28382700		
H		-5.09043500	
-4.43620800	4.06983300		
H		-3.11205400	
-3.67654600	-1.15331900		
H		-2.46425600	

	IMD		-3.33678100	-0.05657300	
C		-1.98157400	C		-4.36521100
3.52164500	0.42338300		-3.80410800	-0.94083200	
C		-3.33134200	C		1.48266800
2.85703300	0.42238300		2.24792600	0.23102100	
O		-3.24041600	C		2.78097500
1.52741000	0.13280200		2.74620200	0.37204100	
Co		-1.55832800	C		3.02079600
0.97432600	-0.49600800		4.13827900	0.59156300	
N		-0.94370900	C		1.94672100
2.67646400	0.16322300		5.02188800	0.70730800	
N		-2.07388400	H		-2.33510700
-0.80857100	-1.12471700		-4.45207200	-2.63976800	
C		-1.13767200	H		-0.38754300
-1.30952800	-1.98494400		-2.89187800	-3.23363000	
C		0.01259400	H		-0.34974200
-0.38892800	-2.28418600		6.48030100	0.97551400	
O		-0.08279900	H		-2.71225900
0.79001500	-1.62750200		5.49158500	0.90572100	
O		0.95816100	H		-4.12918400
-0.70424600	-3.05669400		-0.14201300	0.48602200	
O		-4.39933900	H		-6.01030900
3.45856200	0.69871100		-1.64158800	1.15184100	
C		-3.16272600	H		-6.17775600
-1.62815100	-0.77535900		-3.97713400	0.23151700	
C		-3.26304900	H		-4.42682100
-2.97308000	-1.32132100		-4.81583700	-1.35853300	
C		-2.25845500	H		1.32140200
-3.44067800	-2.22553800		1.17870900	0.07608900	
C		-1.19692600	H		3.62463500
-2.60448300	-2.55744900		2.05074800	0.31168700	
C		0.37009100	H		4.04900000
3.14054400	0.30580200		4.50388700	0.68558500	
C		0.60083600	H		2.11432100
4.54823600	0.58885800		6.08657800	0.90766800	
C		-0.52180300	C		3.90379700
5.41734800	0.77277400		-0.67207900	-1.43774600	
C		-1.81363200	C		4.18914700
4.89567800	0.72562500		-1.30163000	-0.19461600	
C		-4.17834400	C		5.54452000
-1.17005900	0.12015400		-1.54387500	0.16600200	
C		-5.23783400	C		6.59273200
-2.01205600	0.46938100		-1.17001800	-0.70066700	
C		-5.33729300	C		4.95687700

-0.29801400	-2.29683800	
H		2.86479000
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H		5.79246900
-1.99239500	1.13658000	
H		7.63249600
-1.35682900	-0.40986900	
H		4.72003400
0.17772800	-3.25435200	
C		-0.66732500
-2.47166800	3.18510500	
C		0.19788000
-3.39740000	3.83998500	
C		1.54271000
-3.55988700	3.44280200	
C		1.98578800
-2.76311500	2.36772300	
C		1.12477500
-1.83094100	1.69124700	
C		-0.21797000
-1.68078200	2.10933400	
H		-1.70301900
-2.37507100	3.52823000	
H		-0.19064700
-3.99405300	4.67260300	
H		2.20044300
-4.27037800	3.95457900	
H		-0.87950700
-0.96571600	1.60790900	
N		1.82835400
-1.17813700	0.65692800	
N		3.21889300
-2.64536800	1.71324300	
H		4.05129700
-3.20343000	1.89087400	
C		3.08143300
-1.68620400	0.69228600	
C		6.30288900
-0.54551600	-1.93644400	
H		7.11700400
-0.25574600	-2.61003600	