Supporting Information

Palladium Complexes with Tridentate *N*-Heterocyclic Carbene Ligands: Selective "Normal" and "Abnormal" Bindings and their Anticancer Activities

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Table of Contents

Table S1. Crystallographic Data

	3a	**3a'**	**4b**
empirical formula	$C_{18}H_{17}ClN_4OPd$	$C_{18}H_{17}ClN_4OPd$	$C_{20}H_{21}ClN_4O_2Pd$
formula weight	447.21	447.21	491.26
crystal system	orthorhombic	trigonal	monoclinic
space group	$P2_12_12_1$	R-3	$P2_1/c$
a, Å	7.821(4)	22.2283(8)	8.8861(6)
b, Å	8.102(4)	22.2283(8)	12.4320(8)
c, Å	26.932(15)	20.4987(8)	17.2003(11)
α, deg	90	90	90
β, deg	90	90	93.214(5)
γ, deg	90	120	90
V, Å^3	1706.6(15)	8771.4(6)	93.214(5)
T, K	150(2)	150(2)	90
Z	4	18	4
no. of unique data	3727	4268	4148
no. of params refined	227	226	255
R_1[a] [$I > 2\sigma I$]	0.0576	0.0300	0.0385
wR_2[b] (all data)	0.0768	0.0746	0.0701

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$. [b] $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)^2/\Sigma(F_o^2)]^{1/2}$

Table S2. Calculated and Observed Bond Distances (Å) in **3a** and **3a'**

3a			**3a'**		
	Observed[a]	Calculated		Observed[a]	Calculated
Pd1—C1	1.992(10)	1.989	Pd1—C2	1.959(3)	1.974
Pd1—Cl1	2.311(2)	2.374	Pd1—Cl1	2.3133(7)	2.362
Pd1—N3	2.046(8)	2.128	Pd1—N3	2.084(2)	2.119
Pd1—N4	1.986(7)	2.022	Pd1—N4	1.992(2)	2.032
C1—N2	1.328(11)	1.353	C2—N2	1.402(3)	1.394
C2—N2	1.349(11)	1.383	C1—N2	1.337(4)	1.337
C2—C3	1.341(12)	1.352	C1—N1	1.317(4)	1.338
C3—N1	1.367(12)	1.385	C3—N1	1.384(3)	1.383
C1—N1	1.329(12)	1.351	C2—C3	1.367(4)	1.371

[a]From the structural data of **2a** and **3a**

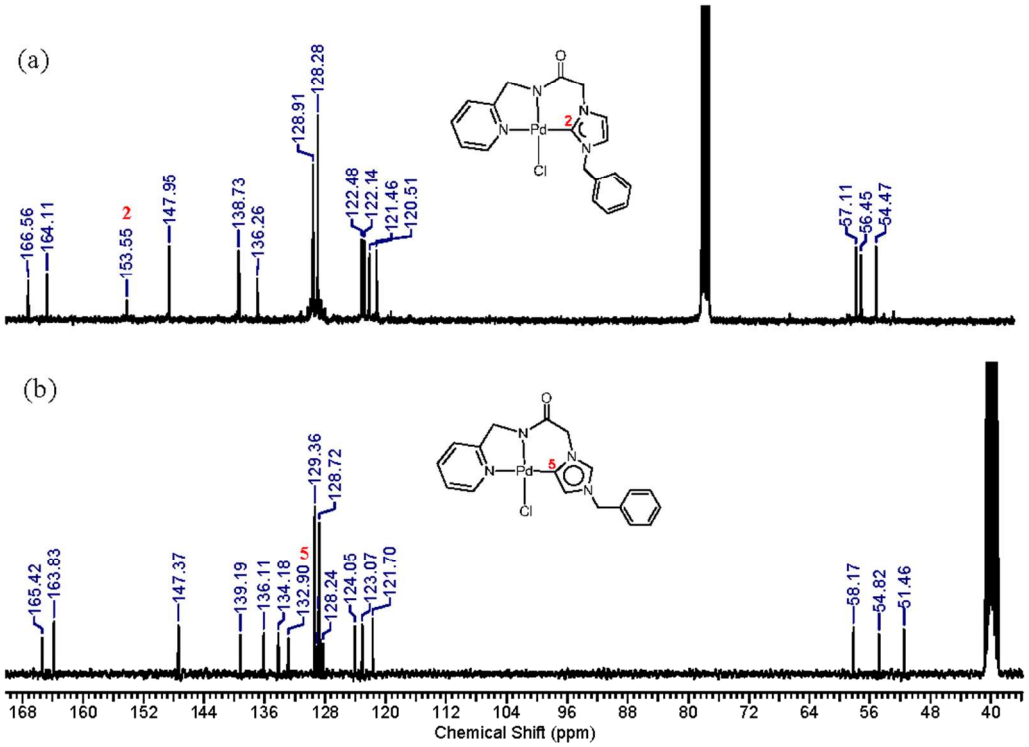

Figure S1. $^{13}C\{^{1}H\}$ NMR spectra of isomeric nNHC complex 3a in $CDCl_3$ and aNHC complex 3a' in d_6-DMSO.

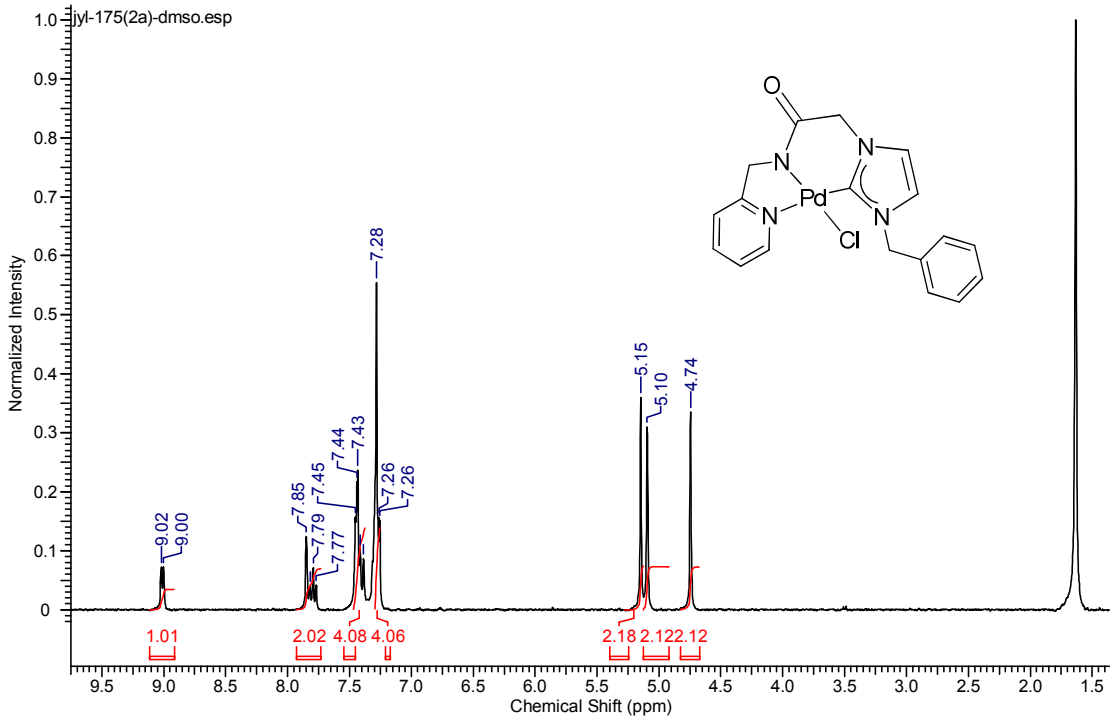

Figure S2. ^{1}H NMR spectrum of 3a in d_6-DMSO (300.13 MHz, 25 °C)

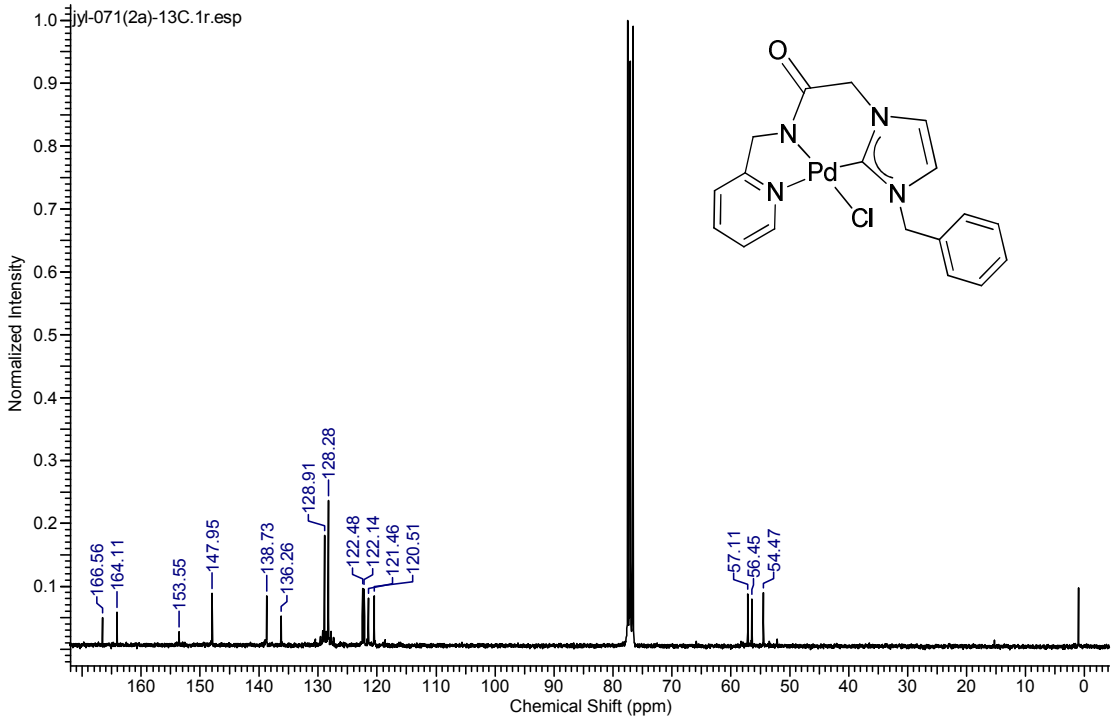

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of 3a in $CDCl_3$ (75.47 MHz; 25 °C)

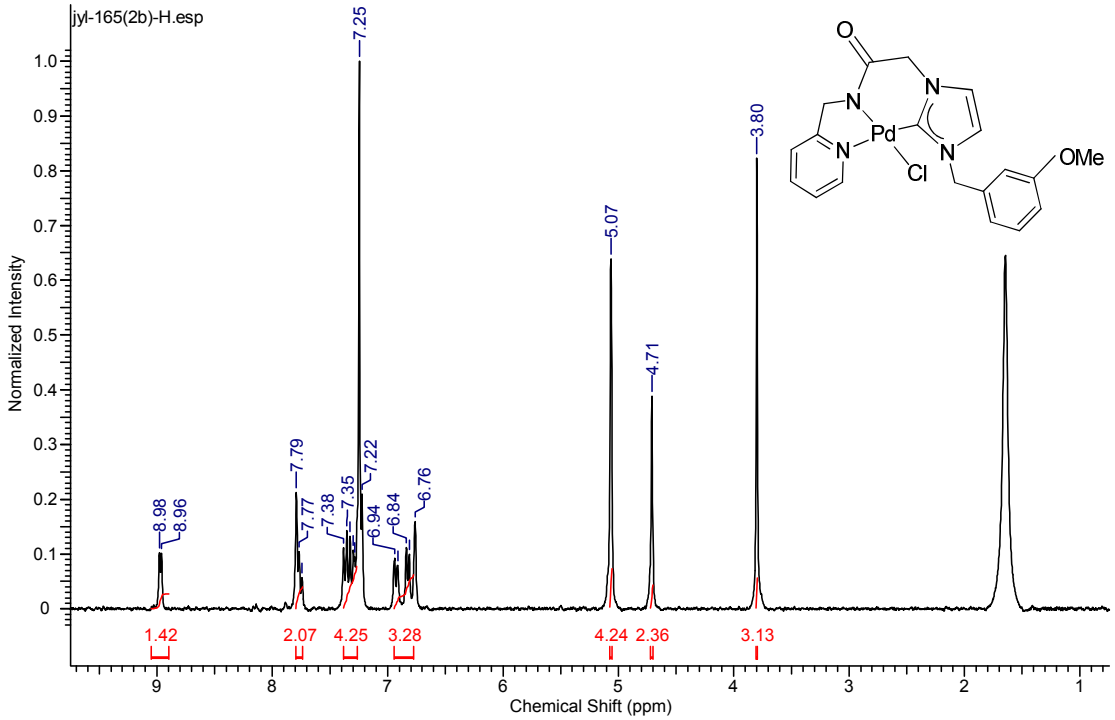

Figure S4. ^{1}H NMR spectrum of 3b in $CDCl_3$ (300.13 MHz, 25 °C)

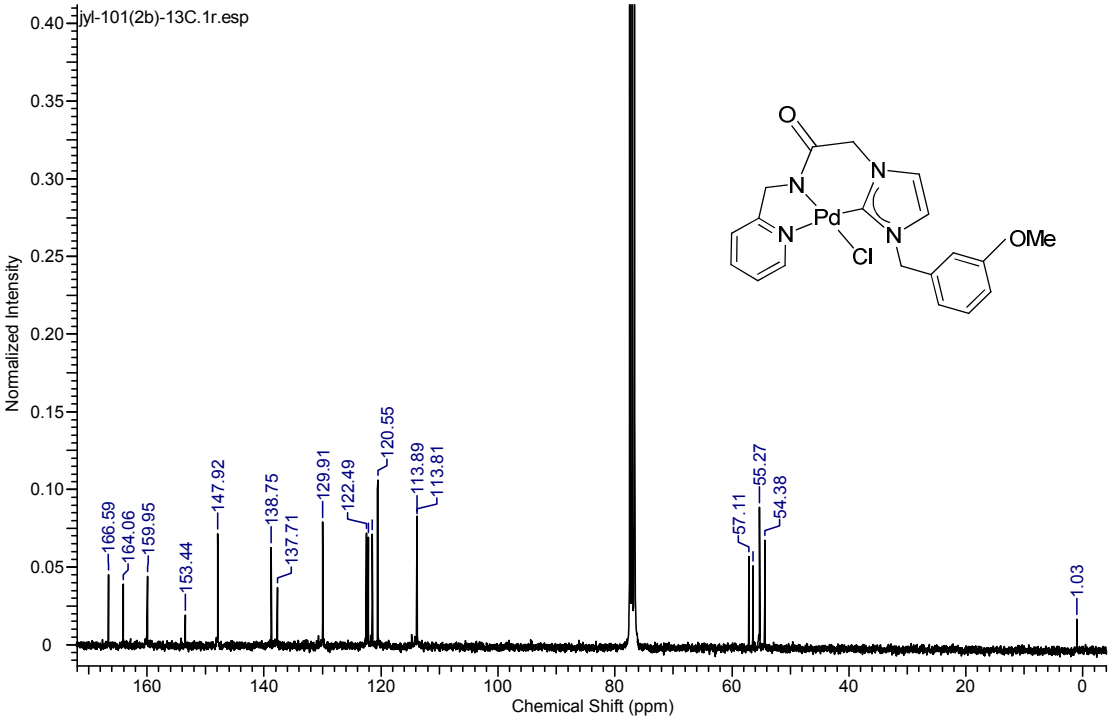

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of 3b in $CDCl_3$ (75.47 MHz; 25 °C)

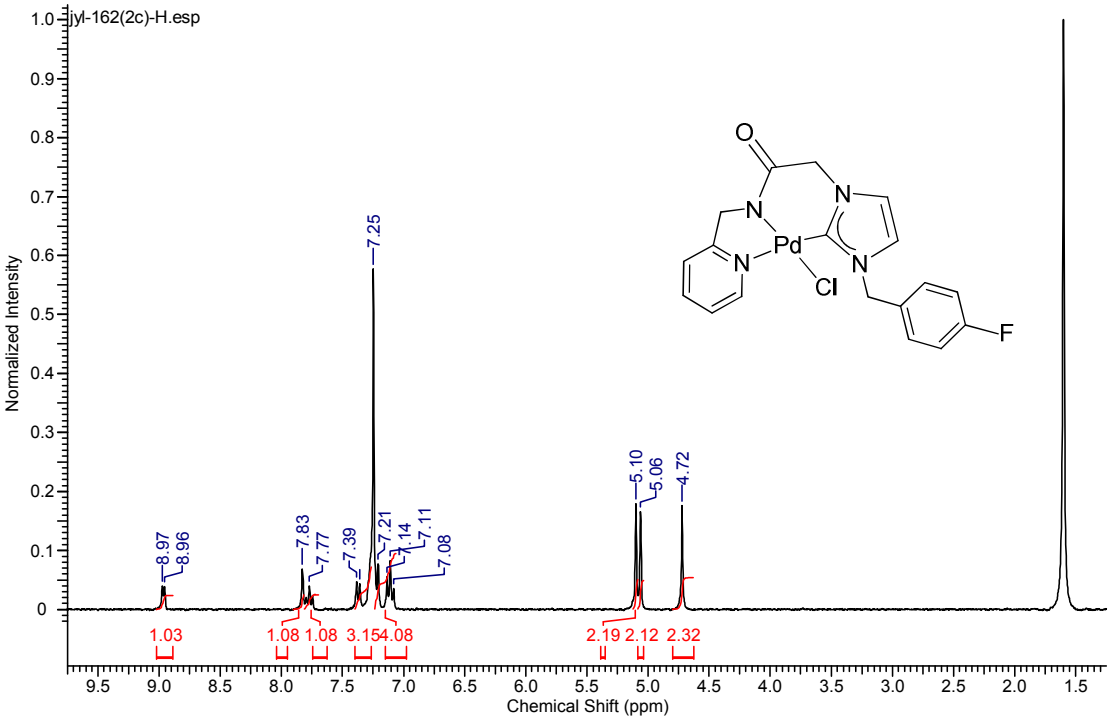

Figure S6. ^{1}H NMR spectrum of 3c in $CDCl_3$ (300.13 MHz, 25 °C)

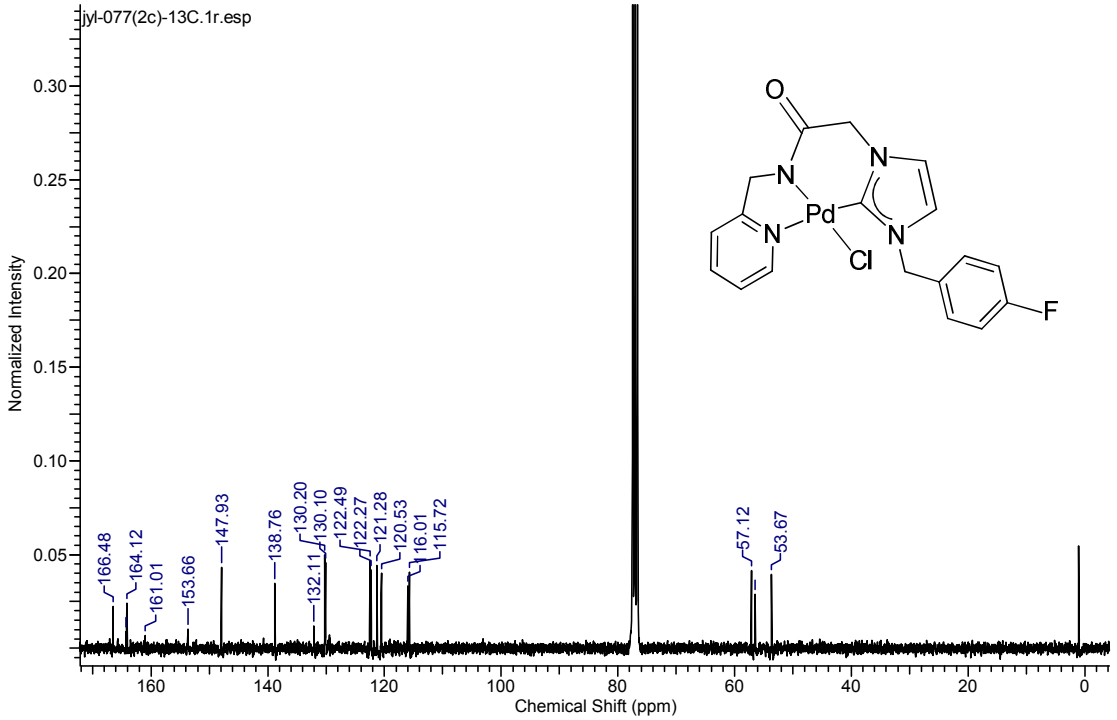

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of 3c in $CDCl_3$ (75.47 MHz; 25 °C)

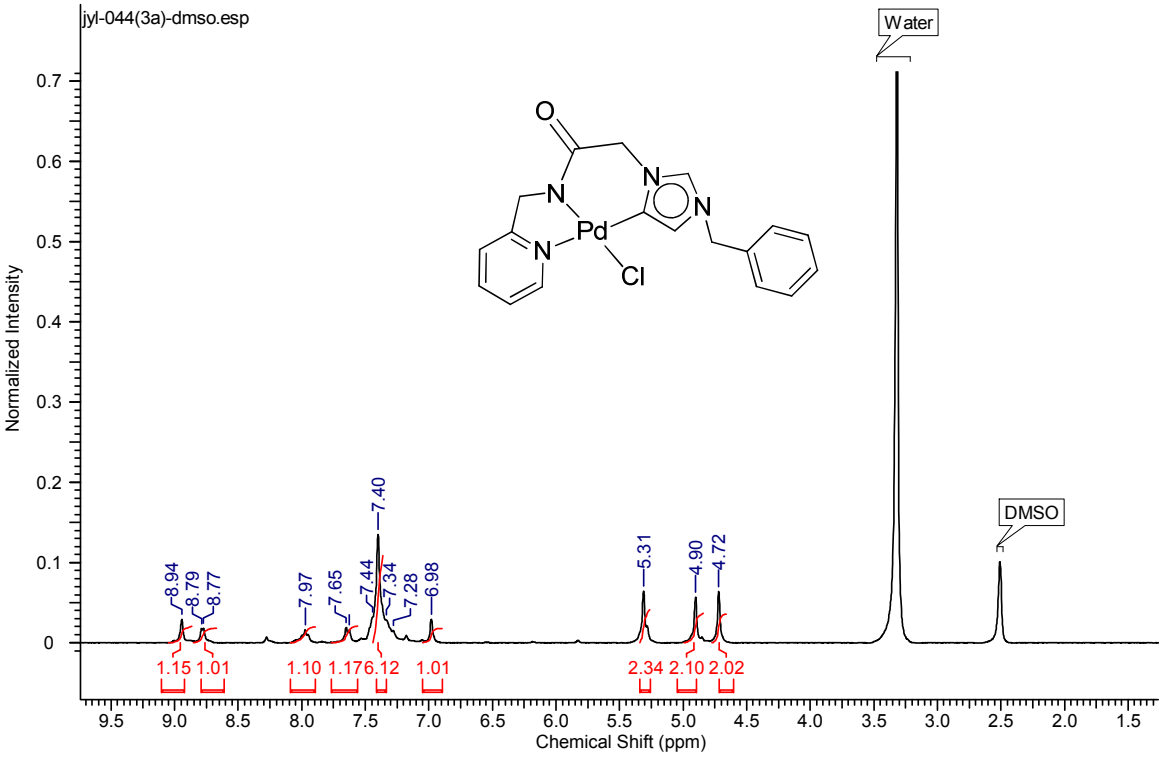

Figure S8. ^{1}H NMR spectrum of 3a' in d_6-DMSO (300.13 MHz, 25 °C)

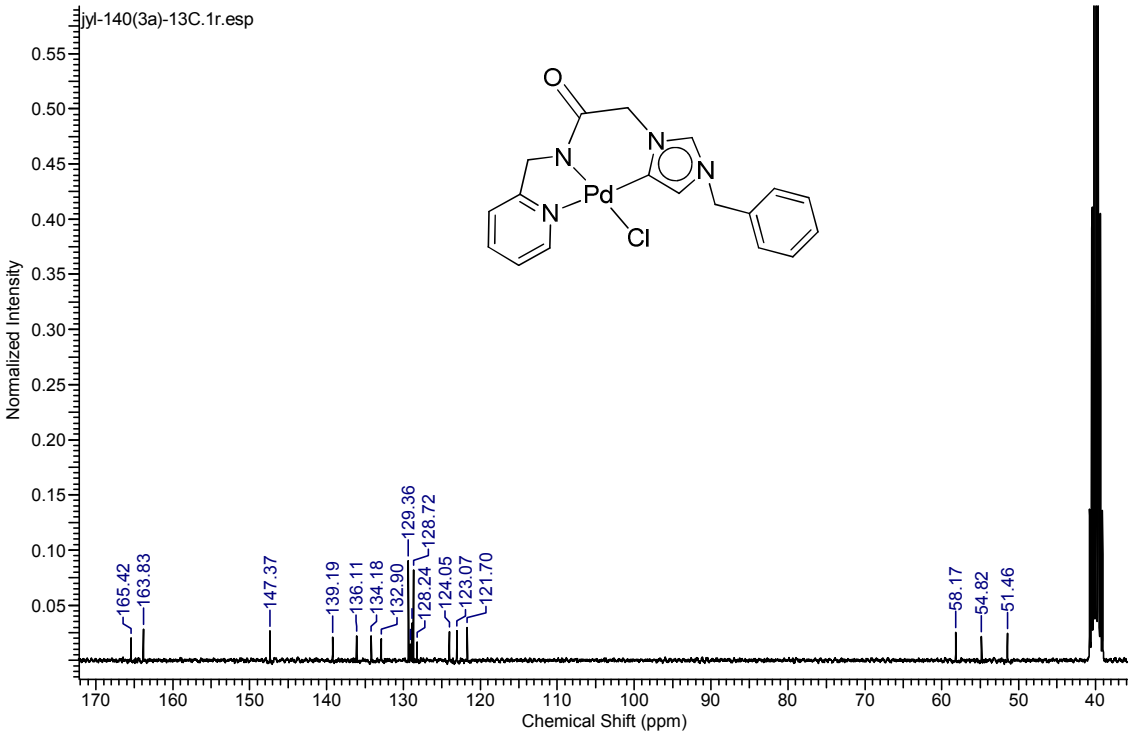

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of 3a' in d_6-DMSO (75.47 MHz; 25 °C)

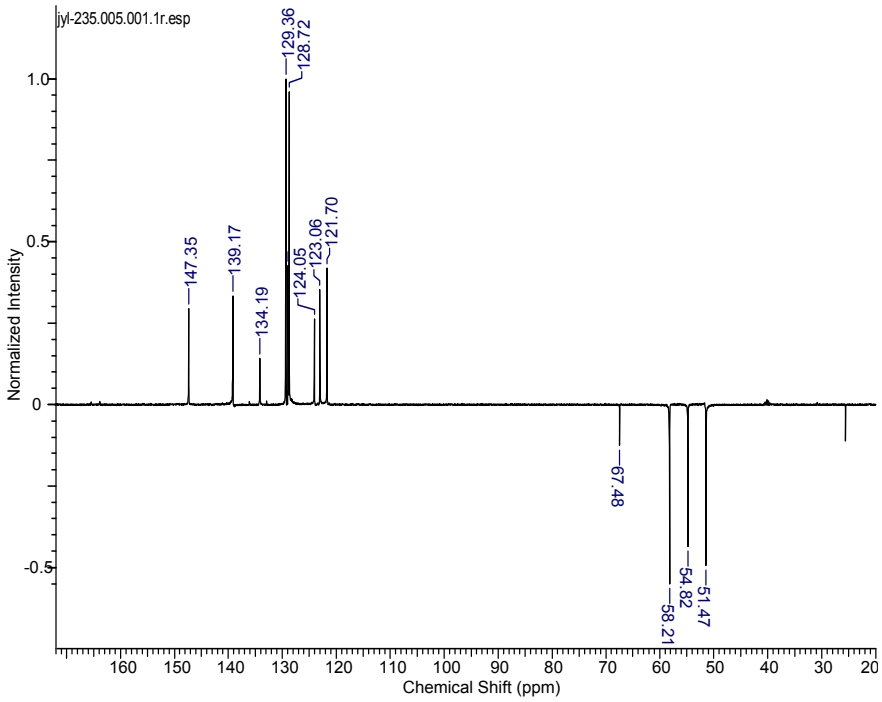

Figure S10. DEPT-135 NMR spectrum of 3a' in d_6-DMSO

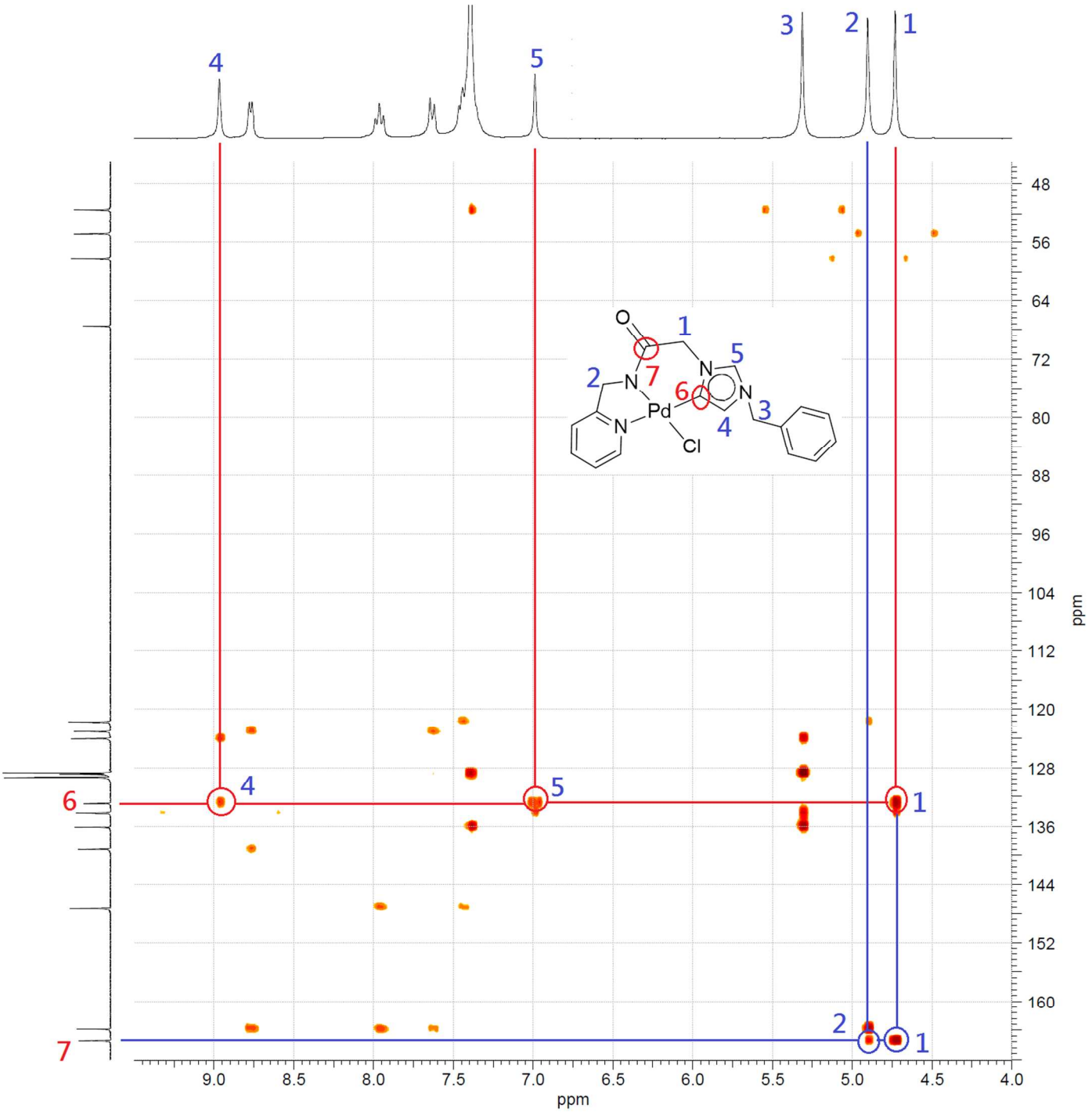

Figure S11. HMBC spectrum of spectrum of 3a' in d_6-DMSO

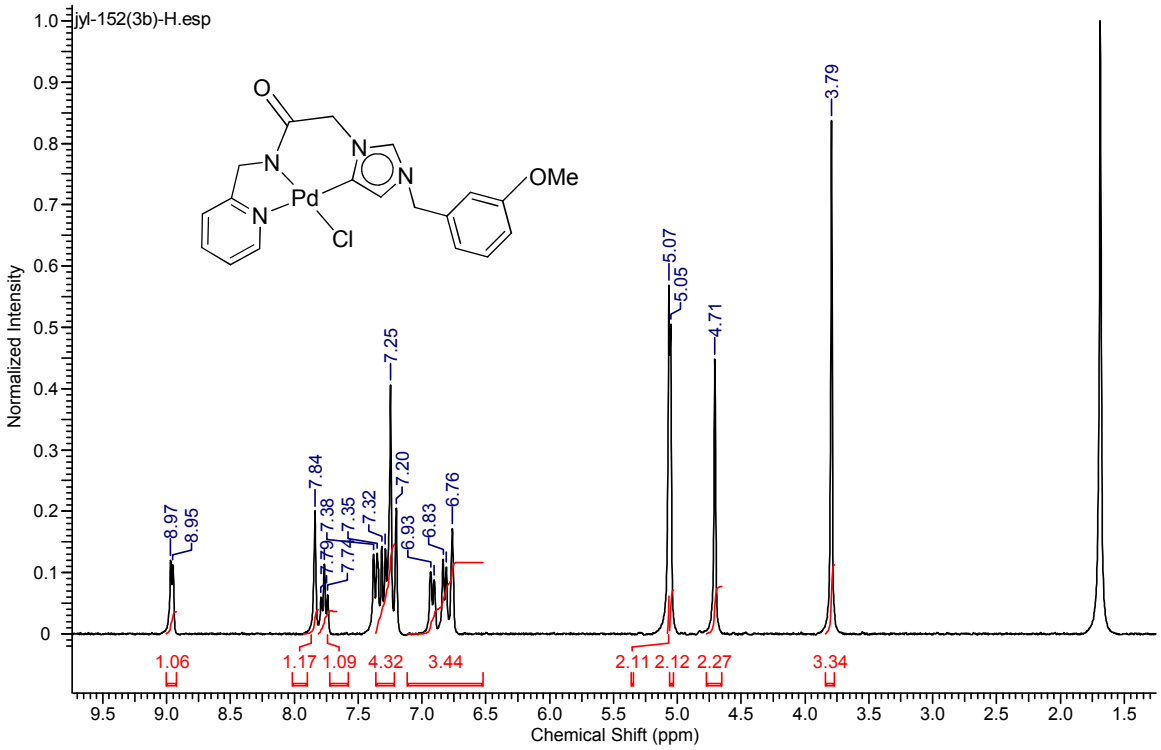

Figure S12. ^{1}H NMR spectrum of 3b' in $CDCl_3$ (300.13 MHz, 25 °C)

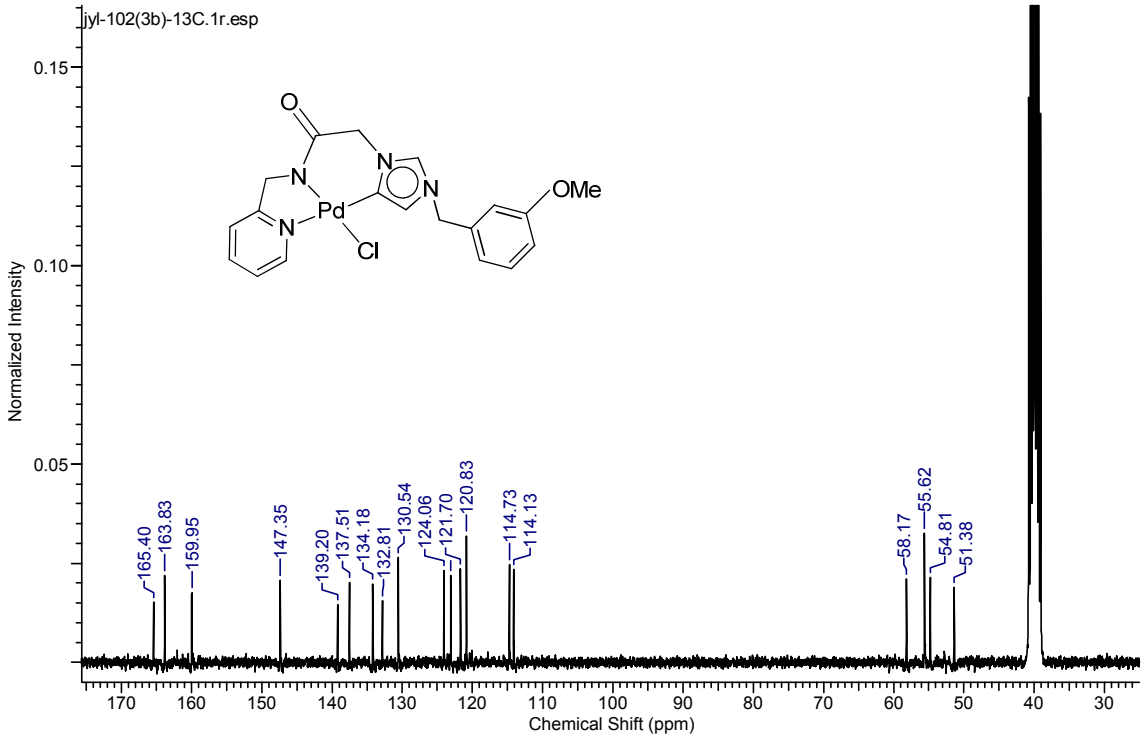

Figure S13. ^{13}C{^{1}H} NMR spectrum of 3b' in d_6-DMSO (75.47 MHz; 25 °C)

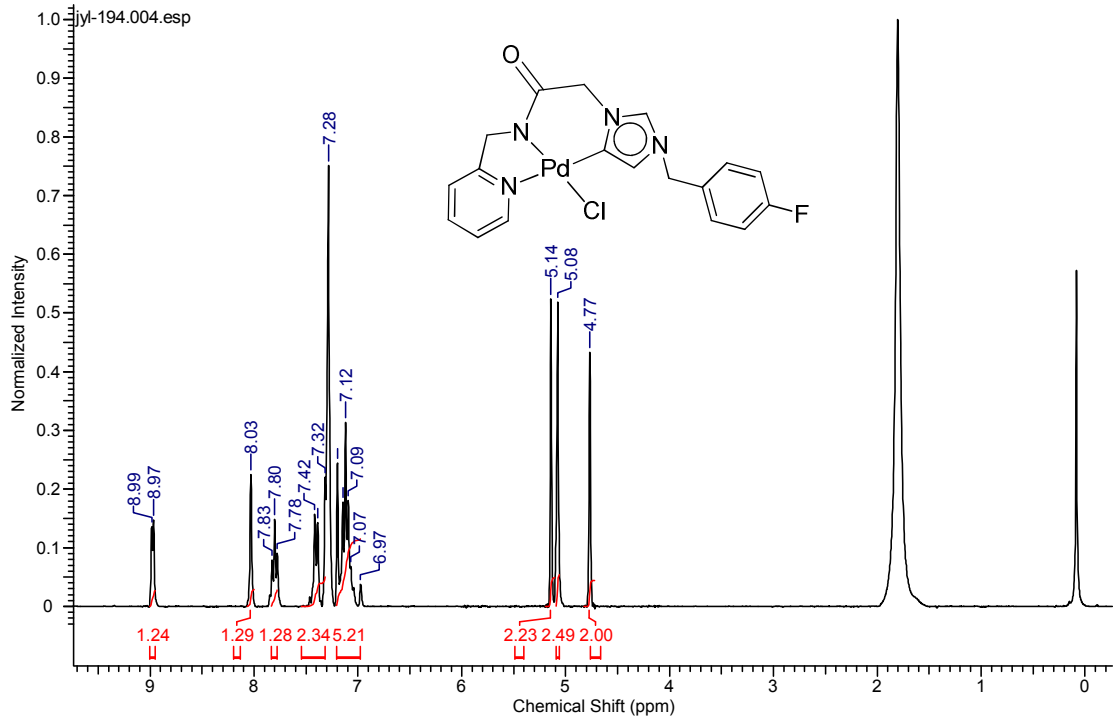

Figure S14. ^{1}H NMR spectrum of 3c' in $CDCl_3$ (300.13 MHz, 25 °C)

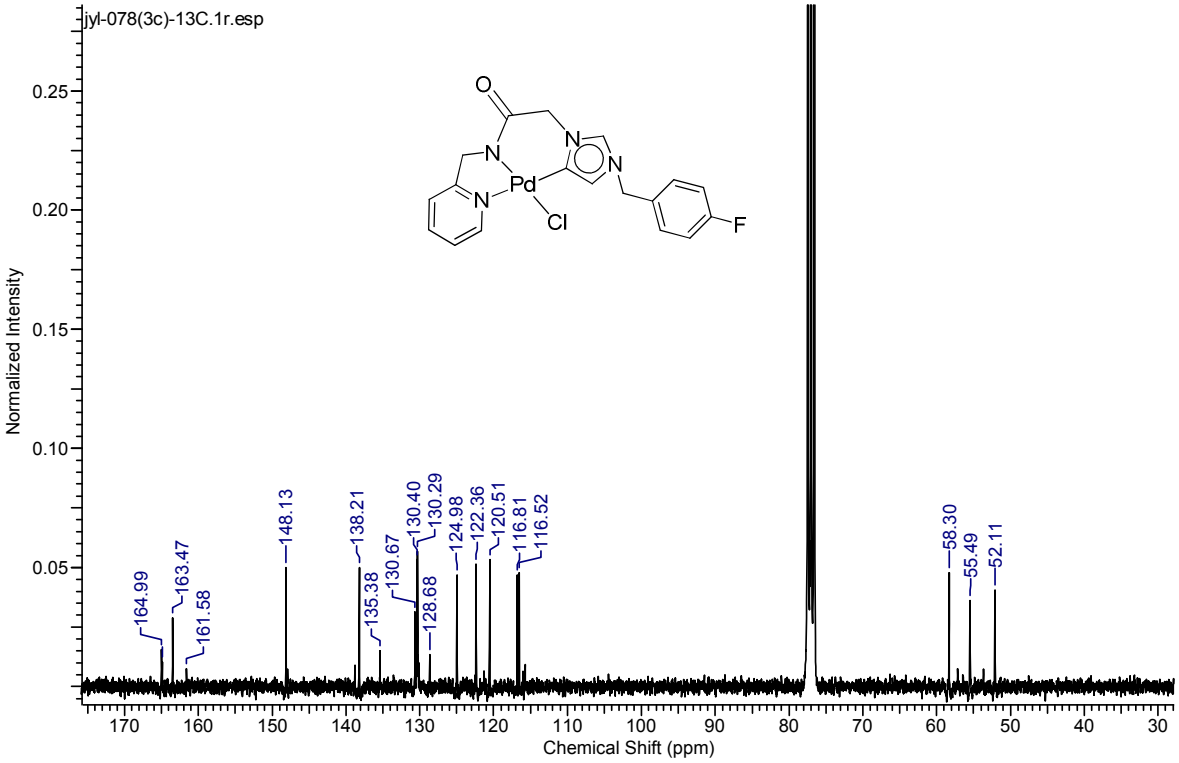

Figure S15. ^{13}C{^{1}H} NMR spectrum of 3c' in $CDCl_3$ (75.47 MHz; 25 °C)

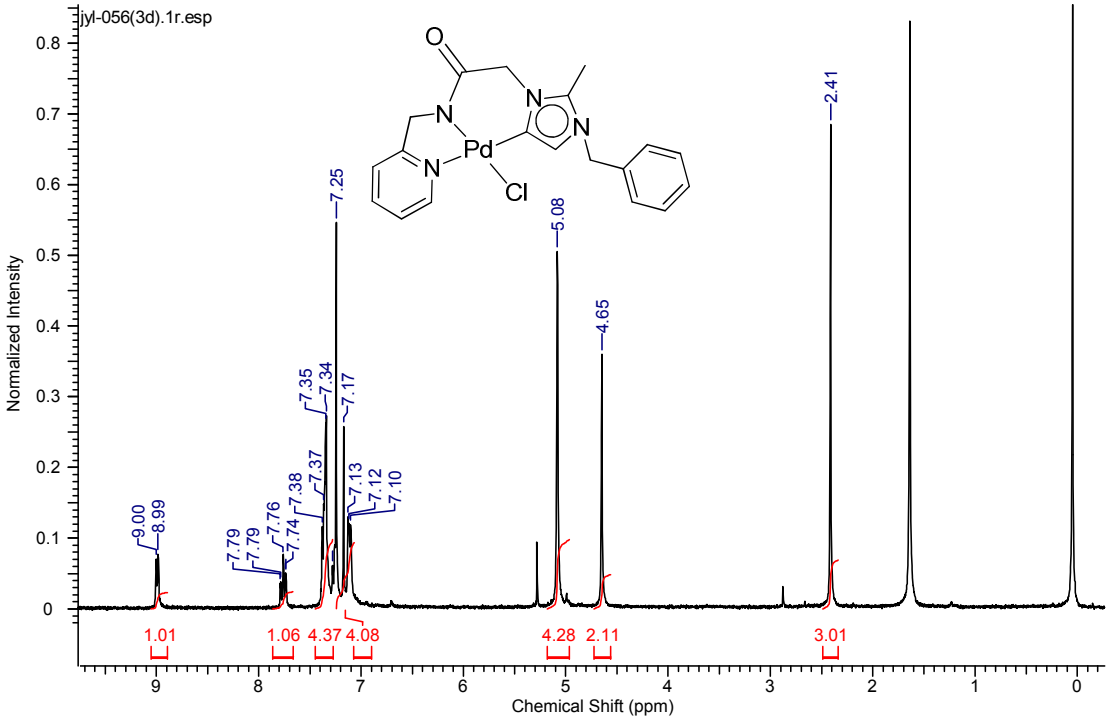

Figure S16. ^{1}H NMR spectrum of 4a in $CDCl_3$ (300.13 MHz, 25 °C)

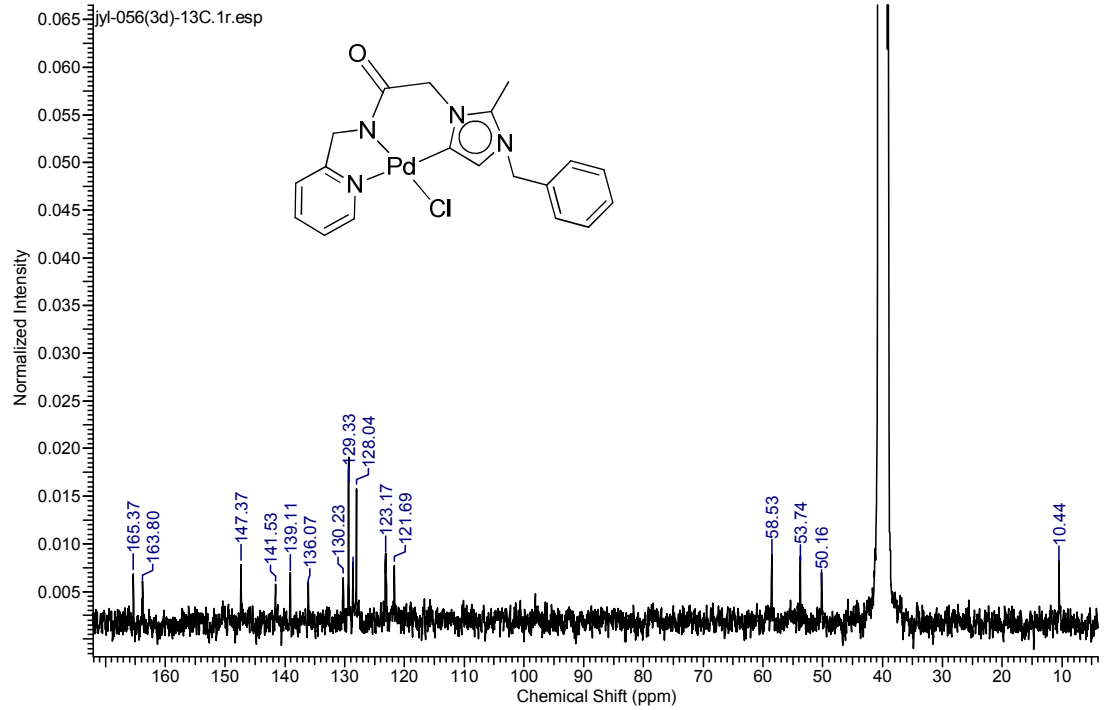

Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of 4a in d_6-DMSO (75.47 MHz; 25 °C)

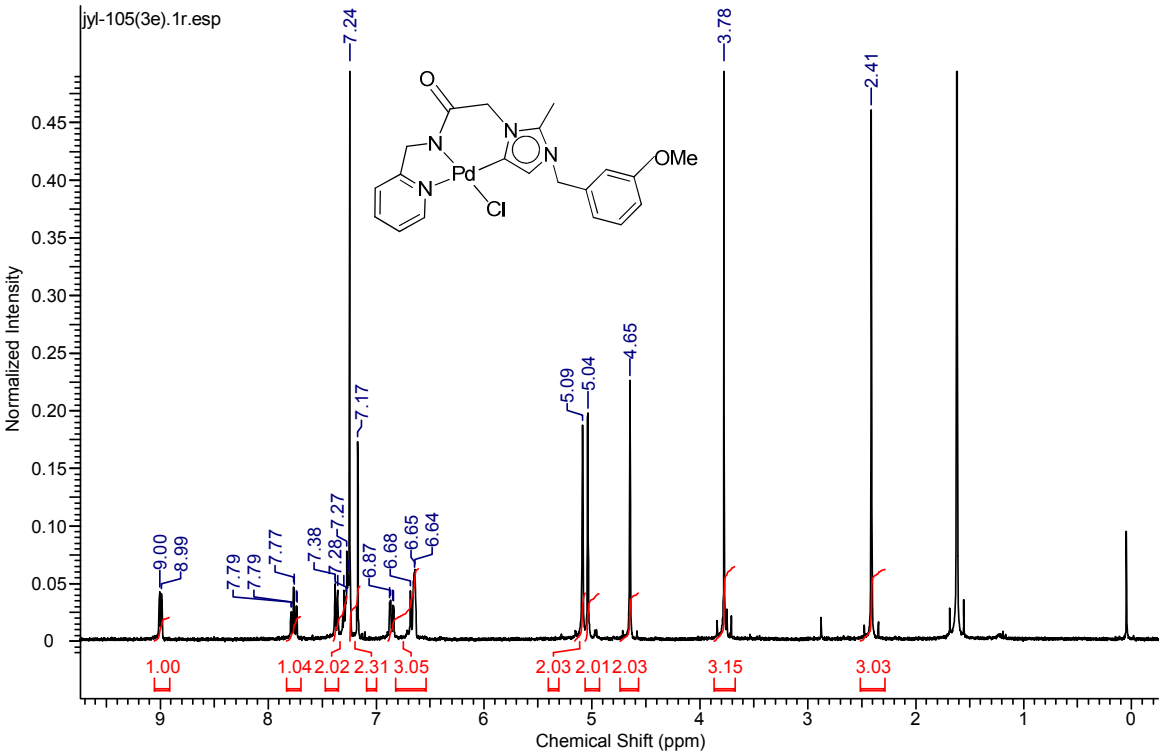

Figure S18. ^{1}H NMR spectrum of 4b in $CDCl_3$ (300.13 MHz, 25 °C)

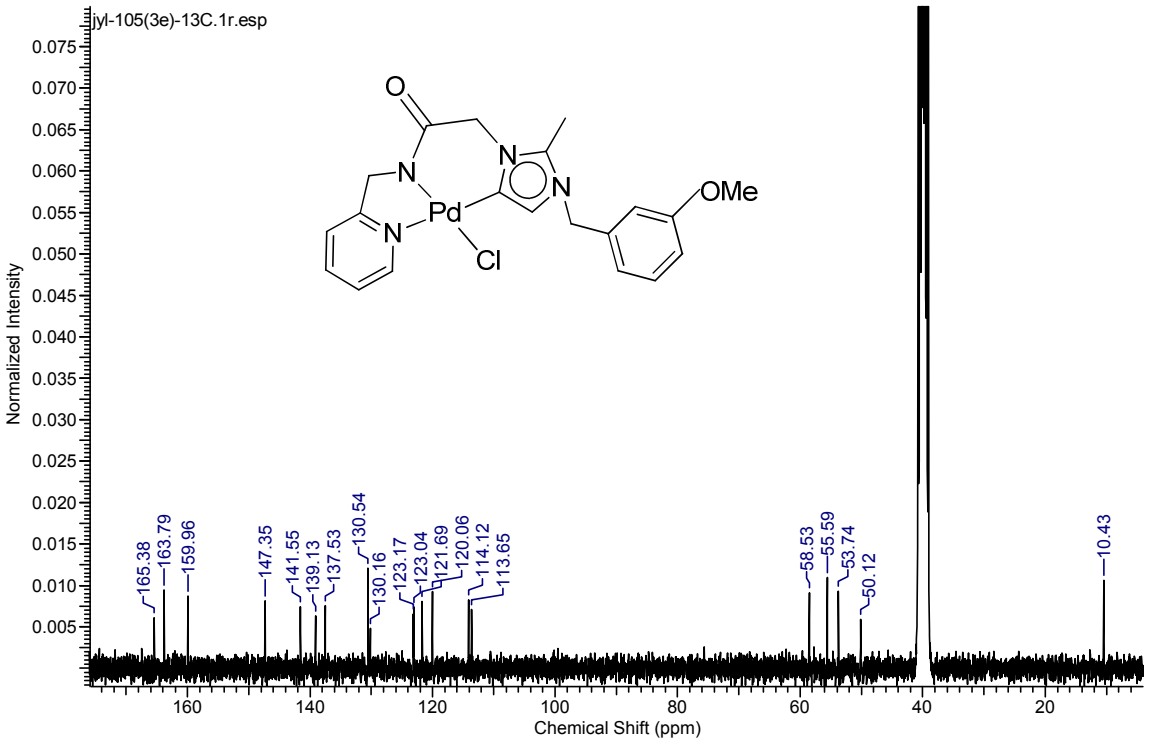

Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of 4b in d_6-DMSO (75.47 MHz; 25 °C)

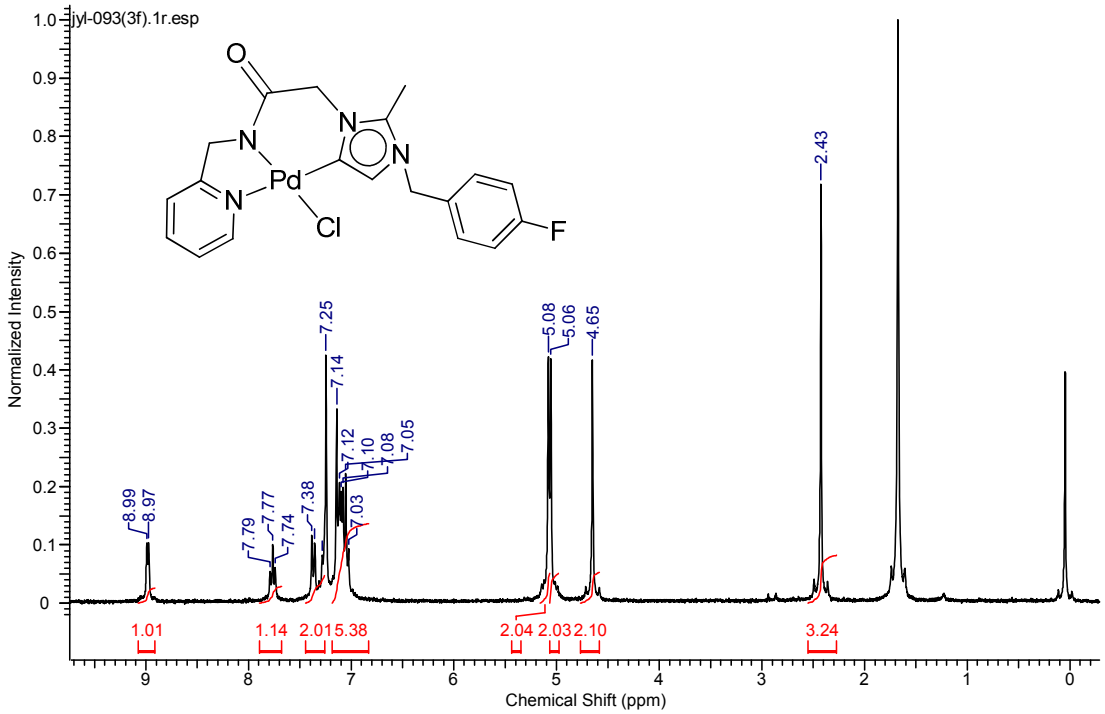

Figure S20. ^{1}H NMR spectrum of 4c in $CDCl_3$ (300.13 MHz, 25 °C)

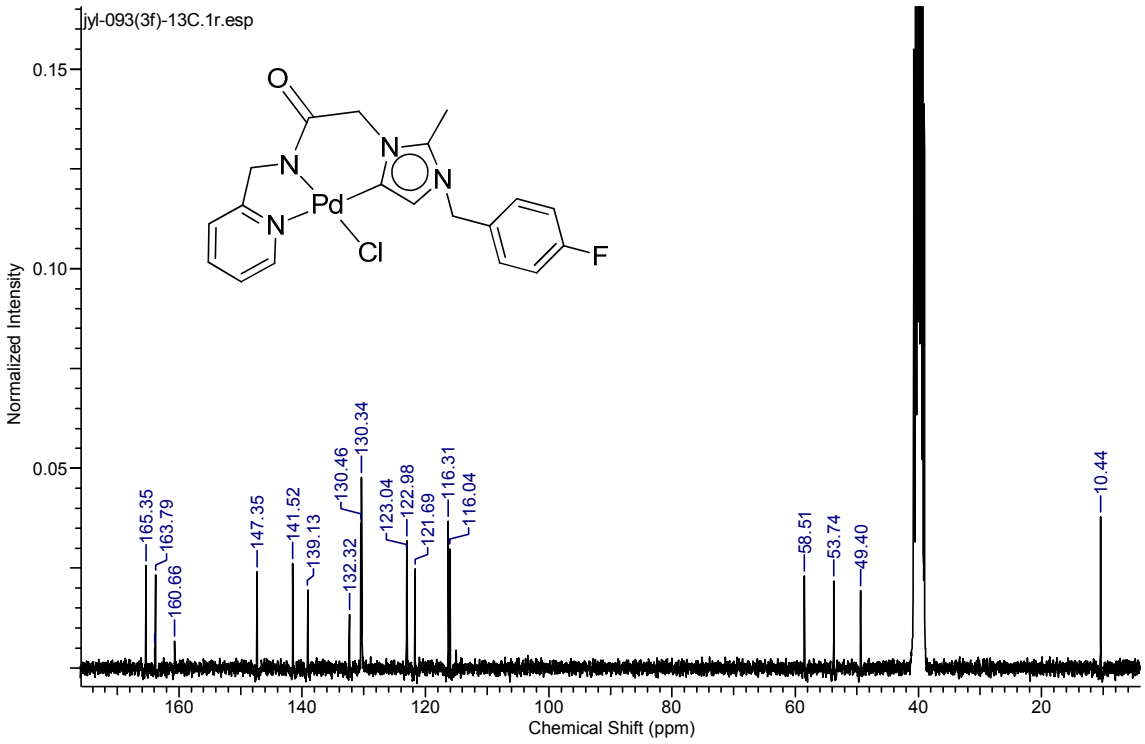

Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of 4c in d_6-DMSO (75.47 MHz; 25 °C)

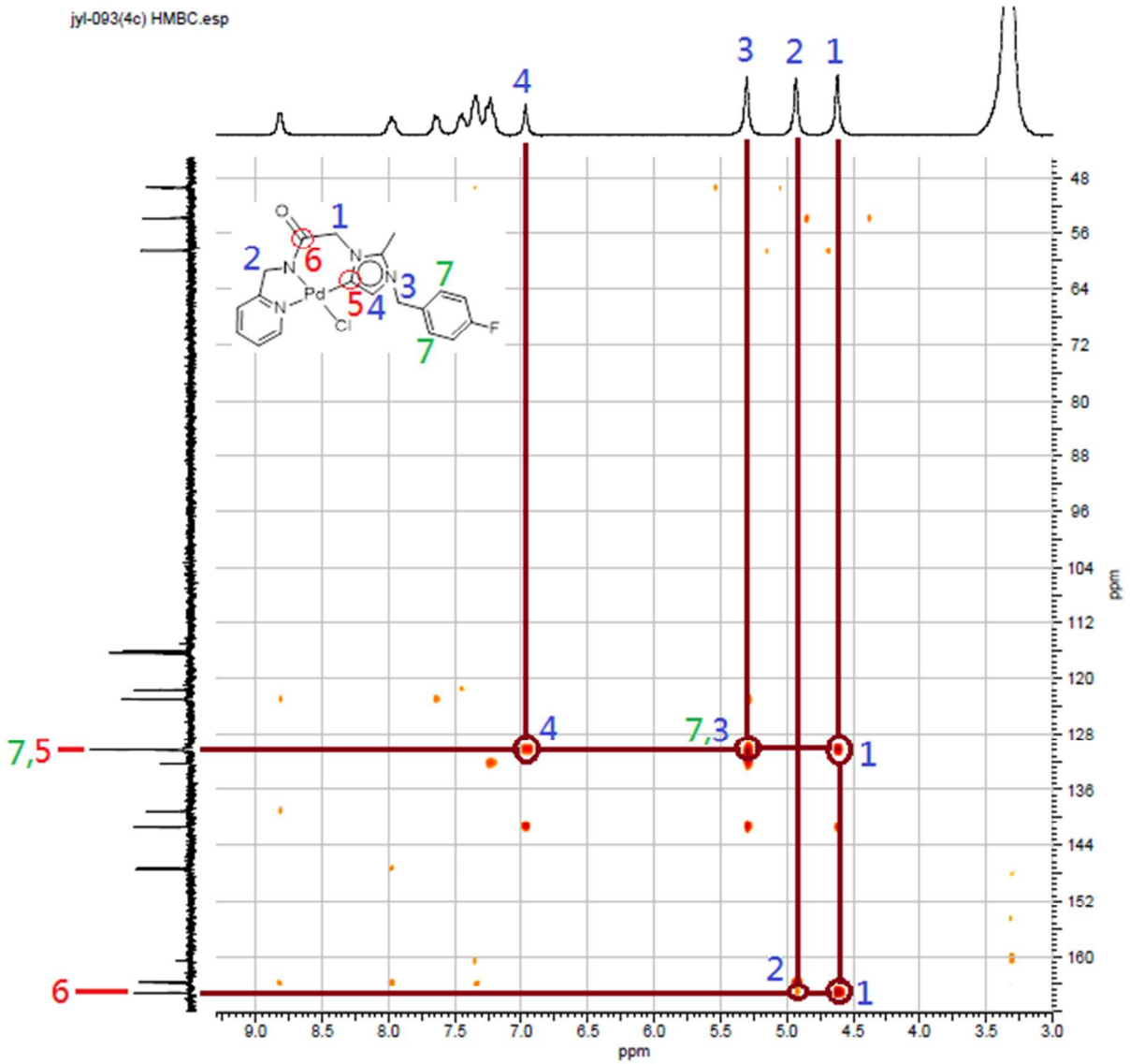

Figure S22. HMBC NMR spectrum of 4c in d_6-DMSO