Supporting Information (SI)

for

Synthesis and Structural Analysis of Palladium(II) Complexes Containing Neutral or Anionic *C*$_2$-Symmetric Bis(oxazoline) Ligands: Effects of Substituents in the 5 Position

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Contents

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1-1. NMR spectra of amino alcohol (6a, 6c).

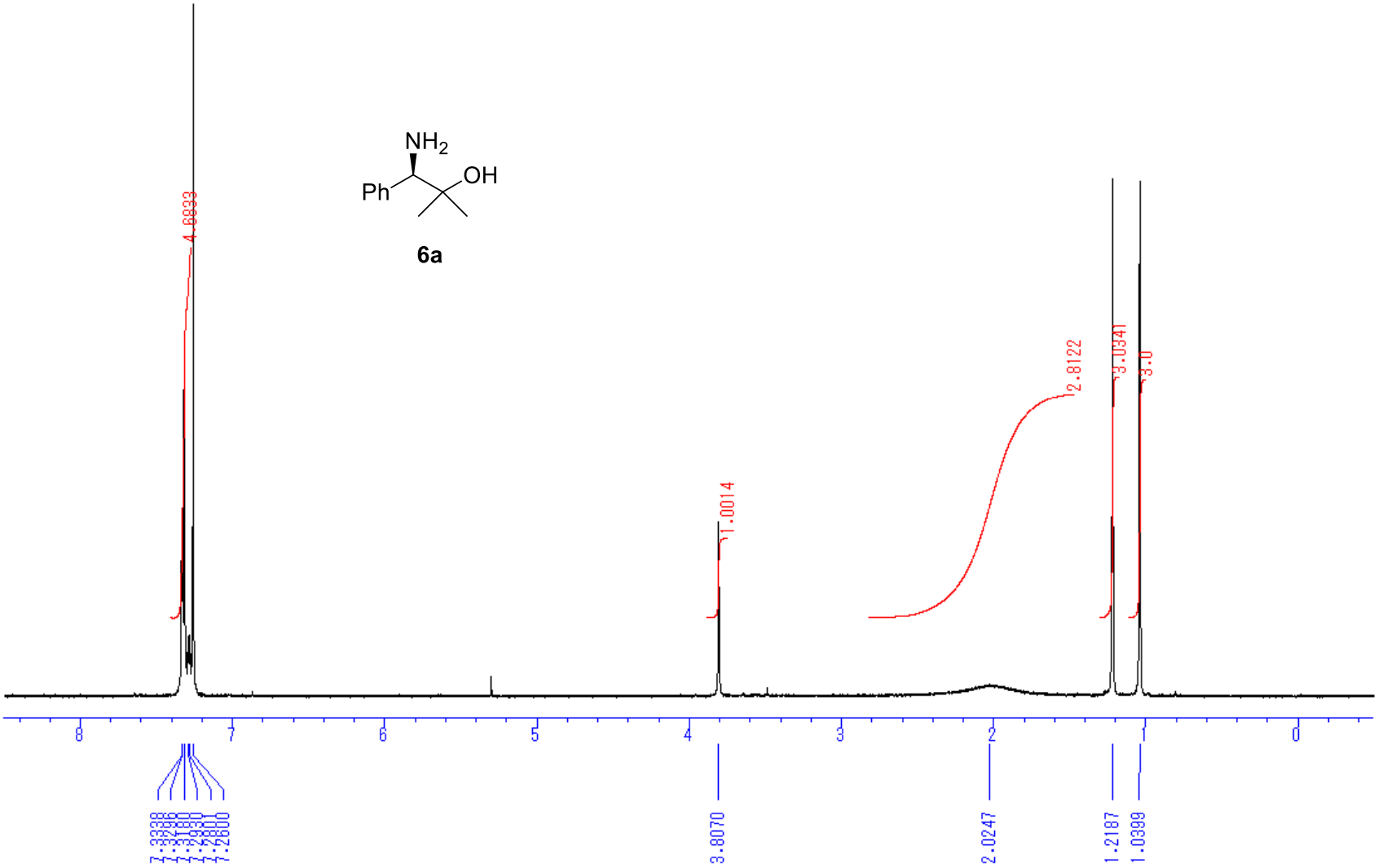

Figure S1. ^{1}H NMR Spectrum of amino alcohol (6a).

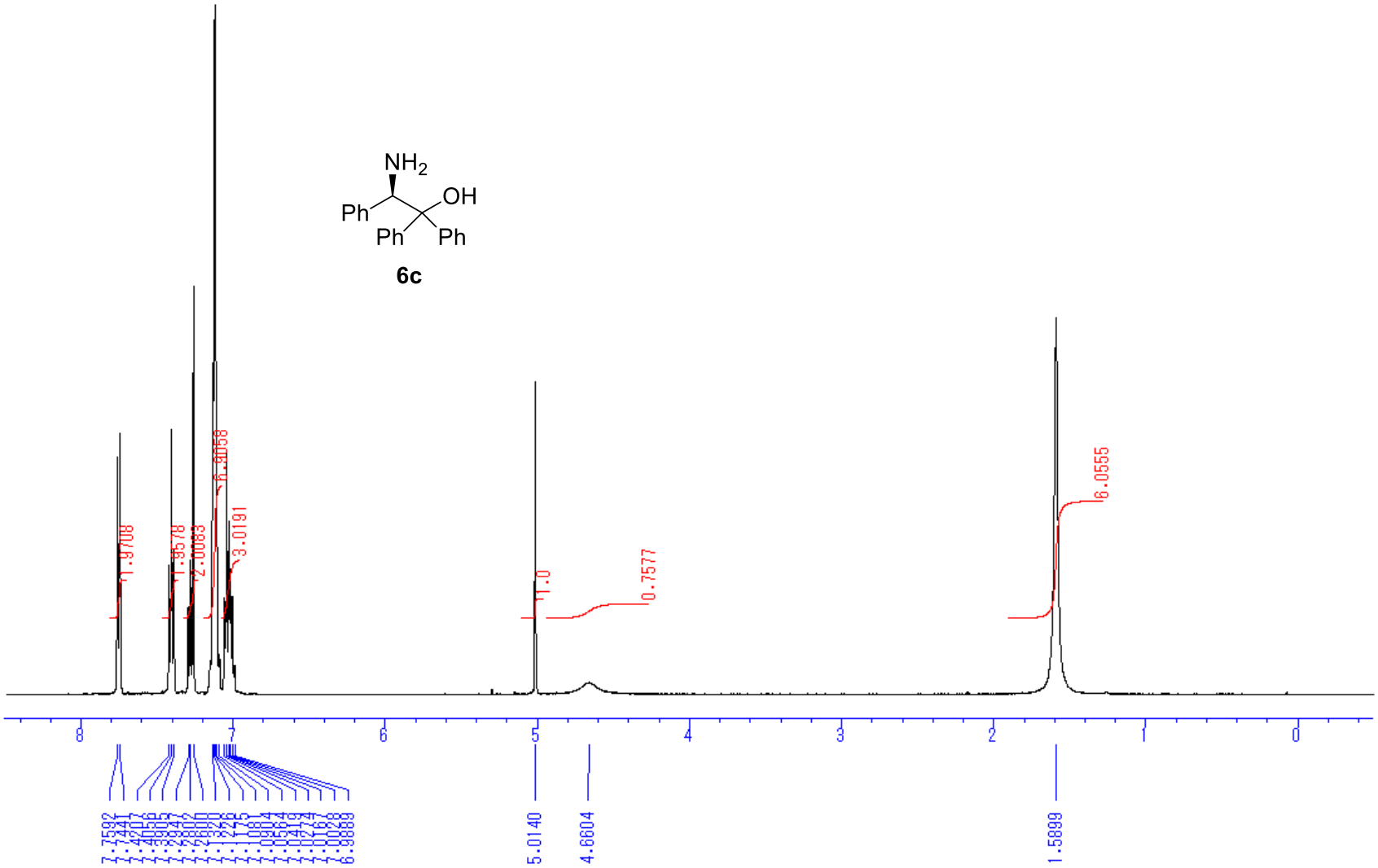

Figure S2. ^{1}H NMR Spectrum of amino alcohol (6c).

1-2. NMR spectra of bisamide alcohol (7a).

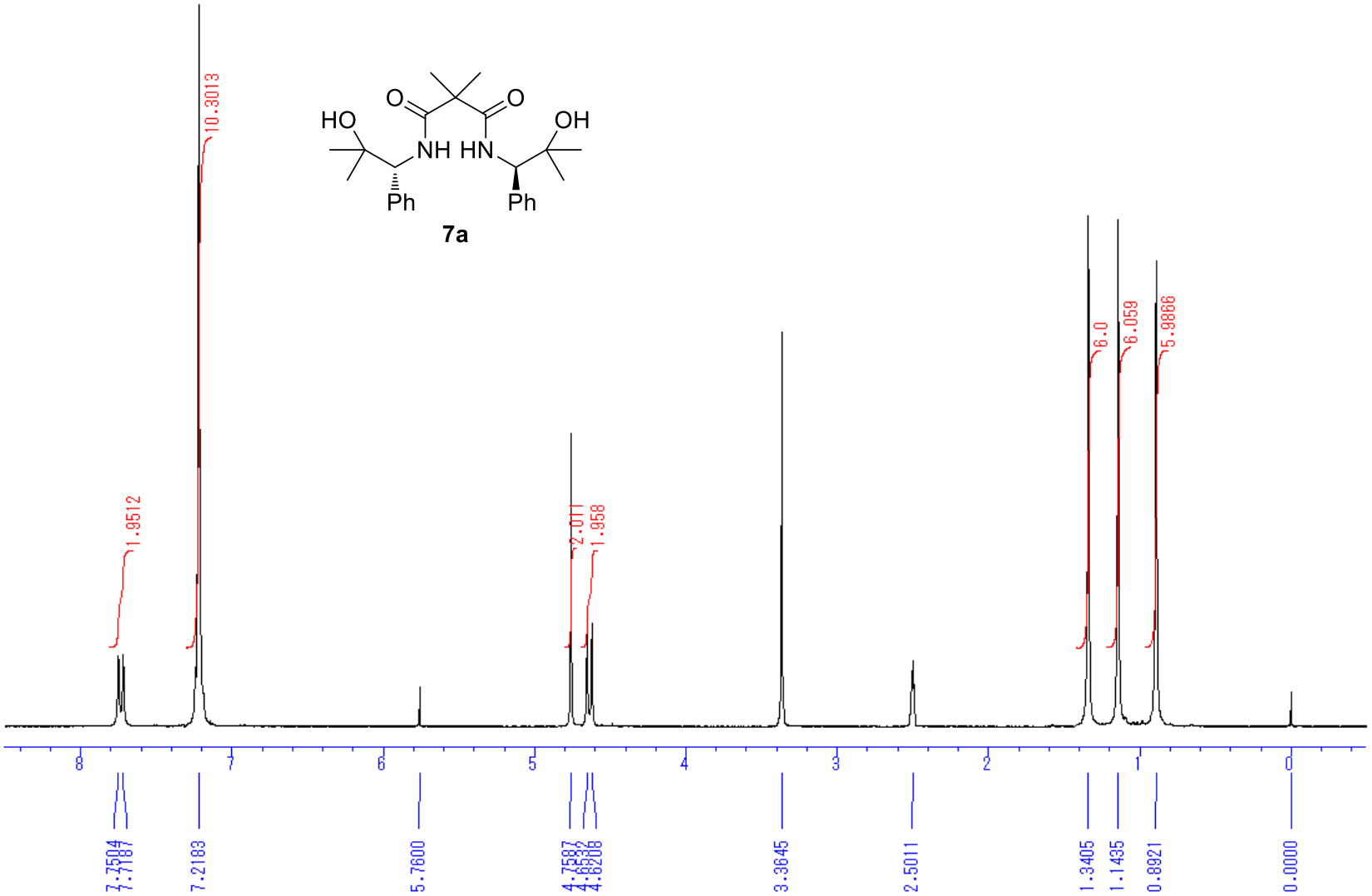

Figure S3. ^{1}H NMR Spectrum of bisamide alcohol (7a).

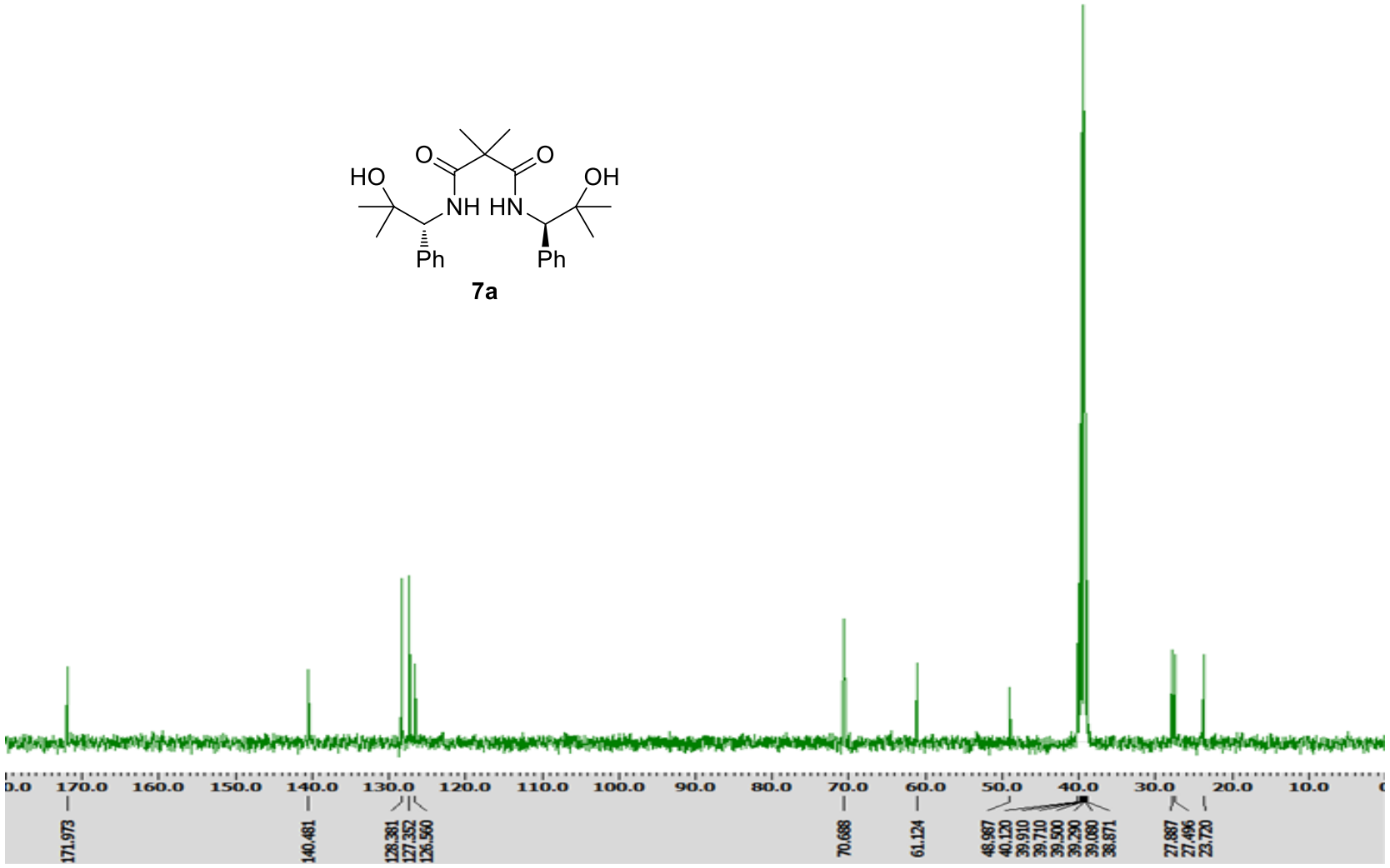

Figure S4. ^{13}C NMR Spectrum of bisamide alcohol (7a).

1-3. NMR spectra of BOX (1a-c).

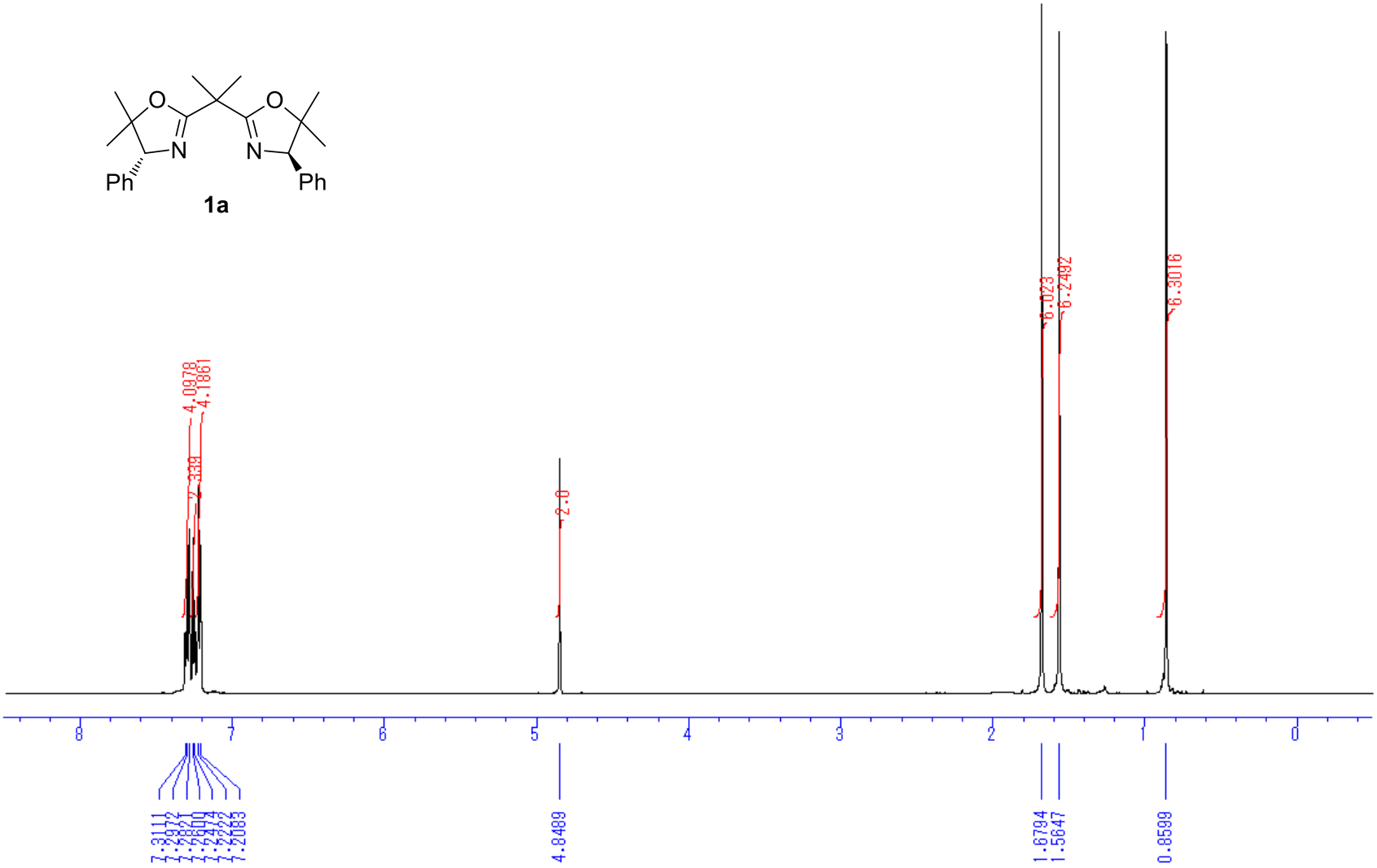

Figure S5. ^{1}H NMR Spectrum of BOX (1a).

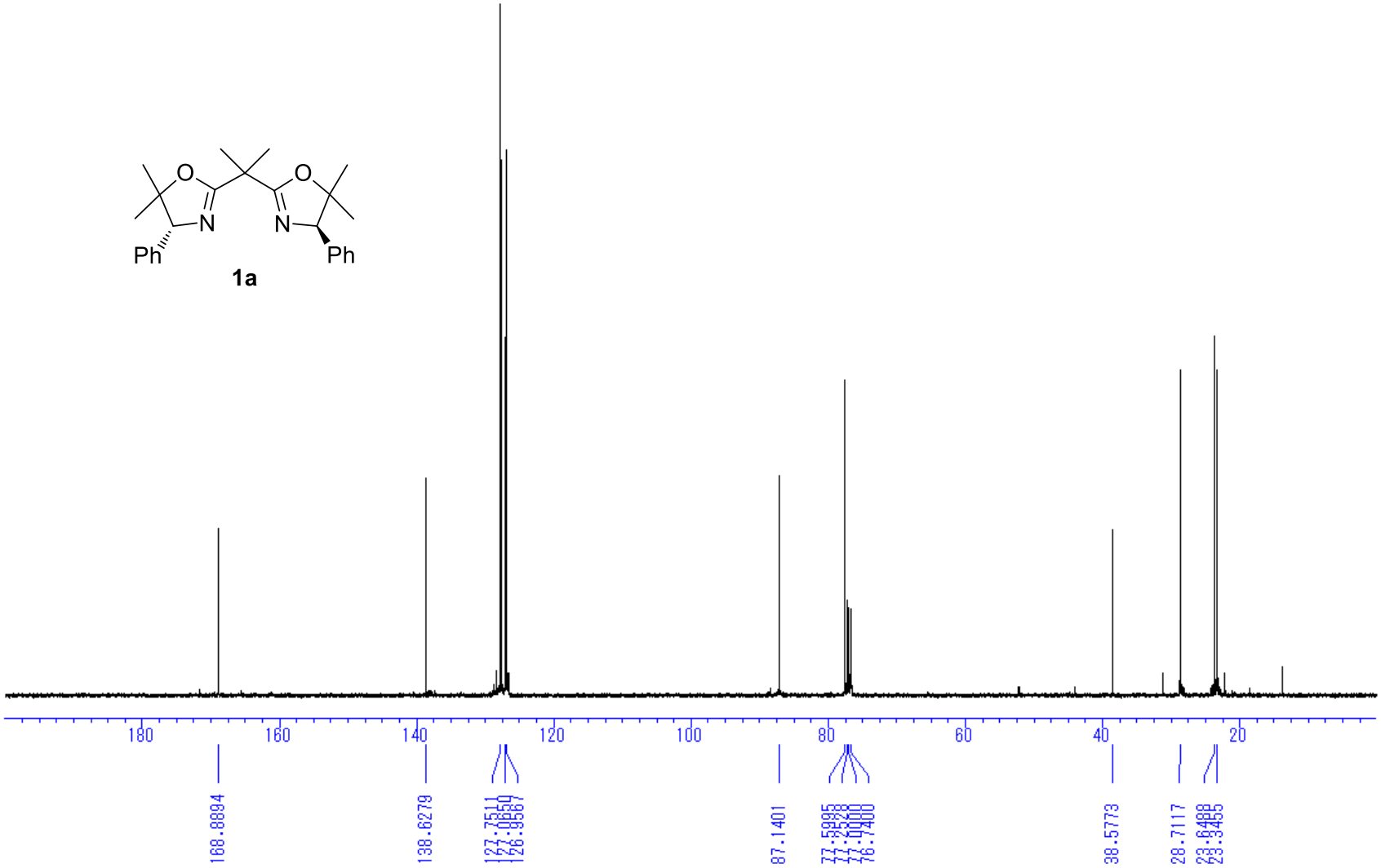

Figure S6. ^{13}C NMR Spectrum of BOX (1a).

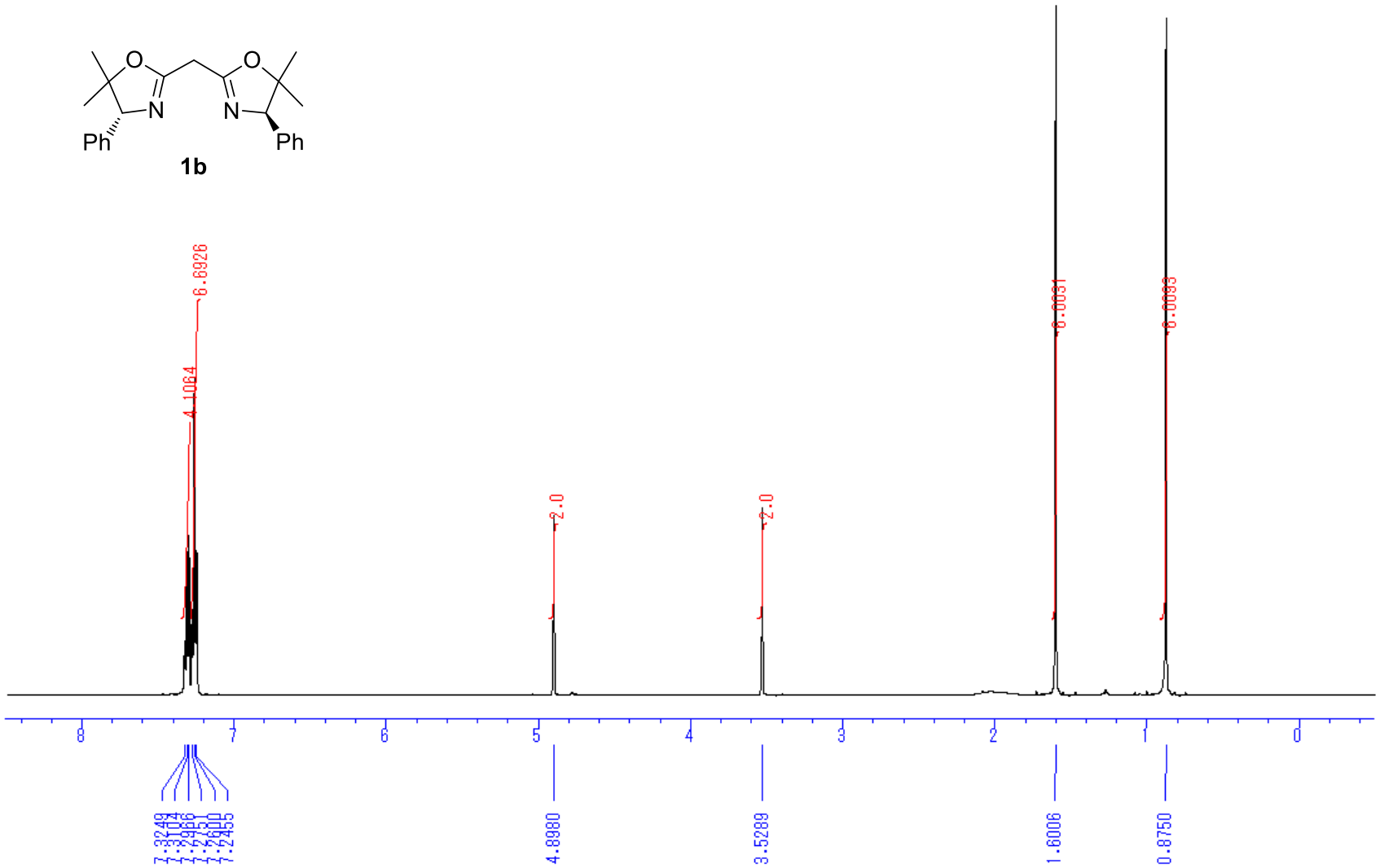

Figure S7. ^{1}H NMR Spectrum of BOX (1b).

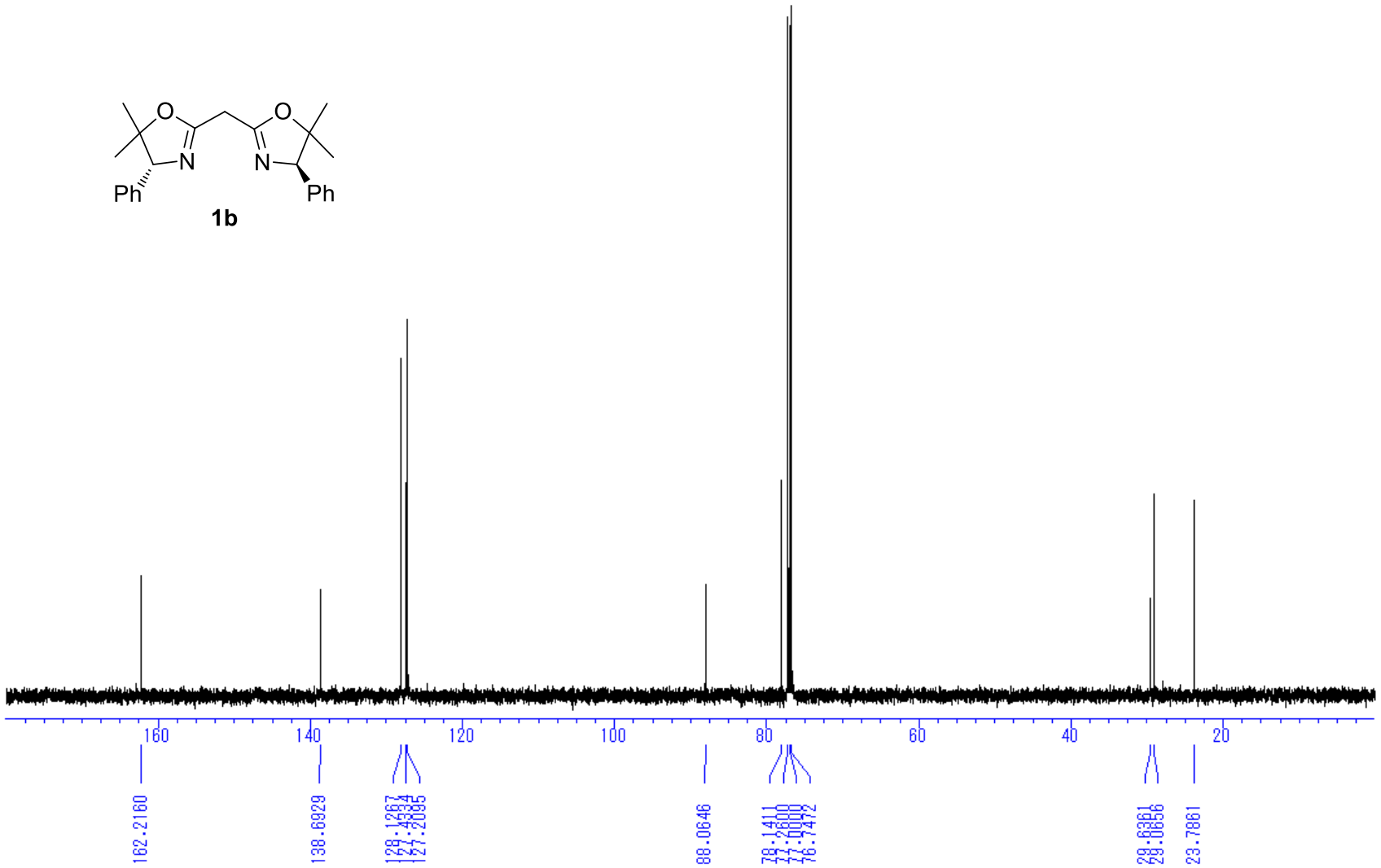

Figure S8. ^{13}C NMR Spectrum of BOX (1b).

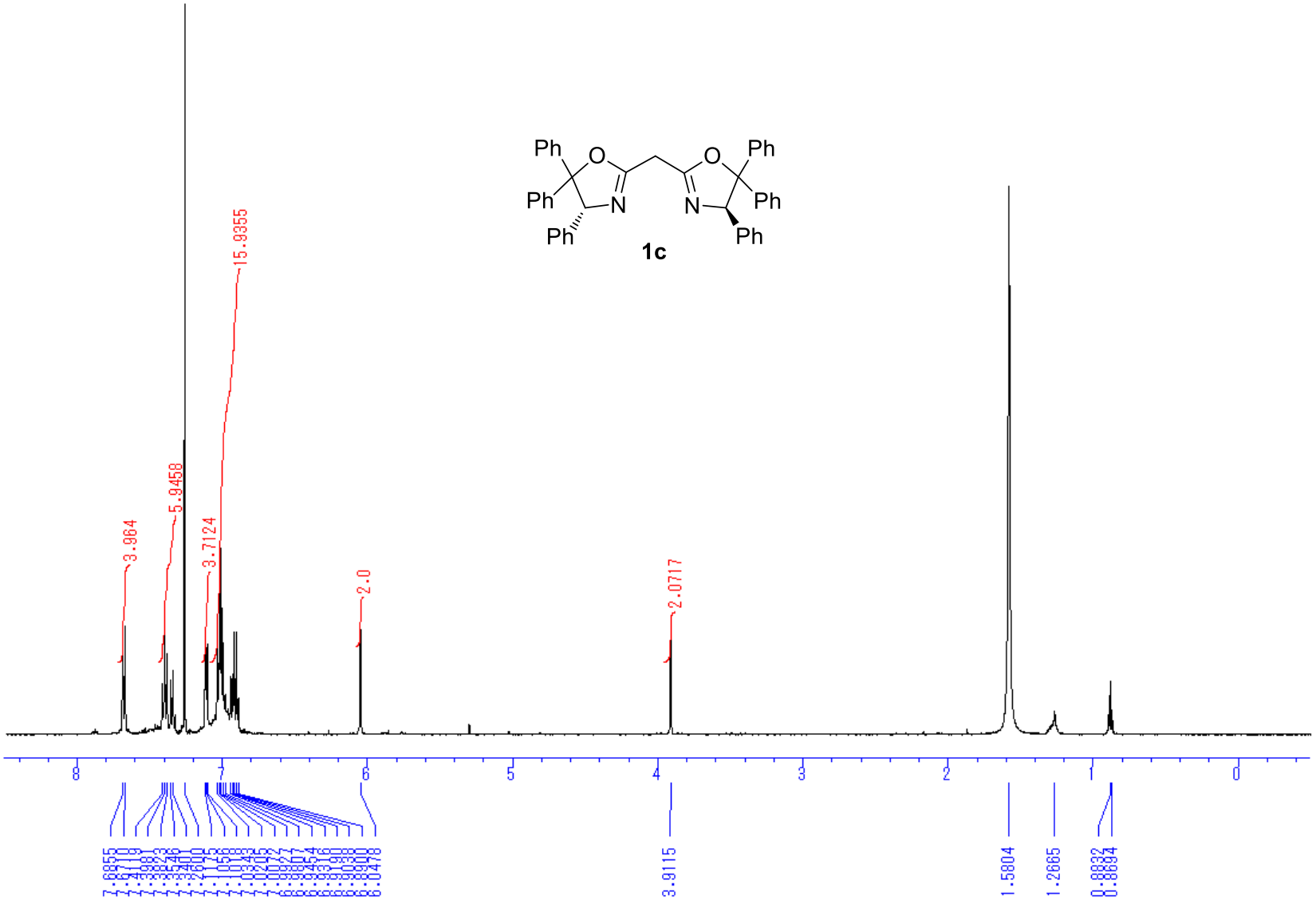

Figure S9. ^{1}H NMR Spectrum of BOX (1c).

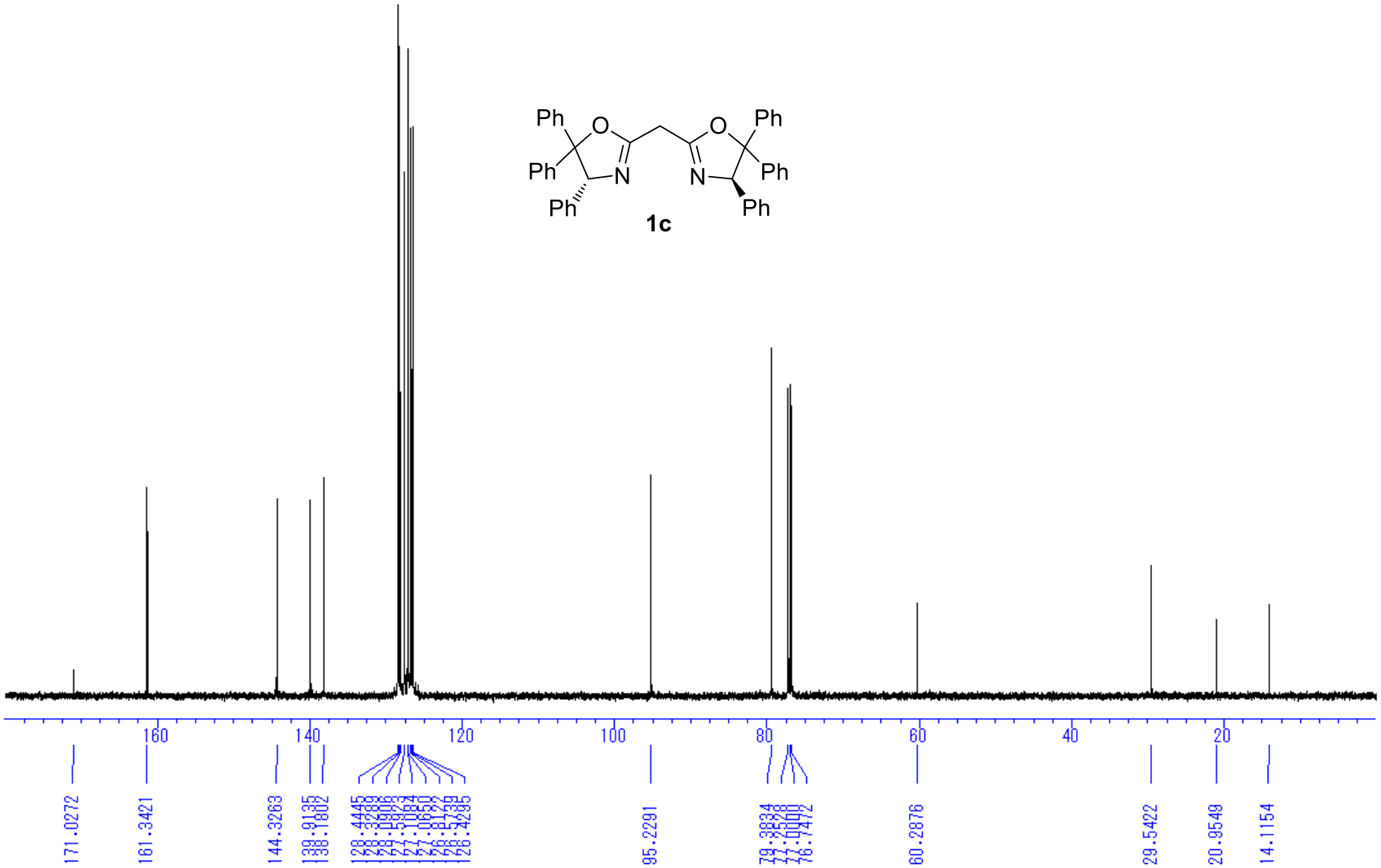

Figure S10. ^{13}C NMR Spectrum of BOX (1c).

1-4. NMR spectra of neutral (BOX)$PdCl_2$ (2a-d).

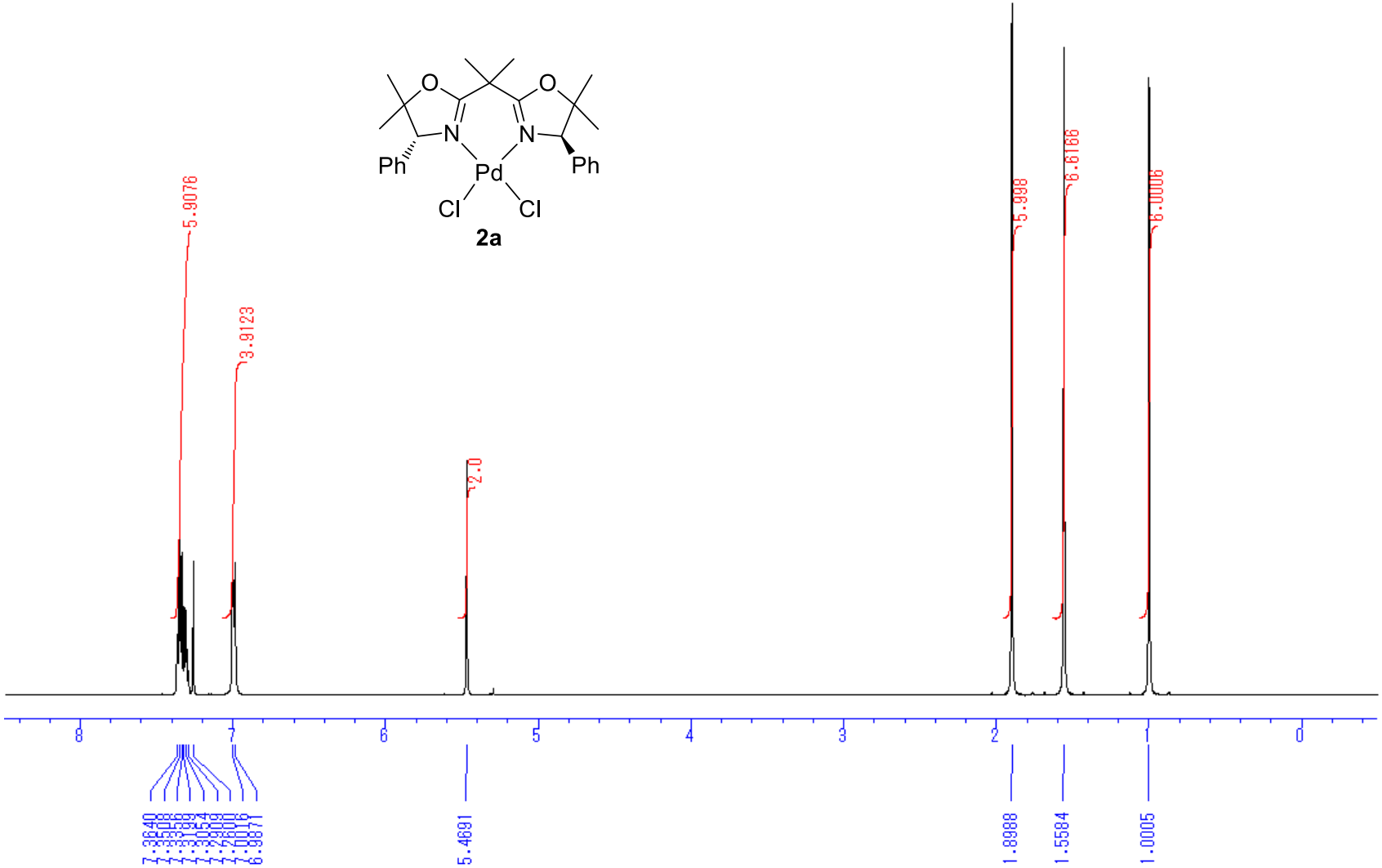

Figure S11. ^{1}H NMR Spectrum of (BOX)$PdCl_2$ (2a).

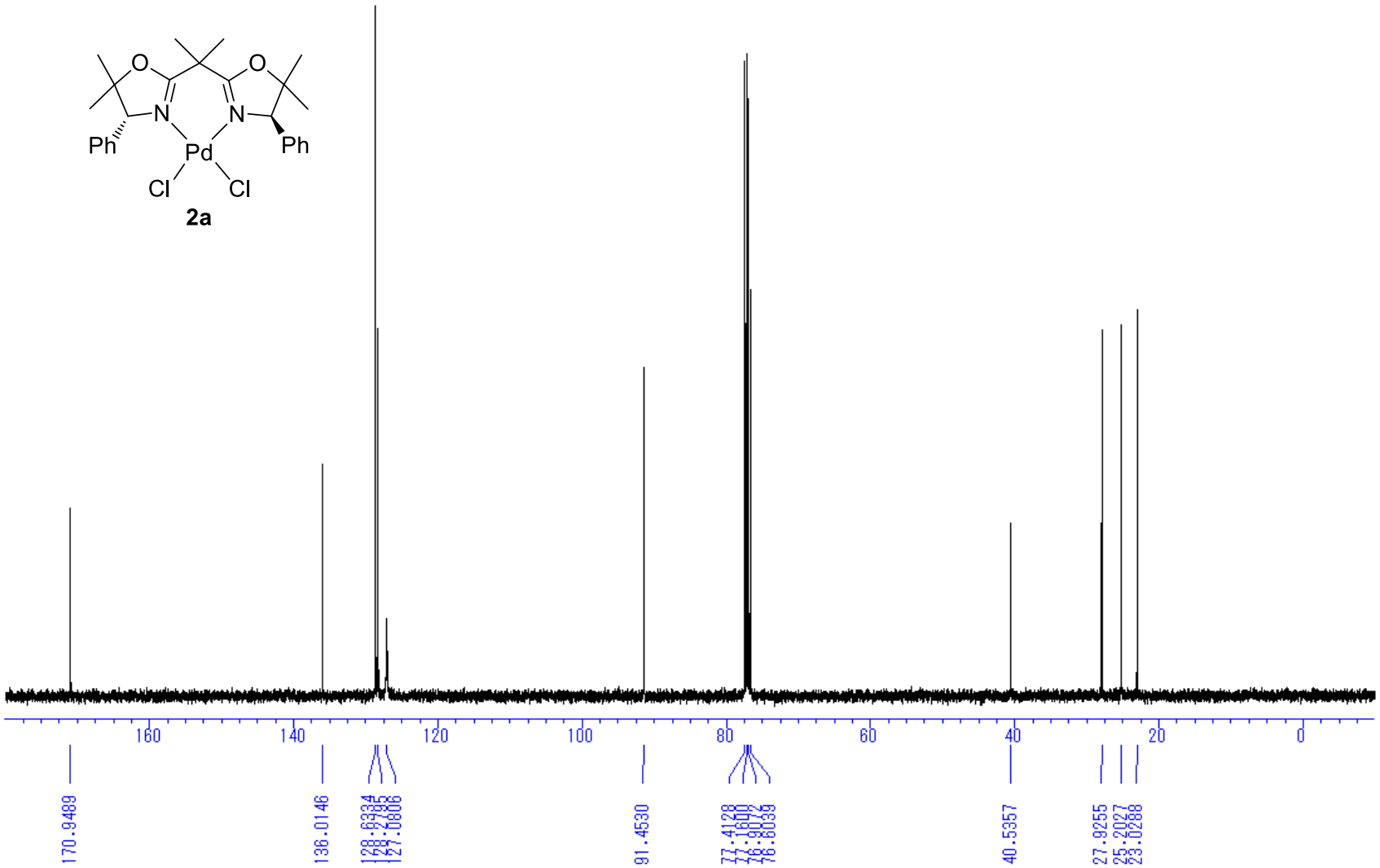

Figure S12. ^{13}C NMR Spectrum of (BOX)PdCl$_2$ (2a).

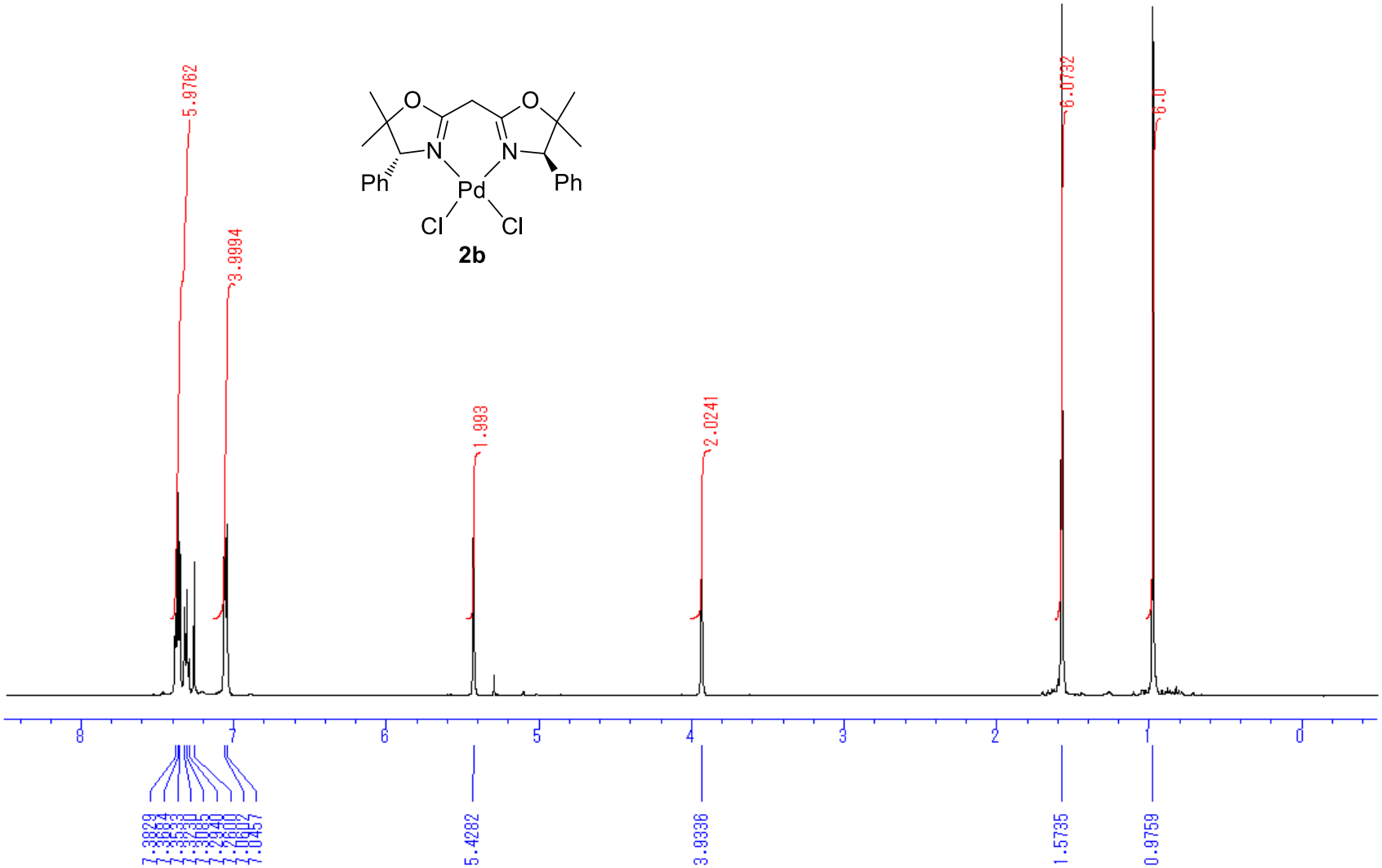

Figure S13. ^{1}H NMR Spectrum of (BOX)PdCl$_2$ (2b).

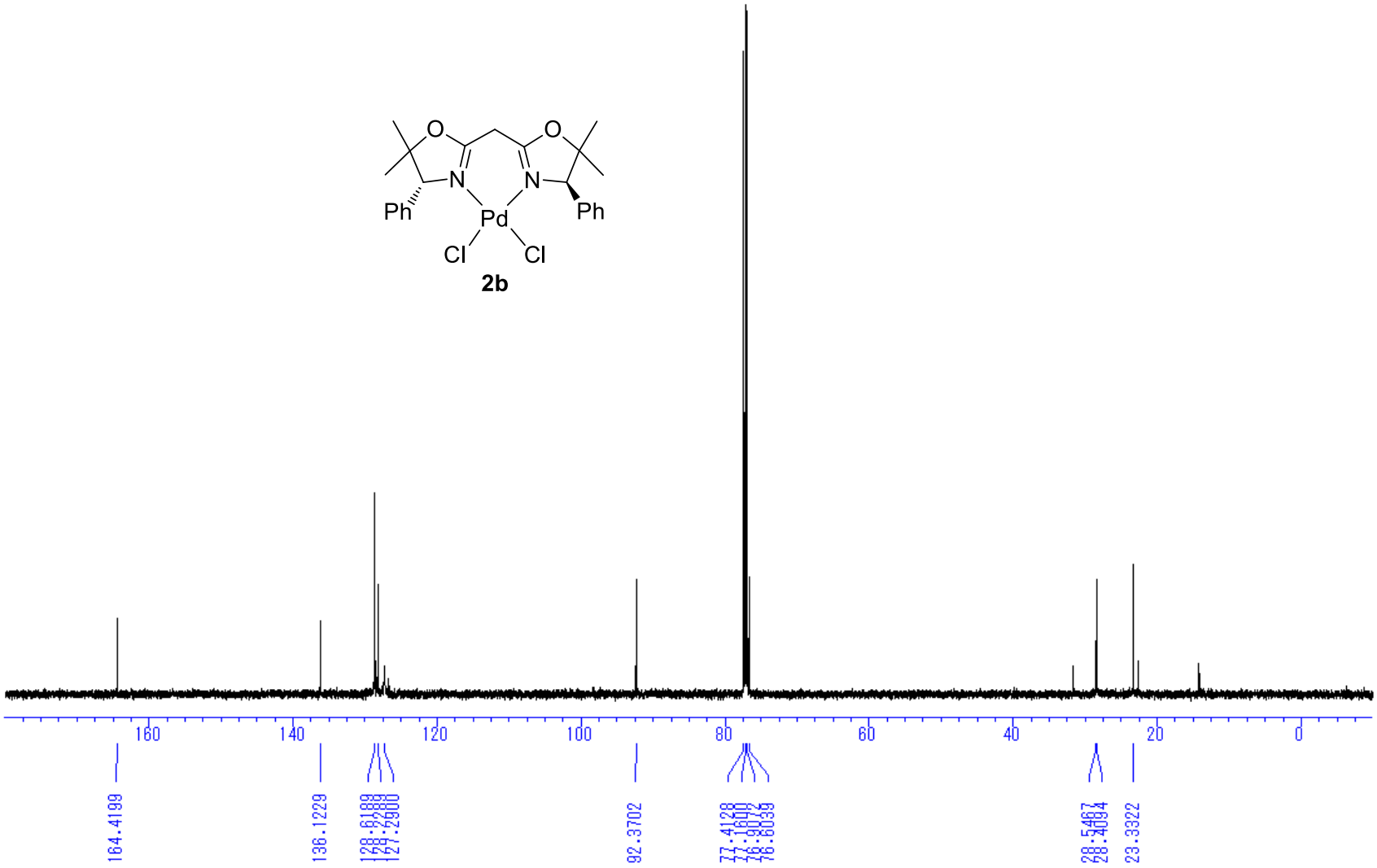

Figure S14. ^{13}C NMR Spectrum of (BOX)PdCl$_2$ (2b).

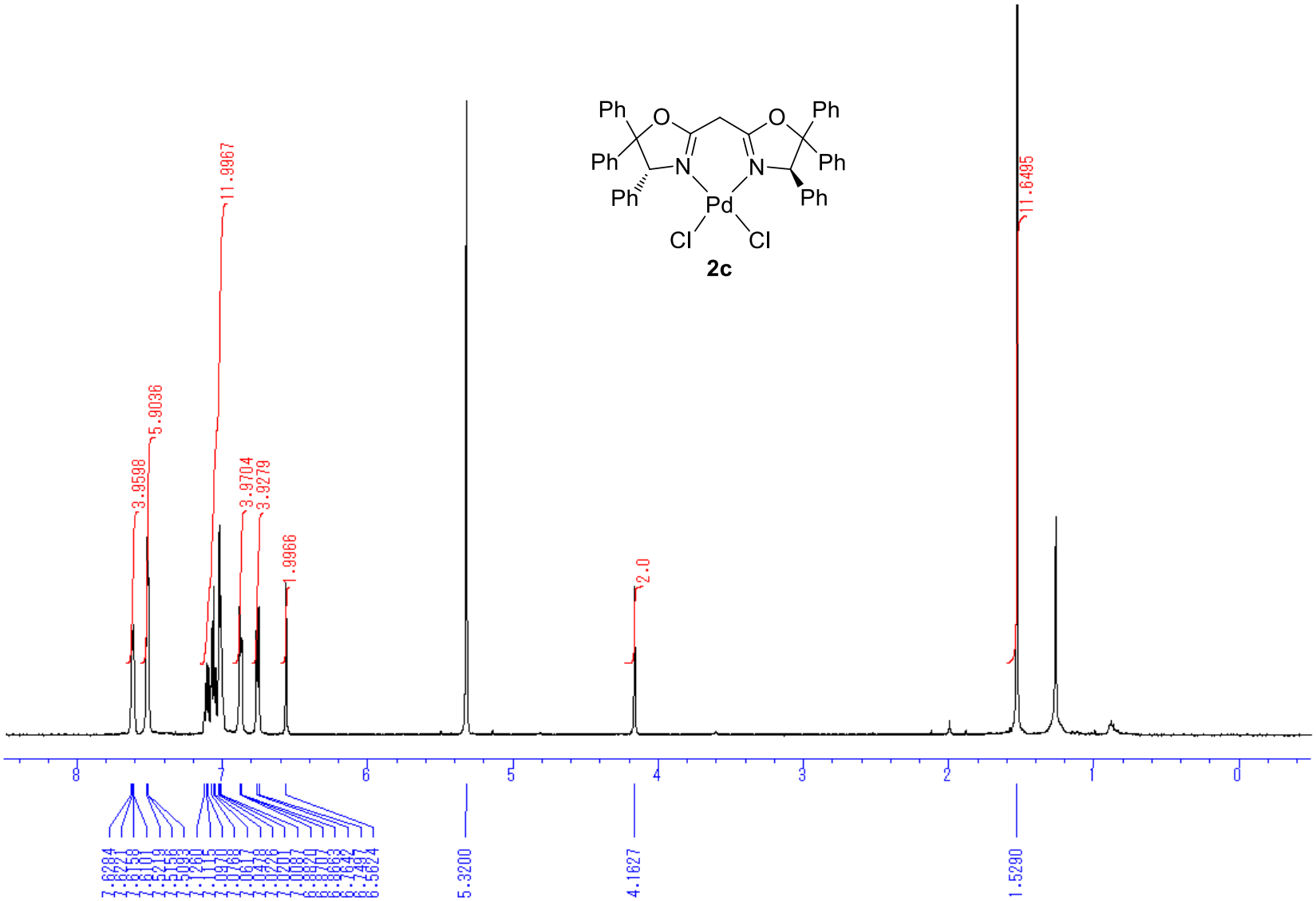

Figure S15. ^{1}H NMR Spectrum of (BOX)PdCl$_2$ (2c).

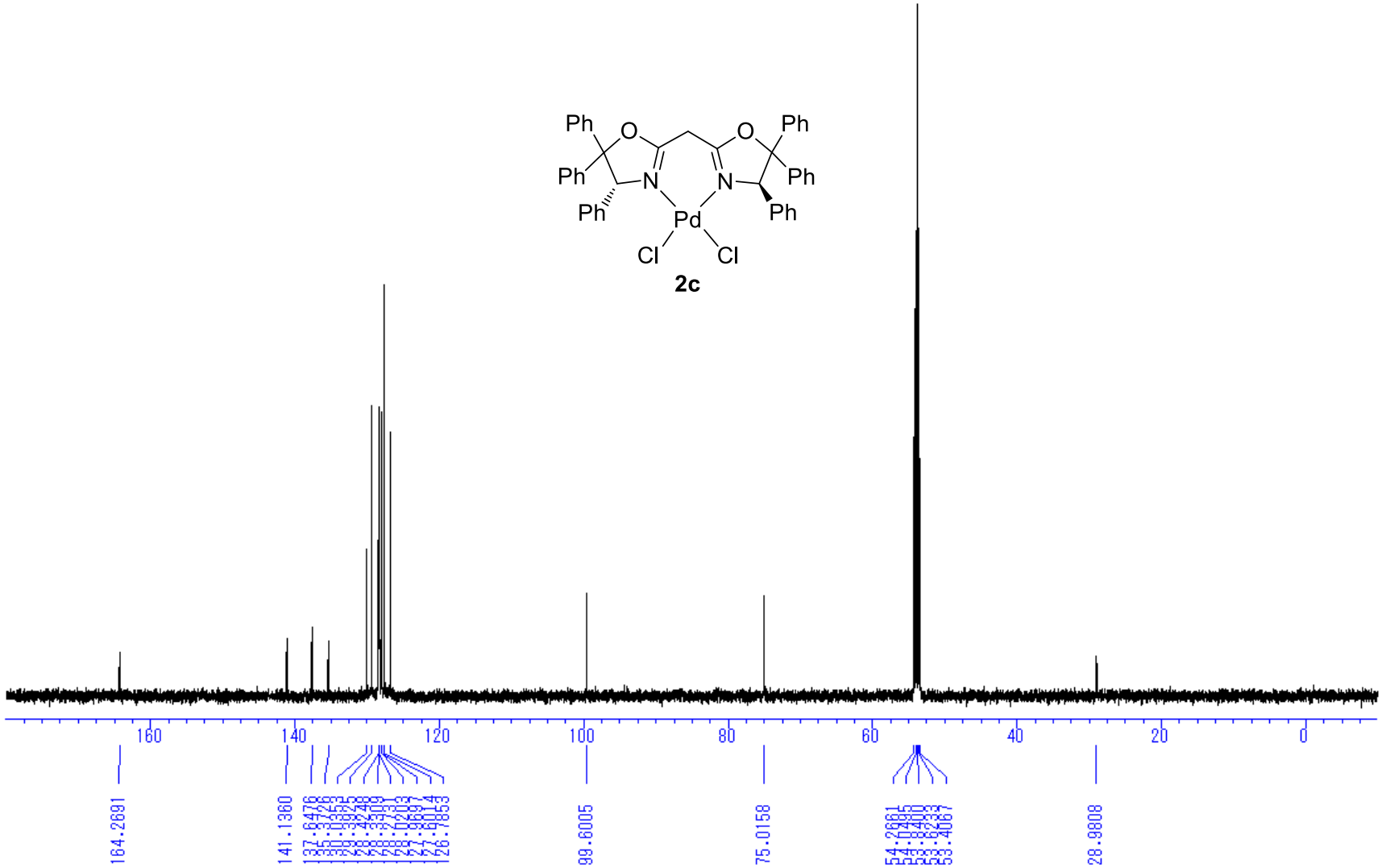

Figure S16. ^{13}C NMR Spectrum of (BOX)PdCl$_2$ (2c).

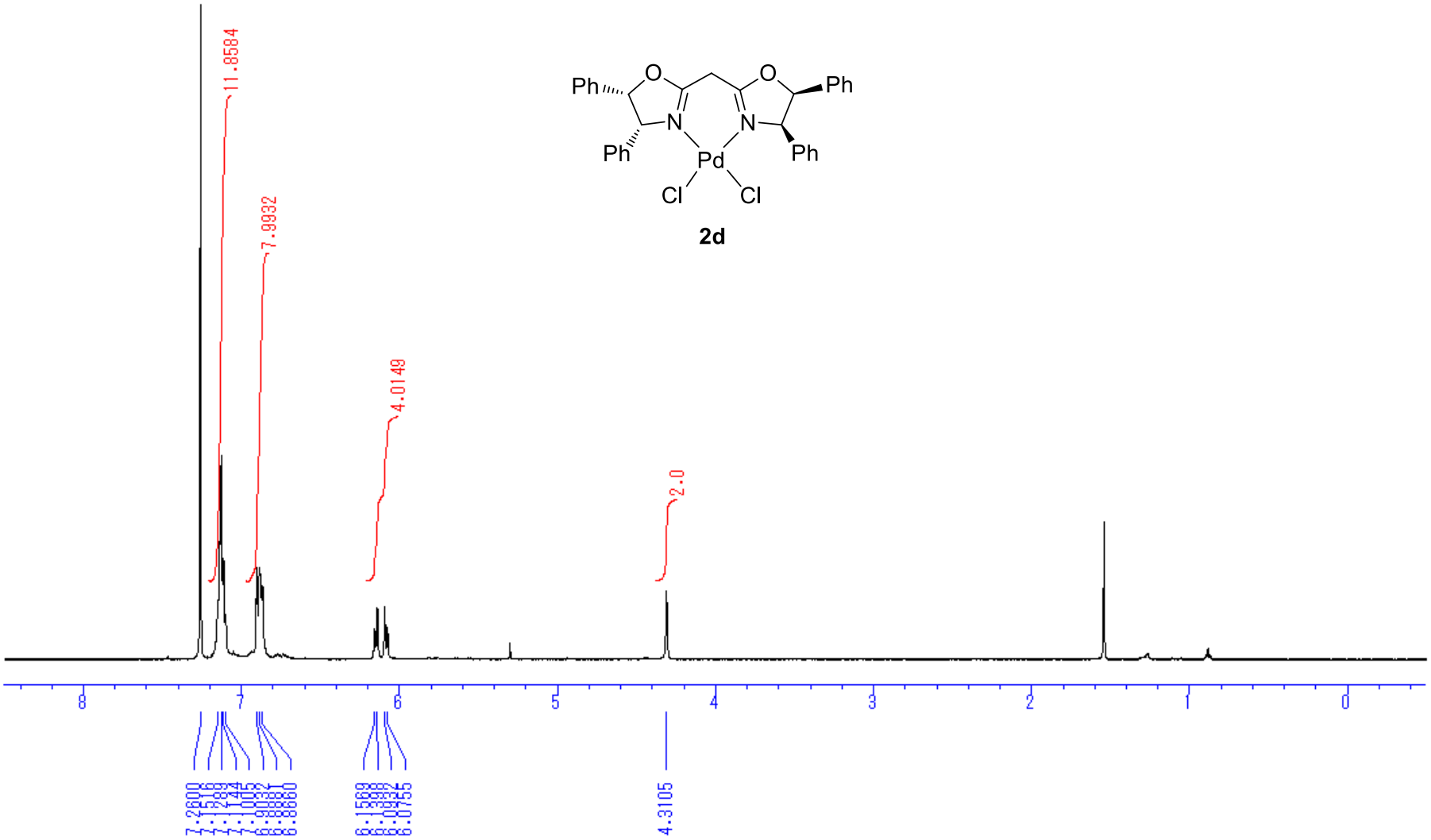

Figure S17. ^{1}H NMR Spectrum of (BOX)PdCl$_2$ (2d).

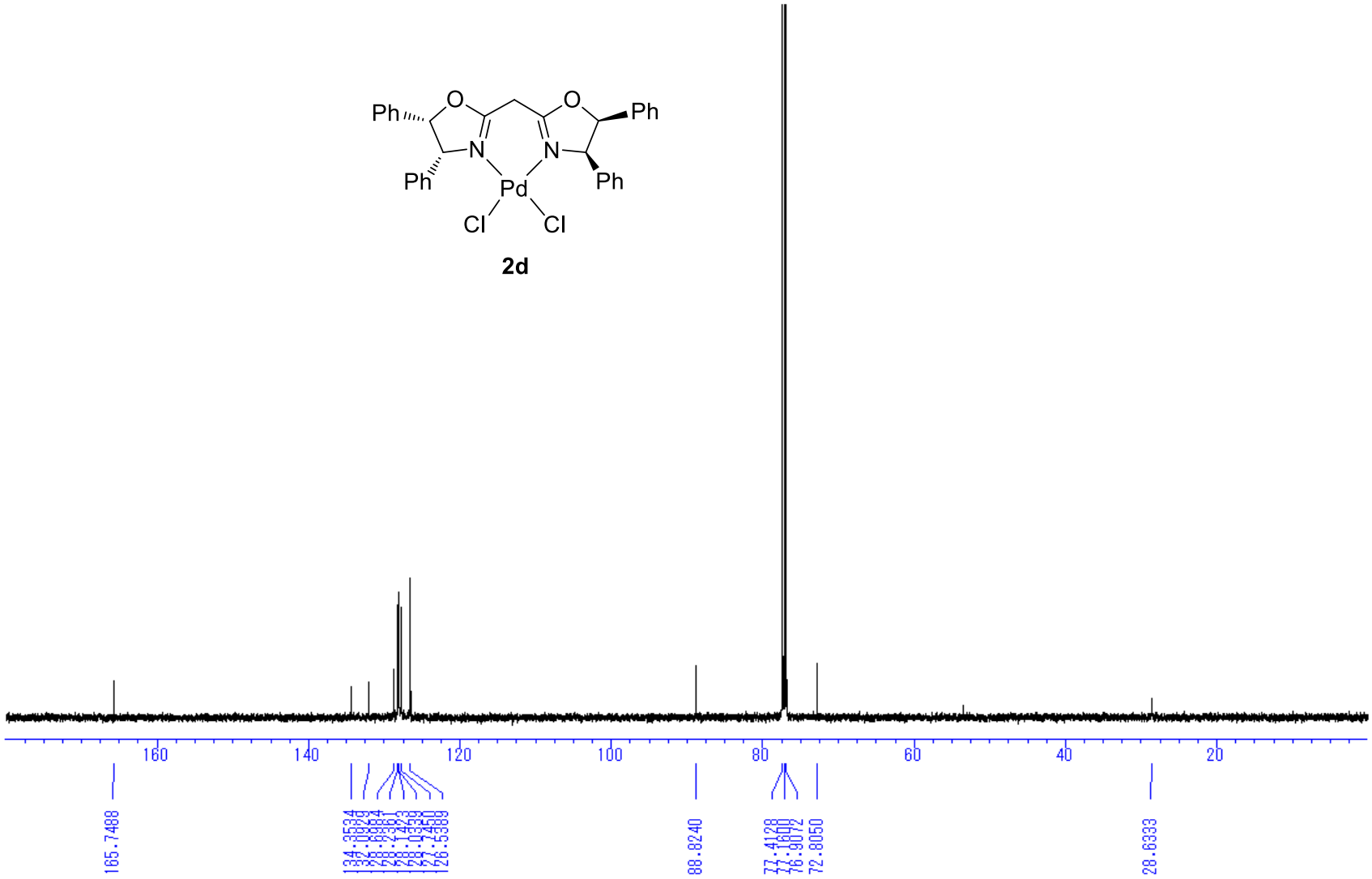

Figure S18. ^{13}C NMR Spectrum of (BOX)PdCl$_2$ (2d).

1-5. NMR spectra of neutral (BOX)PdMeCl (3a-d).

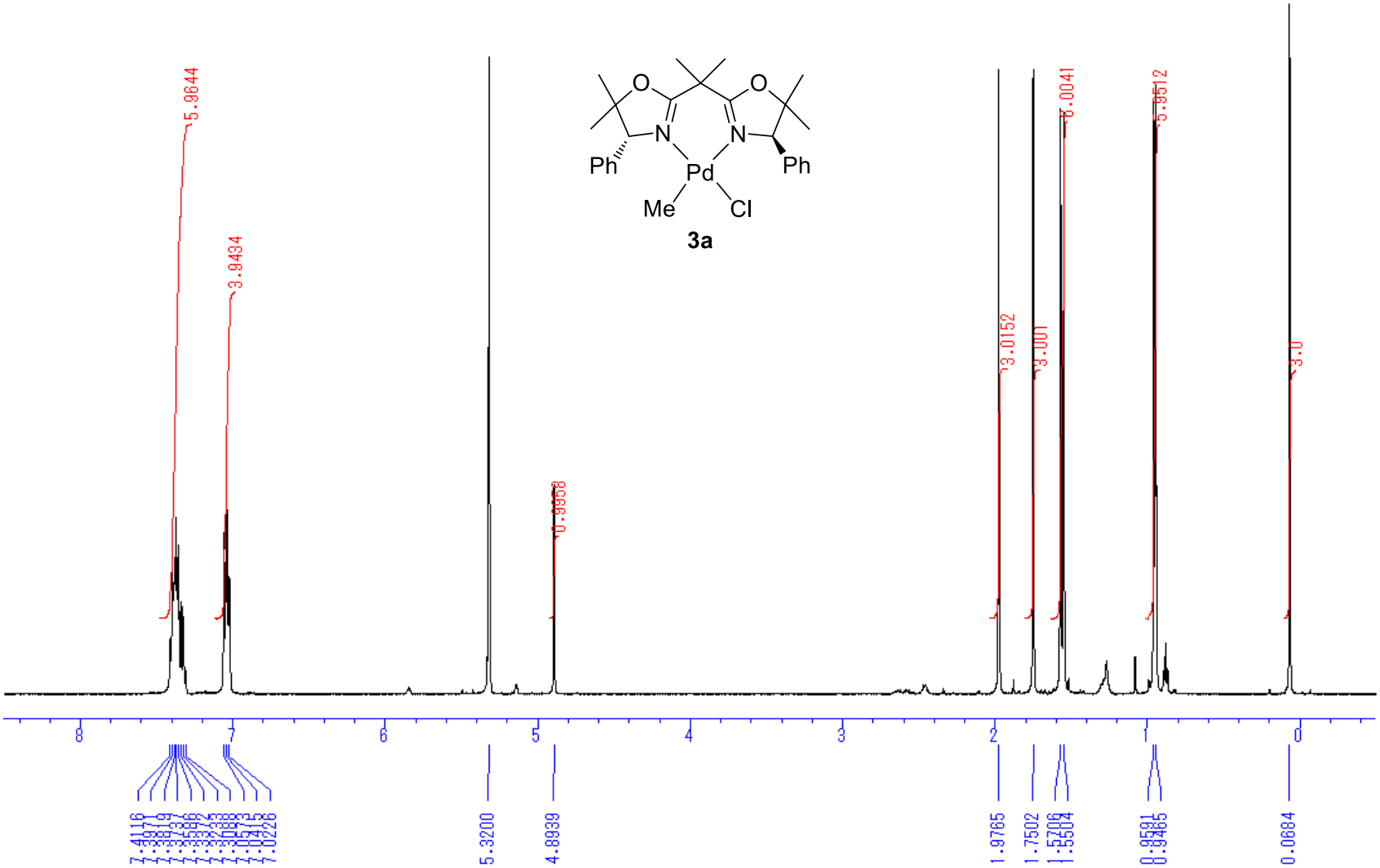

Figure S19. ^{1}H NMR Spectrum of (BOX)PdMeCl (3a).

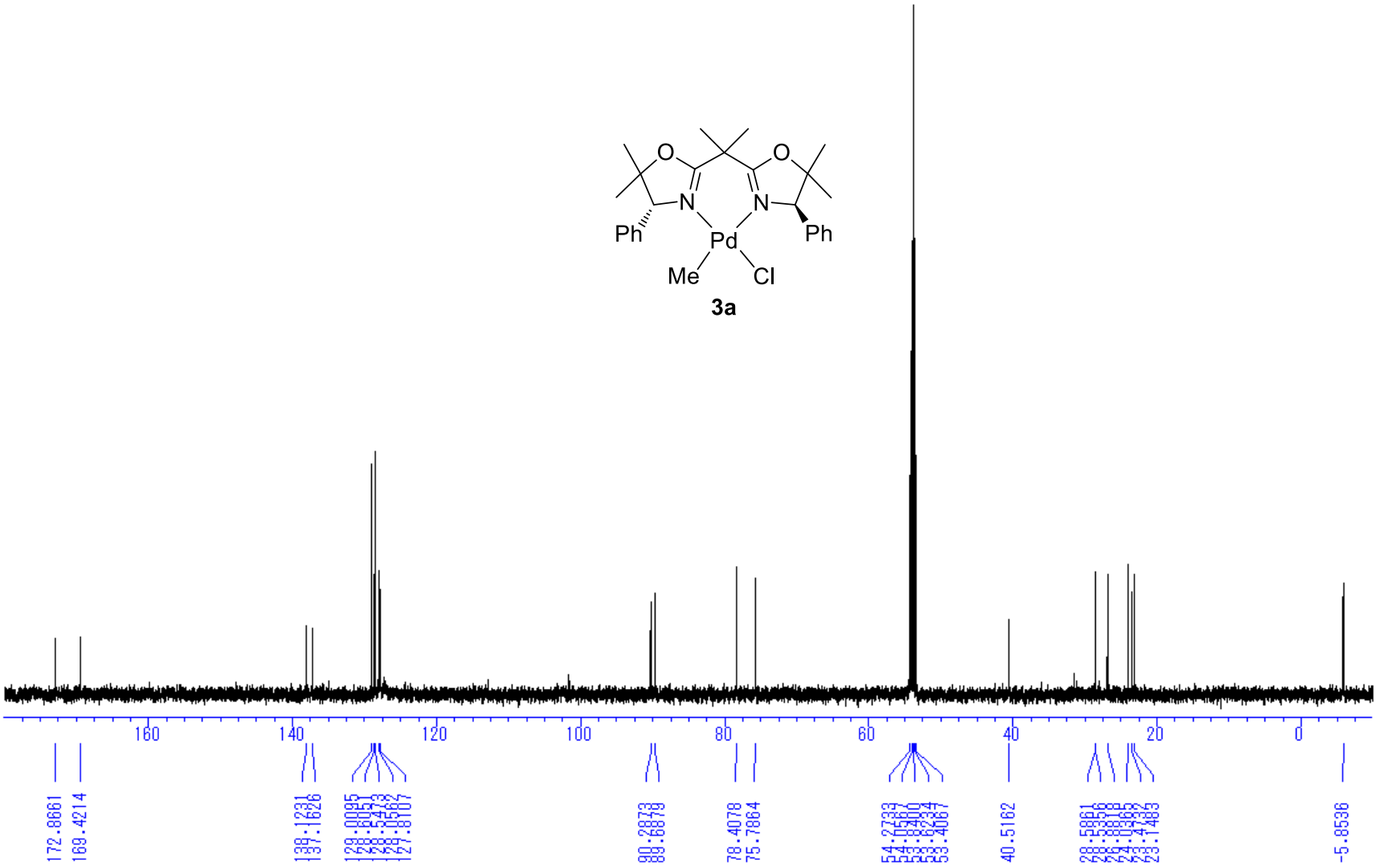

Figure S20. ^{13}C NMR Spectrum of (BOX)PdMeCl (3a).

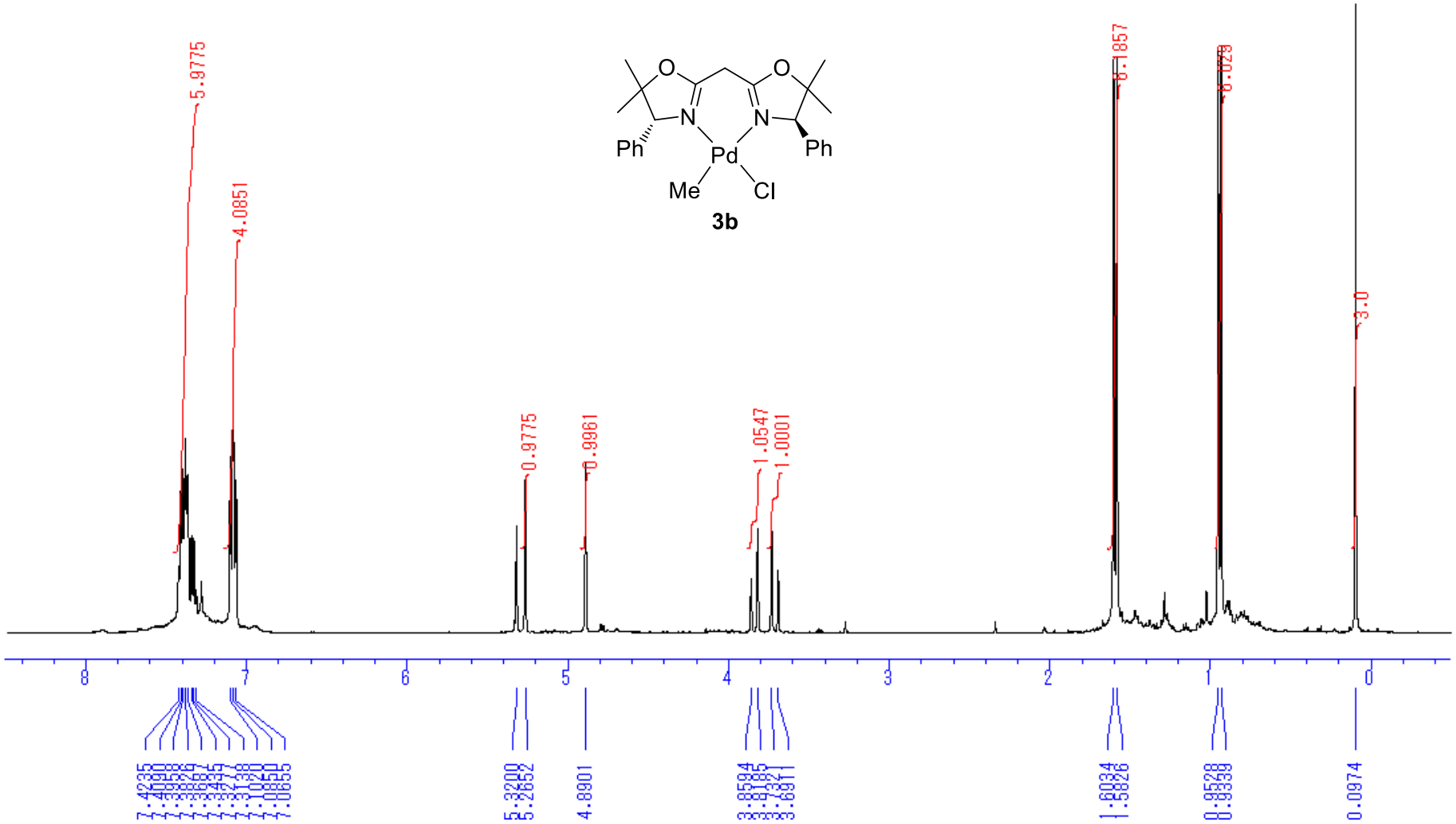

Figure S21. ^{1}H NMR Spectrum of (BOX)PdMeCl (3b).

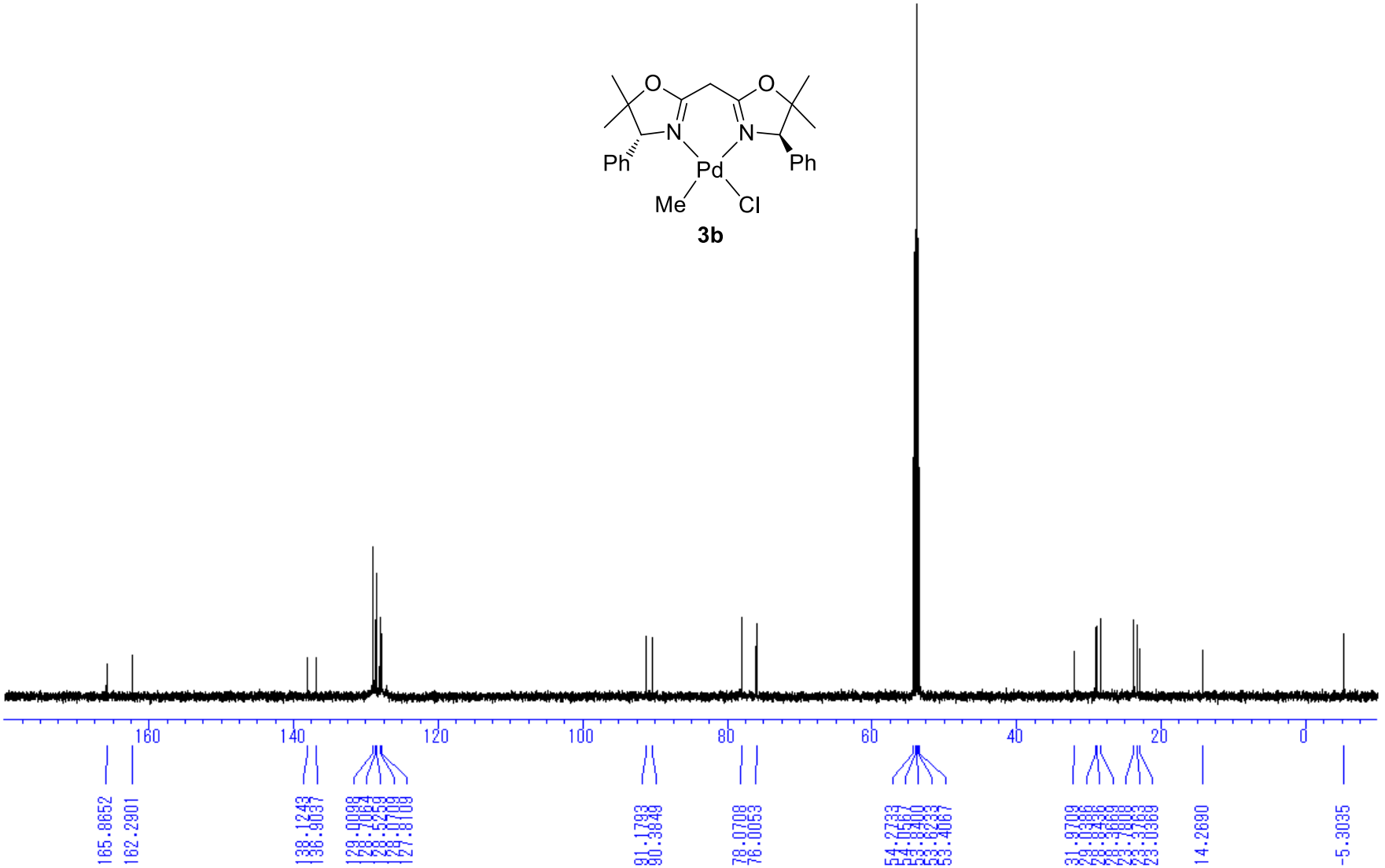

Figure S22. ^{13}C NMR Spectrum of (BOX)PdMeCl (3b).

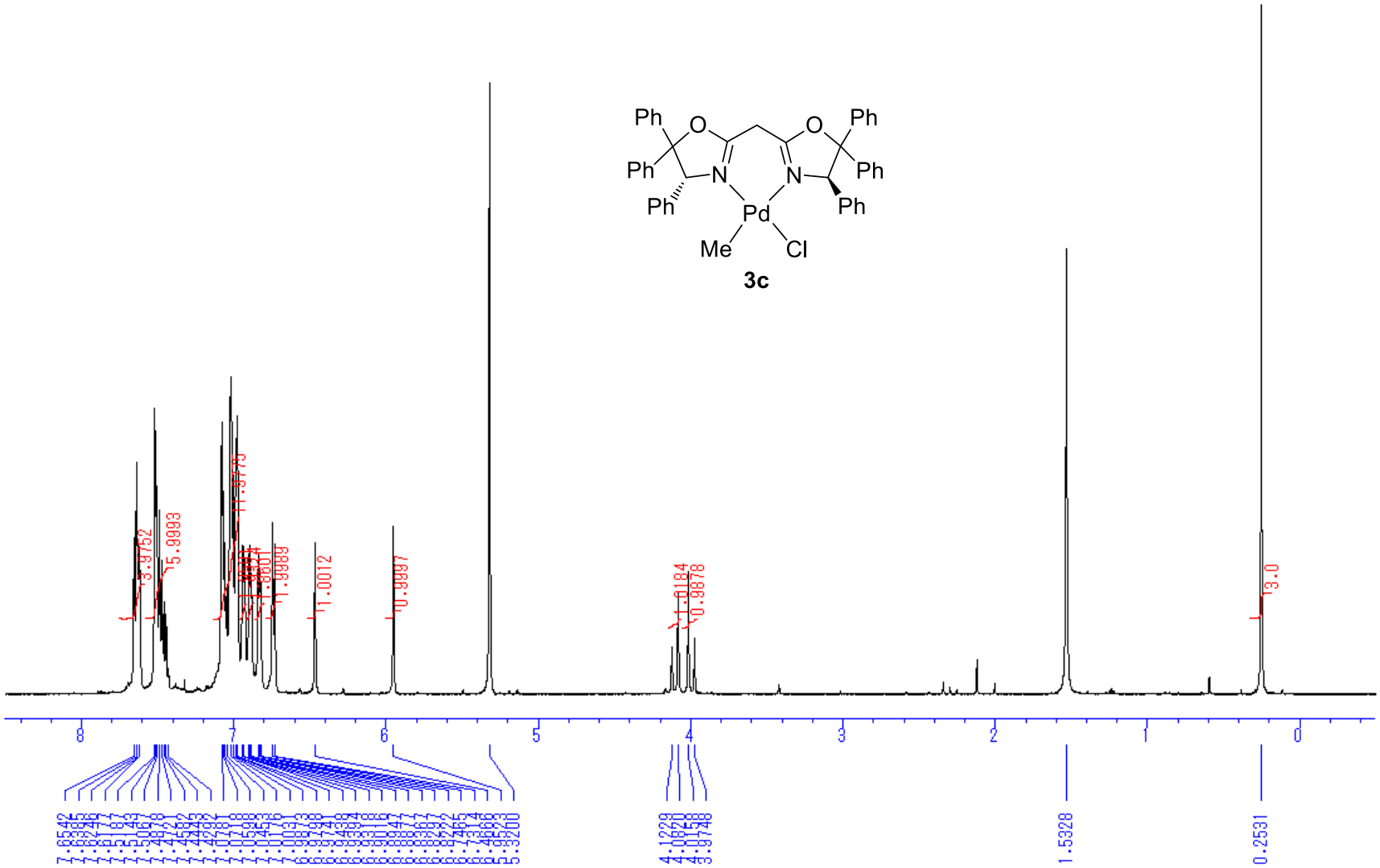

Figure S23. ^{1}H NMR Spectrum of (BOX)PdMeCl (3c).

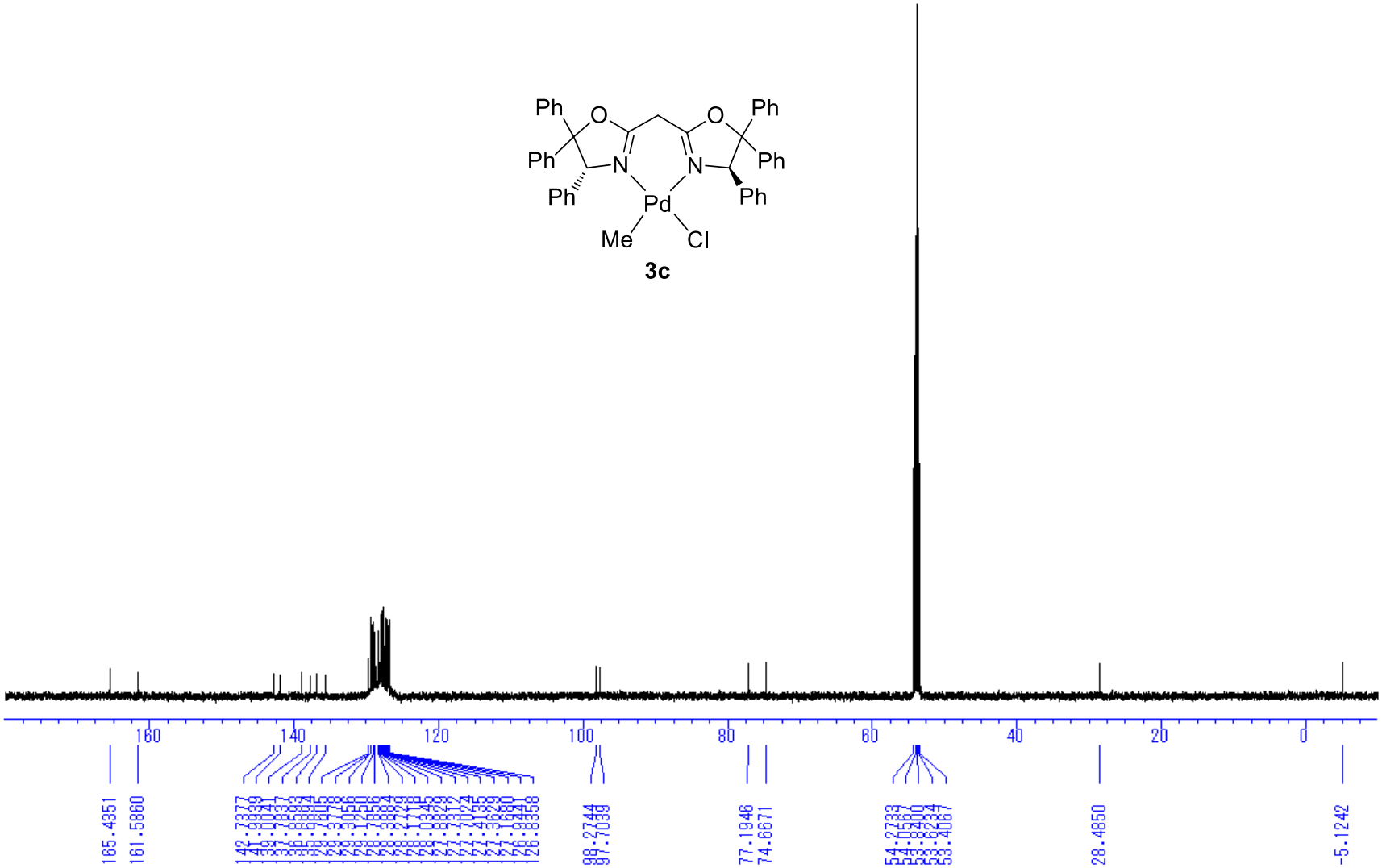

Figure S24. ^{13}C NMR Spectrum of (BOX)PdMeCl (3c).

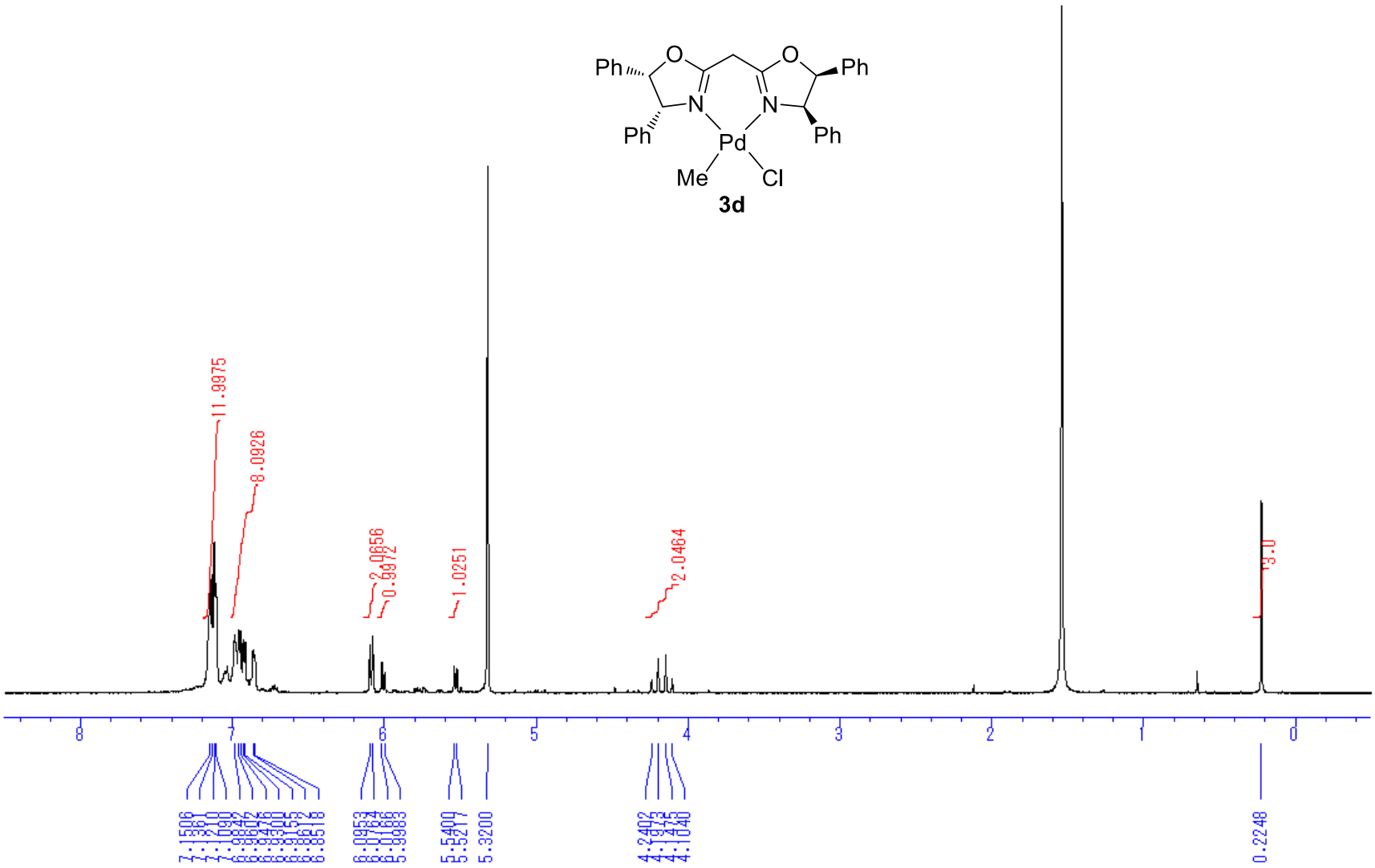

Figure S25. ^{1}H NMR Spectrum of (BOX)PdMeCl (3d).

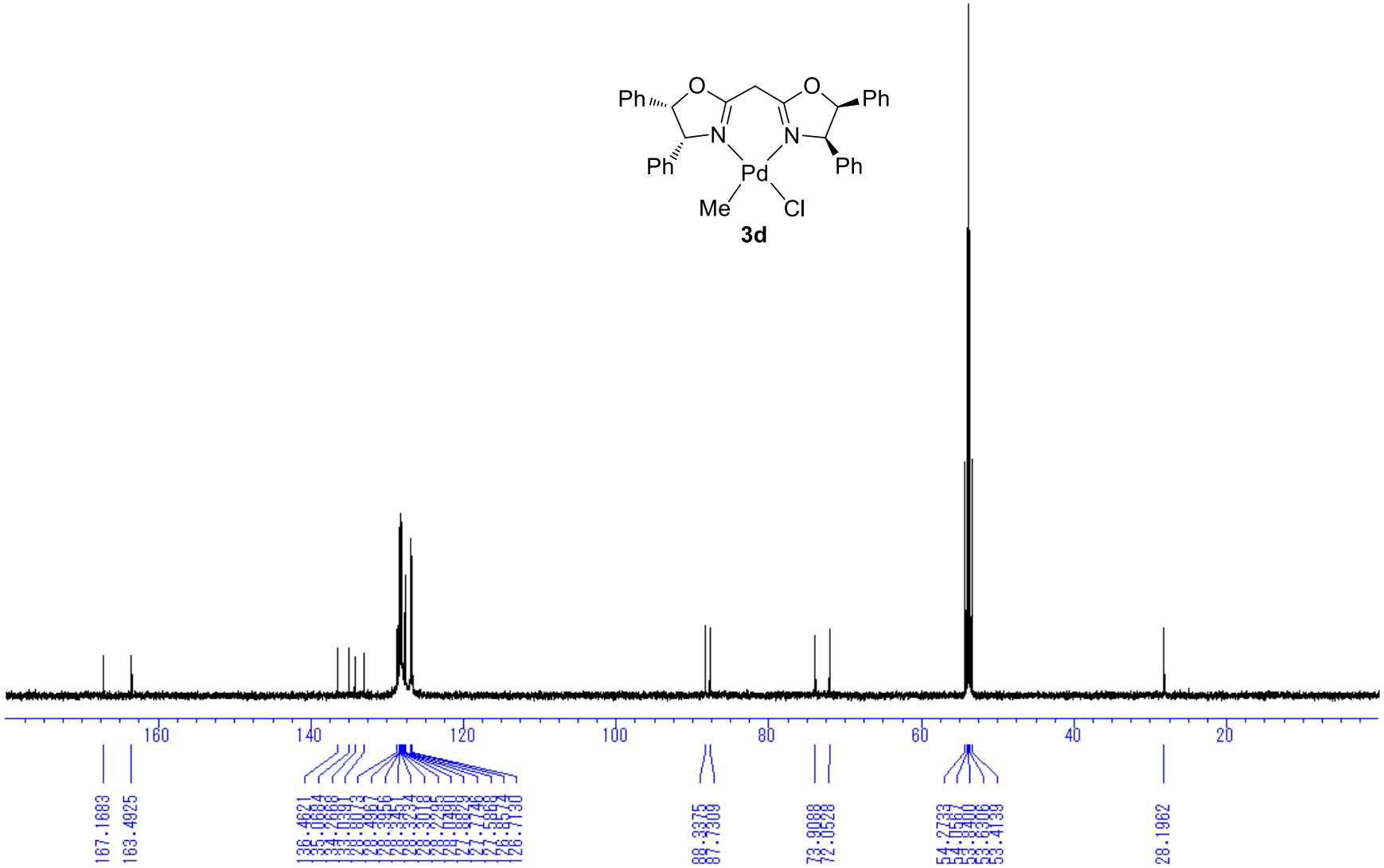

Figure S26. ^{13}C NMR Spectrum of (BOX)PdMeCl (3d).

1-6. NMR spectra of cationic [(BOX)PdMe(2,6-$Me_2C_5H_3N$)]$^+PF_6^-$ (4a-d).

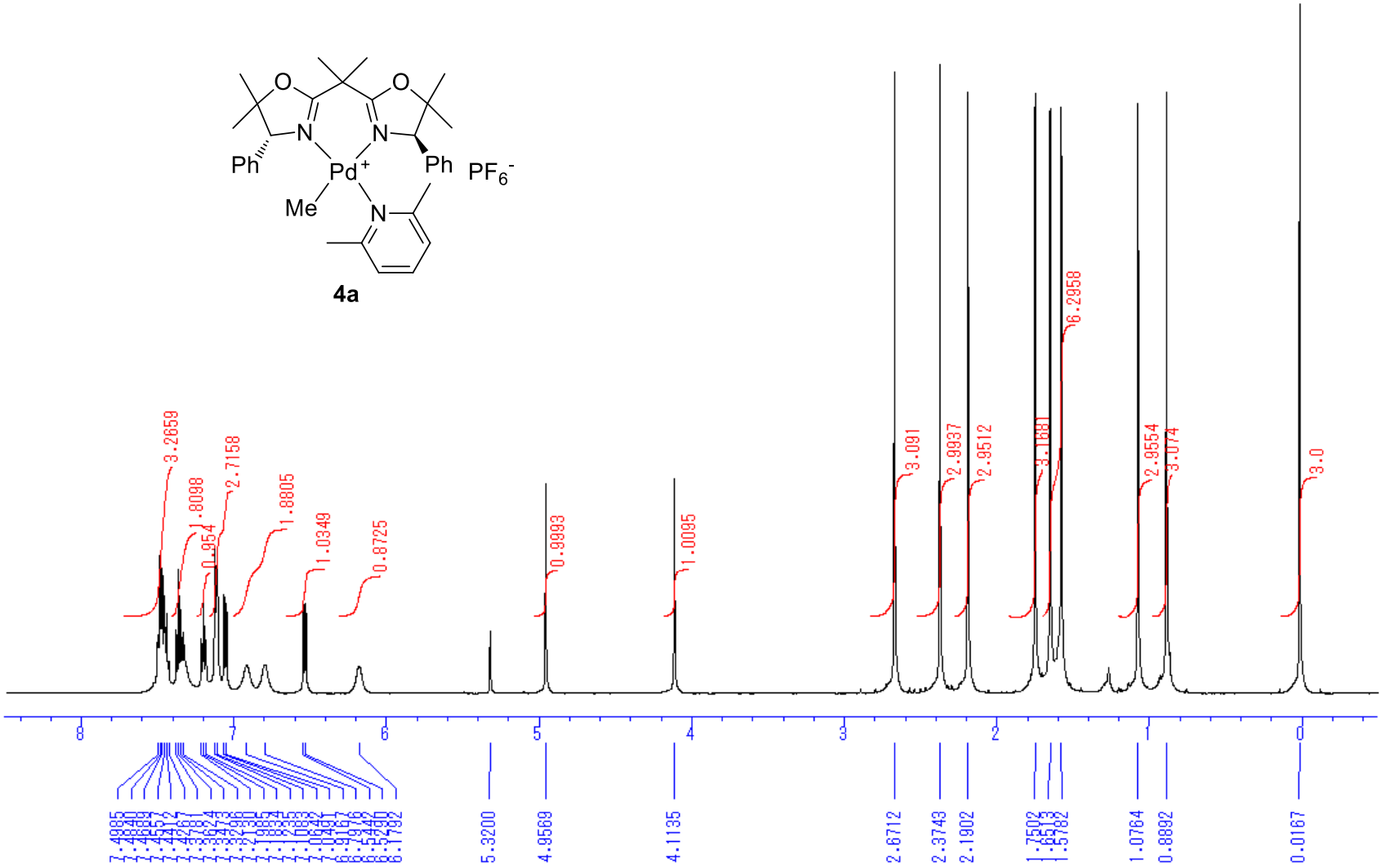

Figure S27. ^{1}H NMR Spectrum of [(BOX)PdMe(2,6-$Me_2C_5H_3N$)]$^+PF_6^-$ (4a).

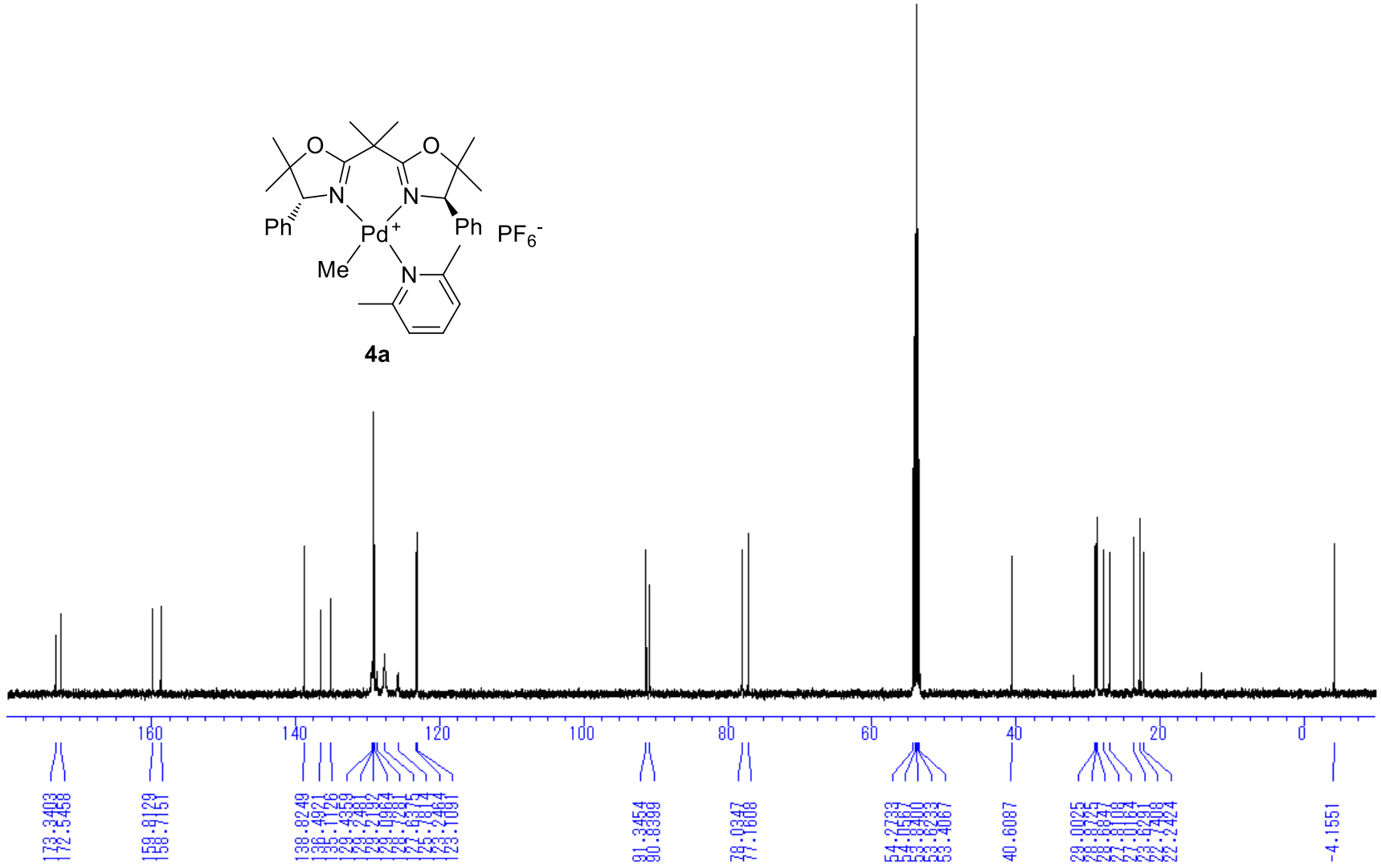

Figure S28. ^{13}C NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4a).

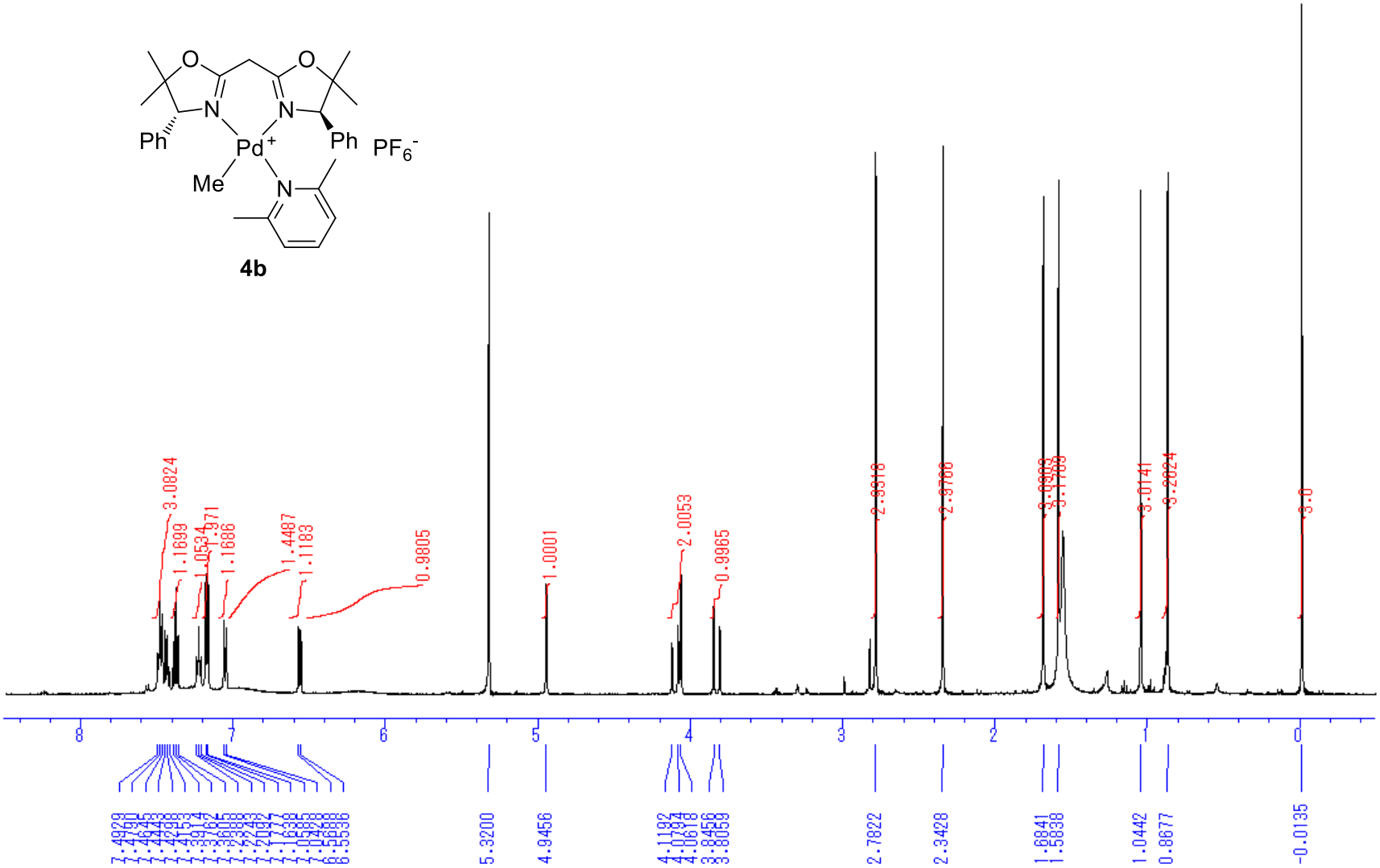

Figure S29. ^{1}H NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^{+}$PF$_6^{-}$ (4b).

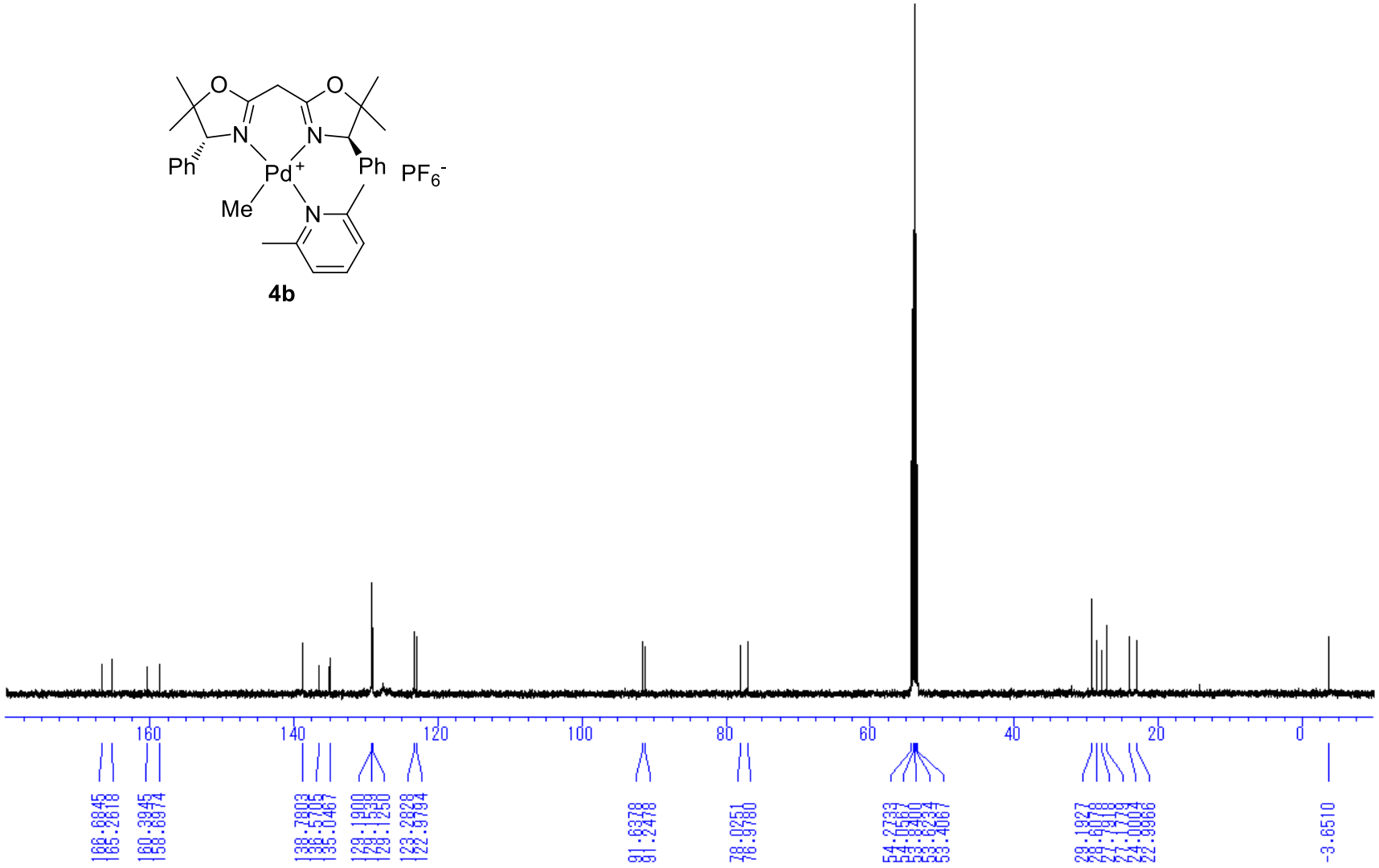

Figure S30. ^{13}C NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4b).

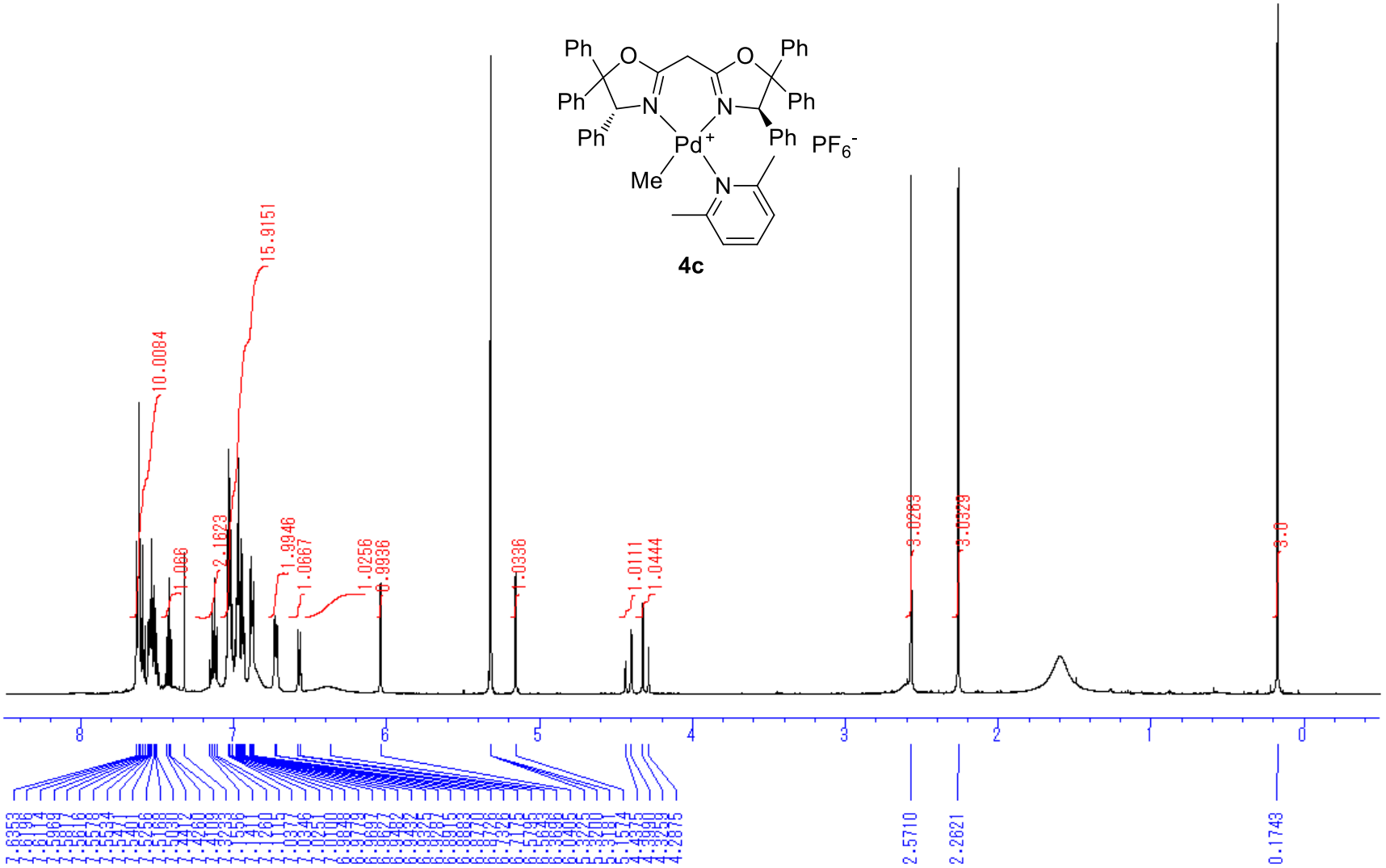

Figure S31. ^{1}H NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4c).

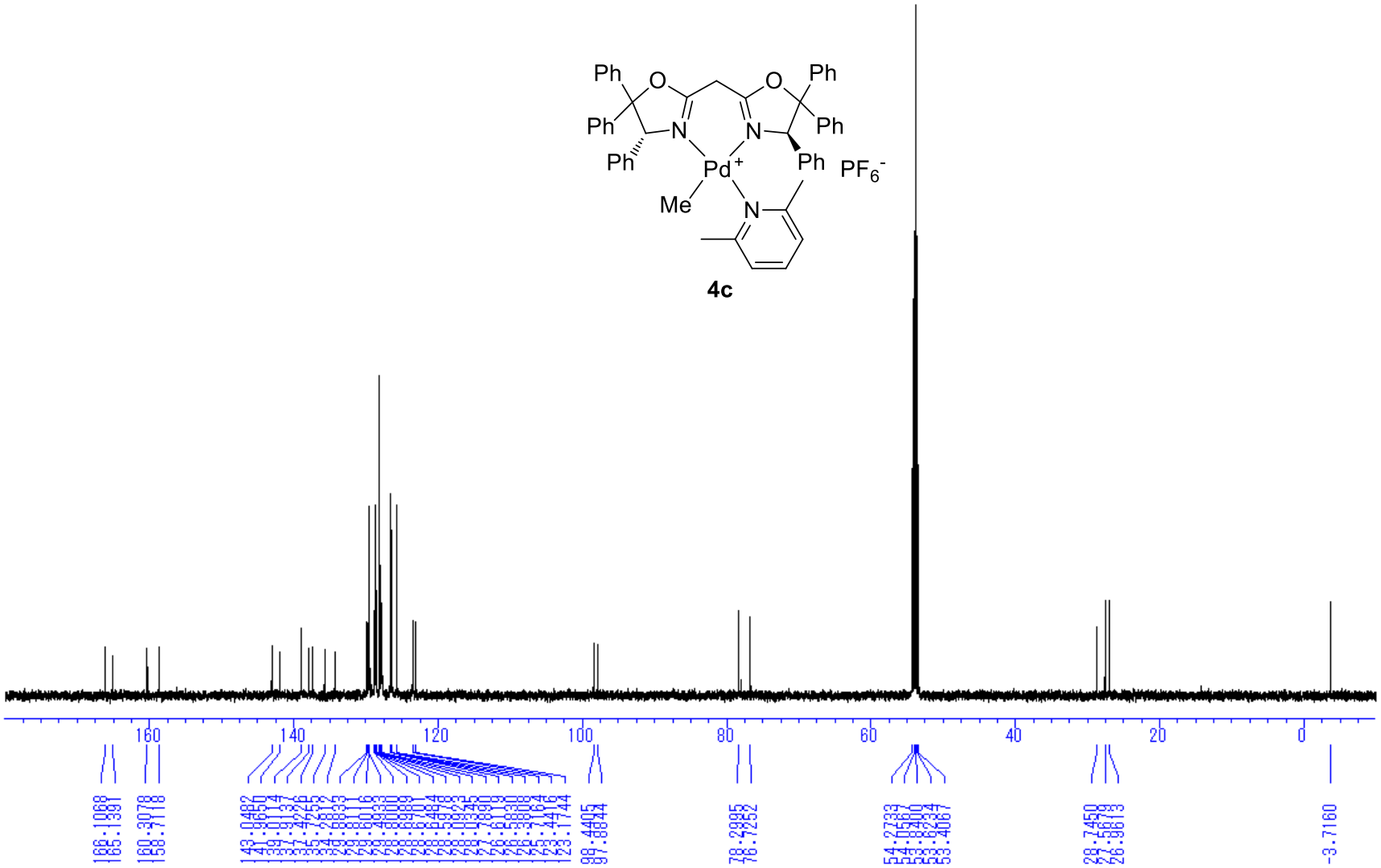

Figure S32. ^{13}C NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4c).

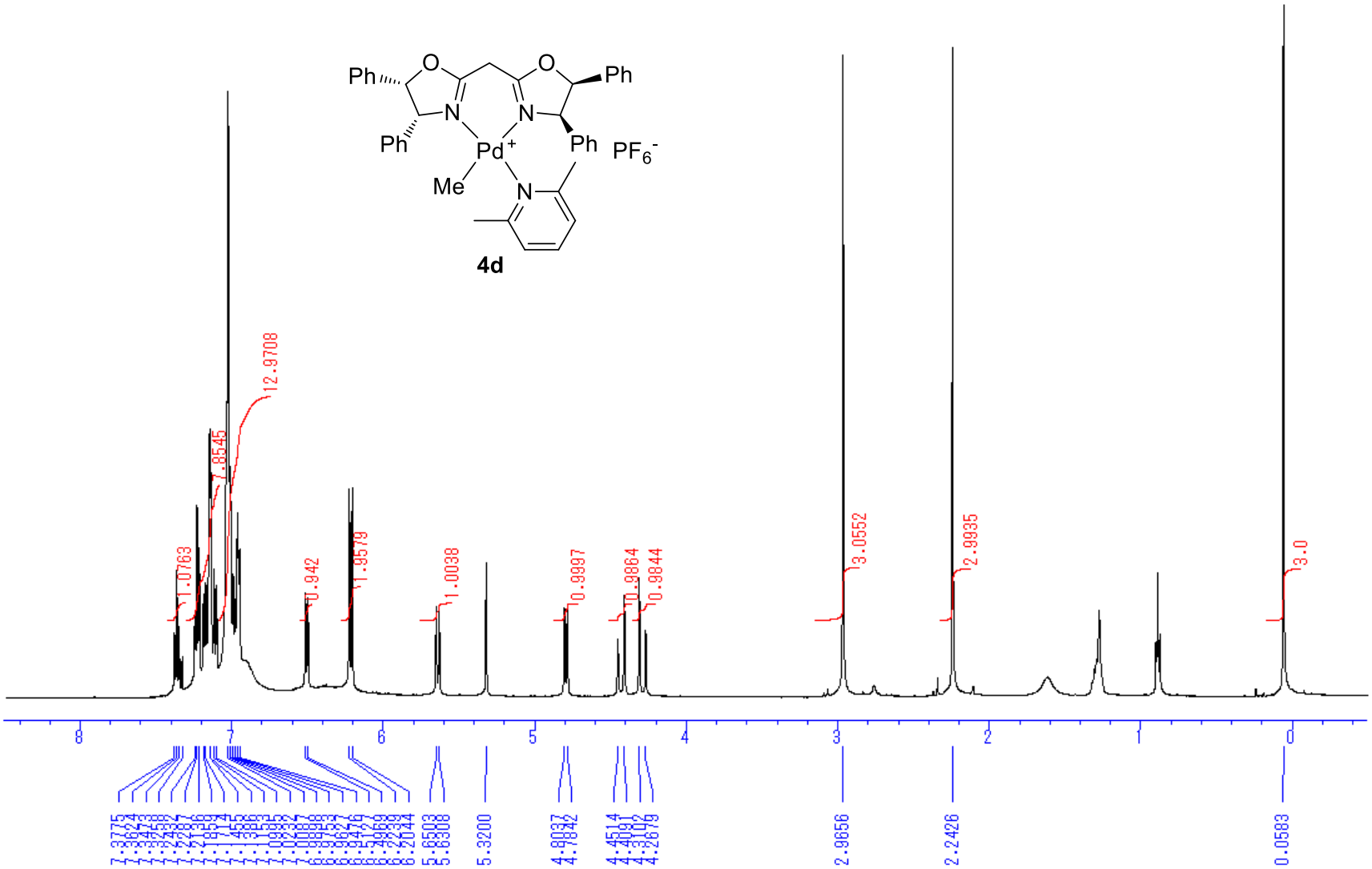

Figure S33. ^{1}H NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4d).

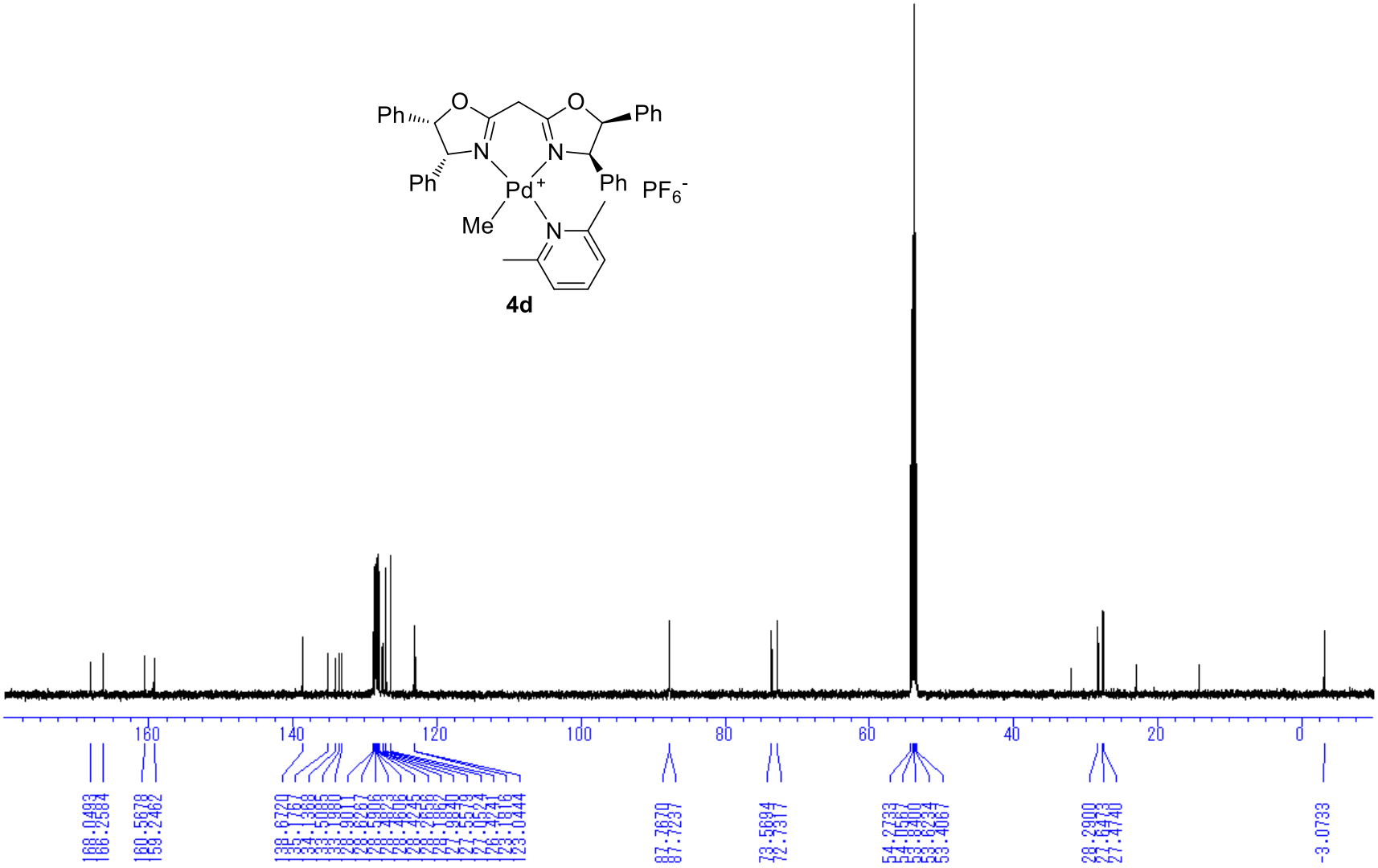

Figure S34. ^{13}C NMR Spectrum of [(BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N)]$^+$PF$_6^-$ (4d).

1-7. NMR spectra of neutral (BOX)PdMe(2,6-$Me_2C_5H_3N$) (5b-d).

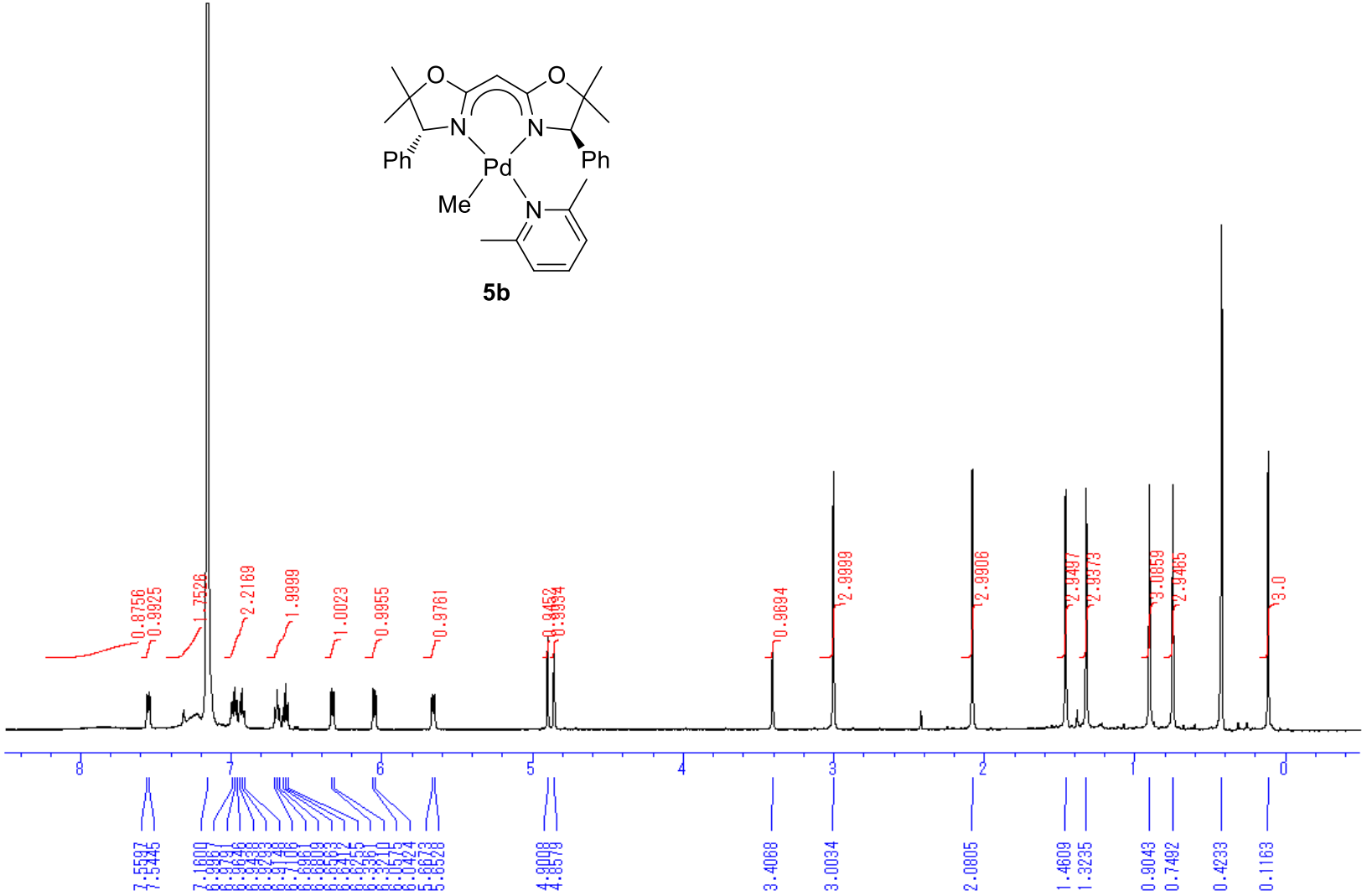

Figure S35. ^{1}H NMR Spectrum of (BOX)PdMe(2,6-$Me_2C_5H_3N$) (5b).

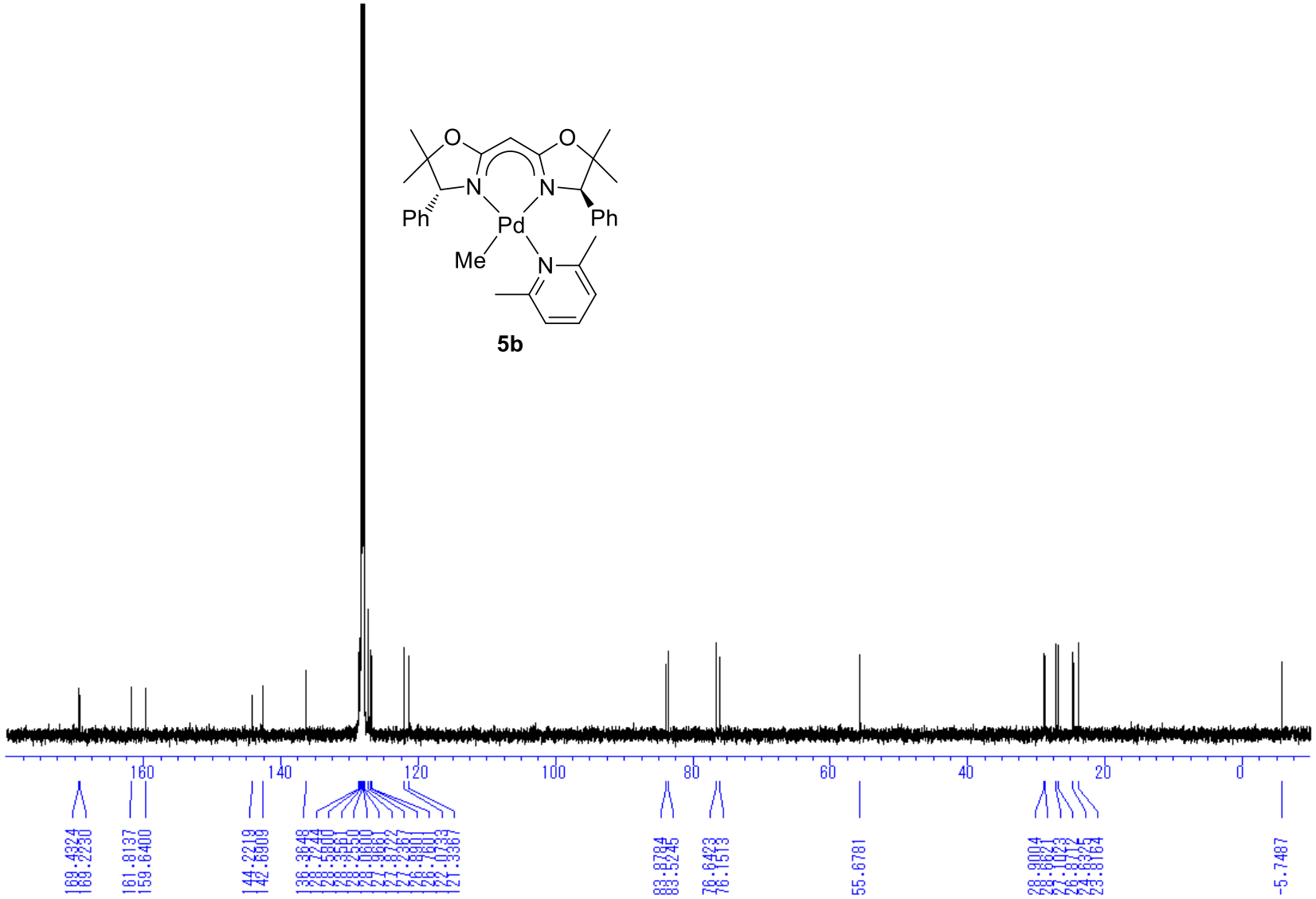

Figure S35. ^{13}C NMR Spectrum of (BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N) (5b).

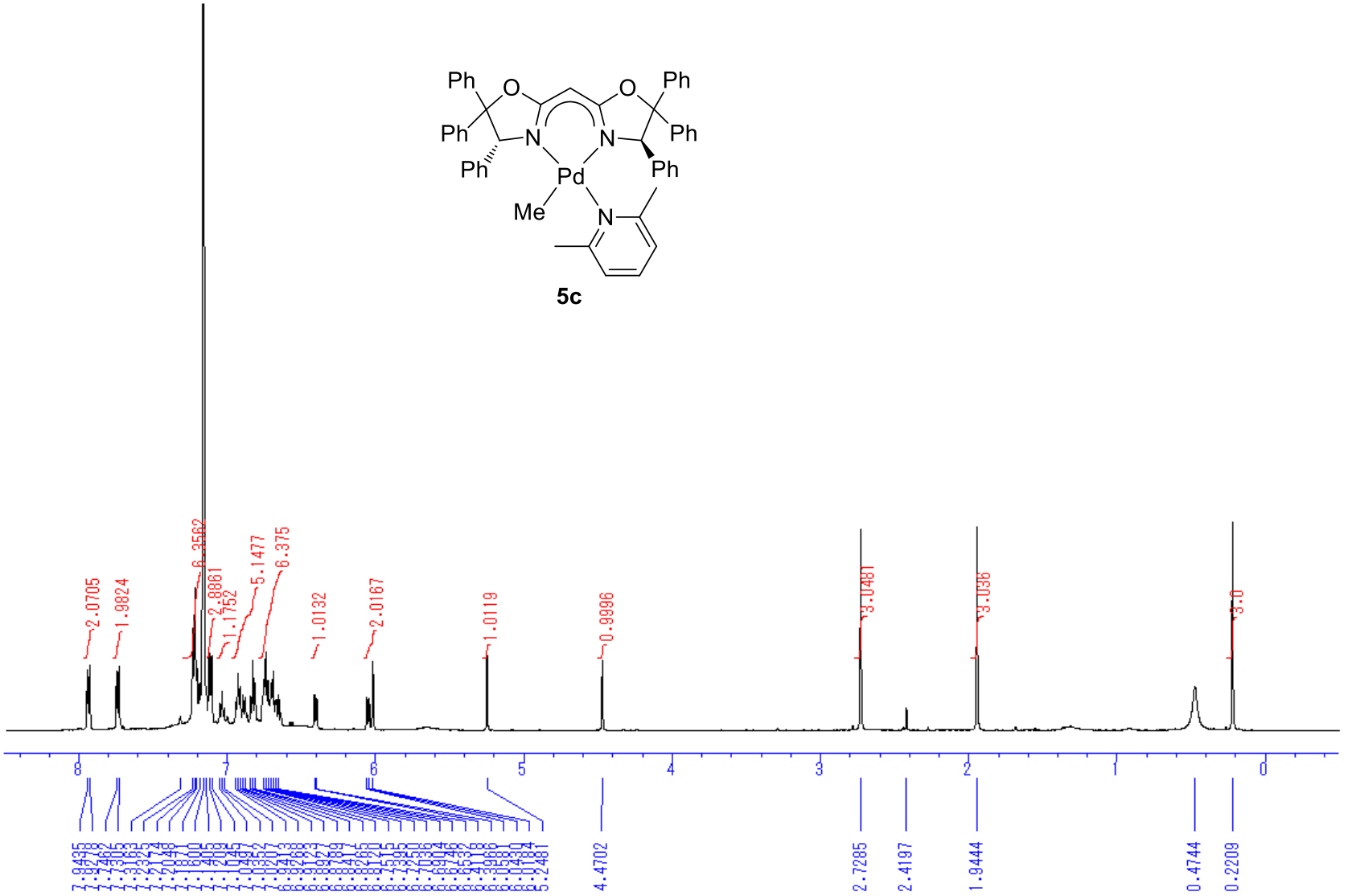

Figure S37. ^{1}H NMR Spectrum of (BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N) (5c).

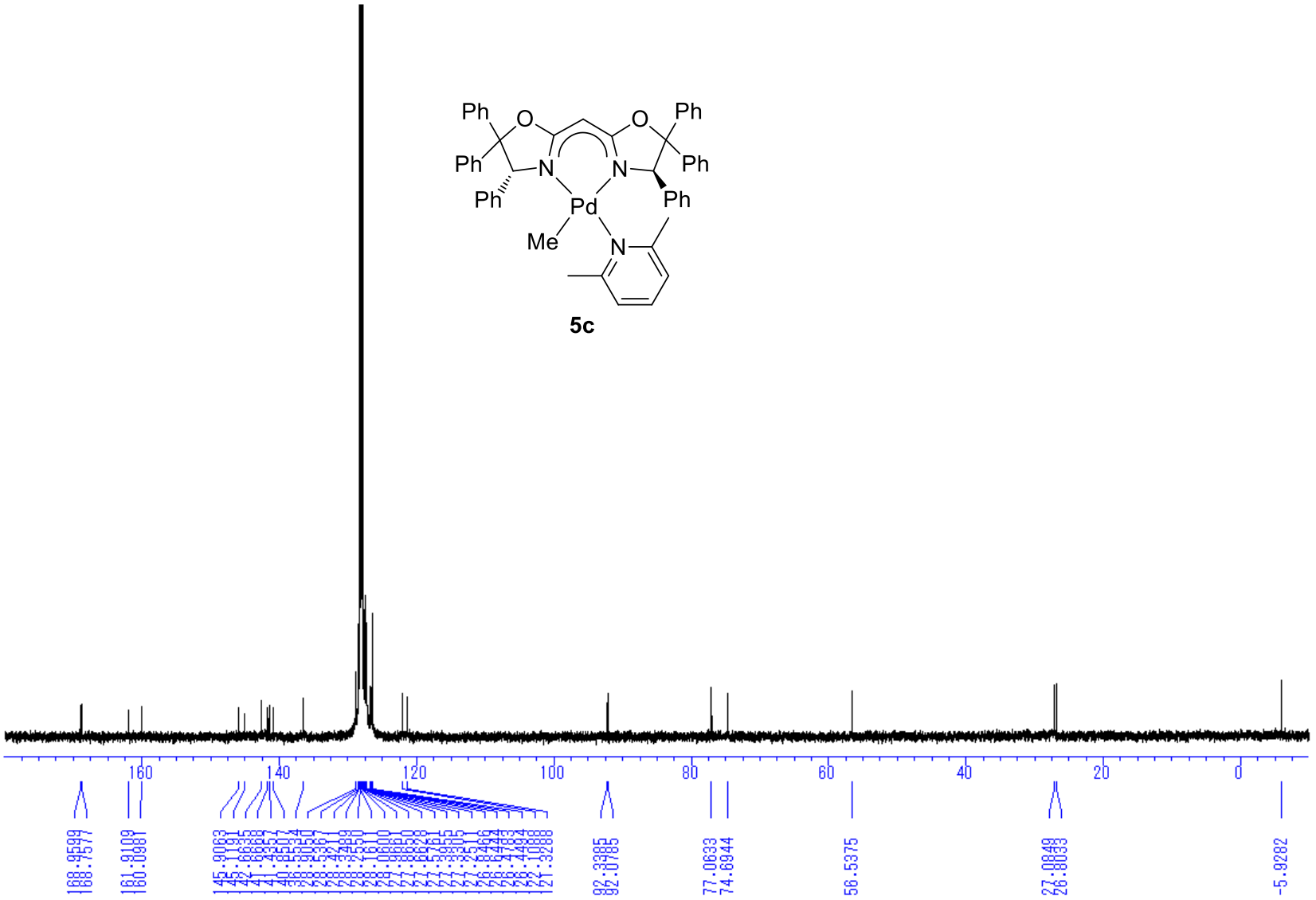

Figure S38. ^{13}C NMR Spectrum of (BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N) (5c).

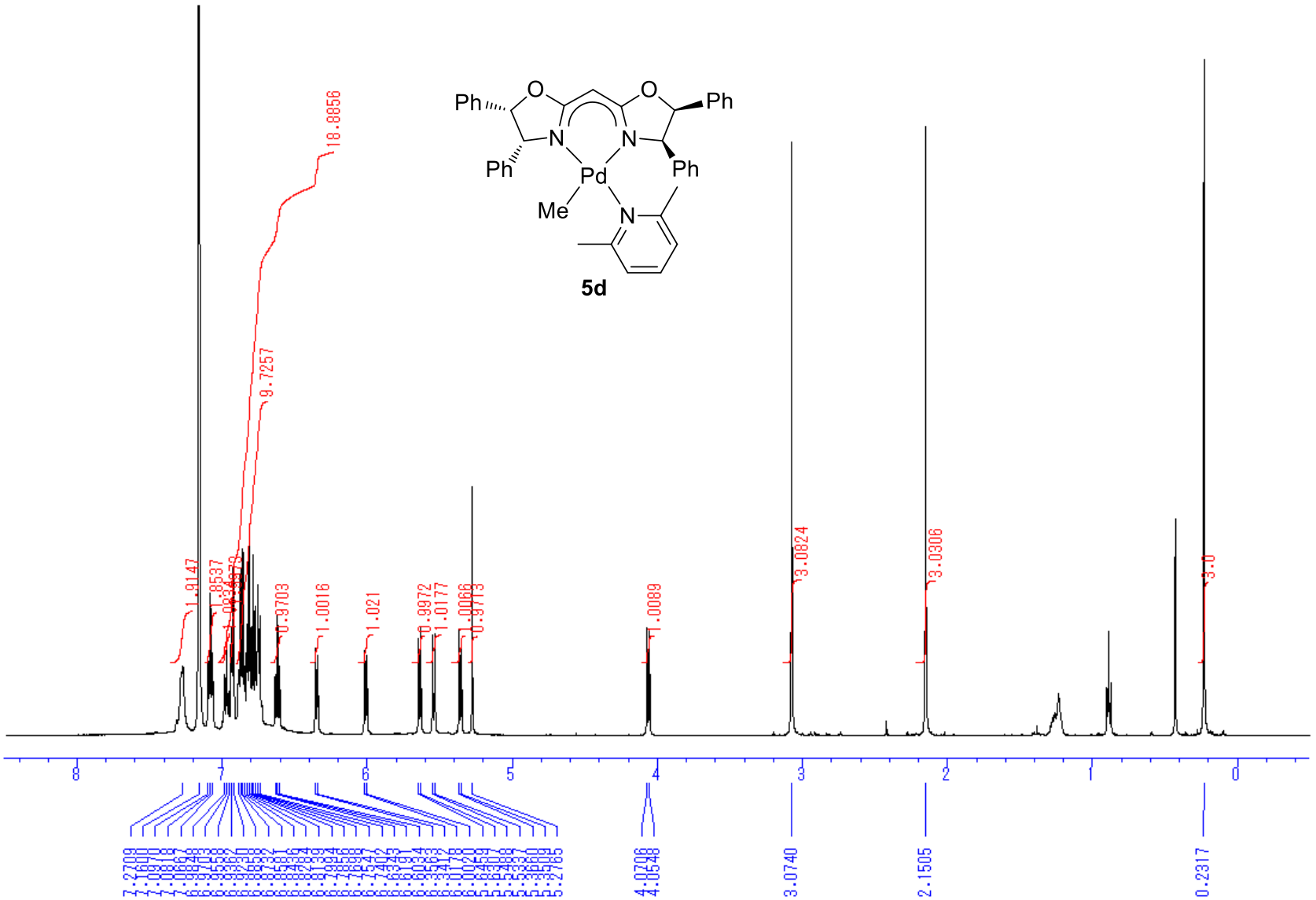

Figure S39. ^{1}H NMR Spectrum of (BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N) (5d).

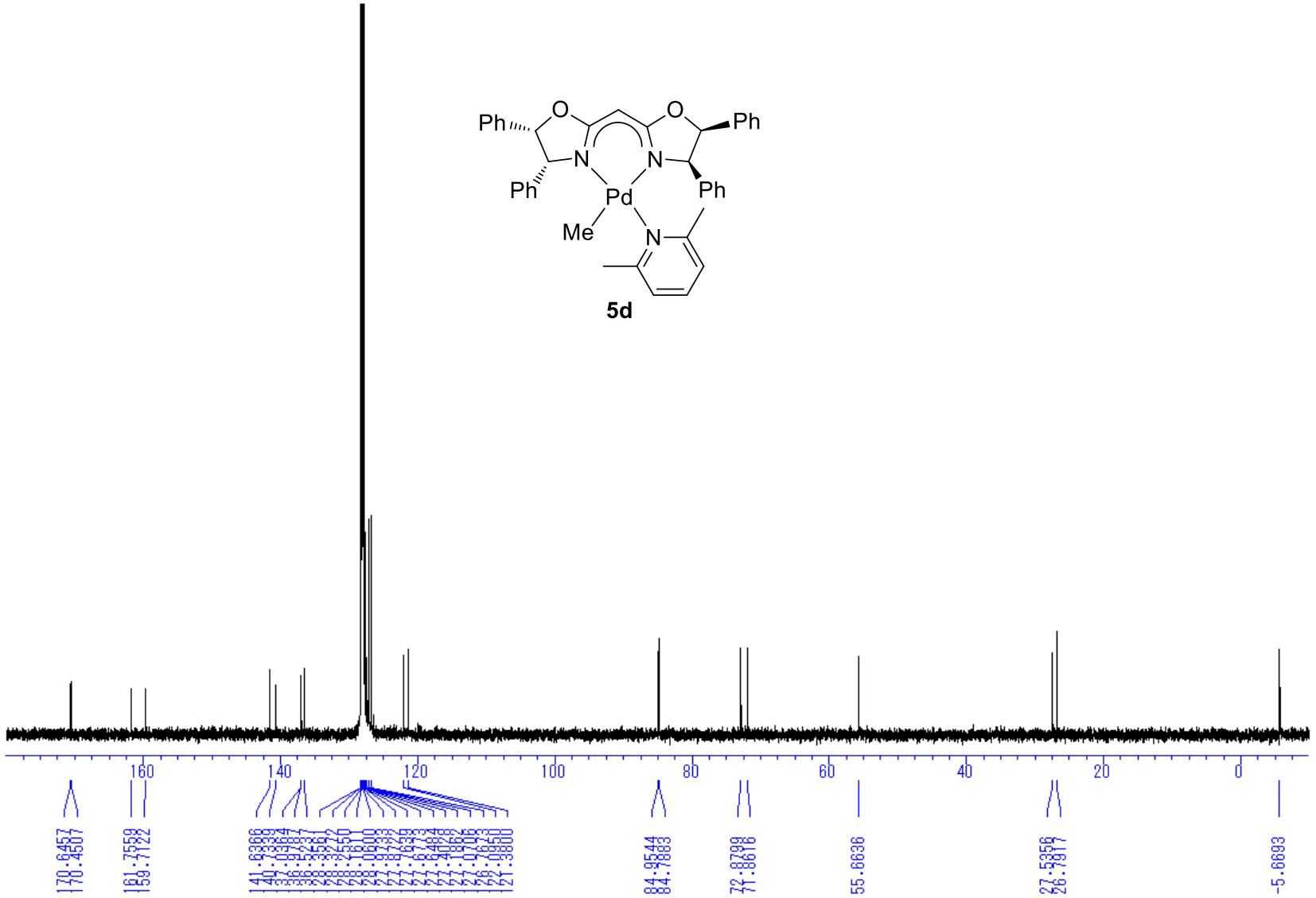

Figure S39. ^{13}C NMR Spectrum of (BOX)PdMe(2,6-Me$_2$C$_5$H$_3$N) (5d).

2. Selected crystal collection parameters for BOX (1b-d), complex 2a-d, 3a, 3c, 4a, 5b.

Table S1. Crystal data and collection parameters of bis(oxazoline) ligands, BOX (**1b**–**d**).

	1b	**1c**	**1d**
Formula	$C_{23}H_{26}N_2O_2$	$C_{43}H_{34}N_2O_2$	$2(C_{31}H_{26}N_2O_2)$
Formula weight	362.47	610.75	917.12
Crystal color, Habit	colorless, prism	colorless, prism	colorless, platelet
Crystal size (mm)	0.460×0.350×0.190	0.270×0.250×0.200	0.780×0.200×0.040
Crystal system	orthorhombic	tetragonal	monoclinic
Space group	$P2_12_12_1$ (#19)	$P4_3$ (#78)	$P2_1$ (#4)
a (Å)	9.576(4)	8.7744(4)	14.65(2)
b (Å)	11.843(4)	8.7744(4)	8.217(8)
c (Å)	17.253(6)	41.560(3)	15.8576(5)
α (deg)	90.0	90.0	90.0
β (deg)	90.0	90.0	103.480(9)
γ (deg)	90.0	90.0	90.0
V (Å^3)	1956.6(13)	3199.7(3)	2464(4)
Z value	4	4	2
D_{calcd} (g/cm^3)	1.230	1.268	1.236
F_{000}	776.00	1288.00	968.00
Temp (K)	93	93	93
μ (MoKα) (cm^{-1})	0.786	0.774	0.774
No. of reflections measured (R_{int})	6866	24001	25775
$2\theta_{max}$ (deg)	54.9	54.9	54.7
No. of observations [$I > 2.00\sigma(I)$]	4431	7075	11073
No. of variables	245	425	688
*R*1 [$I > 2.00\sigma(I)$]	0.0336	0.0343	0.0449
*wR*2 [All reflections]	0.0854	0.0790	0.1097
Goodness of Fit	1.086	1.049	1.100

Table S2. Crystal data and collection parameters of (BOX)$PdCl_2$ (**2a-d**).

	2a	**2b**	**2c**	**2d**
Formula	$C_{25}H_{30}Cl_2N_2O_2Pd$	4[$C_{23}H_{26}Cl_2N_2O_2$ Pd]	$C_{43}H_{34}Cl_2N_2O_2Pd$, 2[CH_2Cl_2]	$C_{31}H_{26}Cl_2N_2O_2Pd$, CH_2Cl_2
Formula weight	567.83	2159.11	957.93	720.80
Crystal color, Habit	yellow, prism	yellow, prism	yellow, prism	yellow, block
Crystal size (mm)	0.480×0.150×0.100	0.340×0.180×0.150	0.230×0.230×0.180	0.310×0.270×0.210
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
Space group	$P2_1$ (#4)	C2 (#5)	C2 (#5)	$P2_12_12_1$ (#19)
a (Å)	9.741(7)	24.590(3)	24.861(10)	7.246(3)
b (Å)	12.154(8)	14.0600(15)	8.317(3)	15.177(6)
c (Å)	11.342(8)	29.311(4)	11.649(5)	27.755(13)
α (deg)	90.0	90.0	90.0	90.0
β (deg)	110.438(7)	111.574(2)	113.088(5)	90.0
γ (deg)	90.0	90.0	90.0	90.0
V (Å^3)	1258(2)	9424(2)	2216(2)	3052(3)
Z value	2	4	2	4
D_{calcd} (g/cm^3)	1.499	1.522	1.436	1.568
F_{000}	580.00	4384.00	972.00	1456.00
Temp (K)	93	93	93	93
μ (MoKα) (cm^{-1})	9.740	10.360	8.187	9.908
No. of reflections measured (R_{int})	13194	77840	11647	31173
$2\theta_{max}$ (deg)	55.0	55.1	54.9	55.0
No. of observations [$I > 2.00\sigma(I)$]	5711	20822	5026	7010
No. of variables	290	1082	259	371
*R*1 [$I > 2.00\sigma(I)$]	0.0279	0.0252	0.0238	0.0246
*wR*2 [All reflections]	0.0731	0.0648	0.0600	0.0571
Goodness of Fit	1.114	1.098	1.040	1.086

Table S3. Crystal data and collection parameters of (BOX)PdMeCl (**3a, c**), cationic $[(BOX)PdMe(2,6\text{-}Me_2C_5H_3N)]^+PF_6^-$ **(4a)**, and neutral (BOX)PdMe(2,6-$Me_2C_5H_3N$) (**5b**).

	3a	**3c**	**4a**	**5b**
Formula	$2[C_{26}H_{33}ClN_2O_2Pd]$	$C_{44}H_{36}ClN_2O_2Pd$, $0.5[H_2O]$	$C_{31}H_{38}F_6N_3O_2PPd$	$C_{31}H_{37}N_3O_2Pd$, C_2H_5OH
Formula weight	1094.82	775.64	736.02	636.12
Crystal color, Habit	yellow, prism	yellow, prism	yellow, prism	colorless, prism
Crystal size (mm)	0.200×0.160×0.070	0.310×0.120×0.060	0.340×0.170×0.130	0.570×0.090×0.070
Crystal system	monoclinic	orthorhombic	orthorhombic	orthorhombic
Space group	$P2_1$ (#4)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)	$P2_12_12_1$ (#19)
a (Å)	9.073(2)	8.7555(18)	12.381(3)	9.5275(8)
b (Å)	14.749(3)	15.173(3)	14.812(3)	13.6026(11)
c (Å)	18.964(4)	29.497(6)	18.603(3)	24.391(2)
α (deg)	90.0	90.0	90.0	90.0
β (deg)	92.462(6)	90.0	90.0	90.0
γ (deg)	90.0	90.0	90.0	90.0
V (Å^3)	2535.4(9)	3918.6(14)	3411.6(12)	3161.0(5)
Z value	2	4	4	4
D_{calcd} (g/cm^3)	1.434	1.315	1.433	1.337
F_{000}	1128.00	1592.00	1504.00	1328.00
Temp (K)	93	93	93	93
μ (MoKα) (cm^{-1})	8.620	5.808	6.549	6.233
No. of reflections measured (R_{int})	20054	36180	14501	13914
$2\theta_{max}$ (deg)	55.0	55.0	55.0	55.0
No. of observations [$I > 2.00\sigma(I)$]	9289	8856	13914	6154
No. of variables	572	457	416	361
*R*1 [$I > 2.00\sigma(I)$]	0.0550	0.0493	0.0257	0.0262
*wR*2 [All reflections]	0.1442	0.1229	0.0649	0.0653
Goodness of Fit	1.022	1.033	1.047	1.142