Supplementary Information for:

Synthesis of Novel *meta*-Benzothiazole and Benzimidazole Functionalised Ni(II)-POCOP Pincer Complexes. Efficient Catalysts in the Production of Diarylketones

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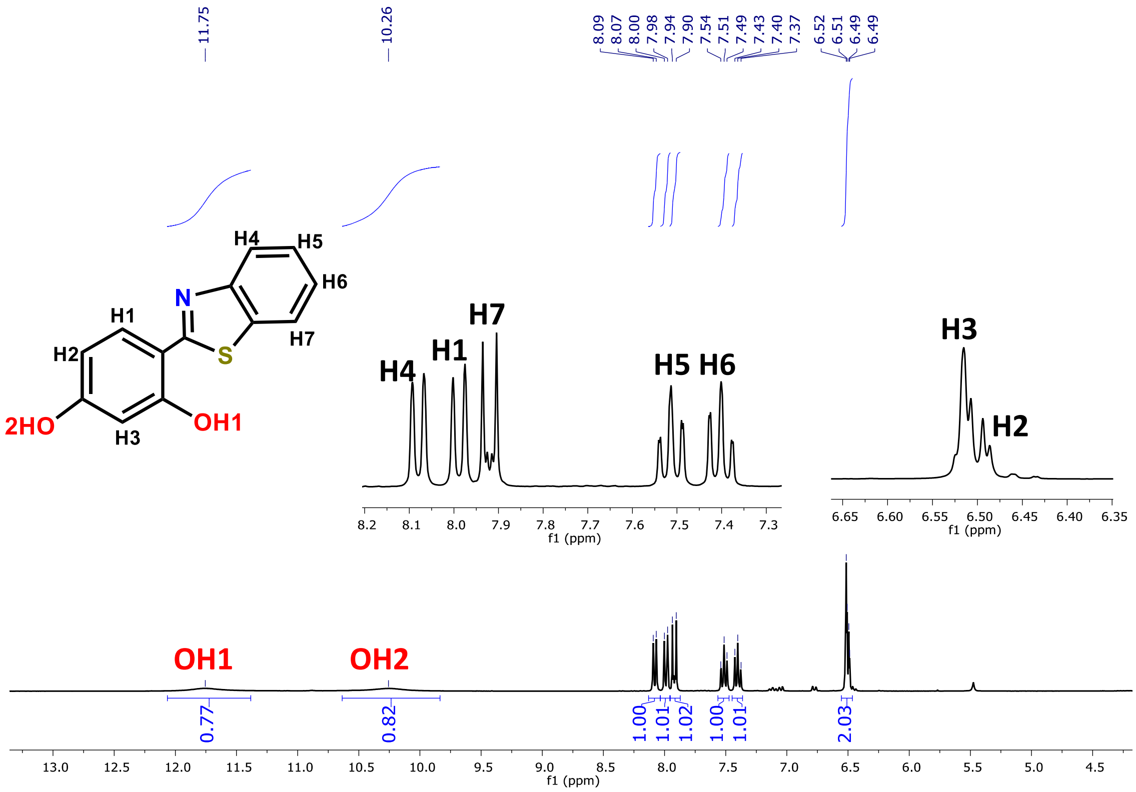


Figure SI**1.** ¹H NMR spectrum of **P1**

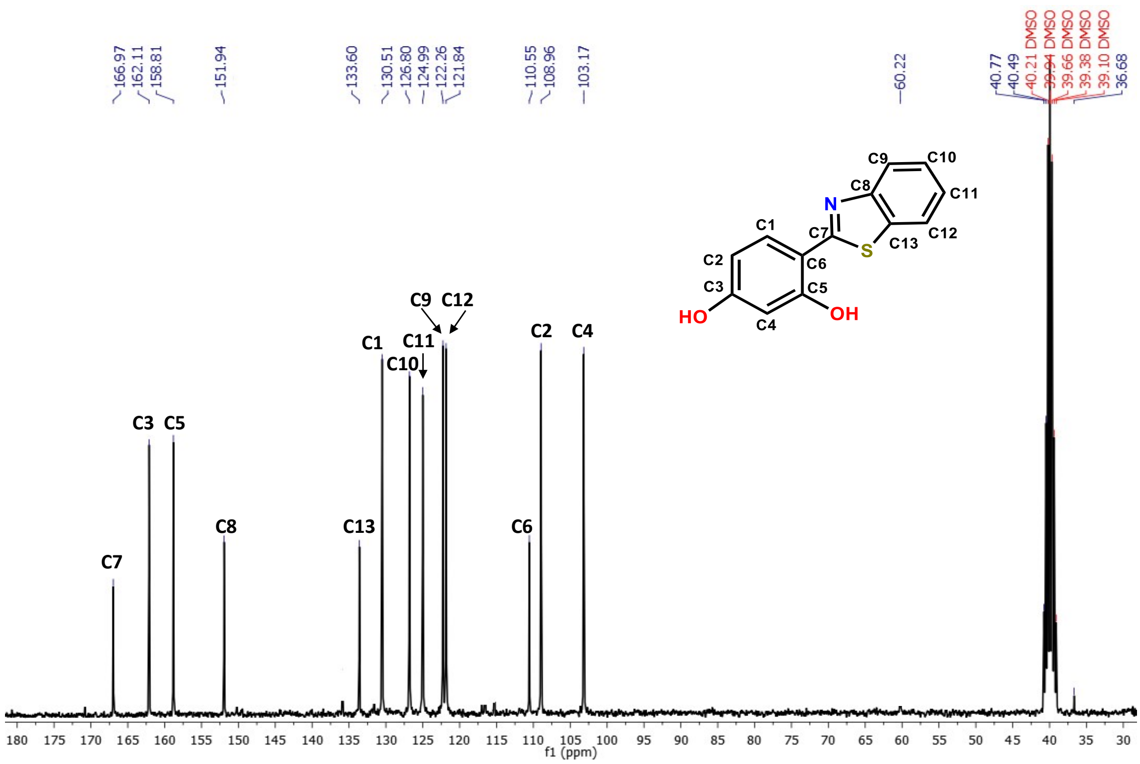


Figure SI**2.** ¹³C{¹H} NMR spectrum of **P1**

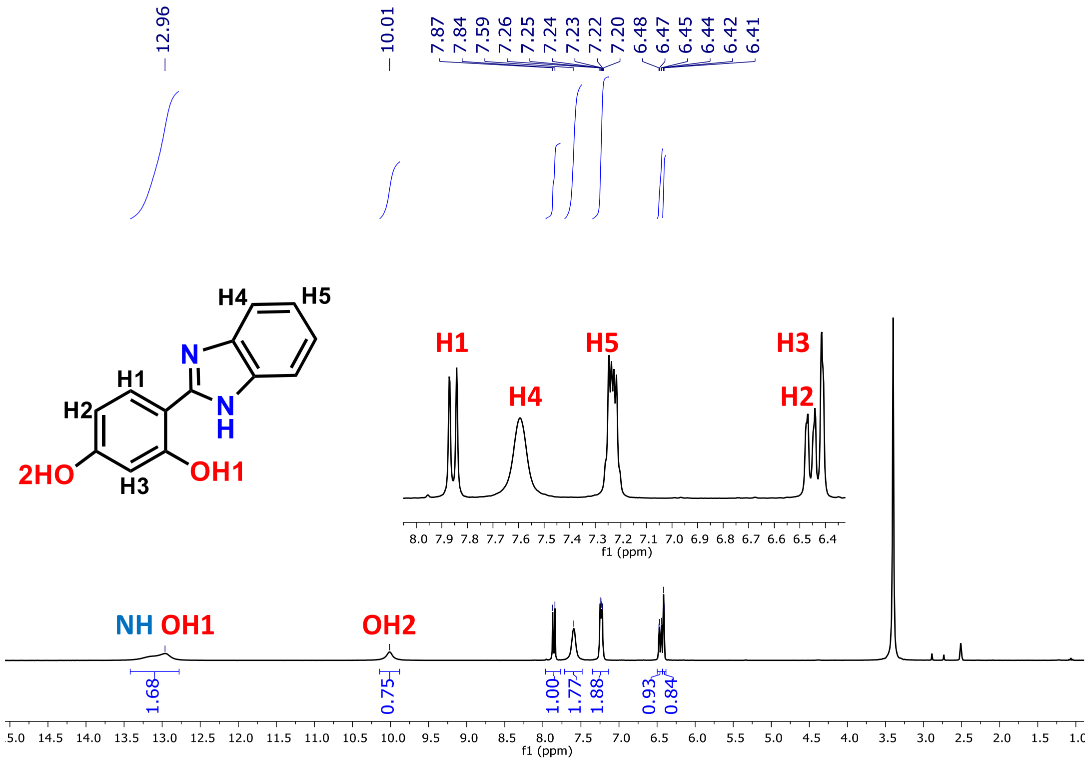


Figure SI**3.** ^{1}H NMR spectrum of **P2**

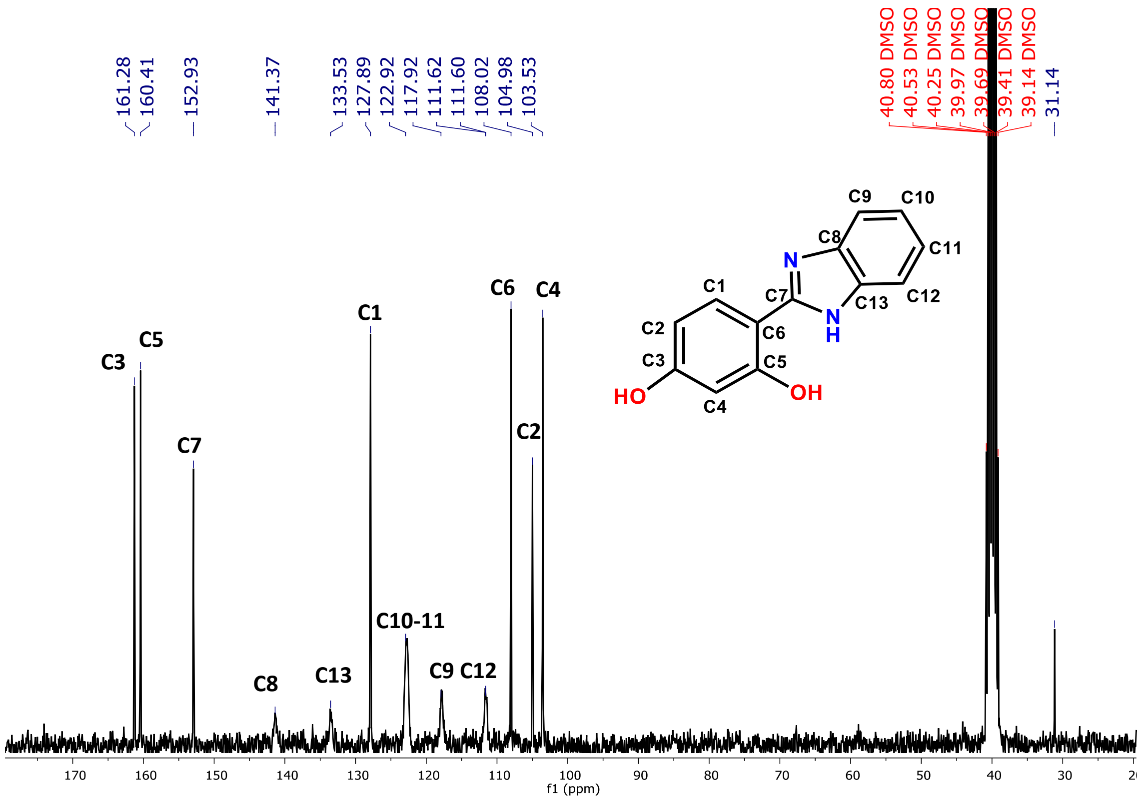


Figure SI**4.** $^{13}C\{^{1}H\}$ NMR spectrum of **P2**

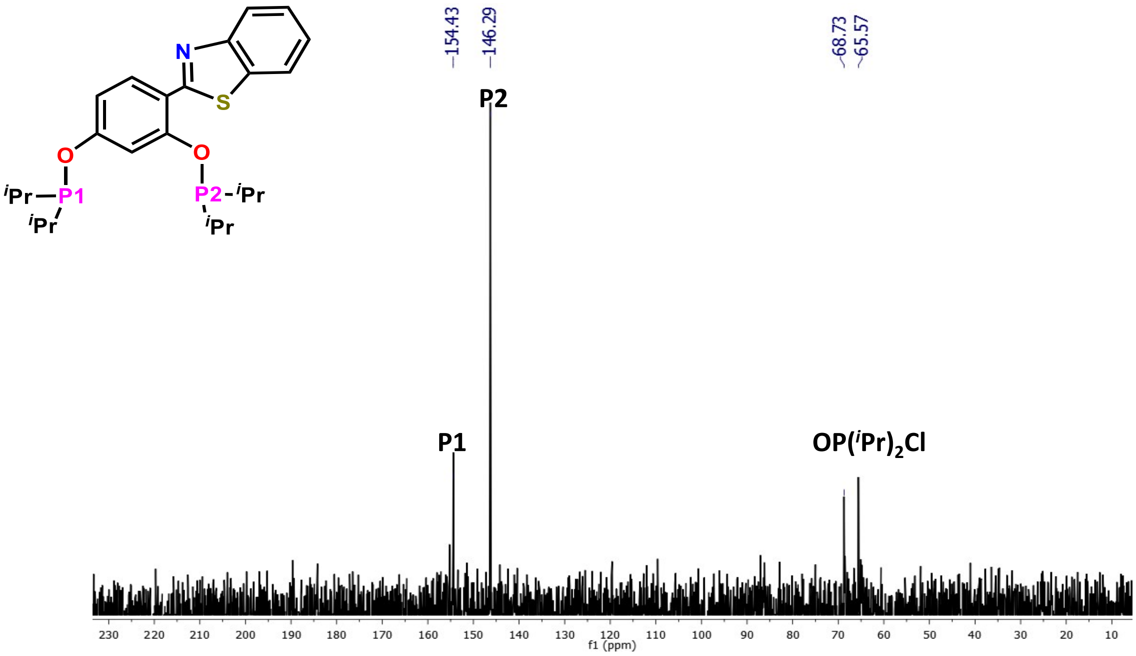


Figure SI**5.** $^{31}P\{^{1}H\}$ NMR spectrum of **L1a**

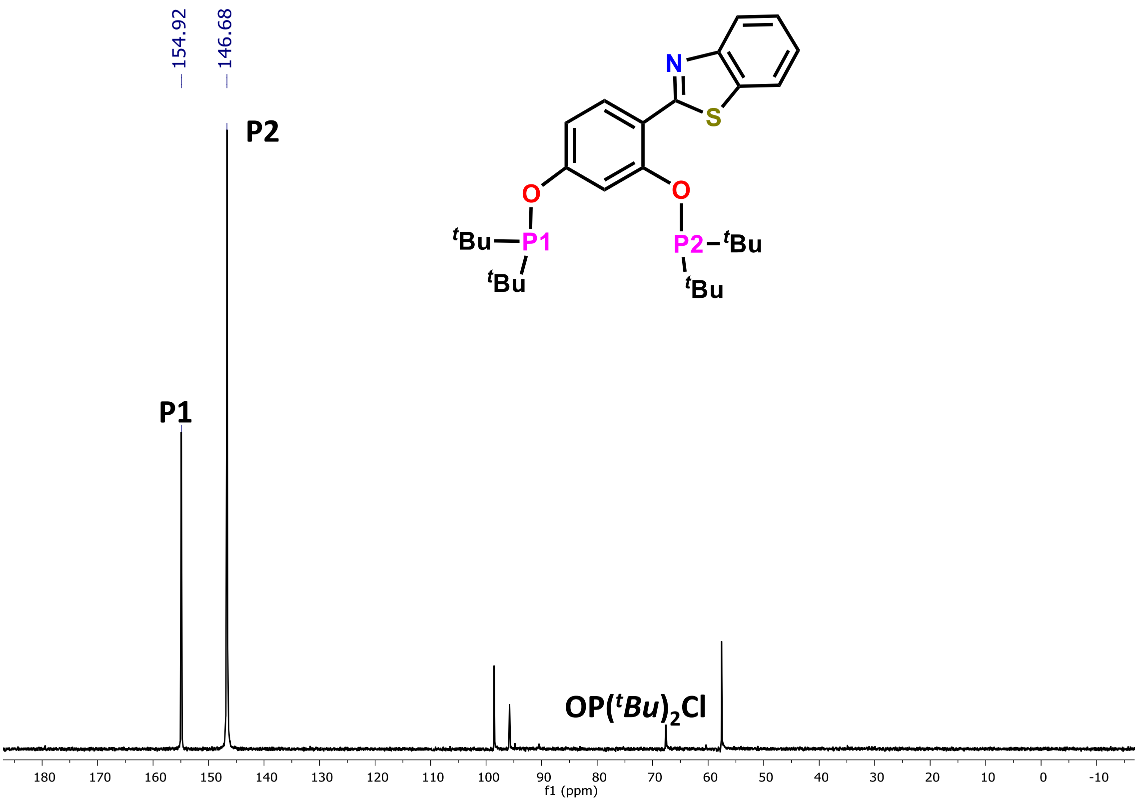


Figure SI**6**. $^{31}P\{^{1}H\}$ NMR spectrum of **L1b**

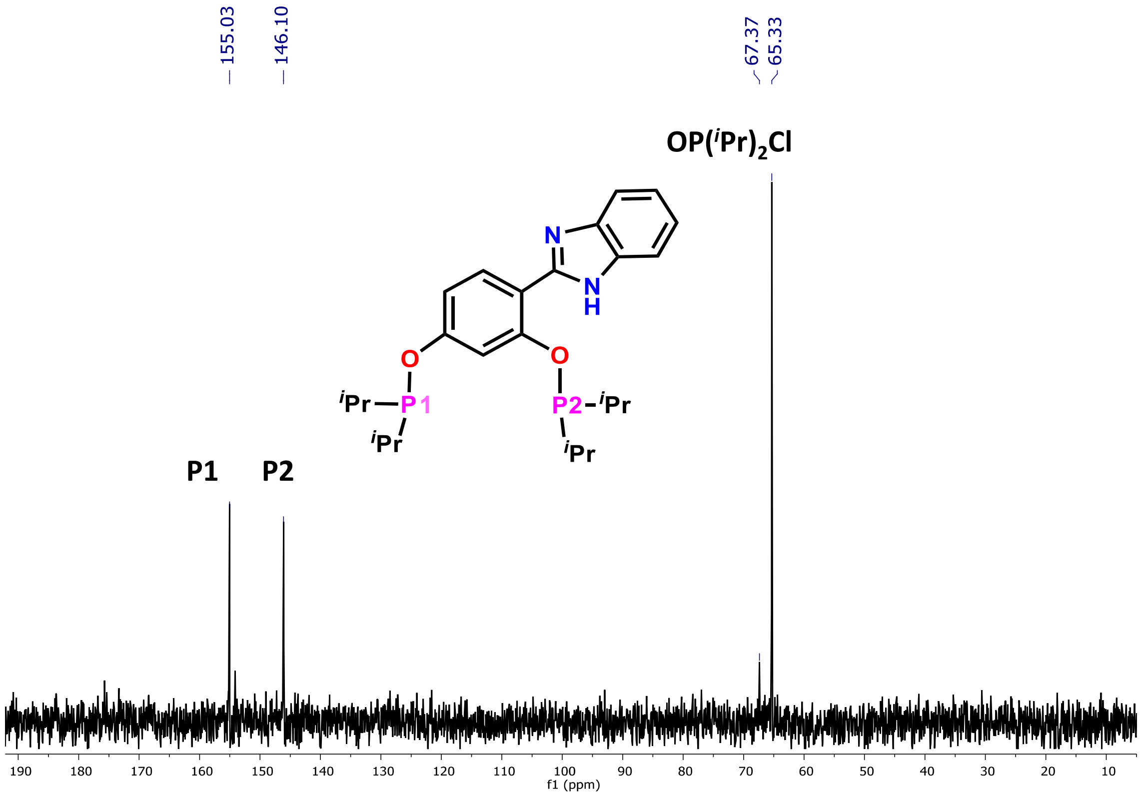


Figure SI**7**. $^{31}P\{^{1}H\}$ NMR spectrum of **L2a**

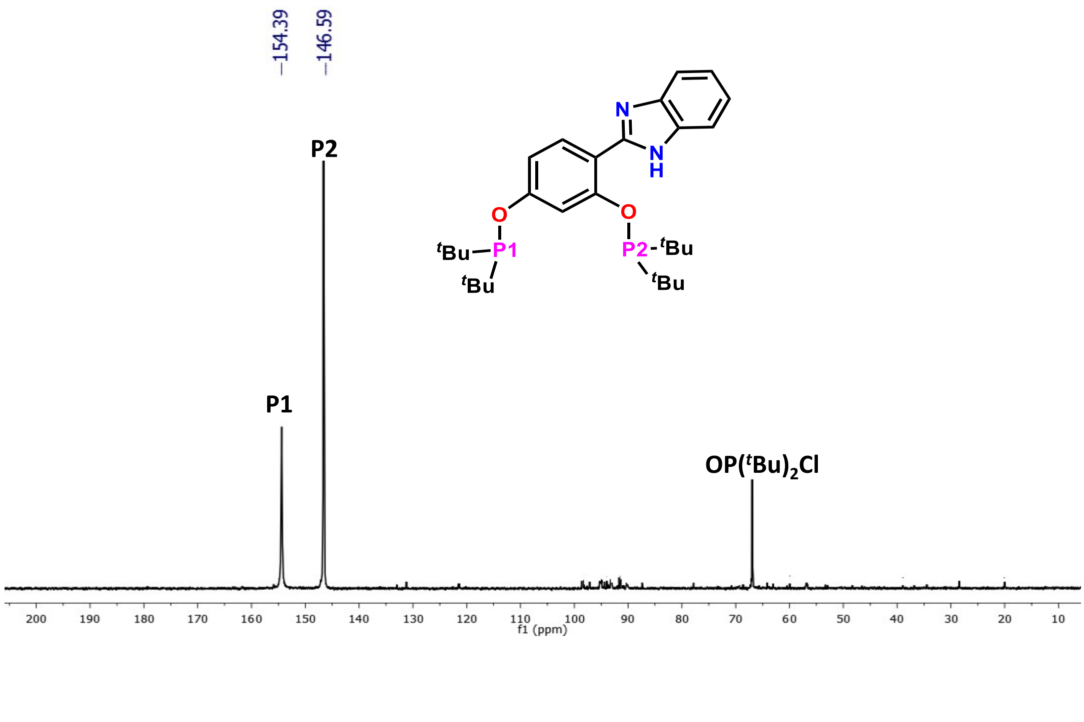


Figure SI**8**. $^{31}P\{^{1}H\}$ NMR spectrum of **L2b**

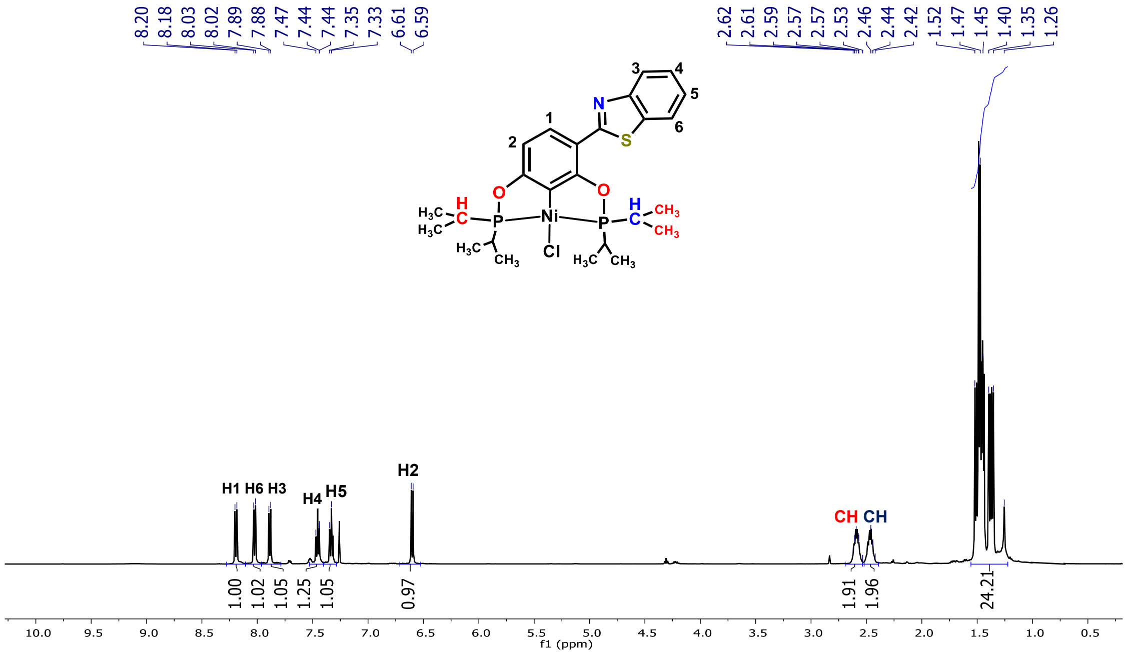


Figure SI**9**. ^{1}H NMR spectrum of **1a**

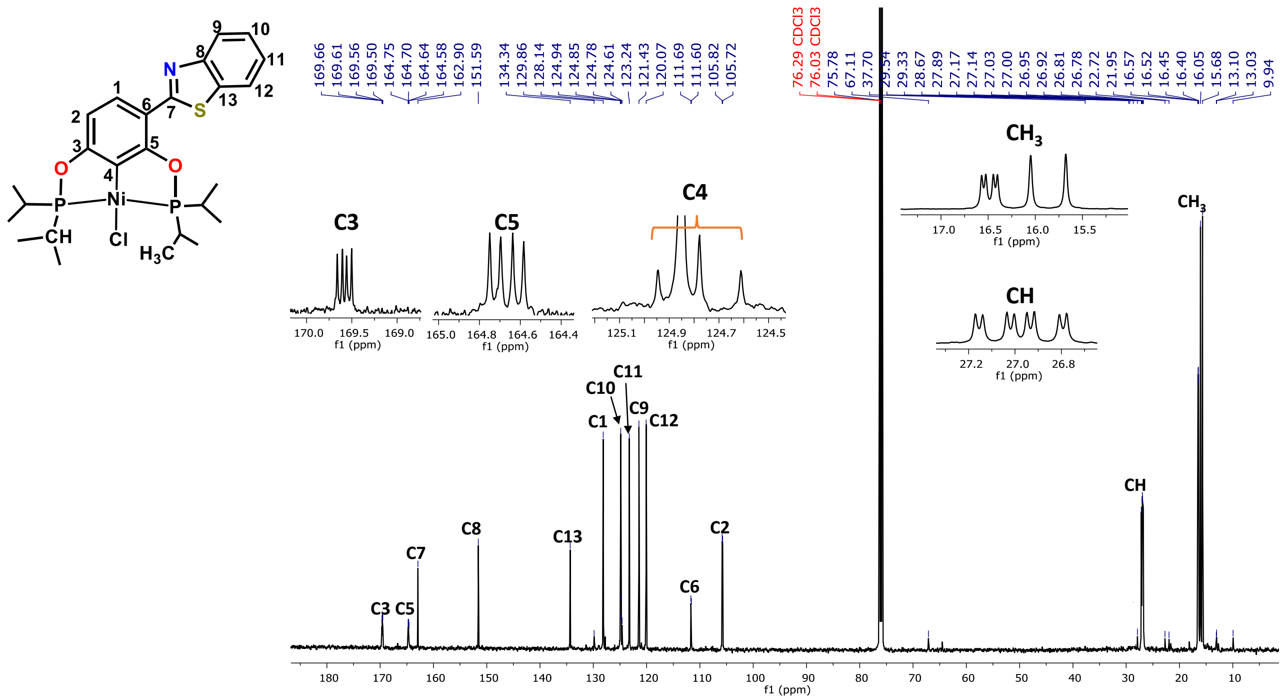


Figure SI**10**. $^{13}C\{^{1}H\}$ NMR spectrum of **1a**

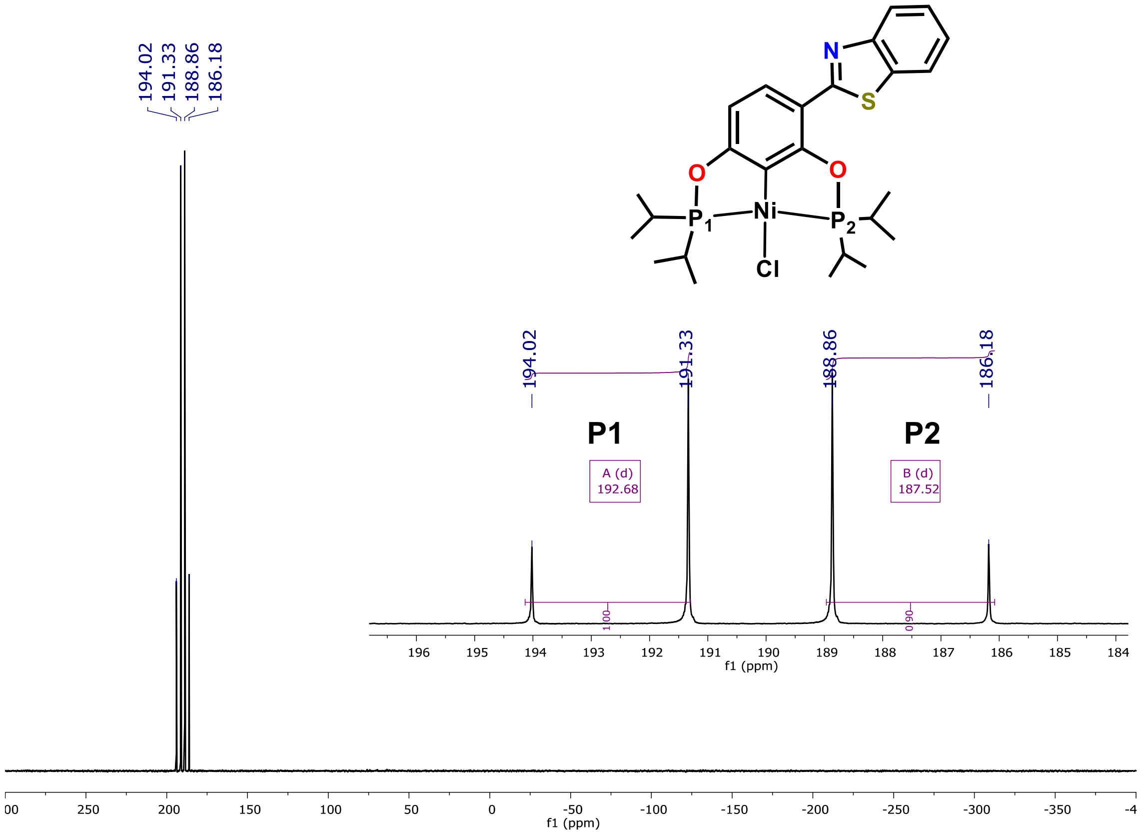


Figure SI**11**. $^{31}P\{^{1}H\}$ spectrum of **1a**

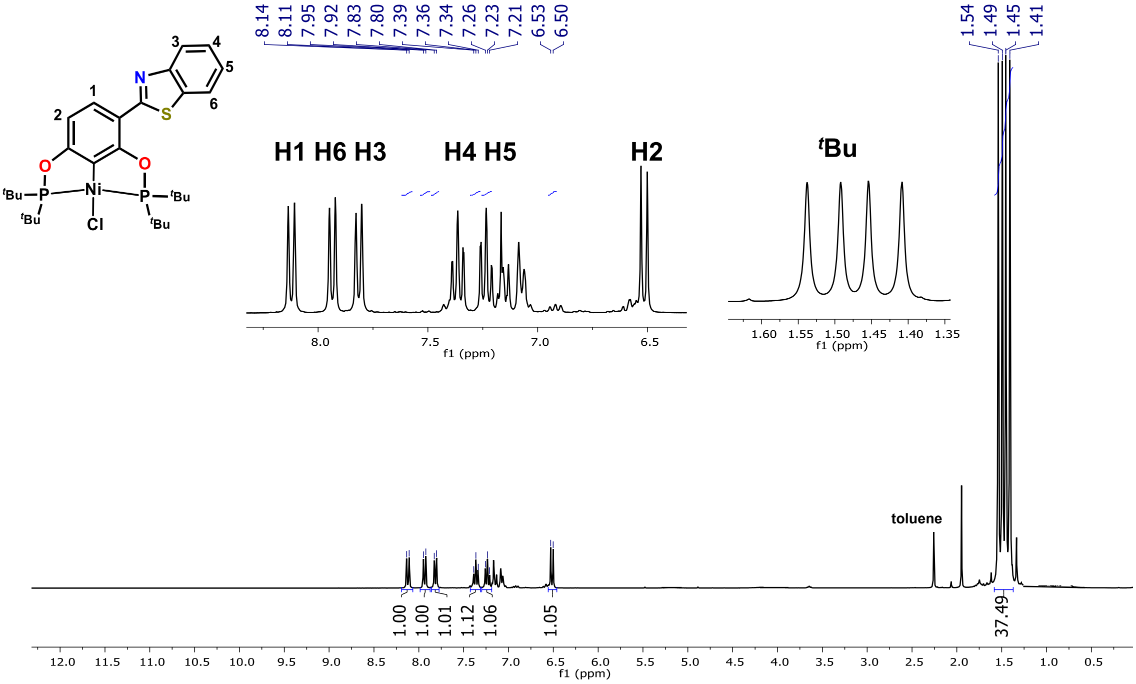


Figure SI**12**. ^{1}H NMR spectrum of **1b**

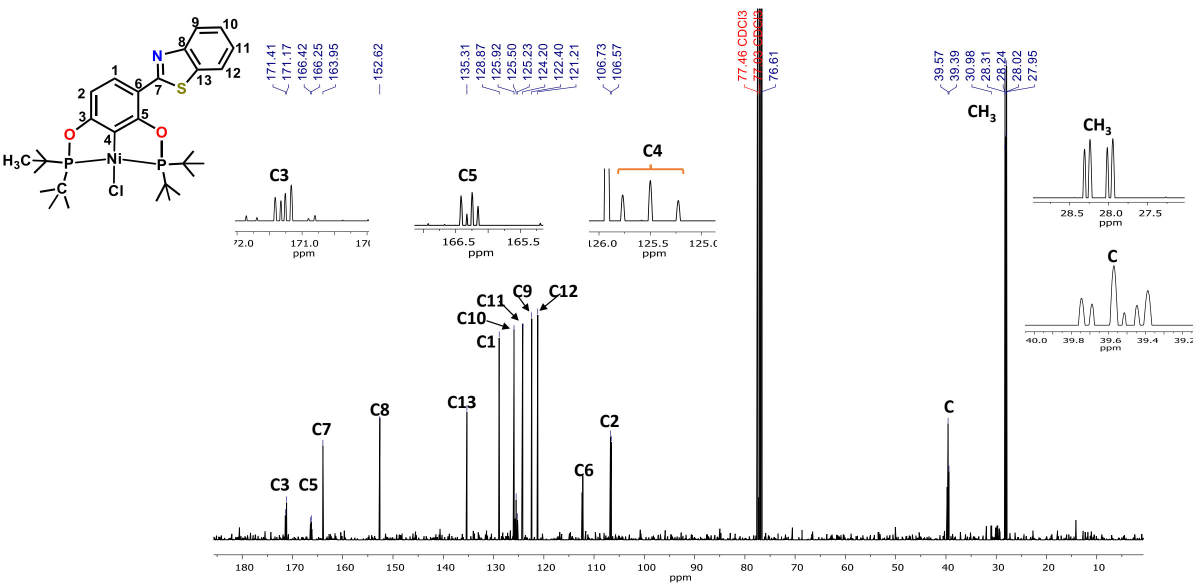


Figure SI**13**. ^{13}C{^{1}H} NMR spectrum of **1b**

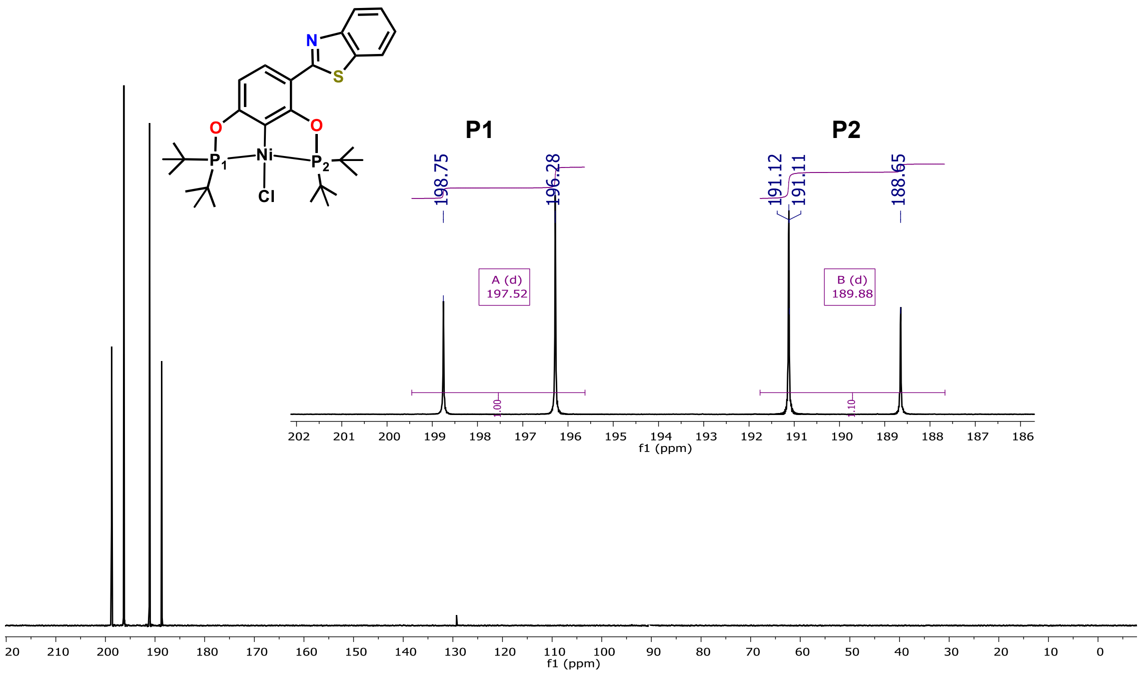


Figure SI**14.** $^{31}P\{^1H\}$ NMR spectrum of **1b**

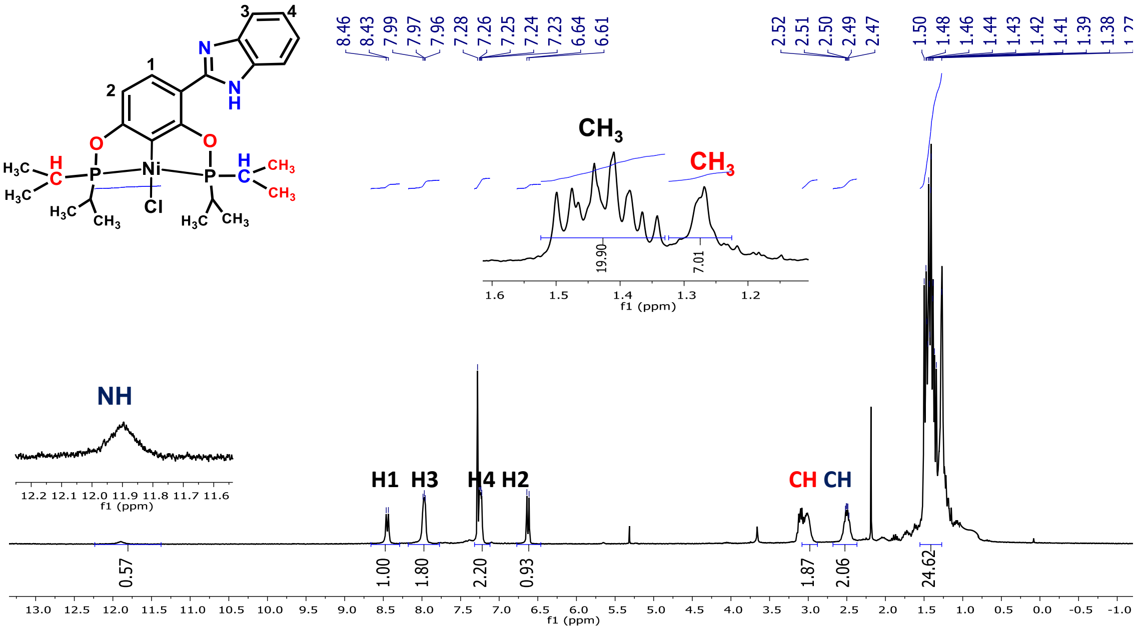


Figure SI**15**. ^{1}H NMR spectrum of **2a**

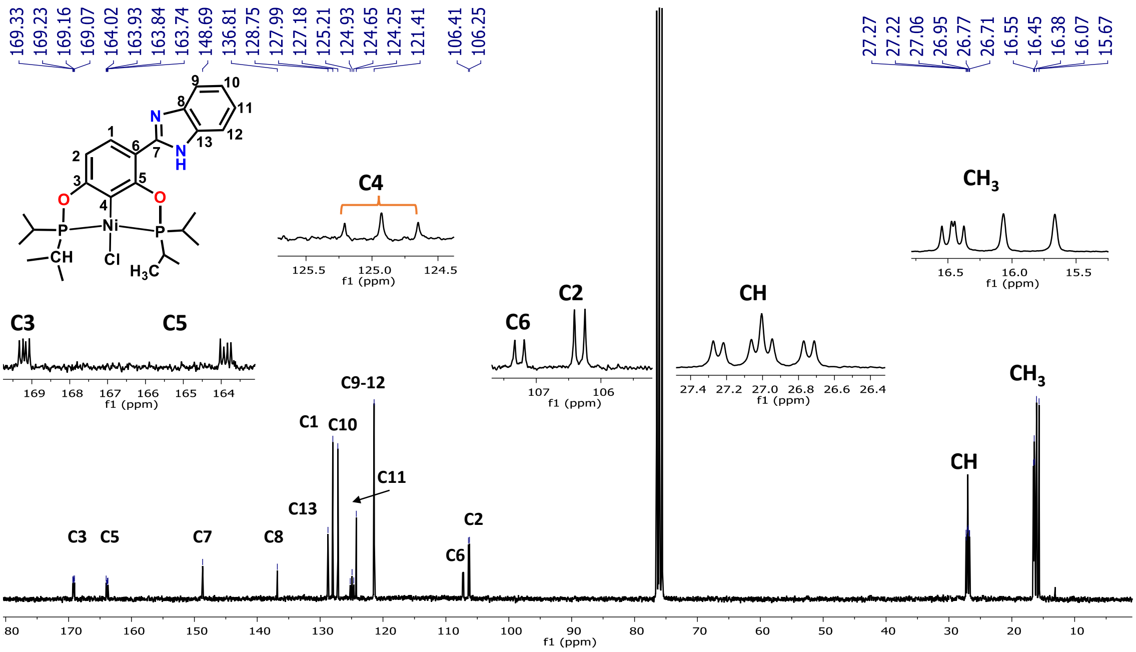


Figure SI**16**. ^{13}C{^{1}H} NMR spectrum of **2a**

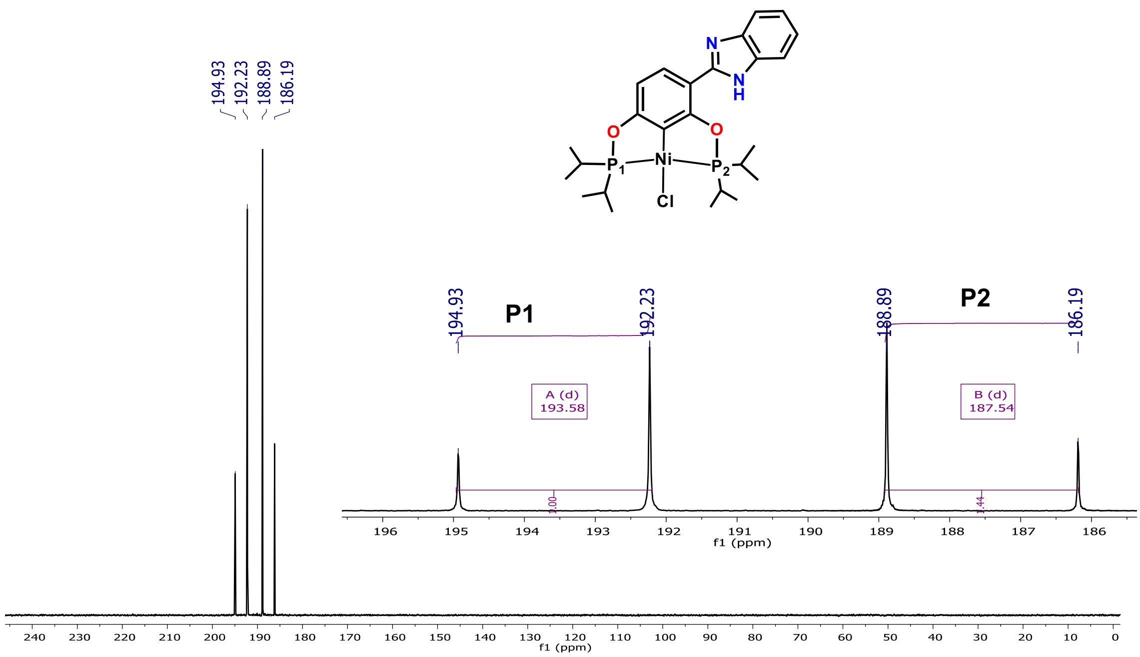


Figure SI**17.** $^{31}P\{^{1}H\}$ NMR spectrum of **2a**

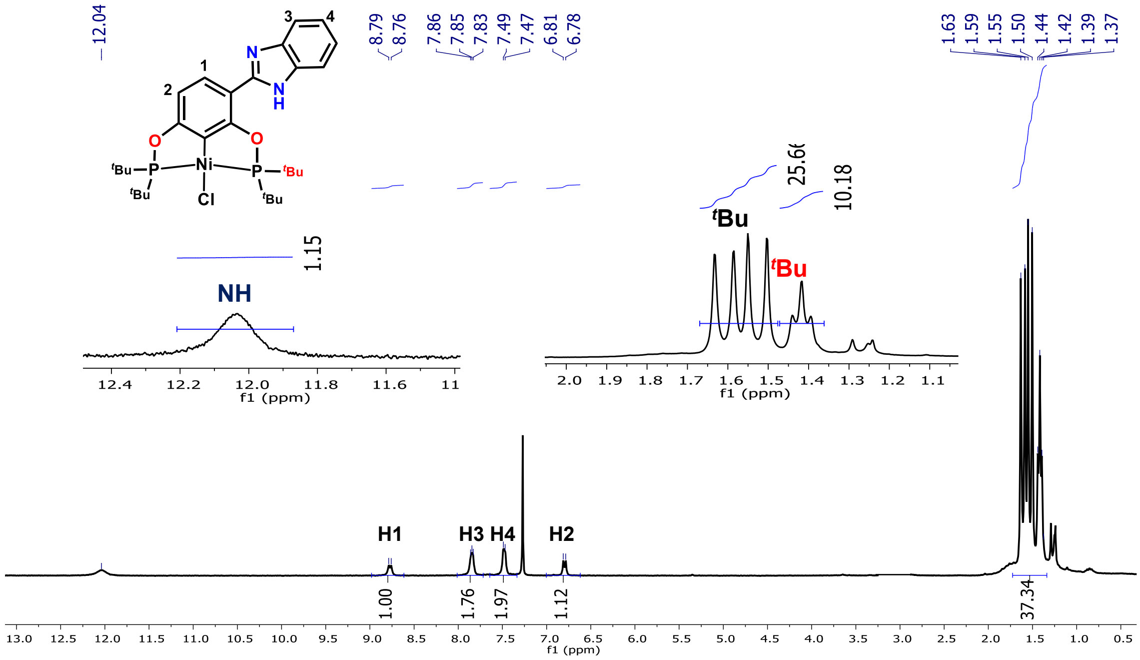


Figure SI**18.** ^{1}H NMR spectrum of **2b**

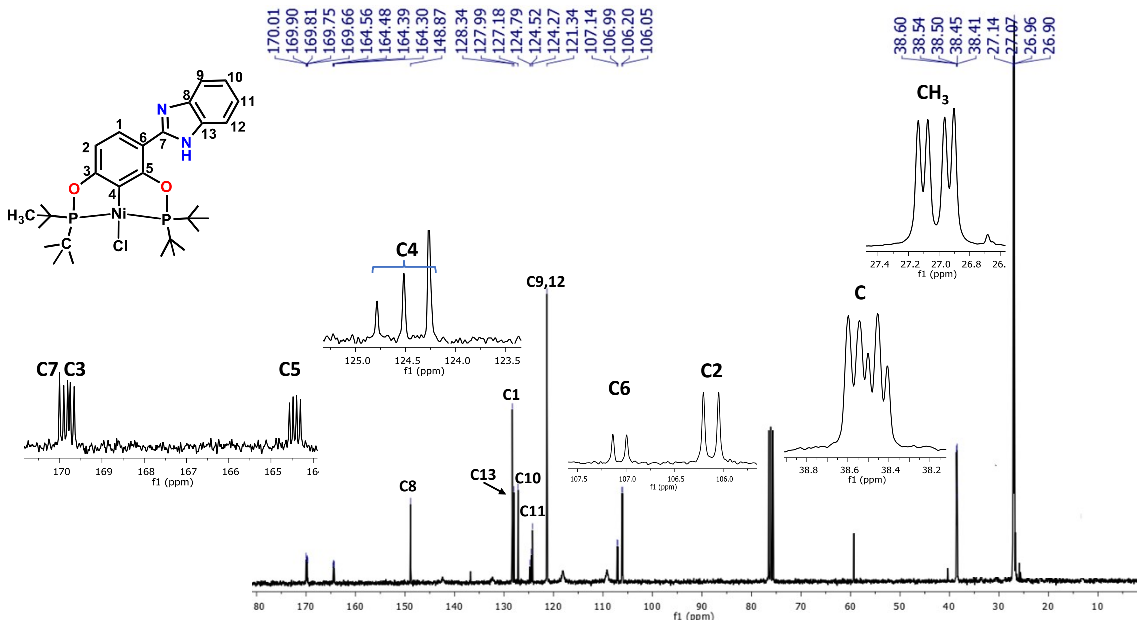


Figure SI**19.** ^{31}P{^{1}H} NMR spectrum of **2b**

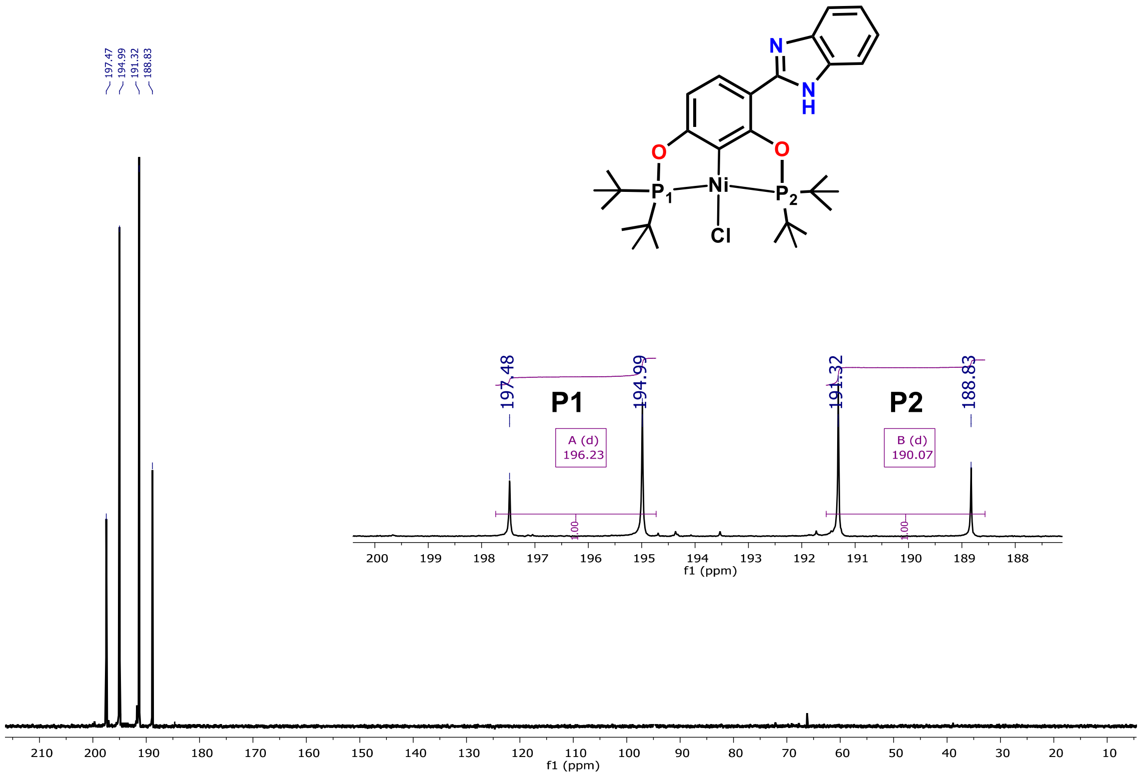
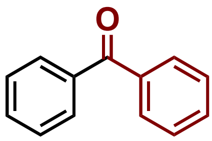


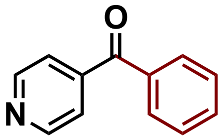
Figure SI**20.** $^{31}P\{^{1}H\}$ NMR spectrum of **2b**

Characterization data for compounds 3a – 3p

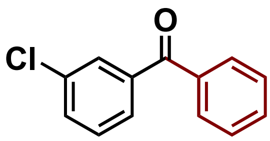
These compounds were characterized by ^{1}H and $^{13}C\{^{1}H\}$ NMR and structurally confirmed by direct comparison of previously reported data.



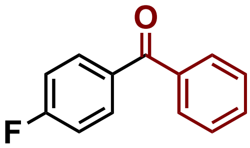
Compound **3a**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.86 (d, *J* = 7.7 Hz, 2H), 7.69 (t, *J* = 7.5 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 196.89, 137.73, 132.54, 130.19, 128.41.[1,4]



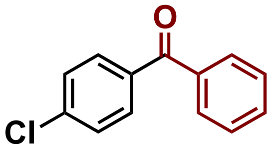
Compound **3b**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.75 (d, *J* = 6.0 Hz, 2H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.58 (t, *J* = 7.60 Hz, 2H), 7.52 (d, *J* = 6.0 Hz, 2H) 7.45 (t, *J* = 7.6 Hz, 2H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 194.9, 150.2, 144.2, 135.4, 133.4, 130.0, 128.5, 122.4.[1]



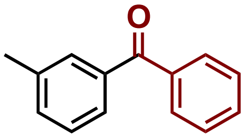
Compound **3c**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.8 – 7.78 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.40 (m, 1H), 7.34 – 7.28 (m, 2H), 7.12 – 7.10 (m, 1H), 6.84 (br s, 1H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 197.5, 156.3, 138.4, 137.4, 132.9, 130.2, 129.6, 128.5, 122.7, 120.3, 116.3.[1]



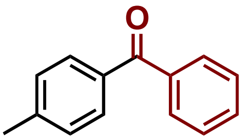
Compound **3d**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79-7.74 (m, 2H), 7.65 (d, J = 7.7 Hz, 2H), 7.65 (t, J = 7.3 Hz, 1 H), 7.47 (t, J = 7.5 Hz, 2H), 7.19 (t, J = 8.3 Hz, 2H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 195.41, 165.52 (d, $J_{C\text{-}F}$ = 252.5 Hz), 137.63, 133.94, 132.80 (d, Hz), 132.61, 130.01, 128.49, 115.68 (d, $J_{C\text{-}F}$ = 21.2 Hz).[3,4]



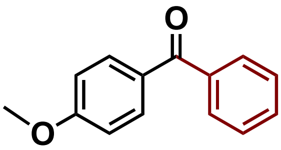
Compound **3e**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.77 (t, J = 7.9 Hz, 4H), 7.60 (t, J = 7.3 Hz, 1H), 7.55-7.42 (m, 4H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 195.6, 139.0, 137.4, 136.3, 132.8, 131.5, 130.1, 128.9, 128.5.[1,2,4]



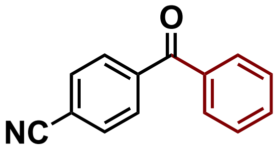
Compound **3f**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.97-7.84 (m, 2H), 7.61-7.58 (m, 1H), 7.48 (t, J = 7.7 Hz, 2H), 7.42 (td, J = 7.5, 1.5 Hz, 1H), 7.34-7.30 (m, 2H), 7.29-7.27 (m, 1H), 2.36 (s, 3H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 198.77, 138.74, 137.86, 136.87, 133.25, 131.12, 130.36, 130.26, 128.64, 128.58, 125.32, 20.12.[1,4]



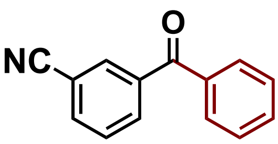
Compound **3g**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.78 (d, J = 8.2 Hz, 2H), 7.73 (d, J = 8.2 Hz, 2H), 7.58 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.5 Hz, 2H), 7.28 (d, J= 7.9 Hz, 2H), 2.44 (s, 3 H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 196.5, 143.4, 138.1, 135.0, 132.3, 130.4, 130.1, 129.1, 128.3, 21.8. [1,2,4]



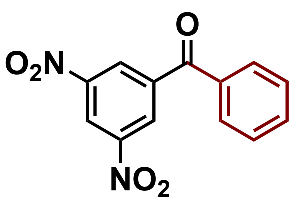
Compound **3h**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.83 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 7.6 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.47 (t, J = 7.4 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 3.89 (s, 3H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 195.6, 163.3, 138.4, 132.7, 132.0, 130.4, 129.7, 128.3, 113.6, 55.5.[1]



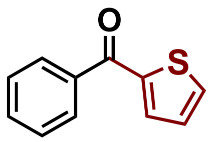
Compound **3i**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.82 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.4 Hz, 4H), 7.61 (t, J = 7.2Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 194.3, 141.1, 136.2, 133.2, 132.4, 130.1, 129.9, 128.1, 117.9, 115.5.[1]



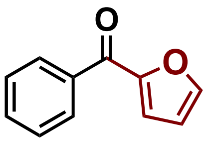
Compound **3j**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (s, 1H), 8.01 (d, J = 8.4 Hz, 1H), 7.85 (d, J = 7.6 Hz, 2H), 7.75 (d, J = 7.6 Hz, 2H), 7.64-7.59 (m, 2H), 7.50 (t, J = 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 193.8, 138.4, 136.0, 135.3, 133.5, 133.2, 133.0, 129.9, 129.4, 128.7, 117.7, 112.6.[1]



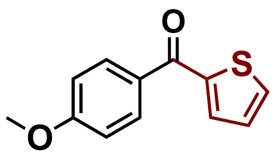
Compound **3k**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.70(s, 1H), 8.68 (s, 1H), 8.32 (s, 1H), 7.80 (d, J = 7.6 Hz, 2H), 7.63 (t, J = 7.6 Hz, 1H), 7.50 (t, J = 7.6 Hz, 2H). ^{13}C{^{1}H} NMR (75.5 MHz, $CDCl_3$): δ 194.8, 149.8, 142.8, 139.8, 136.3, 130.7, 130.1, 128.7, 123.5.



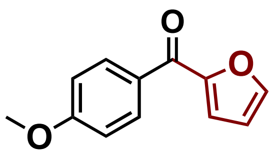
Compound **3l**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.80 (d, *J* = 7.2 Hz, 2H), 7.67 (d, *J* = 5.2 Hz 1H), 7.62 (d, *J* = 3.6 Hz, 1H), 7.55 (t, *J* = 7.2 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2 H), 7.14 (t, *J* = 4.4 Hz, 1 H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 188.1, 143.6, 138.4, 135.0, 134.1, 132.4, 129.1, 128.0, 127.7. [1,2,3]



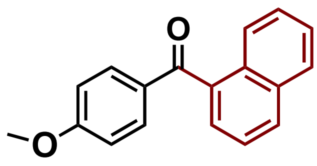
Compound **3m**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.95 – 7.92 (m, 2H), 7.70 – 7.68 (m, 1H), 7.61 – 7.59 (m, 1H), 7.49 (t, *J* = 7.5 Hz, 2H), 7.23 (d, *J* = 3.5 Hz, 1H), 6.59 (dd, *J* = 3.5, 1.6 Hz, 1H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 182.7, 151,9, 147.2, 137.0, 132.7, 129.8, 128.9, 120.7, 112.0.[1,2,3]



Compound **3n**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.99 (d, *J* = 8.9, 2H), 7.67 (d, *J* = 4.9 Hz, 1H), 7.59 (d, *J* = 4.1 Hz, 1H), 7.10 – 7.08 (m, 1H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.85 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 187.1, 163.0, 143.8, 134.0, 133.1, 131.5, 130.8, 127.7, 113.5, 55.3.[1,2,3]



Compound **3o**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.0 (d, *J* = 8.9, 2H), 7.68 (d, *J* = 0.7 Hz, 1H), 7.22 (d, *J* = 3.5 Hz , 1H), 6.98 (d, *J* = 8.9 Hz, 2H), 6.59-6.57 (m, 1H), 3.88 (s, 3H); $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 181.0, 163.2, 152.5, 146.5, 131.6, 129.7, 119.6, 113.6, 112.0, 55.4.[1,2,3]



Compound **3p**, ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.97 (t, *J* = 8.2 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.58 – 7.41 (m, 4H), 6.92 (d, *J* = 8.6 Hz, 2H), 3.87 (s, 3H). $^{13}C\{^{1}H\}$ NMR (75.5 MHz, $CDCl_3$): δ 196.5, 163.5, 136.7, 133.5, 132.2, 130.9, 130.6, 130.5, 128.2, 126.8, 126.7, 126.1, 125.4, 124.2, 113.5, 55.3.[2]

[1] J. Karthikeyan, K. Parthasarathy and C.-H. Cheng, *Chem. Commun.*, 2011, **47**, 10461-10463.
[2] G. Mora, S. Darses and J.-P. Genet, *Advanced Synthesis & Catalysis*, 2007, **349**, 1180-1184.
[3] M. Pucheault, S. Darses and J.-P. Genet, *J. Am. Chem. Soc.*, 2004, **126**, 15356-15357.
[4] S. Shi and M. Szostak, *Org. Lett.*, 2016, **18**, 5872-5875.