Supporting Information

Sugar-boronate ester scaffold tethered pyridyl-imine palladium(II) complexes: Synthesis and their *in vitro* anticancer evaluation

Eda Rami Reddy,[a] Rajiv Trivedi,[*,a] Akella Venkata Subrahmanya Sarma,[b] Balasubramanian Sridhar,[c] Hasitha Shilpa Anantharaju,[d] Dharmarajan Sriram,[d] Perumal Yogeeswari[d], and Narayana Nagesh[*,e]

***,**[a] Inorganic and Physical Chemistry Division, CSIR-IICT, Hyderabad-500007, India. Fax: +91-40-27160921. Tel: +91-40- 27191667.
E-mail: trivedi@iict.res.in, rtrajiv401@gmail.com

Contents of Supporting Information

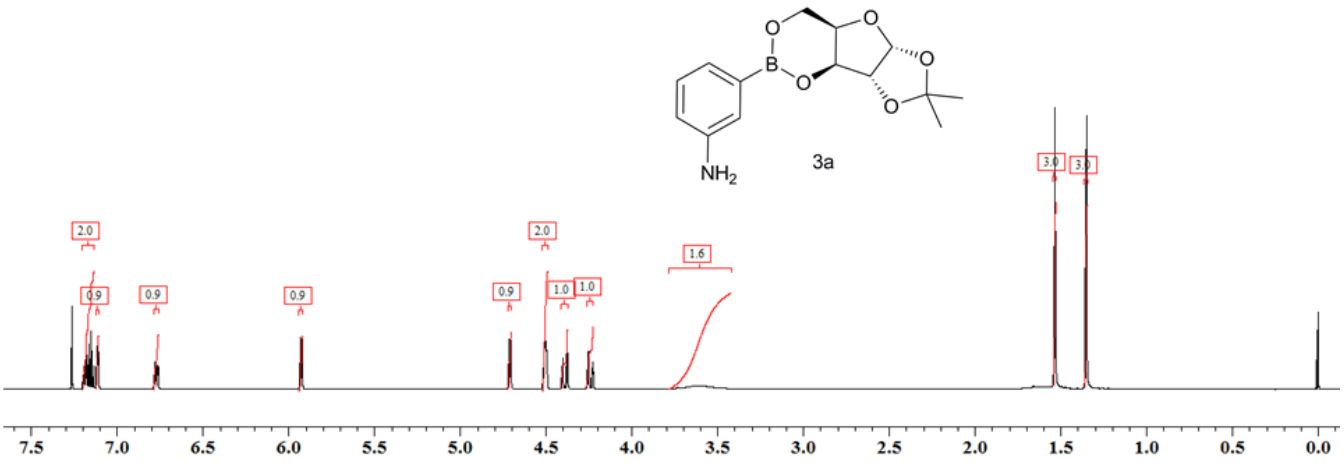

Figure S1: ^{1}H NMR spectrum of compound **3a**.

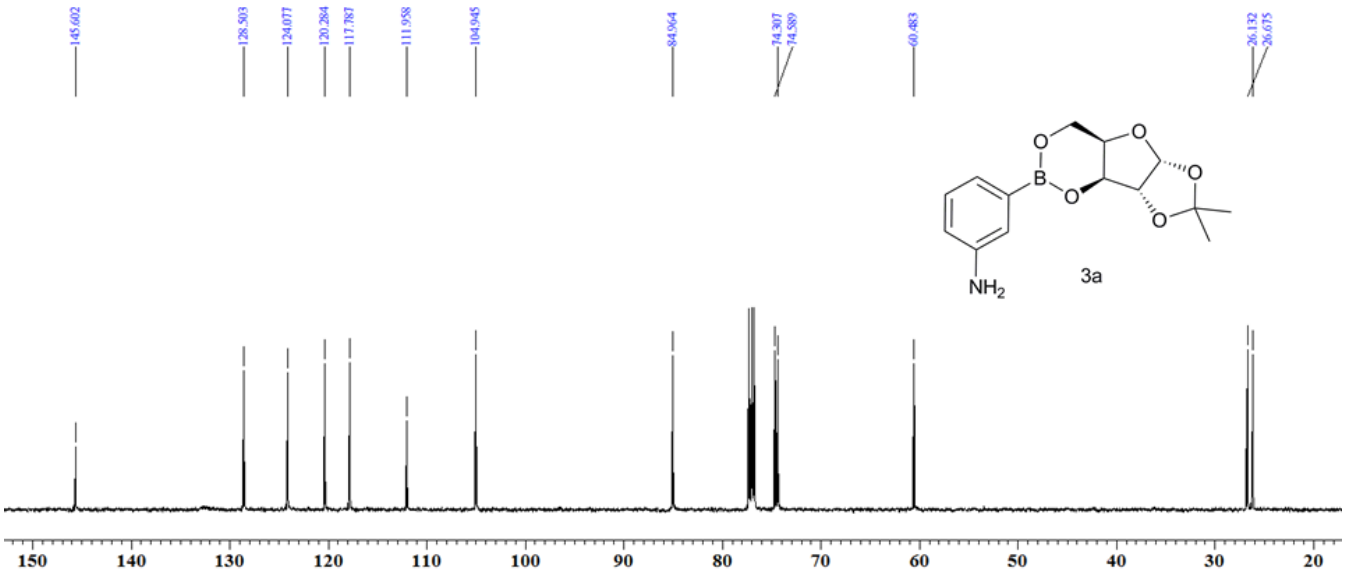

Figure S2: ^{13}C NMR spectrum of compound **3a**.

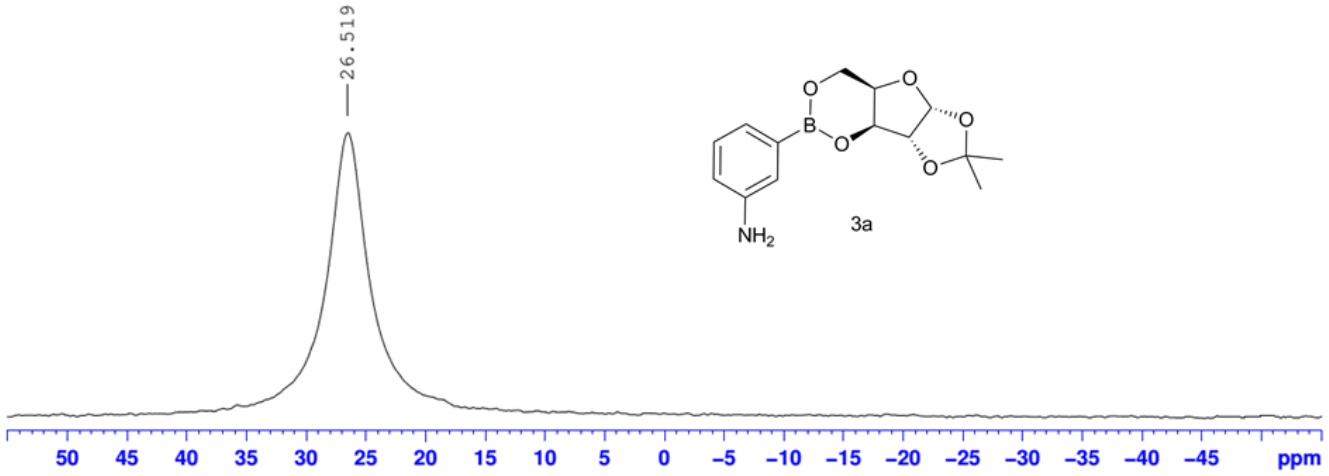

Figure S3: ^{11}B NMR spectrum of compound **3a**.

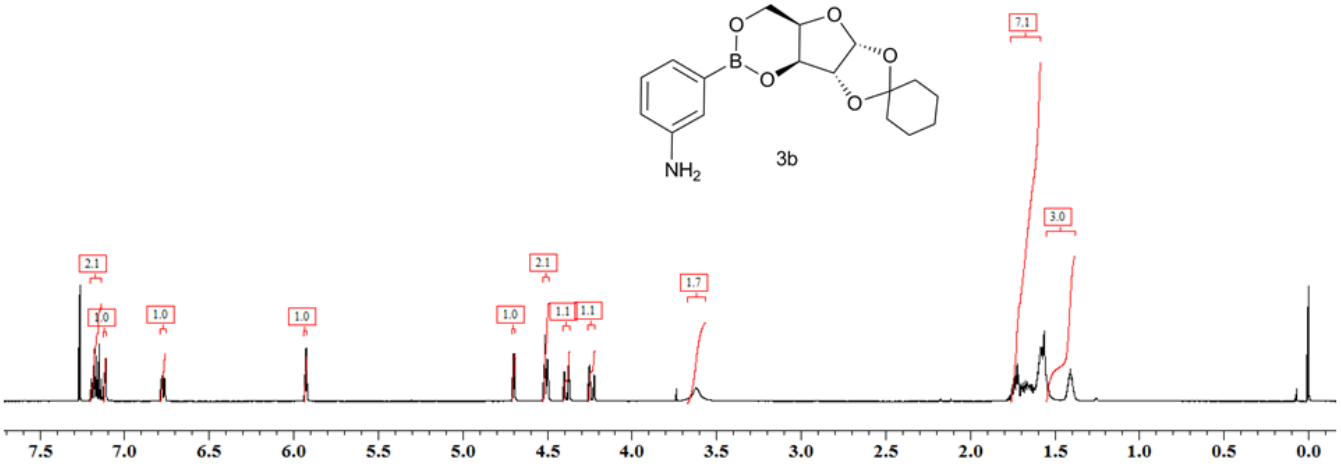

Figure S4: ^{1}H NMR spectrum of compound **3b**. (Note: Moisture peak was observed at δ1.57-1.59 ppm)

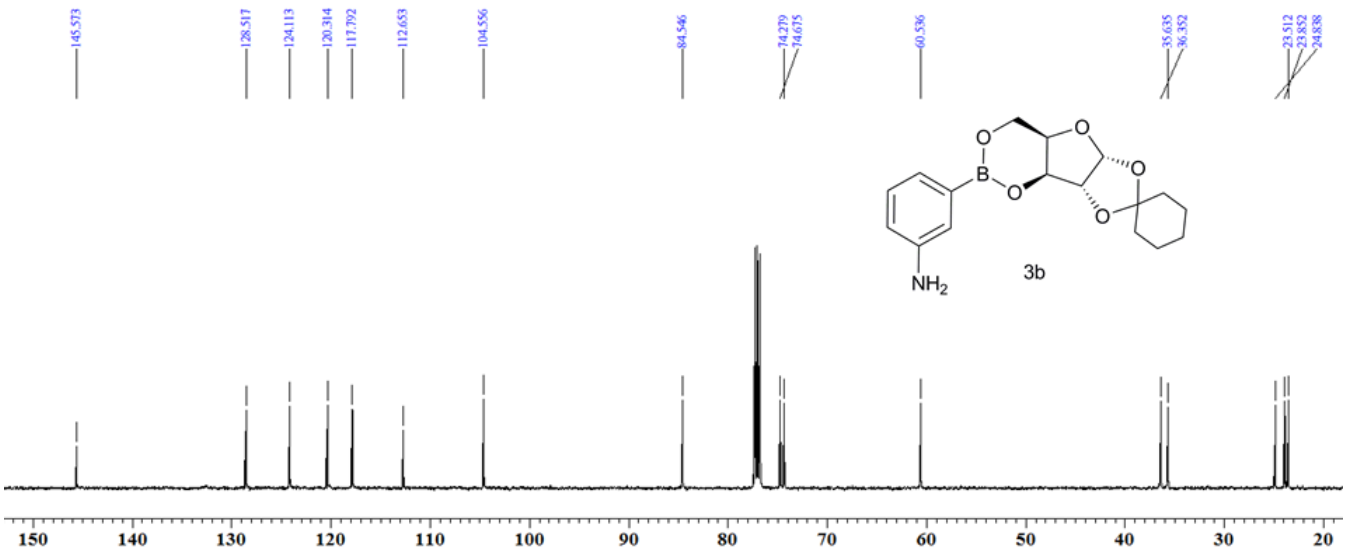

Figure S5: ^{13}C NMR spectrum of compound **3b**.

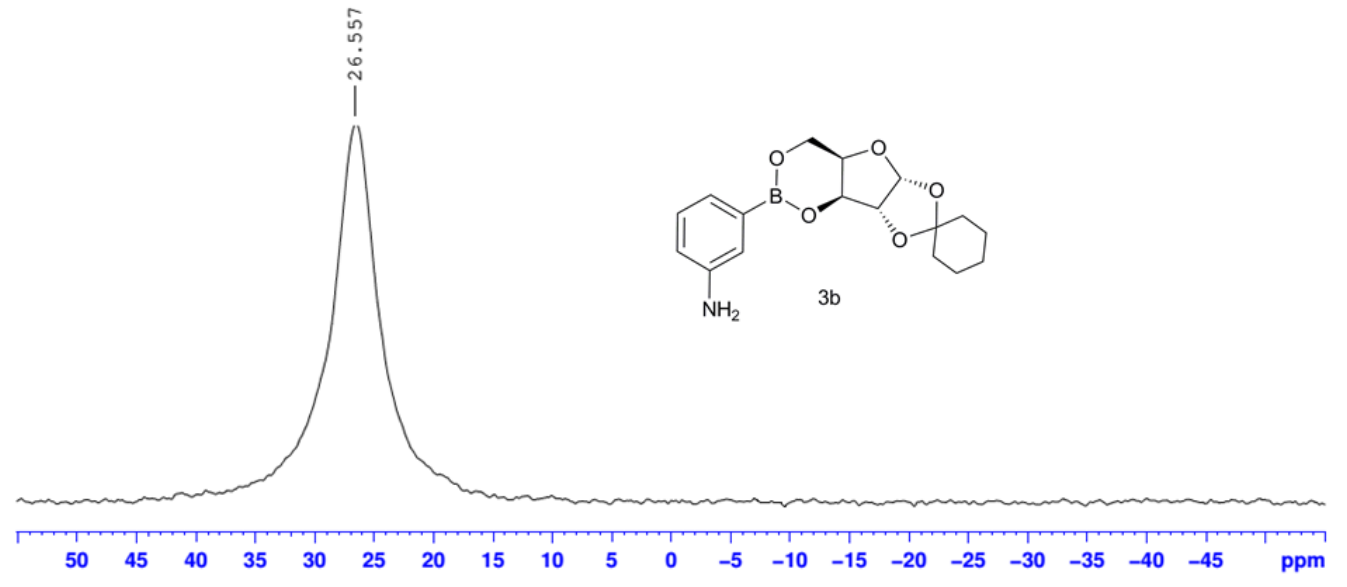

Figure S6: ^{11}B NMR spectrum of compound **3b**.

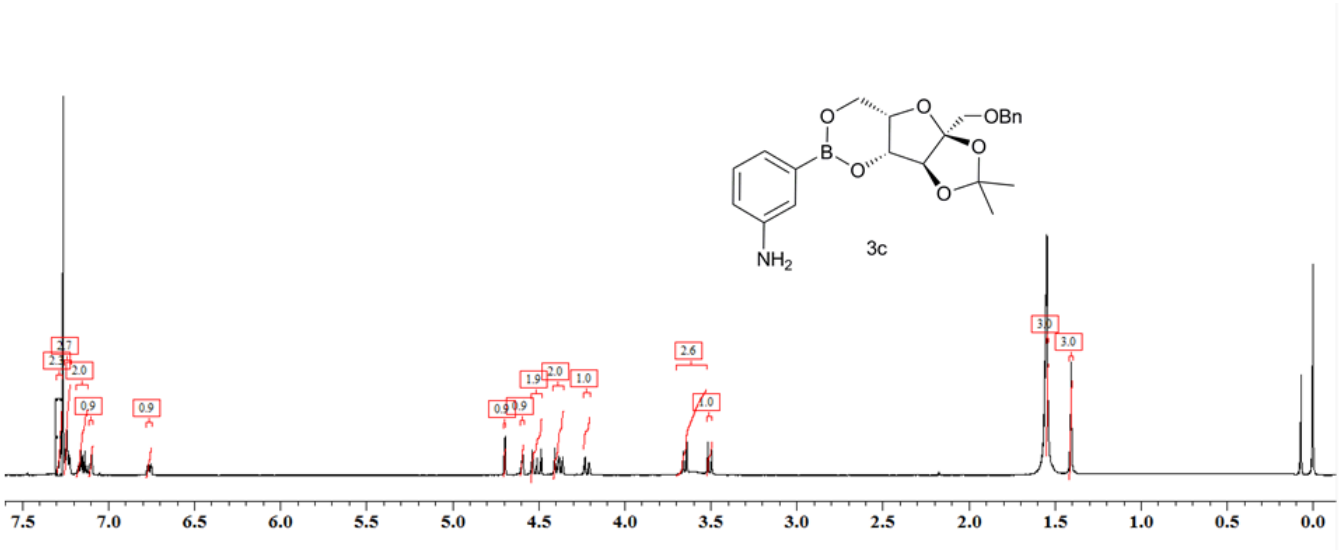

Figure S7: ^{1}H NMR spectrum of compound **3c** (Note: Moisture peak was observed at δ1.54-1.59 ppm)

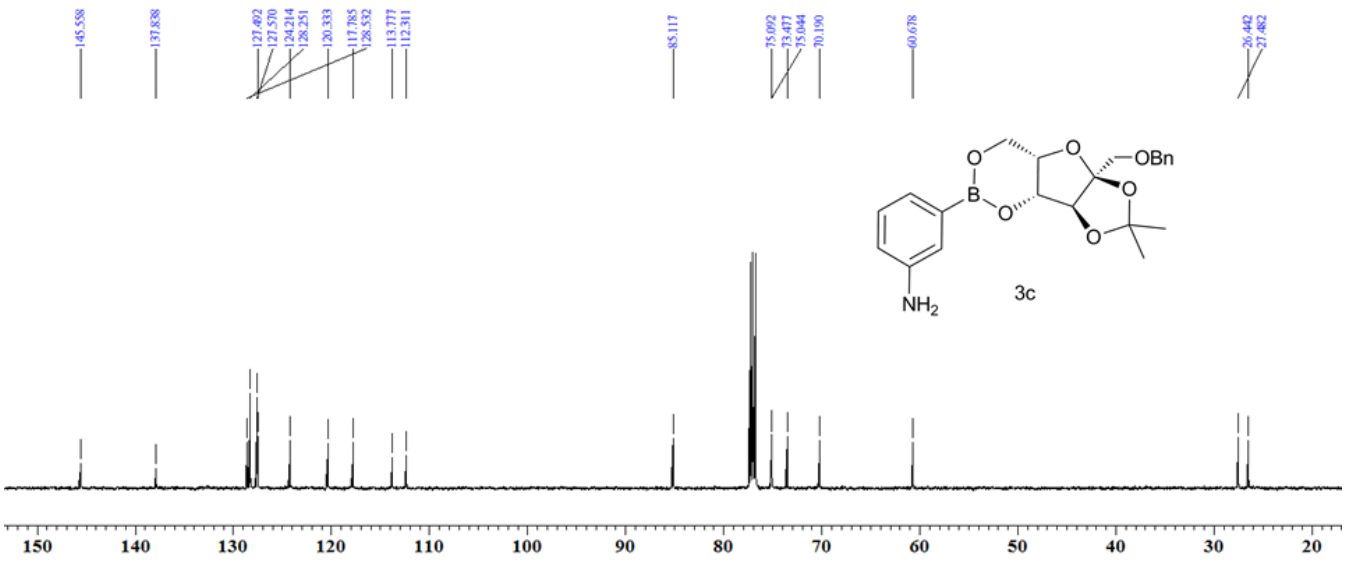

Figure S8: ^{13}C NMR spectrum of compound **3c**.

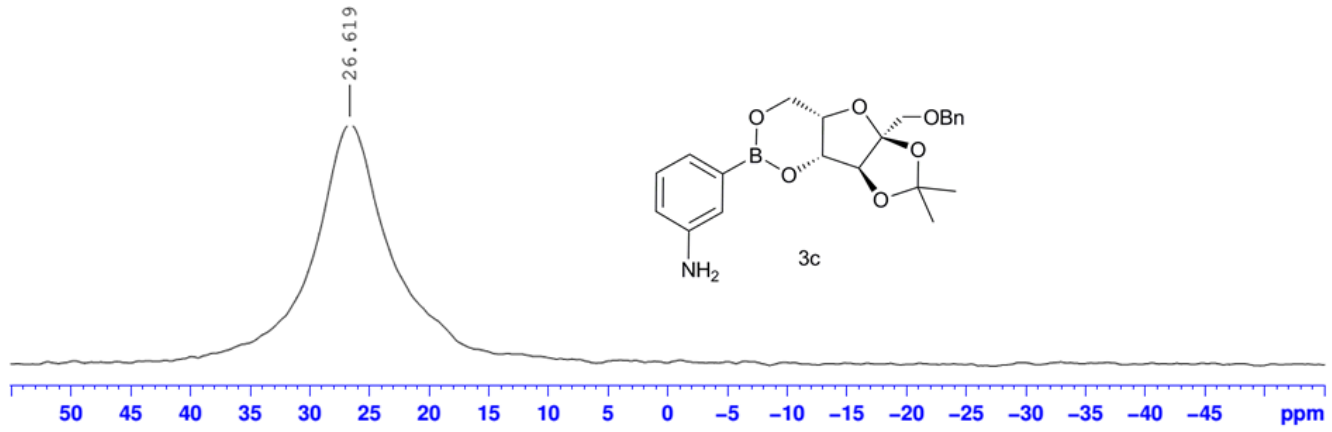

Figure S9: ^{11}B NMR spectrum of compound **3c**.

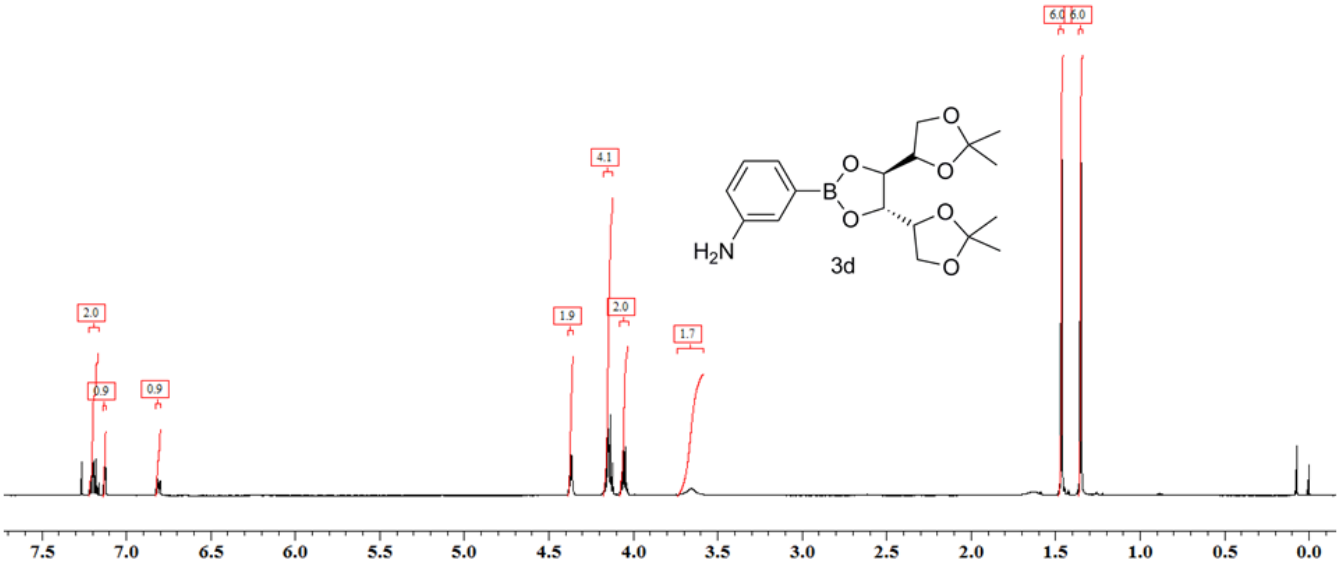

Figure S10: ^{1}H NMR spectrum of compound **3d**.

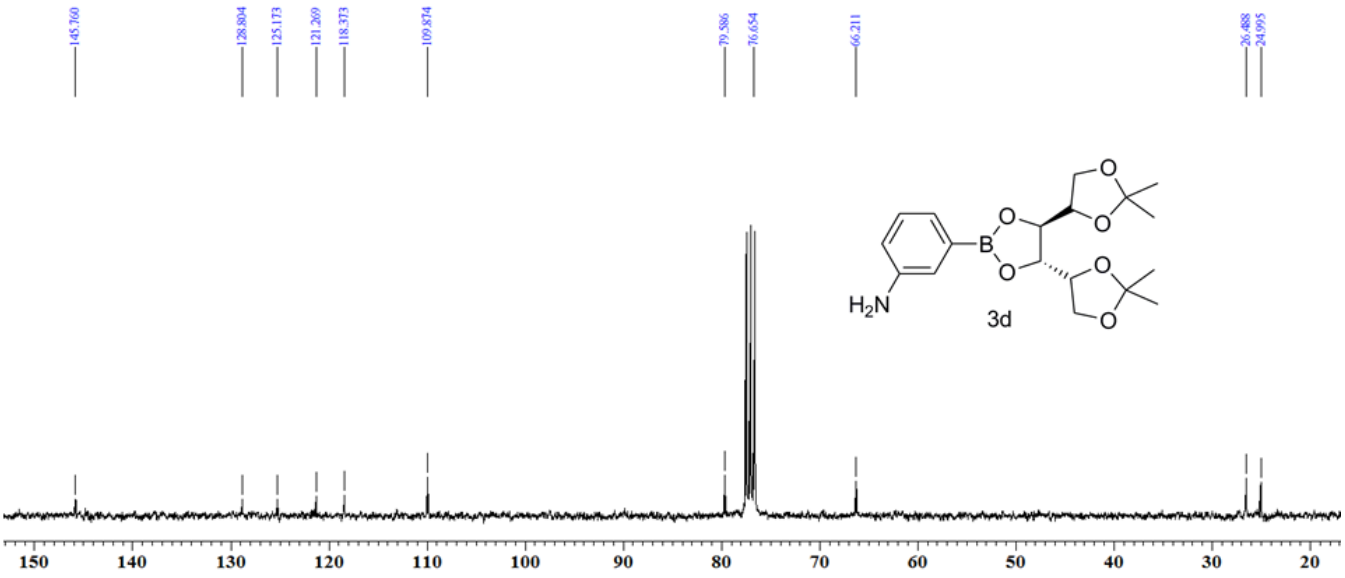

Figure S11: ^{13}C NMR spectrum of compound **3d**.

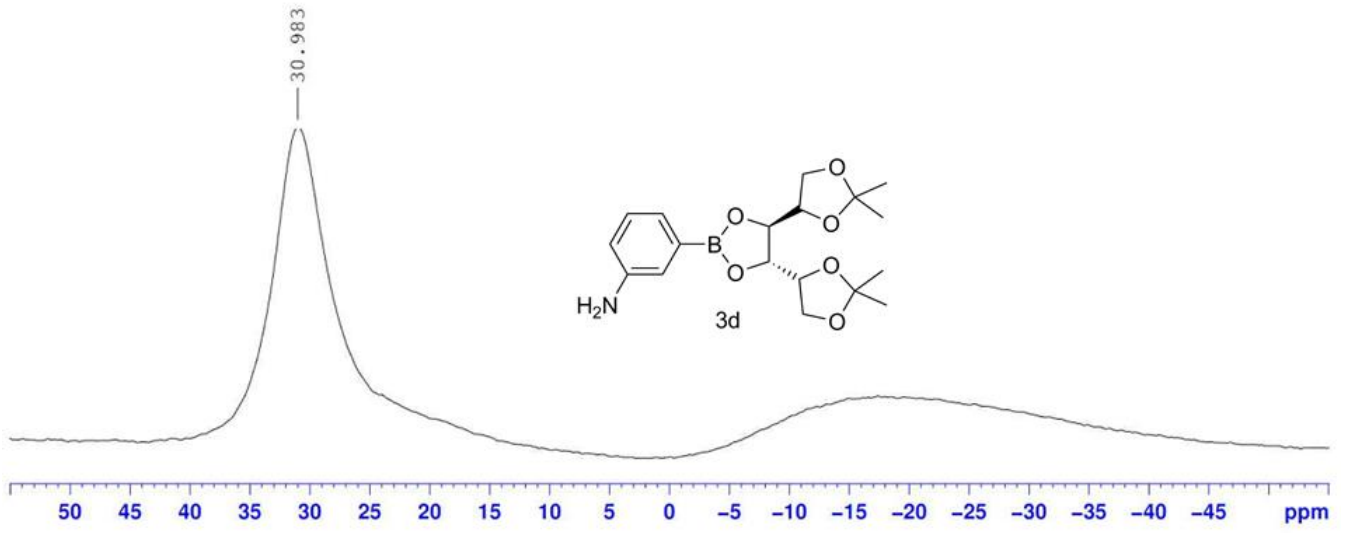

Figure S12: ^{11}B NMR spectrum of compound **3d**.

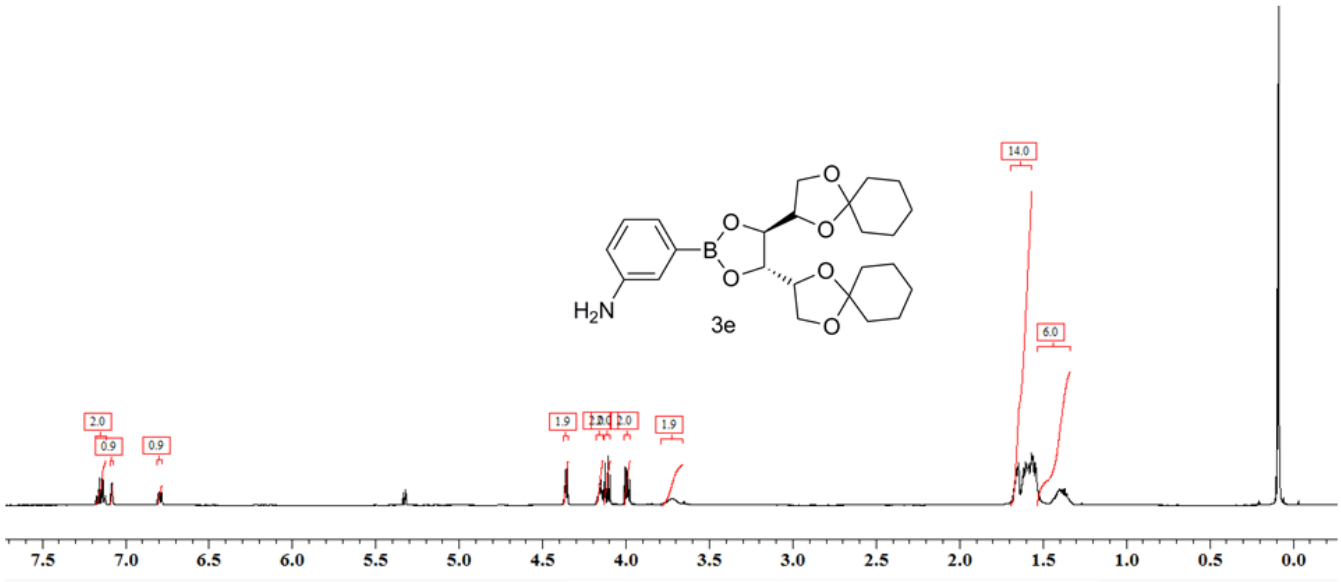

Figure S13: ^{1}H NMR spectrum of compound **3e**. (Note: Moisture peak was observed at δ1.57-1.59 ppm)

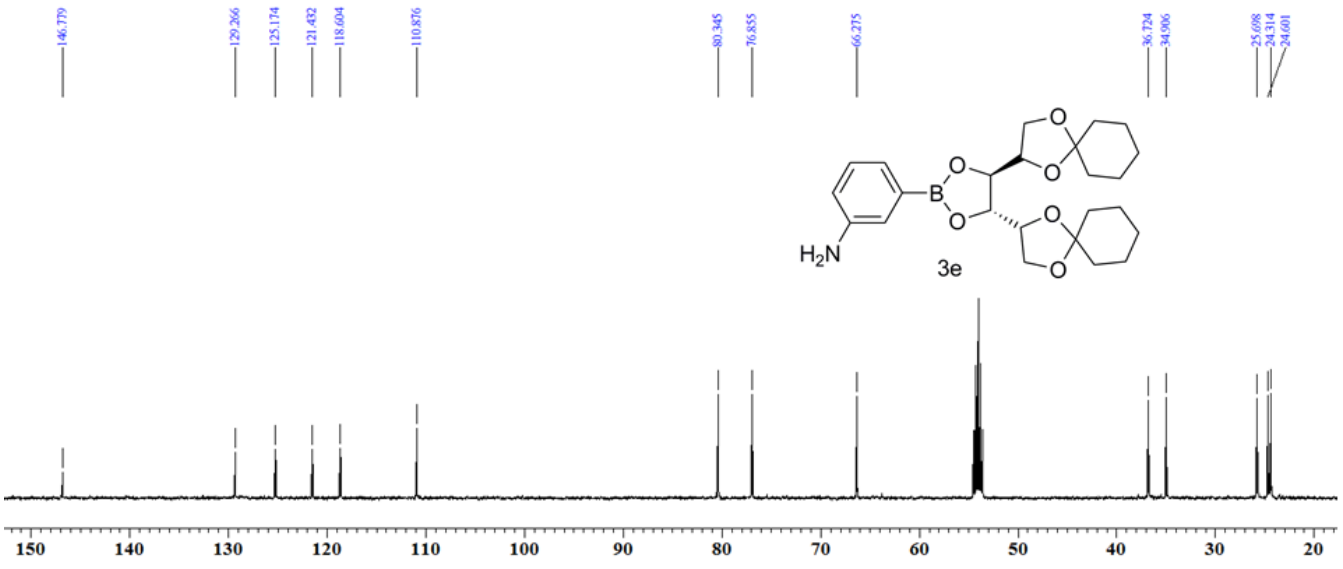

Figure S14: ^{13}C NMR spectrum of compound **3e**.

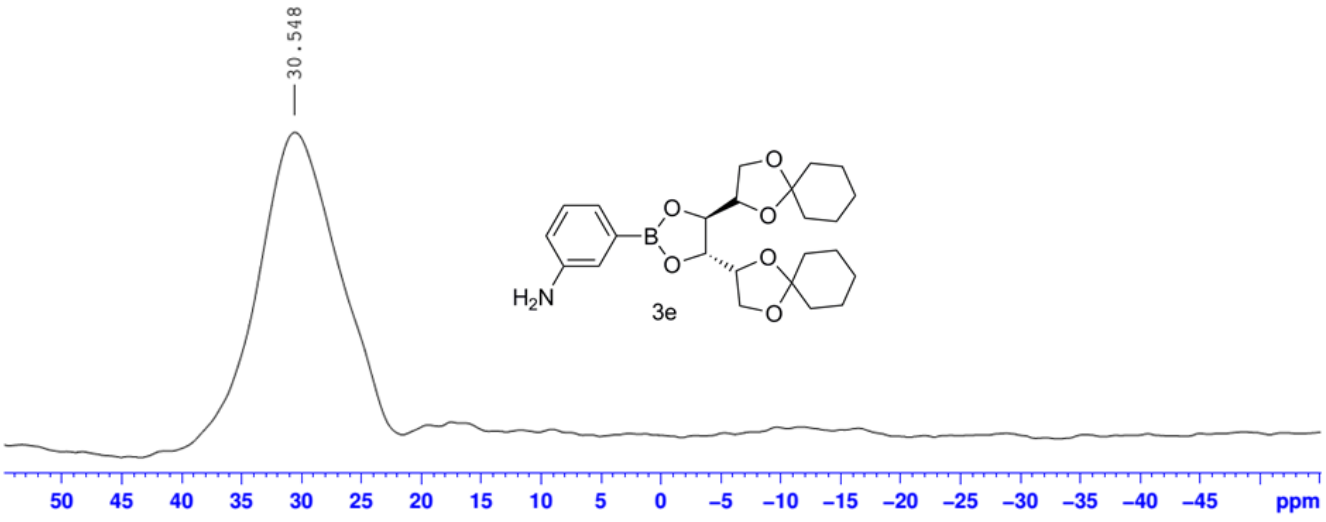

Figure S15: ^{11}B NMR spectrum of compound **3e**.

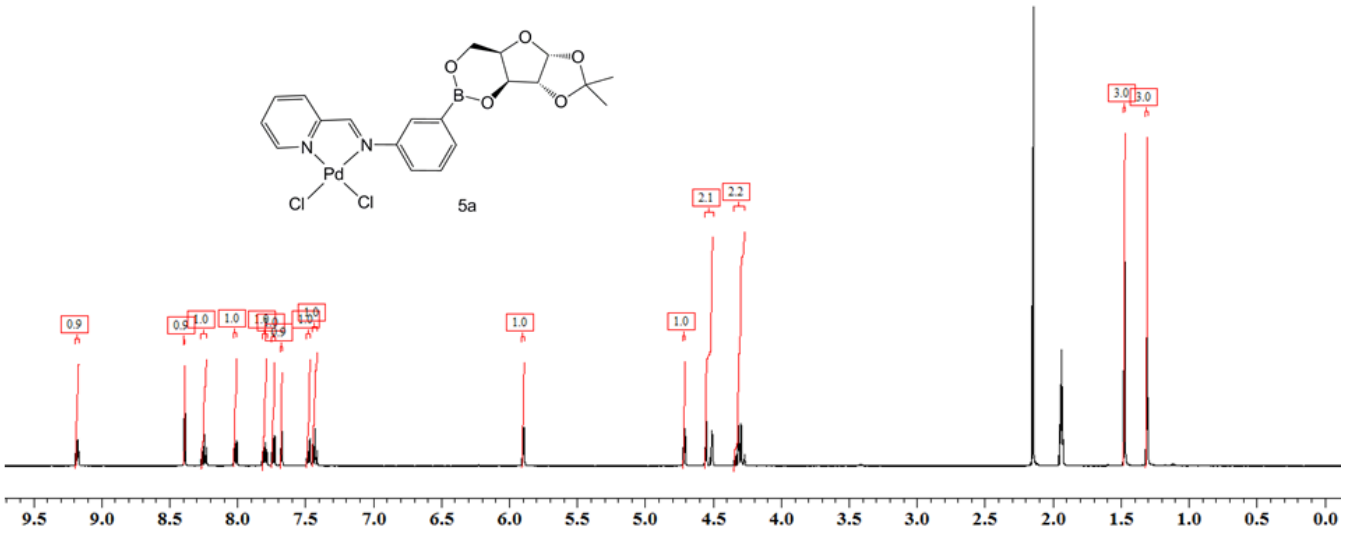

Figure S16: ^{1}H NMR spectrum of compound **5a.**

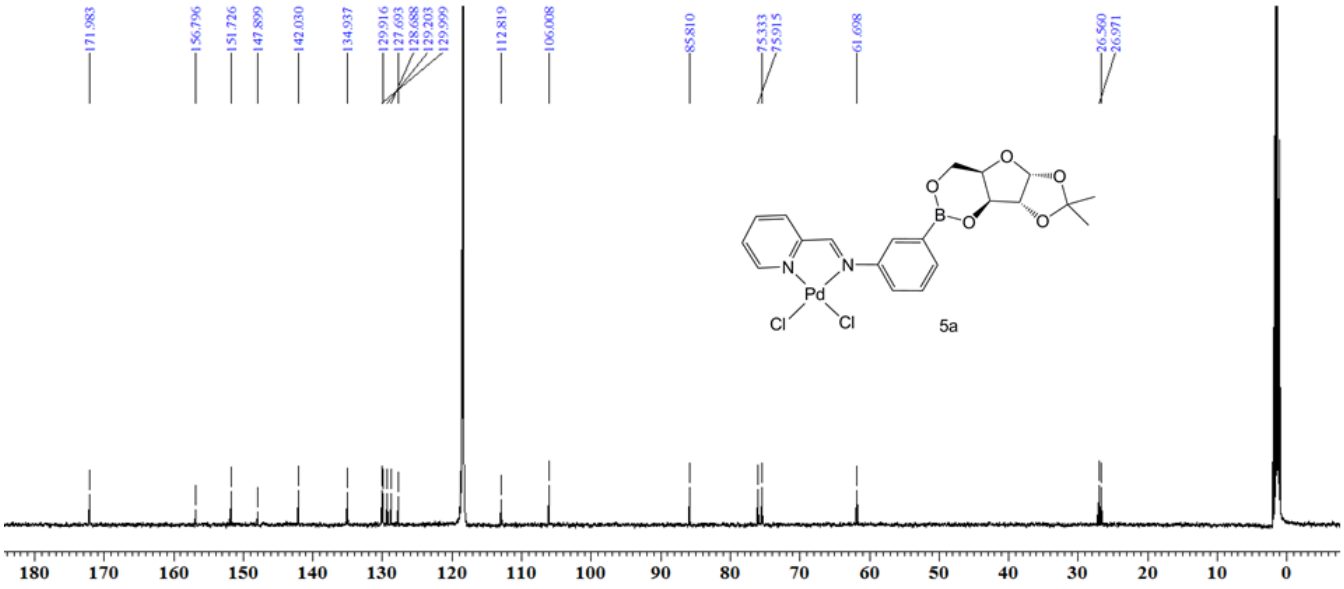

Figure S17: ^{13}C NMR spectrum of compound **5a**.

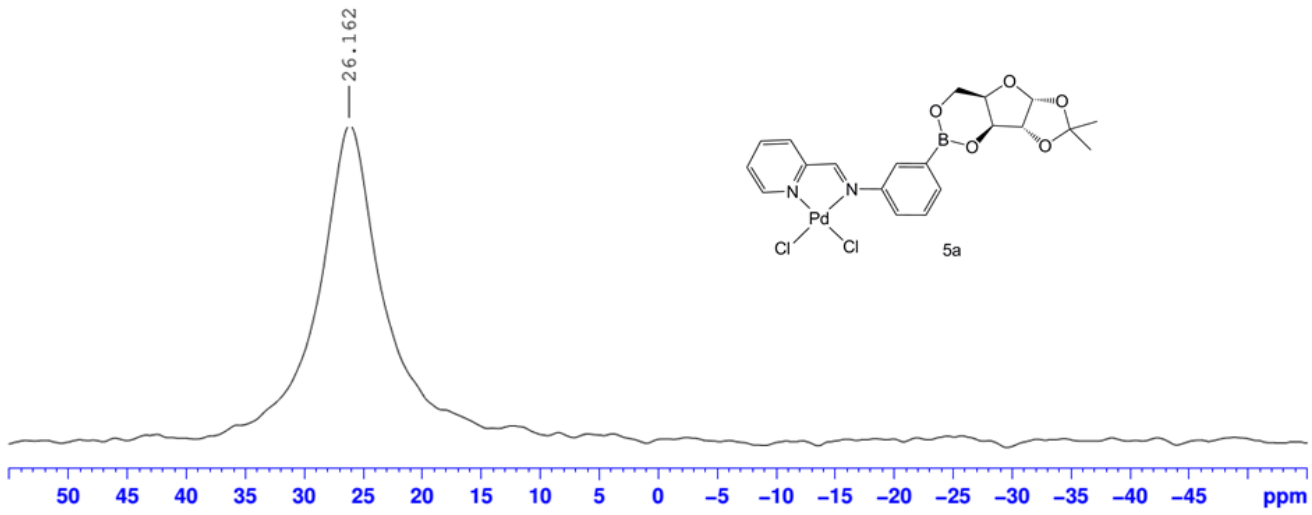

Figure S18: ^{11}B NMR spectrum of compound **5a**.

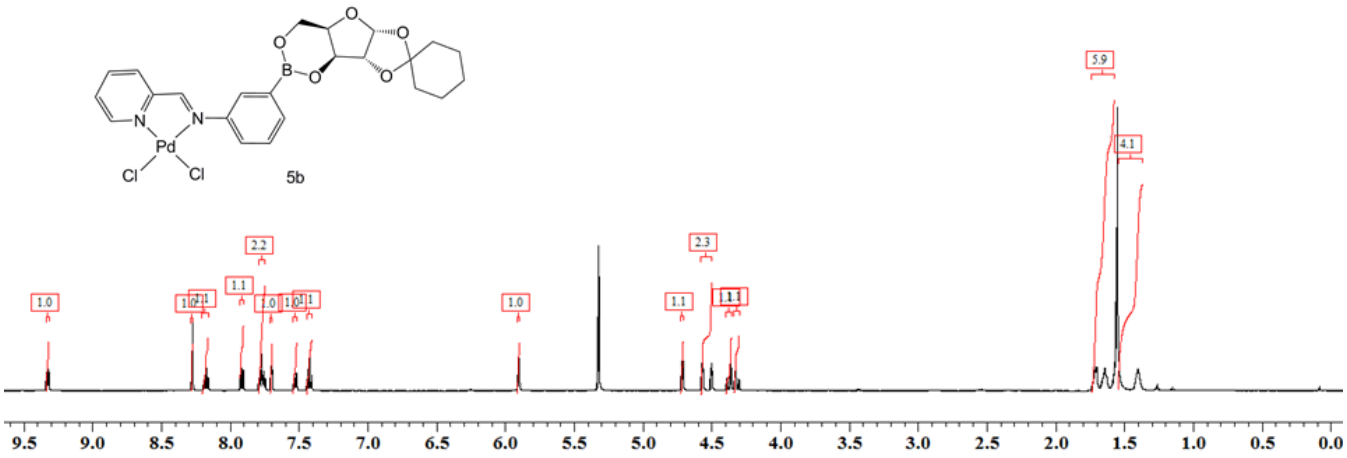

Figure S19: ^{1}H NMR spectrum of compound **5b.** (Note: Moisture peak was observed at δ1.57-1.59 ppm)

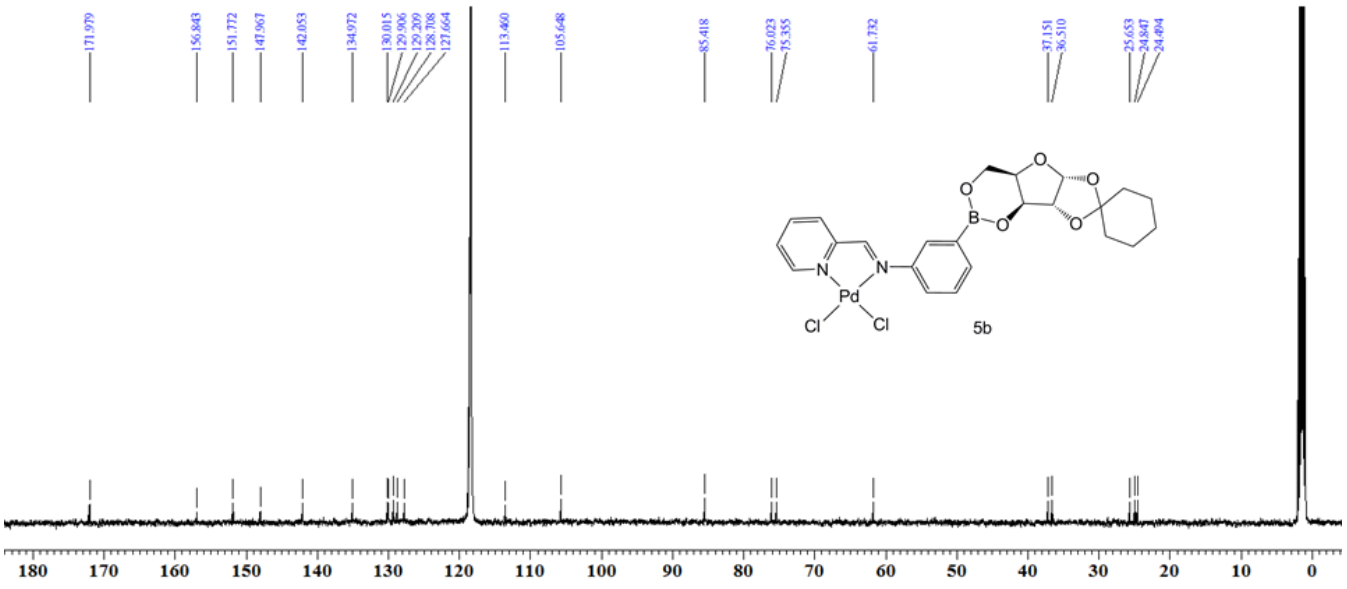

Figure S20: ^{13}C NMR spectrum of compound **5b**.

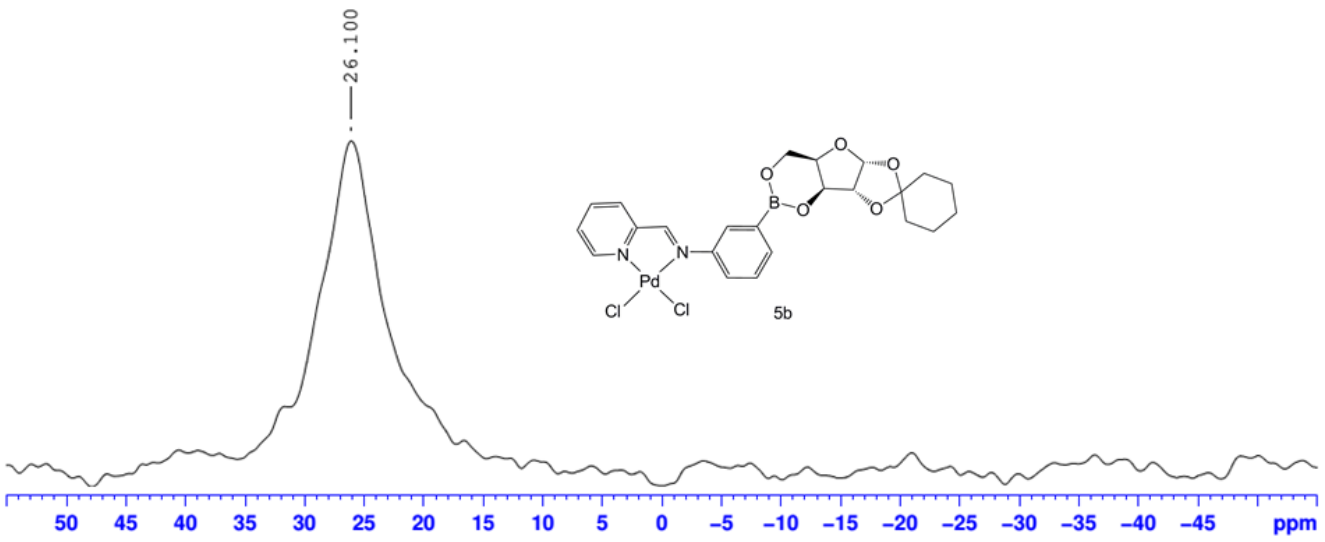

Figure S21: ^{11}B NMR spectrum of compound **5b**.

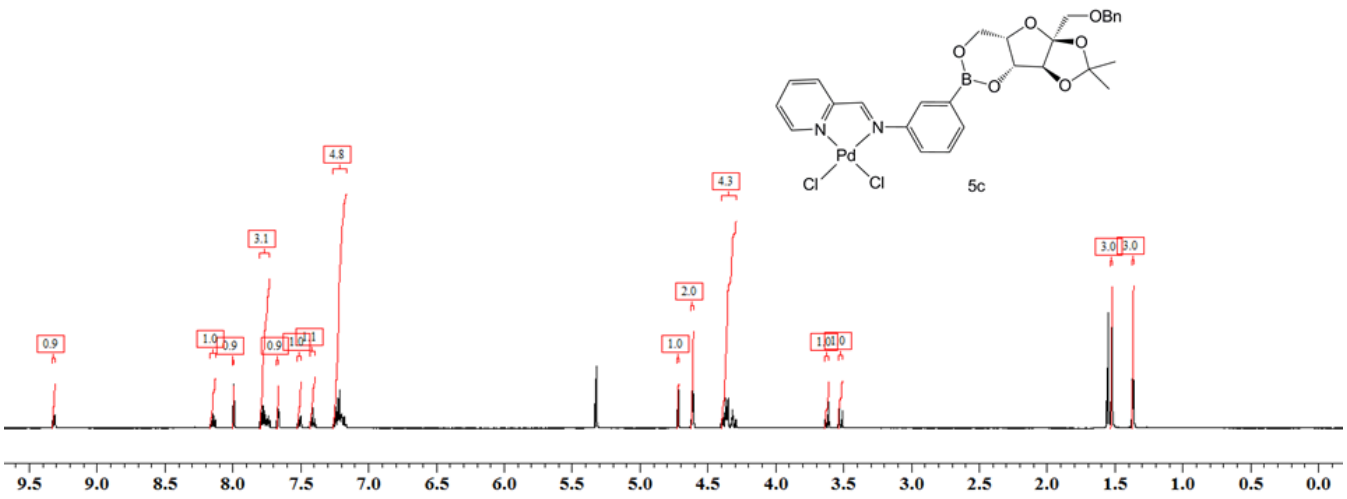

Figure S22: ^{1}H NMR spectrum of compound **5c.**

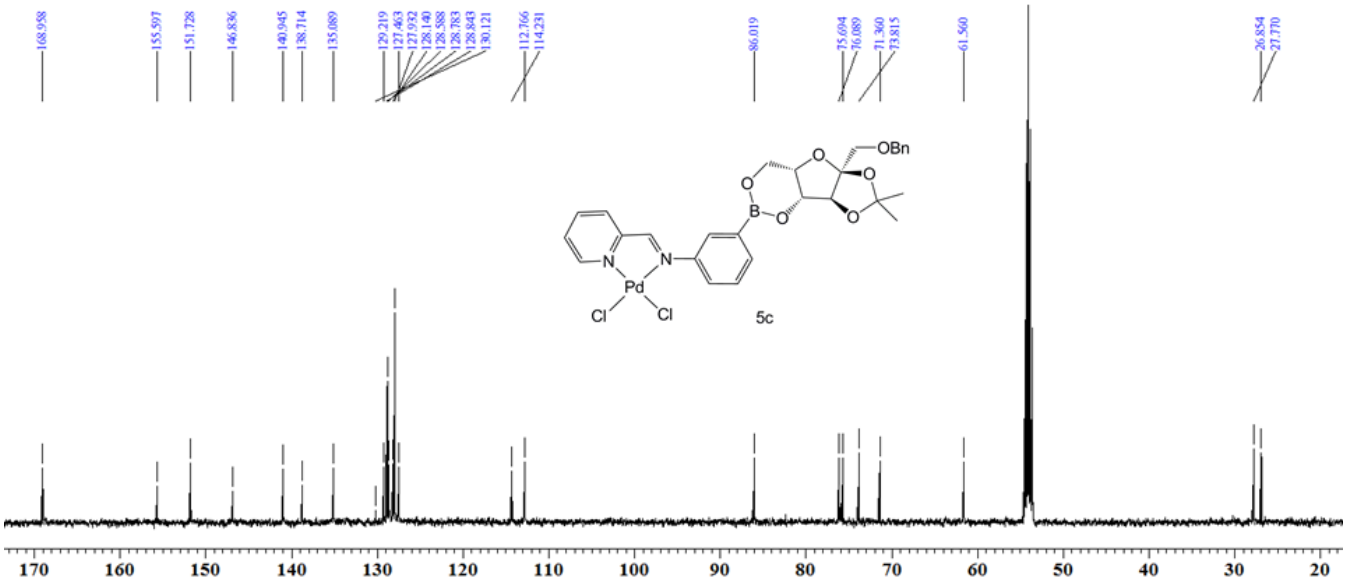

Figure S23: ^{13}C NMR spectrum of compound **5c**.

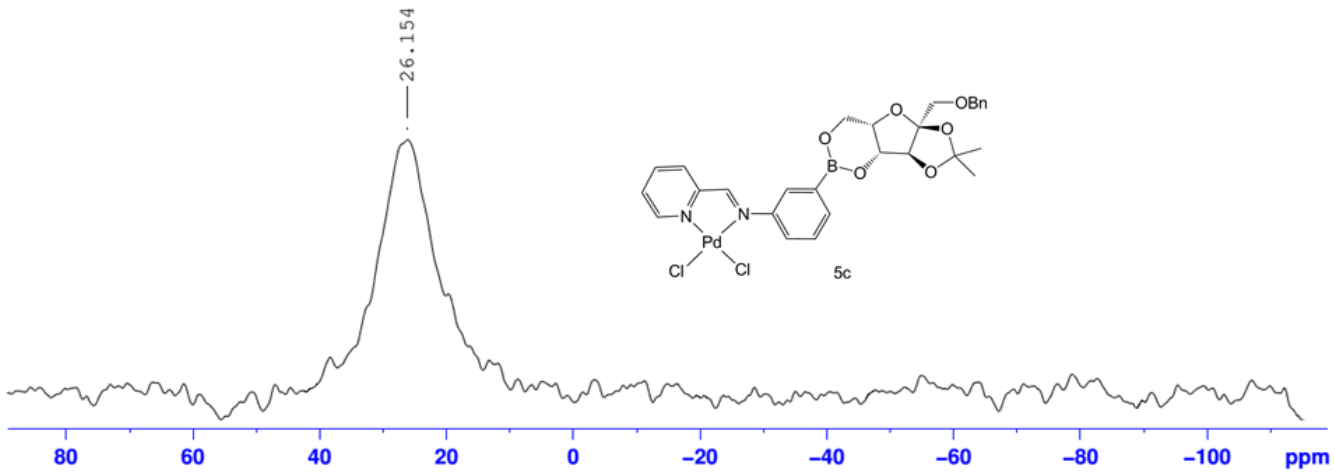

Figure S24: ^{11}B NMR spectrum of compound **5c**.

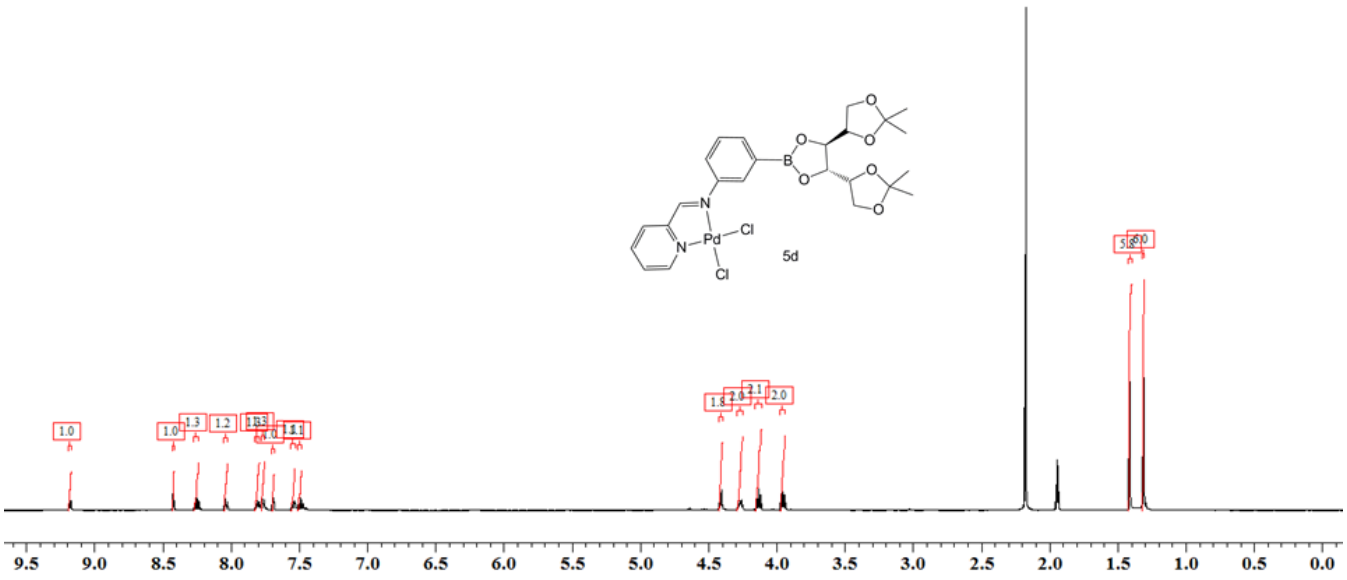

Figure S25: ^{1}H NMR spectrum of compound **5d.**

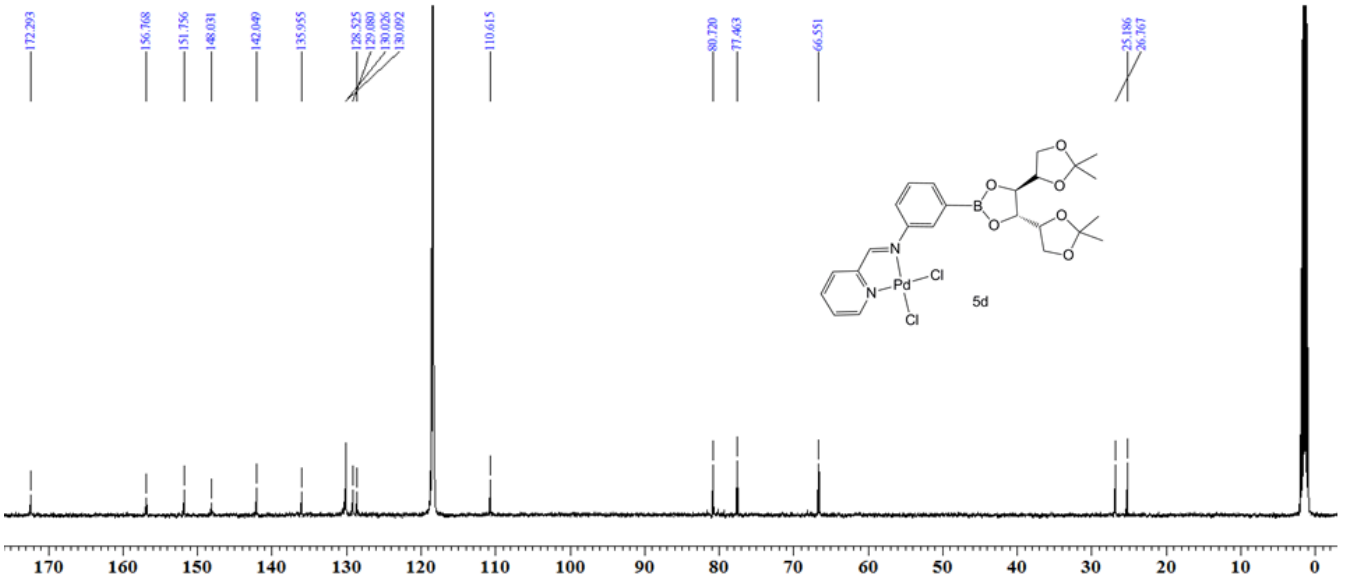

Figure S26: ^{13}C NMR spectrum of compound **5d**.

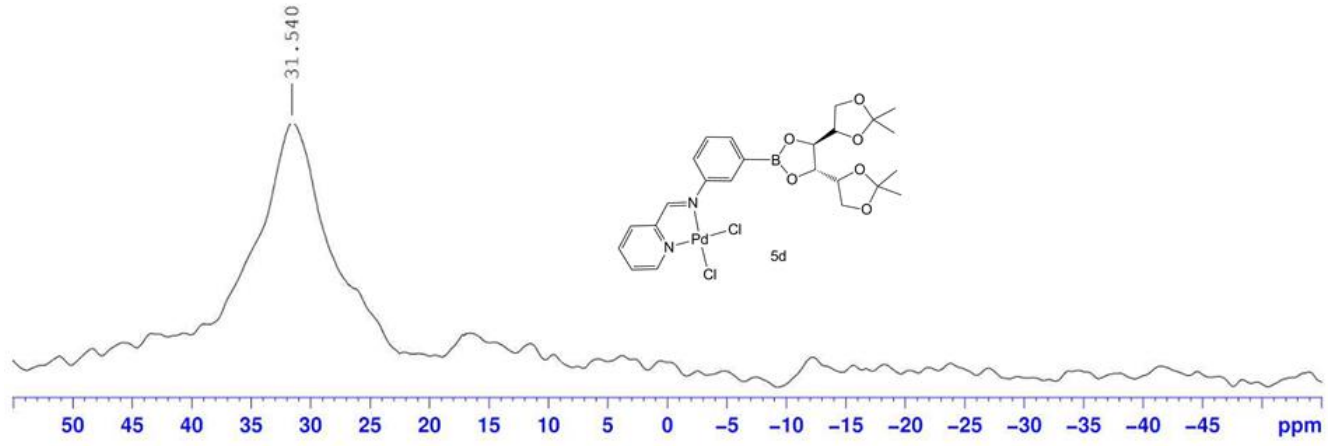

Figure S27: ^{11}B NMR spectrum of compound **5d**.

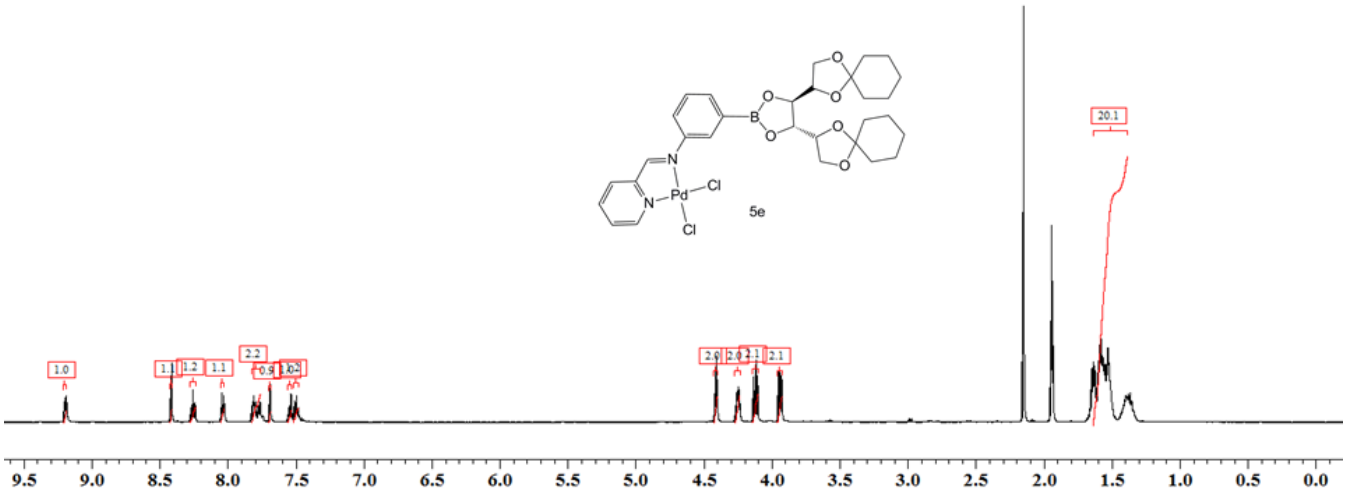

Figure S28: ^{1}H NMR spectrum of compound **5e.**

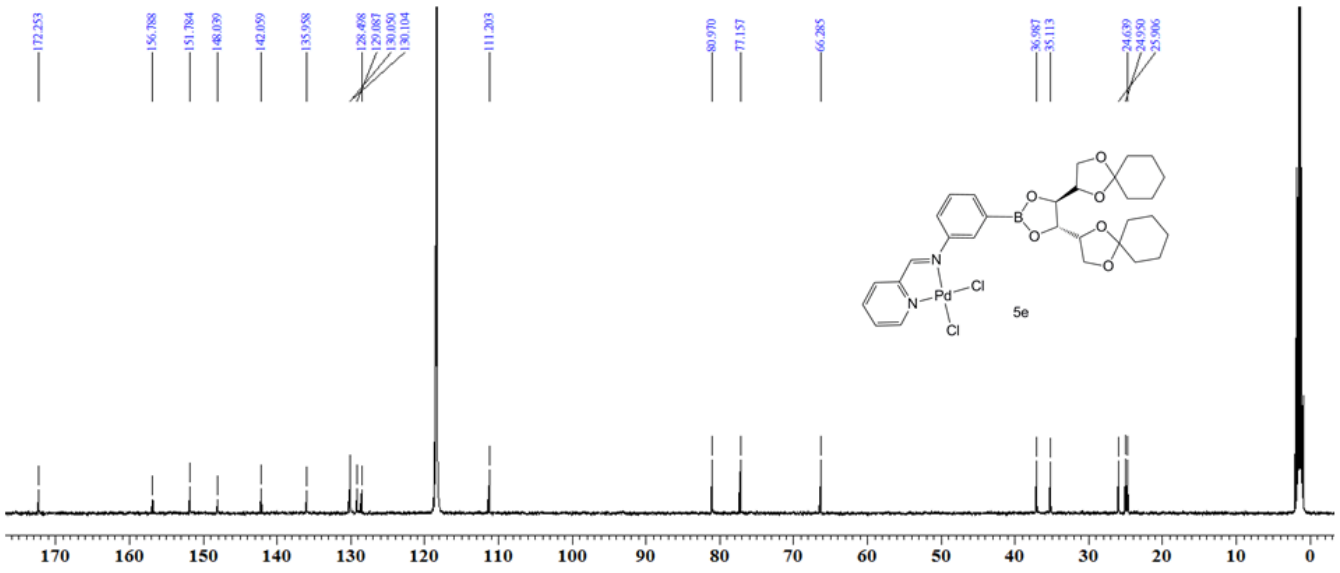

Figure S29: ^{13}C NMR spectrum of compound **5e**.

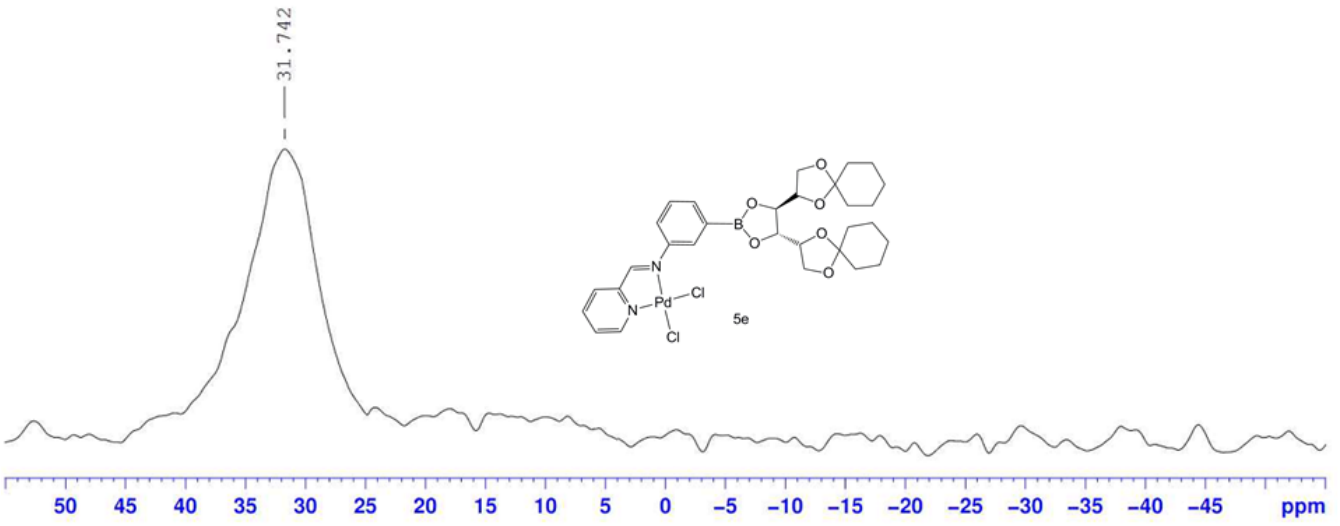

Figure S30: ^{11}B NMR spectrum of compound **5e**.

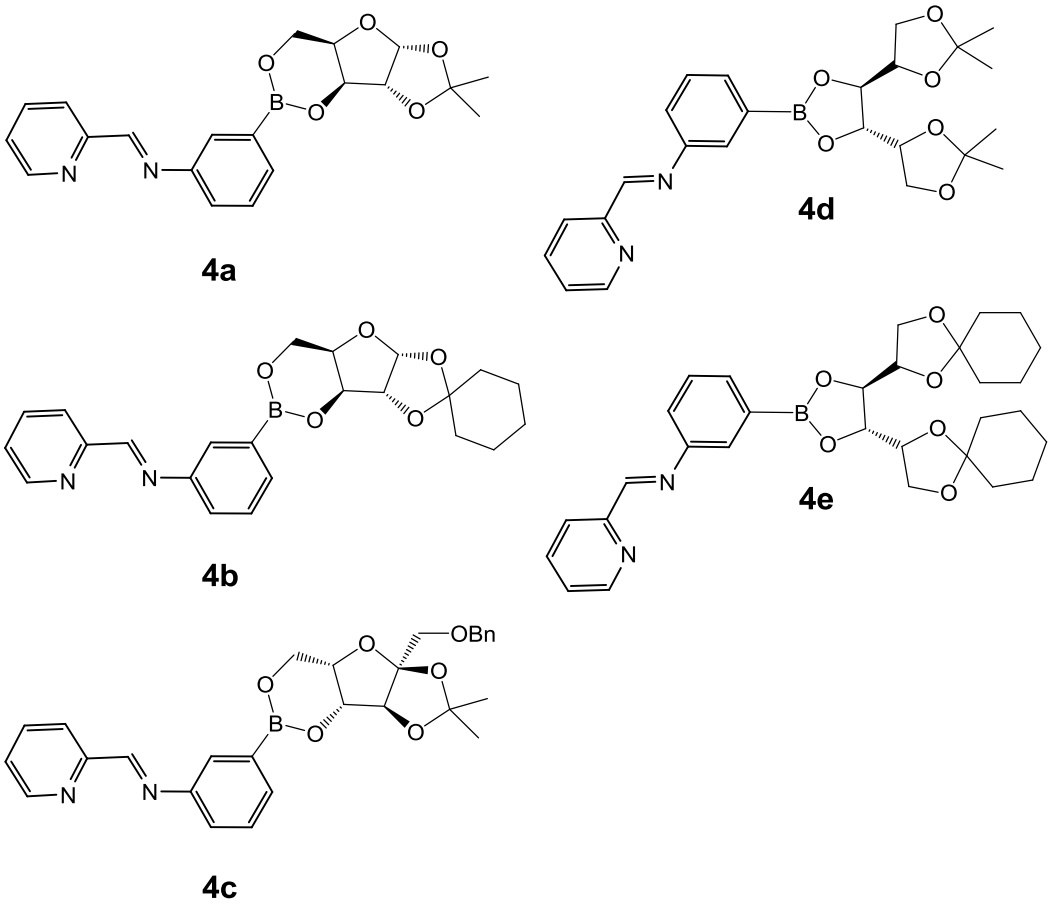

Chart S1. Structures of ligands (generated *in situ*) **4a-e**

Stability studies of complex 5a

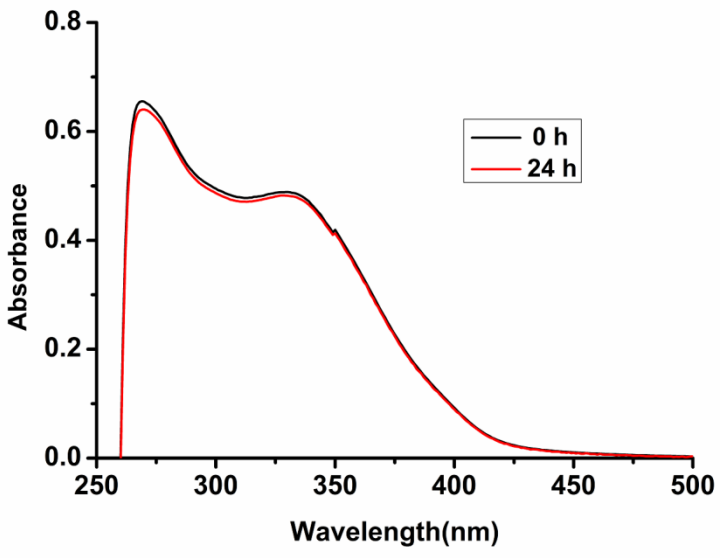

Figure S31. UV-visible spectra of **5a** in DMSO /10% DMEM medium (1:1) solution (pH = 7.4) at 25ºC.

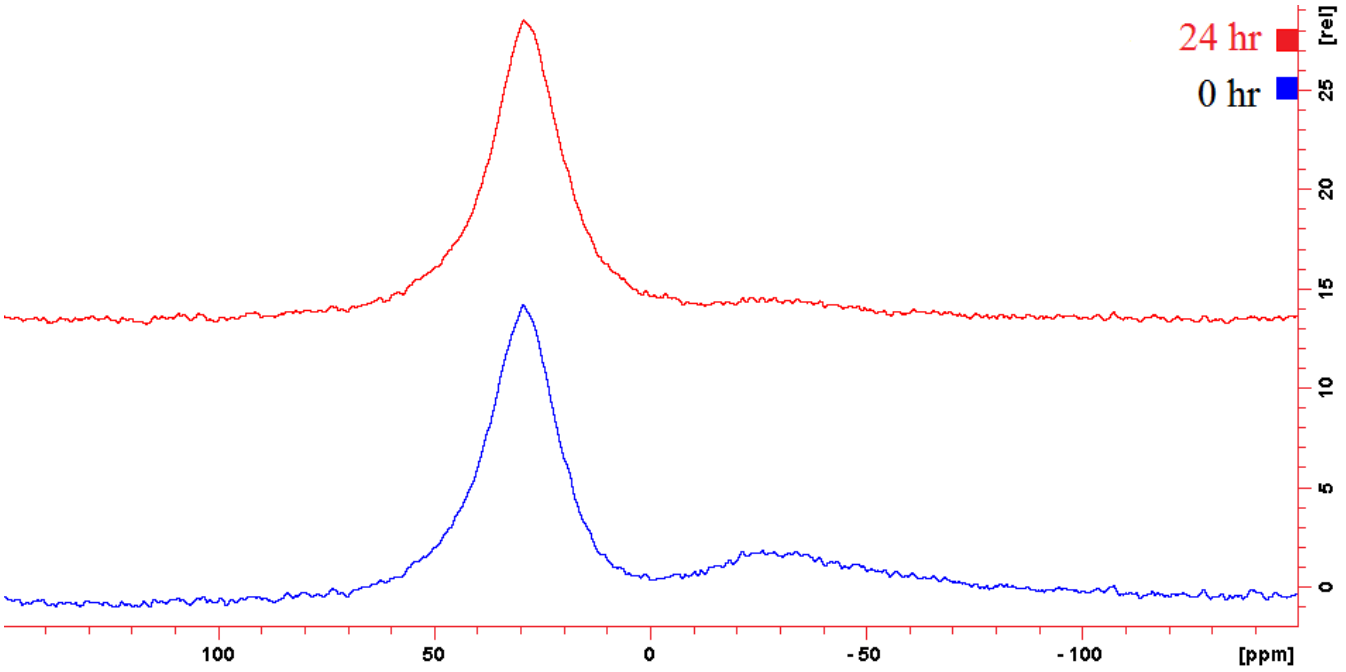

Figure S32.[11]B NMR Spectra of **5a** in DMSO-d_6/10% DMEM medium (2:1) solution (pH = 7.4) at 25ºC

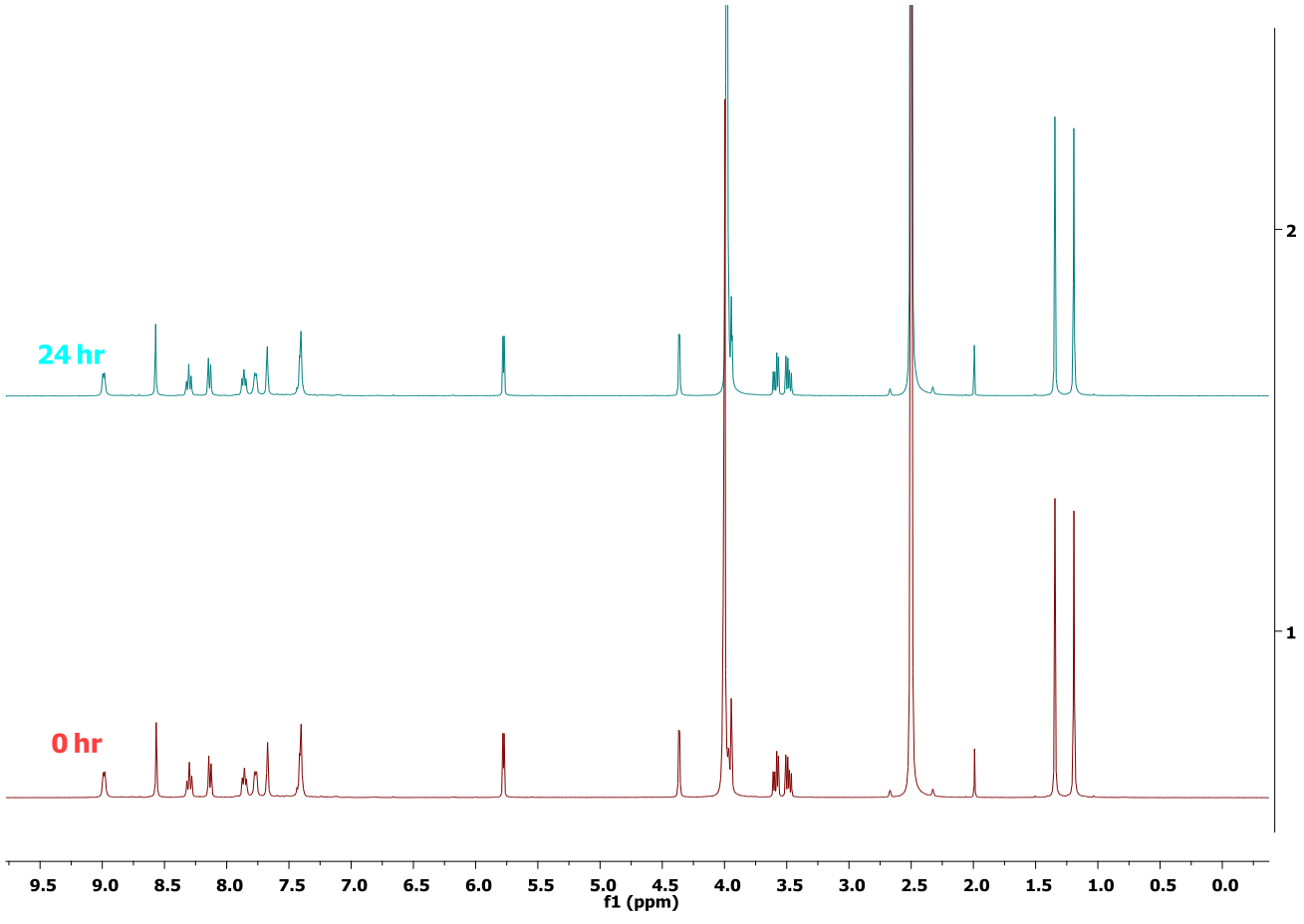

Figure S33.[1]H NMR Spectra of **5a** in DMSO-d_6/D_2O (2:1) solution (pH = 7.0) at 25ºC

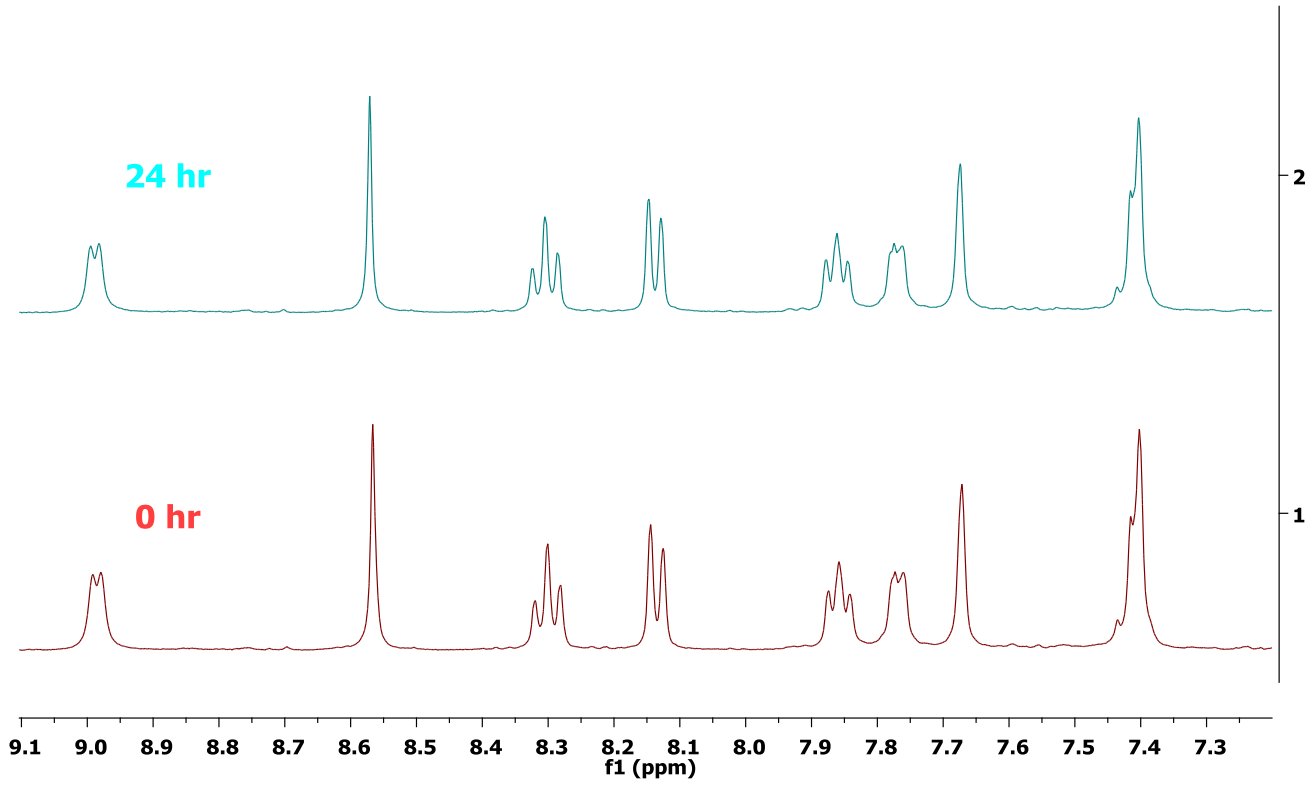

Figure S34. Aromatic region expansion of ^{1}H NMR Spectra of **5a** in DMSO-d_6/D_2O (2:1) solution (pH = 7.0) at 25ºC

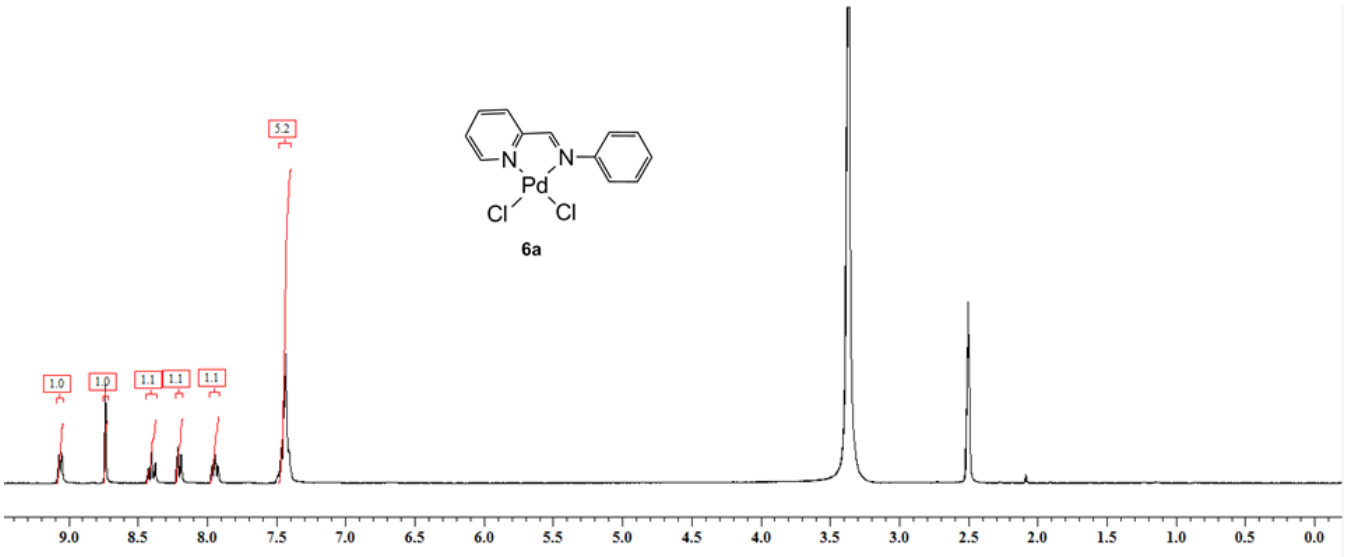

Figure S35: ^{1}H NMR spectrum of compound **6a.**

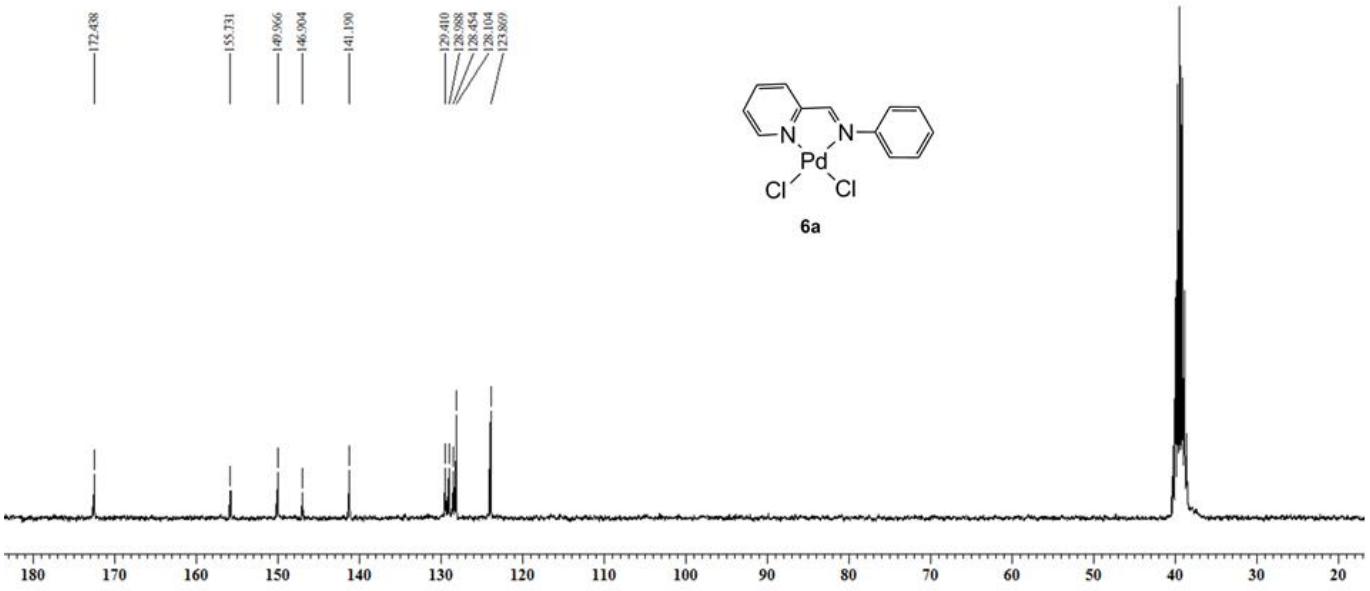

Figure S36: ^{13}C NMR spectrum of compound **6a.**

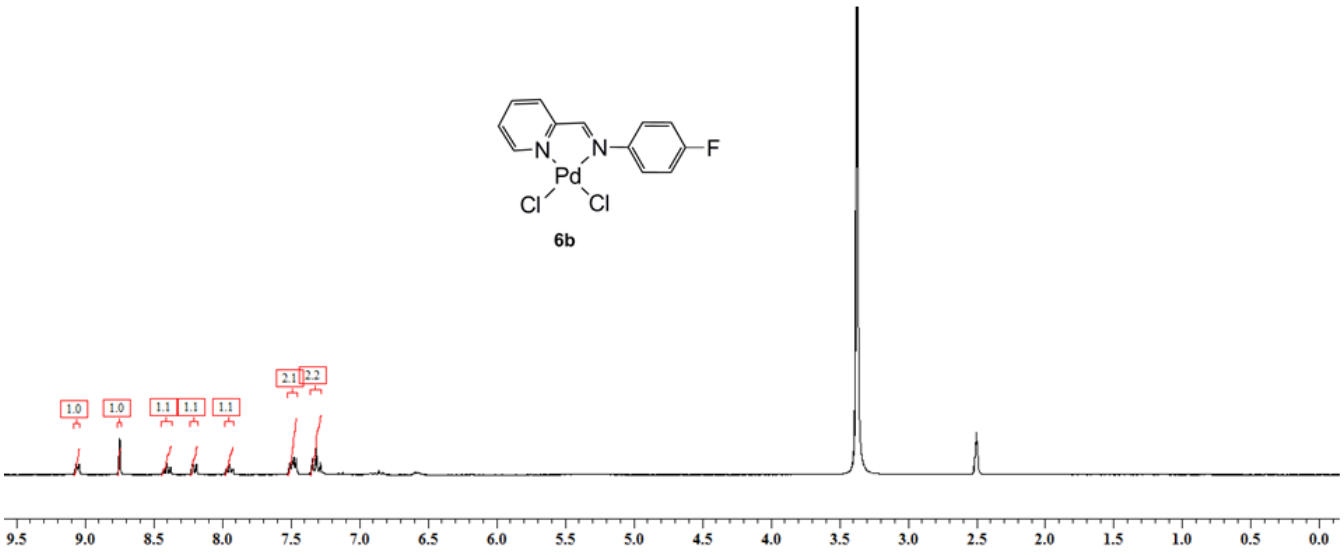

Figure S37: ^{1}H NMR spectrum of compound **6b.**

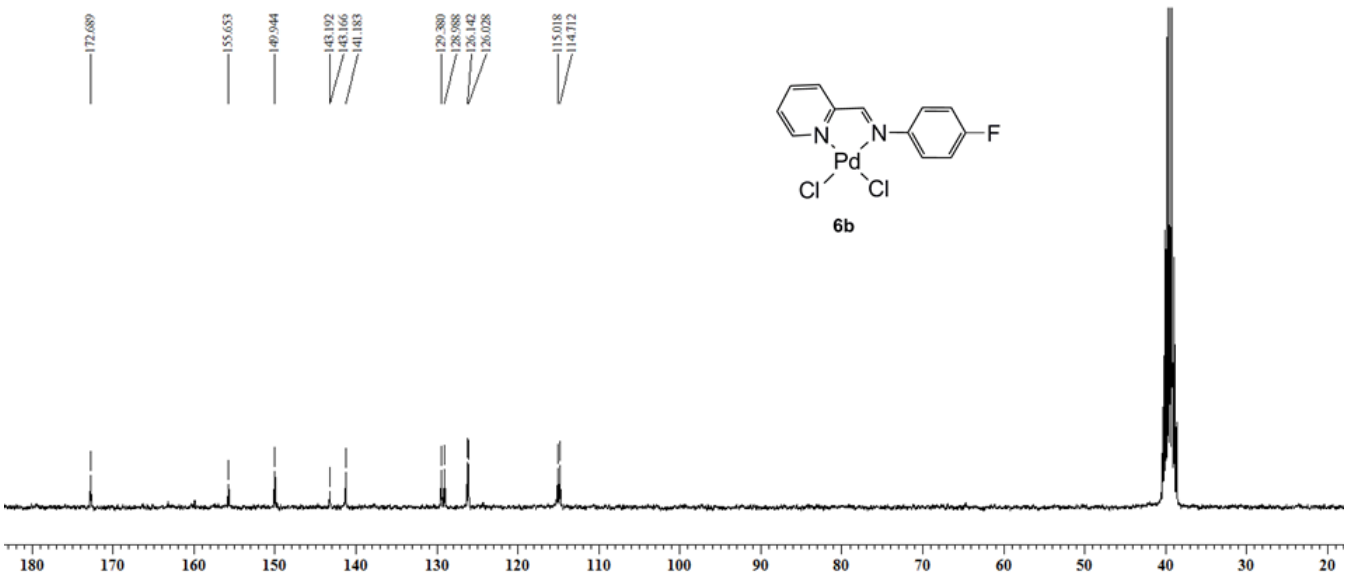

Figure S38: ^{13}C NMR spectrum of compound **6b.**

Table S1. Bond lengths [Å] and angles [°] for **3a**.

B(1)-O(5)	1.349(3)
B(1)-O(3)	1.365(2)
B(1)-C(9)	1.558(3)
C(1)-O(4)	1.397(2)
C(1)-O(1)	1.416(2)
C(1)-C(2)	1.531(3)
C(1)-H(1)	0.9800
C(2)-O(2)	1.420(2)
C(2)-C(3)	1.514(3)
C(2)-H(2)	0.9800
C(3)-O(3)	1.427(2)
C(3)-C(4)	1.500(3)
C(3)-H(3)	0.9800
C(4)-O(4)	1.433(3)
C(4)-C(5)	1.506(3)
C(4)-H(4)	0.9800
C(5)-O(5)	1.426(3)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700

C(6)-O(1)	1.421(2)
C(6)-O(2)	1.427(2)
C(6)-C(7)	1.497(3)
C(6)-C(8)	1.509(3)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(10)	1.391(3)
C(9)-C(14)	1.394(3)
C(10)-C(11)	1.386(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.385(3)
C(11)-N(1)	1.398(2)
C(12)-C(13)	1.374(3)
C(12)-H(12)	0.9300
C(13)-C(14)	1.376(3)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
N(1)-H(1N)	0.90(2)
N(1)-H(2N)	0.87(2)

O(5)-B(1)-O(3)	123.2(2)
O(5)-B(1)-C(9)	118.21(18)
O(3)-B(1)-C(9)	118.53(18)
O(4)-C(1)-O(1)	111.46(14)
O(4)-C(1)-C(2)	107.39(14)
O(1)-C(1)-C(2)	104.56(14)
O(4)-C(1)-H(1)	111.1
O(1)-C(1)-H(1)	111.1
C(2)-C(1)-H(1)	111.1
O(2)-C(2)-C(3)	109.87(16)
O(2)-C(2)-C(1)	104.18(14)
C(3)-C(2)-C(1)	102.97(15)
O(2)-C(2)-H(2)	113.0
C(3)-C(2)-H(2)	113.0
C(1)-C(2)-H(2)	113.0
O(3)-C(3)-C(4)	111.54(15)

O(3)-C(3)-C(2)	106.89(16)
C(4)-C(3)-C(2)	102.07(15)
O(3)-C(3)-H(3)	111.9
C(4)-C(3)-H(3)	111.9
C(2)-C(3)-H(3)	111.9
O(4)-C(4)-C(3)	103.48(16)
O(4)-C(4)-C(5)	109.85(18)
C(3)-C(4)-C(5)	113.42(16)
O(4)-C(4)-H(4)	110.0
C(3)-C(4)-H(4)	110.0
C(5)-C(4)-H(4)	110.0

O(5)-C(5)-C(4)	112.12(17)
O(5)-C(5)-H(5A)	109.2
C(4)-C(5)-H(5A)	109.2
O(5)-C(5)-H(5B)	109.2
C(4)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
O(1)-C(6)-O(2)	104.77(13)
O(1)-C(6)-C(7)	109.00(19)
O(2)-C(6)-C(7)	108.93(17)
O(1)-C(6)-C(8)	109.74(18)
O(2)-C(6)-C(8)	110.18(19)
C(7)-C(6)-C(8)	113.8(2)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(14)	117.63(18)
C(10)-C(9)-B(1)	121.40(17)
C(14)-C(9)-B(1)	120.97(17)
C(11)-C(10)-C(9)	122.14(18)

C(11)-C(10)-H(10)	118.9
C(9)-C(10)-H(10)	118.9
C(12)-C(11)-C(10)	118.49(17)
C(12)-C(11)-N(1)	120.36(18)
C(10)-C(11)-N(1)	121.02(18)
C(13)-C(12)-C(11)	120.45(19)
C(13)-C(12)-H(12)	119.8
C(11)-C(12)-H(12)	119.8
C(12)-C(13)-C(14)	120.54(19)
C(12)-C(13)-H(13)	119.7
C(14)-C(13)-H(13)	119.7
C(13)-C(14)-C(9)	120.73(17)
C(13)-C(14)-H(14)	119.6
C(9)-C(14)-H(14)	119.6
C(11)-N(1)-H(1N)	111.2(15)
C(11)-N(1)-H(2N)	112.7(14)
H(1N)-N(1)-H(2N)	119(2)
C(1)-O(1)-C(6)	109.44(13)
C(2)-O(2)-C(6)	106.74(14)
B(1)-O(3)-C(3)	121.49(16)
C(1)-O(4)-C(4)	108.44(14)
B(1)-O(5)-C(5)	120.26(16)

Table S2. Bond lengths [Å] and angles [°] for **5a**.

B(1)-O(5)	1.362(3)
B(1)-O(3)	1.378(3)
B(1)-C(9)	1.578(3)
C(1)-O(1)	1.400(3)
C(1)-O(4)	1.415(3)
C(1)-C(2)	1.532(3)
C(1)-H(1)	0.9800
C(2)-O(2)	1.427(3)
C(2)-C(3)	1.522(3)
C(2)-H(2)	0.9800
C(3)-O(3)	1.438(3)
C(3)-C(4)	1.525(3)

C(3)-H(3)	0.9800
C(4)-O(4)	1.440(3)
C(4)-C(5)	1.509(3)
C(4)-H(4)	0.9800
C(5)-O(5)	1.441(3)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-O(1)	1.430(4)
C(6)-O(2)	1.430(4)
C(6)-C(8)	1.514(4)
C(6)-C(7)	1.526(4)
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(14)	1.396(3)
C(9)-C(10)	1.412(3)
C(10)-C(11)	1.394(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.382(3)
C(11)-N(1)	1.449(2)
C(12)-C(13)	1.403(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.383(4)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300
C(15)-N(1)	1.287(3)
C(15)-C(16)	1.464(3)
C(15)-H(15)	0.9300
C(16)-N(2)	1.362(3)
C(16)-C(17)	1.386(3)
C(17)-C(18)	1.392(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.371(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.391(4)
C(19)-H(19)	0.9300
C(20)-N(2)	1.352(3)

C(20)-H(20)	0.9300
Cl(1)-Pd(1)	2.2953(6)
Cl(2)-Pd(1)	2.2921(6)
N(1)-Pd(1)	2.0441(16)
N(2)-Pd(1)	2.0362(17)

O(5)-B(1)-O(3)	123.7(2)
O(5)-B(1)-C(9)	116.18(19)
O(3)-B(1)-C(9)	120.10(18)
O(1)-C(1)-O(4)	112.5(2)
O(1)-C(1)-C(2)	105.3(2)
O(4)-C(1)-C(2)	106.84(18)
O(1)-C(1)-H(1)	110.7
O(4)-C(1)-H(1)	110.7
C(2)-C(1)-H(1)	110.7
O(2)-C(2)-C(3)	108.9(2)
O(2)-C(2)-C(1)	103.73(19)
C(3)-C(2)-C(1)	103.59(18)
O(2)-C(2)-H(2)	113.2
C(3)-C(2)-H(2)	113.2
C(1)-C(2)-H(2)	113.2
O(3)-C(3)-C(2)	107.60(17)
O(3)-C(3)-C(4)	111.80(18)
C(2)-C(3)-C(4)	101.57(17)
O(3)-C(3)-H(3)	111.8
C(2)-C(3)-H(3)	111.8
C(4)-C(3)-H(3)	111.8
O(4)-C(4)-C(5)	109.9(2)
O(4)-C(4)-C(3)	103.11(16)
C(5)-C(4)-C(3)	114.21(18)
O(4)-C(4)-H(4)	109.8
C(5)-C(4)-H(4)	109.8
C(3)-C(4)-H(4)	109.8
O(5)-C(5)-C(4)	112.61(17)
O(5)-C(5)-H(5A)	109.1
C(4)-C(5)-H(5A)	109.1
O(5)-C(5)-H(5B)	109.1
C(4)-C(5)-H(5B)	109.1
H(5A)-C(5)-H(5B)	107.8
O(1)-C(6)-O(2)	105.9(2)

O(1)-C(6)-C(8)	110.3(3)
O(2)-C(6)-C(8)	108.7(3)
O(1)-C(6)-C(7)	108.4(3)
O(2)-C(6)-C(7)	111.2(3)
C(8)-C(6)-C(7)	112.1(3)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(14)-C(9)-C(10)	117.7(2)
C(14)-C(9)-B(1)	119.96(19)
C(10)-C(9)-B(1)	122.38(19)
C(11)-C(10)-C(9)	120.1(2)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	121.40(19)
C(12)-C(11)-N(1)	117.41(19)
C(10)-C(11)-N(1)	121.2(2)
C(11)-C(12)-C(13)	118.9(2)
C(11)-C(12)-H(12)	120.5
C(13)-C(12)-H(12)	120.5
C(14)-C(13)-C(12)	119.8(2)
C(14)-C(13)-H(13)	120.1
C(12)-C(13)-H(13)	120.1
C(13)-C(14)-C(9)	122.1(2)
C(13)-C(14)-H(14)	119.0
C(9)-C(14)-H(14)	119.0
N(1)-C(15)-C(16)	118.18(18)
N(1)-C(15)-H(15)	120.9
C(16)-C(15)-H(15)	120.9
N(2)-C(16)-C(17)	122.3(2)
N(2)-C(16)-C(15)	114.06(18)

C(17)-C(16)-C(15)	123.4(2)
C(16)-C(17)-C(18)	118.6(2)
C(16)-C(17)-H(17)	120.7
C(18)-C(17)-H(17)	120.7
C(19)-C(18)-C(17)	119.2(2)
C(19)-C(18)-H(18)	120.4
C(17)-C(18)-H(18)	120.4
C(18)-C(19)-C(20)	119.9(2)
C(18)-C(19)-H(19)	120.0
C(20)-C(19)-H(19)	120.0
N(2)-C(20)-C(19)	121.5(2)
N(2)-C(20)-H(20)	119.3
C(19)-C(20)-H(20)	119.3
C(15)-N(1)-C(11)	118.49(16)
C(15)-N(1)-Pd(1)	113.68(13)
C(11)-N(1)-Pd(1)	127.71(13)
C(20)-N(2)-C(16)	118.35(19)
C(20)-N(2)-Pd(1)	128.37(16)
C(16)-N(2)-Pd(1)	113.24(13)
C(1)-O(1)-C(6)	111.2(2)
C(2)-O(2)-C(6)	109.8(2)
B(1)-O(3)-C(3)	120.78(17)
C(1)-O(4)-C(4)	109.34(17)
B(1)-O(5)-C(5)	120.72(18)
N(2)-Pd(1)-N(1)	80.25(7)
N(2)-Pd(1)-Cl(2)	173.00(6)
N(1)-Pd(1)-Cl(2)	95.10(5)
N(2)-Pd(1)-Cl(1)	93.83(5)
N(1)-Pd(1)-Cl(1)	173.61(5)
Cl(2)-Pd(1)-Cl(1)	91.01(3)