Supporting Information

1,2,3-Triazole based bisphosphine, 5-(diphenylphosphanyl)-1-(2-(diphenylphosphanyl)-phenyl)-4-phenyl-1H-1,2,3-triazole: An ambidentate ligand with switchable coordination modes

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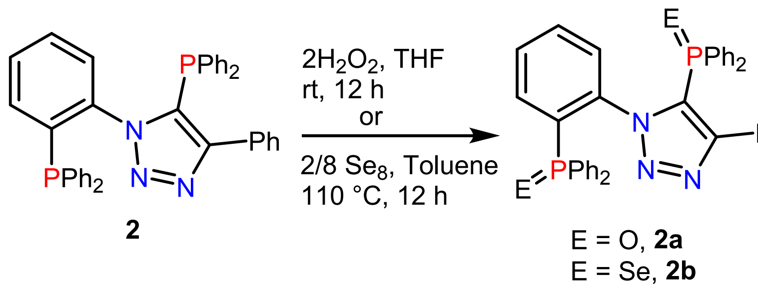
(1). Synthesis of chalcogenide derivatives of 2



Scheme S1 Synthesis of chalcogenide derivatives of **2**

Synthesis of [*o*-$Ph_2P(O)(C_6H_4)$\{1,2,3-N_3C(Ph)C((O)PPh_2)\}] (2a)

A 30% aqueous solution of H_2O_2 (0.0064 g, 0.102 mmol) was added to a THF (10 mL) solution of **2** (0.03 g, 0.051 mmol) at room temperature. The reaction mixture was stirred for 12 h. The solvent was removed under vacuum and residue washed with diethyl ether to obtain analytically pure solid compound **2a**. Yield 92 % (0.029 g). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (dd, *J* = 12.0, 7.7 Hz, 4H), 7.68 – 7.58 (m, 5H), 7.57 – 7.43 (m, 8H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.24 – 7.09 (m, 8H), 7.05 (q, *J* = 6.0 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$) δ 28.52, 12.75. HRMS (ES) m/z calcd for $C_{38}H_{30}N_3P_2O_2$ ([M+H]$^+$) 622.1808; found 622.1809.

Synthesis of [*o*-$Ph_2P(Se)(C_6H_4)$\{1,2,3-N_3C(Ph)C((Se)PPh_2)\}] (2b)

The round bottom flask charged with bisphosphine ligand **2** (0.03 g, 0.051 mmol) and Se_8 (8.8 mg, 0.0139 mmol) in Toluene (15 mL) at room temperature. The reaction mixture was refluxed for 12 h and excess of se was filtered off through celite containing frit. The solvent was completely removed under reduced pressure and residue was washed with petroleum ether to obtain analytically pure solid compound **2b** Yield: 93 % (0.035 g) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.29 (d, *J* = 10.4 Hz, 2H), 8.19 (dd, *J* = 7.6, 4.4 Hz, 1H), 8.04 (dd, *J* = 14.6, 7.6 Hz, 2H), 7.80 – 7.69 (m, 4H), 7.50 (dd, *J* = 25.9, 14.6 Hz, 8H), 7.36 (t, *J* = 7.7 Hz, 1H), 7.20 – 7.06 (m, 7H), 7.06 – 6.99

(m, 3H), 6.88 (dd, J = 13.4, 6.8 Hz, 1H).^{31}P NMR (202 MHz, $CDCl_3$) δ 31.70 (s), 18.53(s). HRMS (ES) m/z calcd for $C_{38}H_{30}N_3P_2Se_2$ ([M+H]$^+$) 750.0248; found 750.0284.

(2). NMR spectral data of compounds a-i and k

a. 2-phenylbenzofuran.[1]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.93 – 7.84 (m, 2H), 7.62 – 7.57 (m, 1H), 7.56 – 7.51 (m, 1H), 7.46 (dd, J = 10.6, 4.8 Hz, 2H), 7.39 – 7.33 (m, 1H), 7.32 – 7.27 (m, 1H), 7.27 – 7.21 (m, 1H), 7.04 (d, J = 0.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.10, 155.07, 130.66, 129.40, 128.97, 128.73, 125.11, 124.44, 123.11, 121.08, 111.36, 101.48.4

b. 2-(2-methoxyphenyl)benzofuran[2]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (dd, J = 7.8, 1.7 Hz, 1H), 7.64 – 7.58 (m, 1H), 7.53 (d, J = 8.0 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.36 – 7.31 (m, 1H), 7.31 – 7.26 (m, 1H), 7.23 (dd, J = 10.8, 4.1 Hz, 1H), 7.10 (td, J = 7.7, 0.8 Hz, 1H), 7.02 (d, J = 8.3 Hz, 1H), 4.01 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.69, 153.52, 152.35, 129.98, 129.43, 127.25, 124.28, 122.81, 121.21, 120.97, 119.53, 111.22, 111.01, 106.50, 55.64.

c. 2-(4-methoxyphenyl)benzofuran[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.73 (m, 2H), 7.59 – 7.55 (m, 1H), 7.53 – 7.50 (m, 1H), 7.25 (dqd, J = 14.5, 7.3, 1.3 Hz, 2H), 7.01 – 6.96 (m, 2H), 6.89 (d, J = 0.8 Hz, 1H), 3.87 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 160.17, 156.24, 154.89, 129.68, 126.60, 123.91, 123.54, 123.01, 120.75, 114.44, 111.16, 99.86, 55.53.

d. 5,7-dimethyl-2-phenylbenzofuran[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.87 (m, 2H), 7.51 (t, J = 7.5 Hz, 2H), 7.40 (dd, J = 10.6, 4.1 Hz, 1H), 7.25 (s, 1H), 6.99 (s, 2H), 2.63 (s, 3H), 2.49 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ

155.74, 152.54, 132.46, 130.99, 128.95, 128.85, 128.41, 126.81, 124.94, 120.93, 118.32, 101.53, 21.44, 15.15.

e. 2-(4-(tert-butyl)phenyl)benzofuran[4]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (t, J = 9.2 Hz, 2H), 7.59 (dd, J = 17.2, 7.7 Hz, 2H), 7.51 (d, J = 8.4 Hz, 2H), 7.35 – 7.23 (m, 2H), 7.01 (s, 1H), 1.40 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.33, 155.00, 151.95, 132.44, 129.54, 127.91, 125.90, 125.65, 124.92, 124.16, 123.01, 120.93, 111.30, 100.85, 34.93, 31.42.

f. 5,7-dimethyl-2-(p-tolyl)benzofuran

White solid. Mp: 81-84 °C ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 8.1 Hz, 2H), 7.27 (d, J = 7.6 Hz, 2H), 7.20 (s, 1H), 6.92 (s, 1H), 6.90 (s, 1H), 2.57 (s, 3H), 2.43 (s, 3H), 2.42 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.04, 152.40, 138.44, 132.40, 129.58, 129.07, 128.27, 126.55, 124.92, 120.89, 118.16, 100.78, 21.55, 21.47, 15.19. Mass m/z (GCMS): 236.1

g. 2-hexyl-5,7-dimethylbenzofuran

Brown liquid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (s, 1H), 6.86 (s, 1H), 6.34 – 6.28 (m, 1H), 2.78 (td, J = 7.7, 2.2 Hz, 2H), 2.50 (3H), 2.42 (3H), 1.83 – 1.71 (m, 2H), 1.37 (dd, J = 6.9, 3.2 Hz, 6H), 0.94 (dd, J = 6.6, 3.4 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.75, 152.21, 131.84, 128.78, 125.46, 120.46, 117.64, 101.81, 77.45, 77.20, 76.95, 31.78, 29.08, 28.71, 27.89, 22.77, 21.41, 15.19, 14.26. Mass m/z (GCMS): 230.1

h. 2-hexylbenzofuran[5]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 – 7.46 (m, 1H), 7.44 – 7.40 (m, 1H), 7.23 – 7.15 (m, 2H), 6.38 (d, J = 0.7 Hz, 1H), 2.80 – 2.71 (m, 2H), 1.75 (dt, J = 15.3, 7.5 Hz, 2H), 1.39 – 1.26 (m, 6H), 0.90 (td, J = 10.3, 5.5 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.96, 154.79, 129.21, 123.17, 122.52, 120.32, 110.87, 101.91, 31.76, 29.06, 28.64, 27.84, 22.75, 14.25.

i. 2-(4-fluorophenyl)benzofuran[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.78 (m, 2H), 7.61 – 7.56 (m, 1H), 7.54 – 7.50 (m, 1H), 7.32 – 7.27 (m, 1H), 7.26 – 7.21 (m, 1H), 7.18 – 7.11 (m, 2H), 6.96 (s, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.29, 161.82, 155.19, 155.02, 129.36, 126.97, 126.89, 124.47, 123.20, 121.07, 116.16, 115.94, 111.31, 101.17, 1.21.

k. 7-methoxy-2-phenylbenzofuran-5-carbaldehyde[6]

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.00 (s, 1H), 7.90 (d, *J* = 8.1 Hz, 2H), 7.71 (s, 1H), 7.46 (t, *J* = 7.6 Hz, 2H), 7.42 – 7.35 (m, 2H), 7.12 – 7.07 (m, 1H), 4.10 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.93, 158.02, 147.87, 146.25, 133.66, 131.02, 129.74, 129.38, 129.05, 125.38, 119.47, 104.81, 102.05, 56.40.

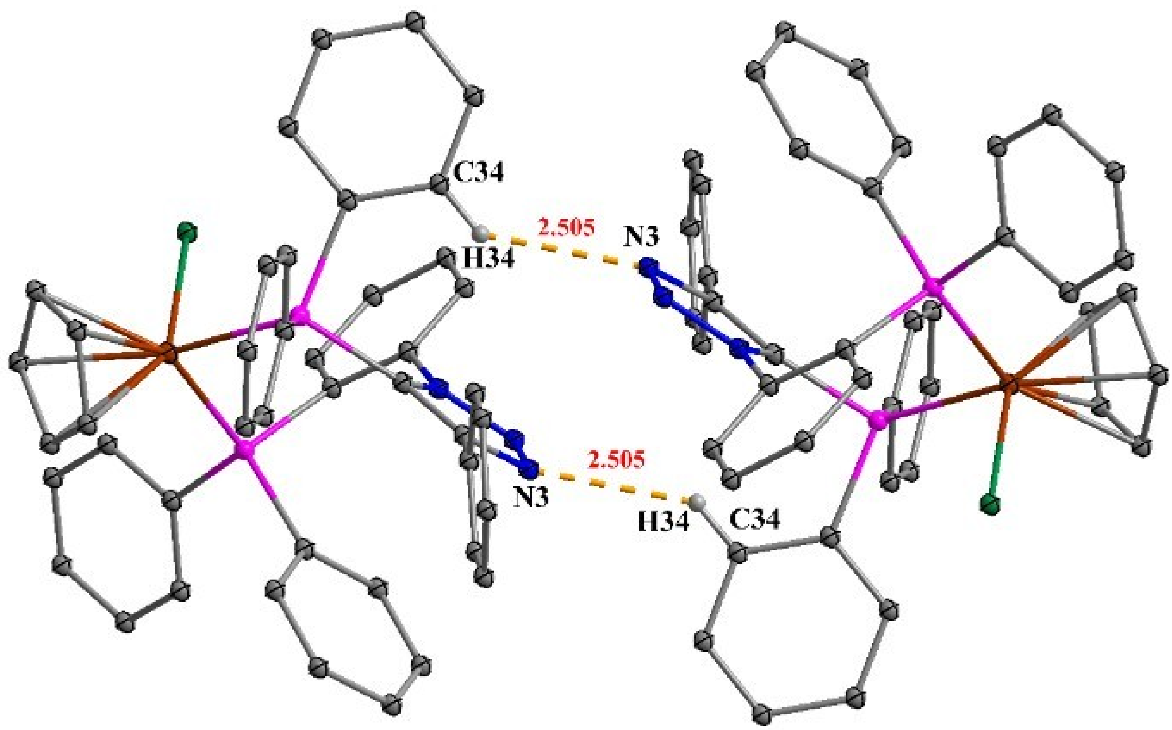


Fig. S1 Molecular structure of **8** showing intermolecular hydrogen bonding.

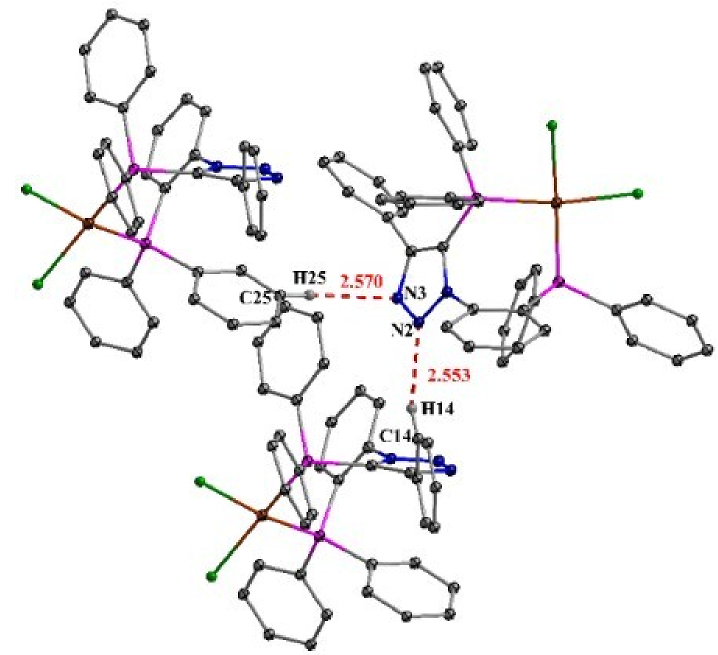
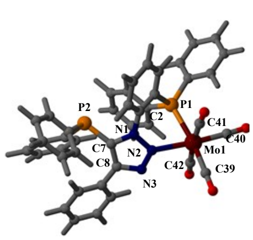
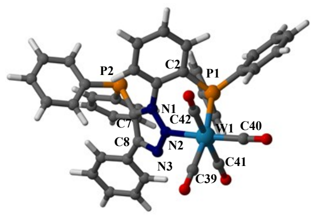


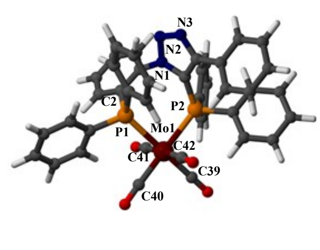
Fig. S2 Molecular structure of **10** showing intermolecular hydrogen bonding

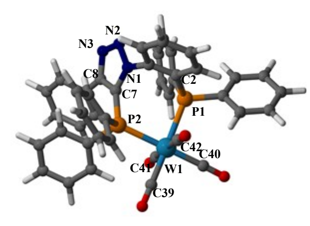
(3). Computational Details

Density functional theory calculations were performed using the Gaussian 09 suite of quantum chemical programs. The optimized molecular structures and determination of energies were calculated by using M06/6-31G**, lanl2dz (Mo, W) level of theory. Molecular orbital analysis have been done to find the HOMO-LUMO energy gap using the iop(6/7=3) at M062X/6-31G** level of theory. Graphical representations of the optimized geometries of compounds **3-6** were created by using CYLView.[7]









3 **4** **5** **6**

Fig. S3 Optimized structures of **3-6** at M062X/6-31G**, lanl2dz level of theory

Table S1 Selected experimental and DFT calculated bond lengths (Å) of compounds **4-6**

	4 (M=W)	DFT **4**	**5** (M=Mo)	DFT **5**	**6** (M=W)	DFT **6**
P1-C2	1.840(4)	1.846	1.846(3)	1.855	1.844(5)	1.856
P2-C7	1.824(4)	1.837	1.834(3)	1.834	1.828(5)	1.836
P1-M	2.5156(11)	2.538	2.5335(9)	2.59	2.5263(13)	2.571
P2-M	-	-	2.5245(9)	2.561	2.5131(13)	2.547
M-C39	1.972(5)	2.004	1.997(4)	2.001	2.000(6)	1.995
M-C40	1.978(5)	1.978	1.998(4)	2.012	2.006(6)	2.004
M-C41	2.039(5)	2.042	2.030(4)	2.06	2.027(5)	2.004
M-C42	2.021(5)	2.047	2.044(4)	2.05	2.039(5)	2.038
N2-N3	1.313(5)	1.297	1.303(4)	1.288	1.311(6)	1.289
M-N2	2.242(3)	2.286	-	-	-	-

Table S2 Selected experimental and DFT calculated bond angels (deg) of compounds **4-6**

	4 (M=W)	DFT **4**	**5** (M=Mo)	DFT **5**	**6** (M=W)	DFT **6**
P1–M–P2	-	-	87.76(3)	87.112	87.81(4)	86.841
P1–M–N2	75.10(9)	75.701	-	-	-	-
P1–M–C40	97.74(15)	97.912	92.21(10)	92.730	92.27(16)	92.961
P2–M–C39	-	-	92.06(10)	91.117	92.27(16)	91.131
N2–M–C39	96.93(18)	94.905	-	-	-	-
P1–M–C39	171.68(15)	169.201	174.34(11)	173.117	173.87(15)	173.082
N2–M–C40	172.32(16)	171.858	-	-	-	-
P2–M–C40	-	-	178.17(10)	177.696	178.09(14)	176.744
C41–M–C42	173.32(17)	174.802	174.19(14)	176.701	174.8(2)	177.709
N1–N2–N3	107.3(3)	108.218	107.4(3)	107.663	107.2(4)	107.652

(4) NMR and mass spectra of 2 and 4-12

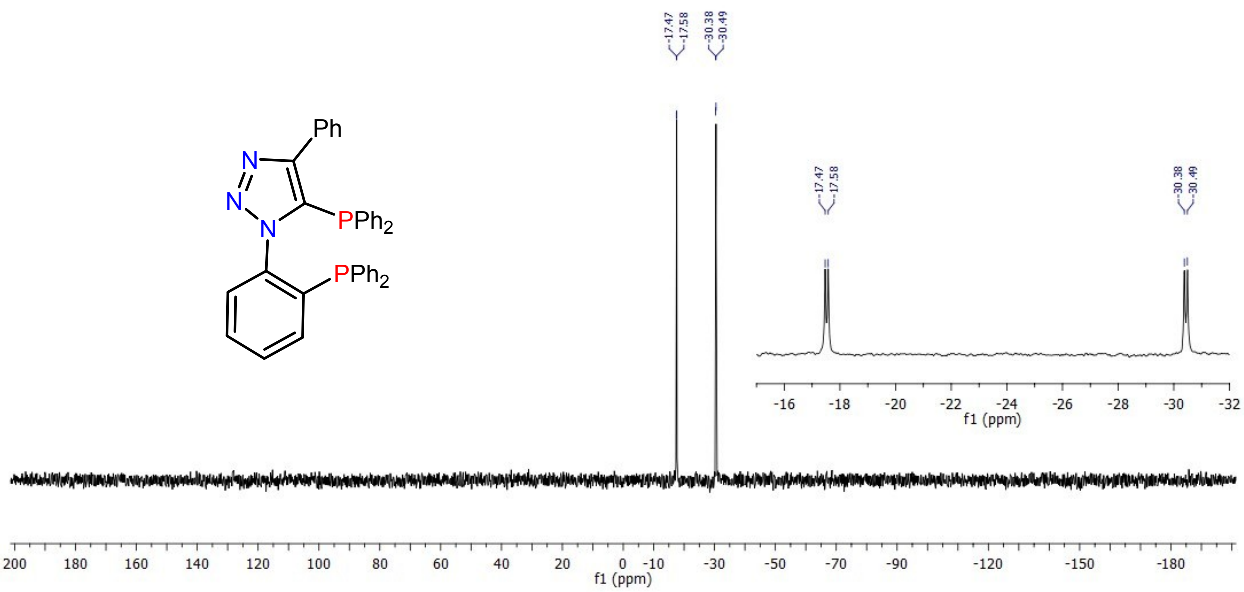


Fig. S4 $^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$ (202 MHz)

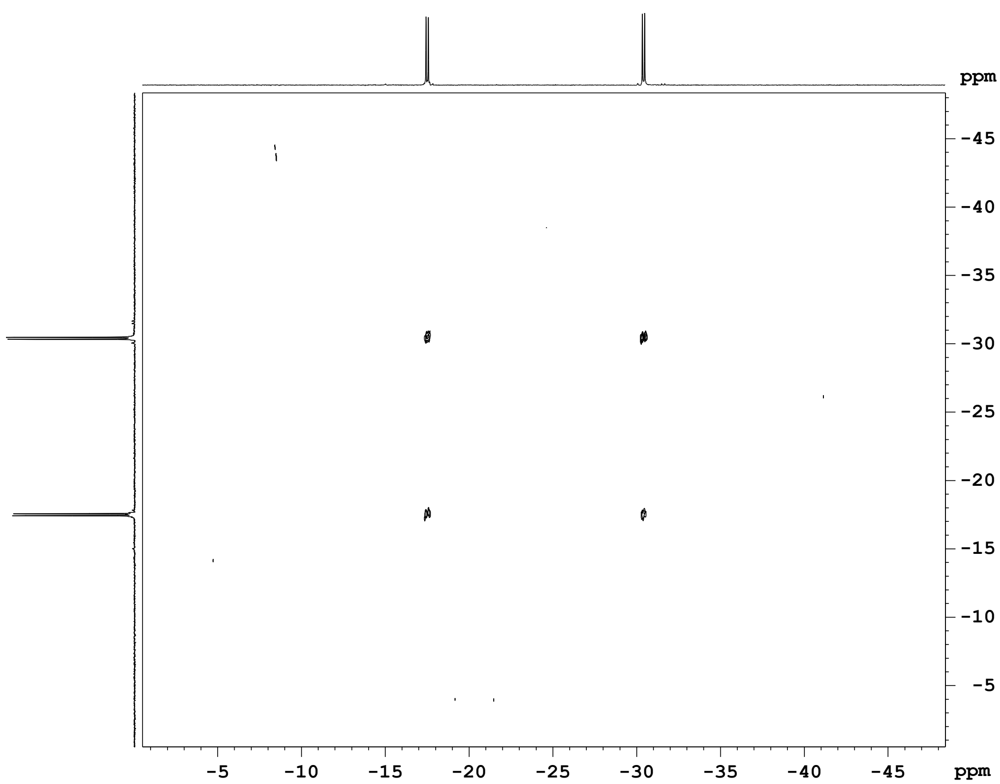


Fig. S5 $^{31}P\{^{1}H\}$-$^{31}P\{^{1}H\}$ COSY NMR spectrum of **2** in $CDCl_3$ (162 MHz)

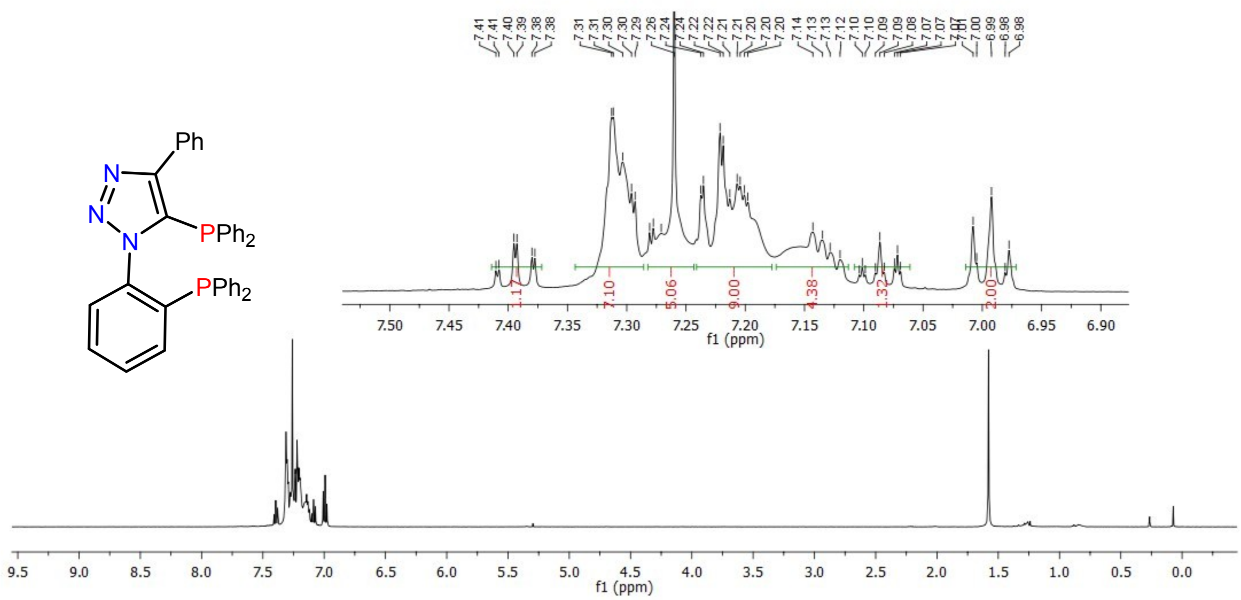


Fig. S6 ^{1}H NMR spectrum of **2** in $CDCl_3$ (500 MHz)

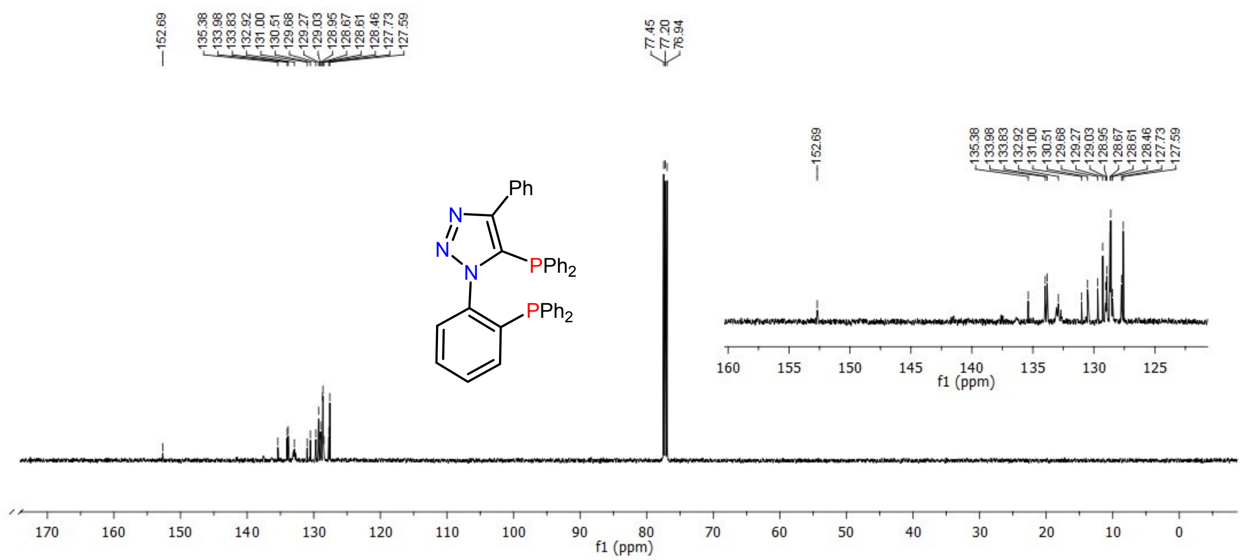
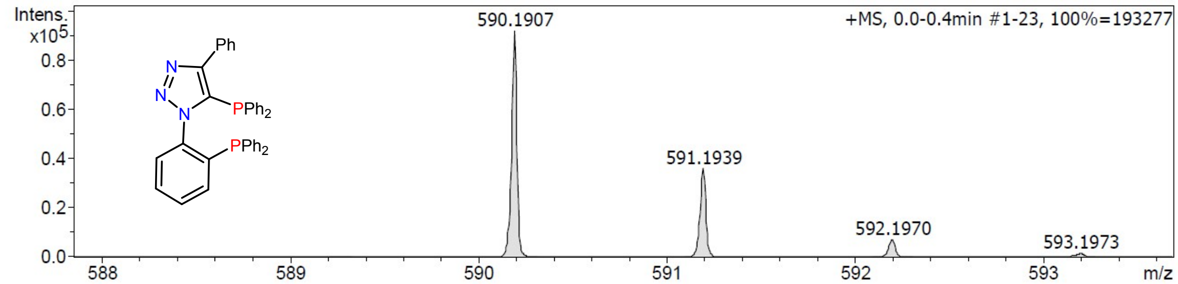


Fig. S7 ^{13}C NMR spectrum of **2** in $CDCl_3$ (126 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
590.1907	1	C38H30N3P2	590.1909	0.5	17.0	1	100.00	26.5	even	ok

Fig. S8 EI mass spectrum of **2**

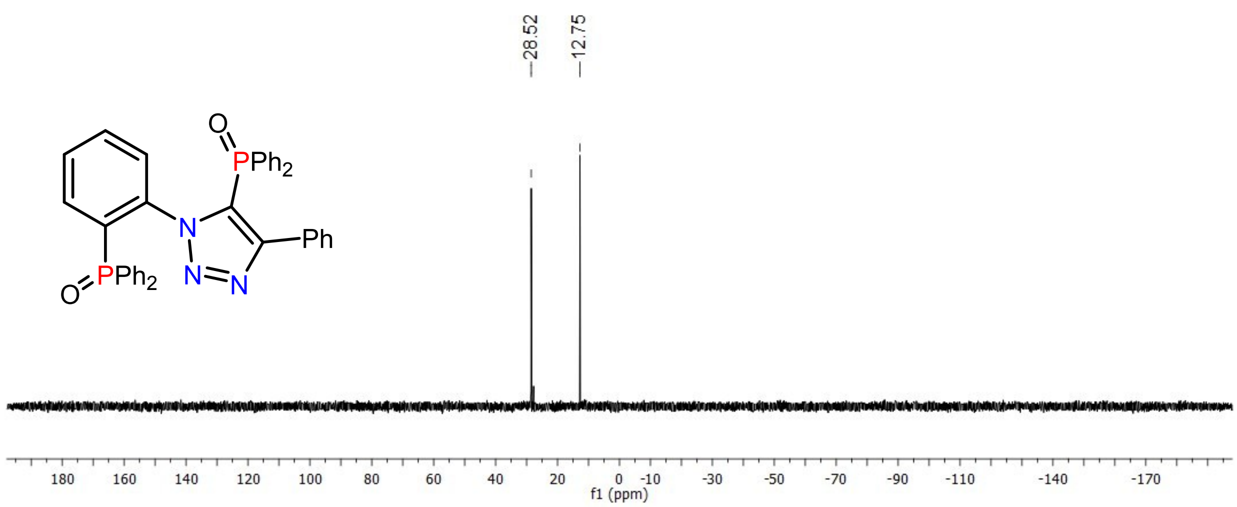


Fig. S9 $^{31}P\{^{1}H\}$ NMR spectrum of **2a** in $CDCl_3$ (162 MHz)

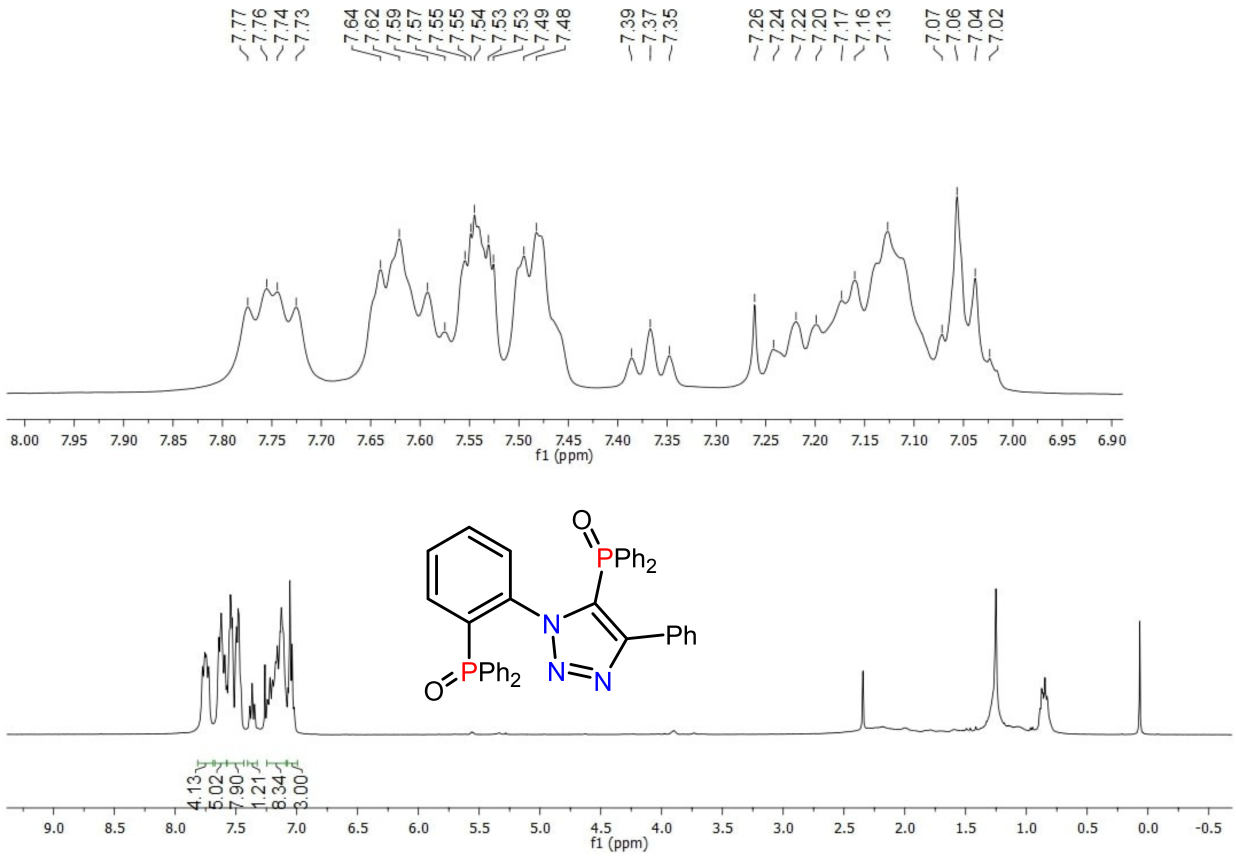
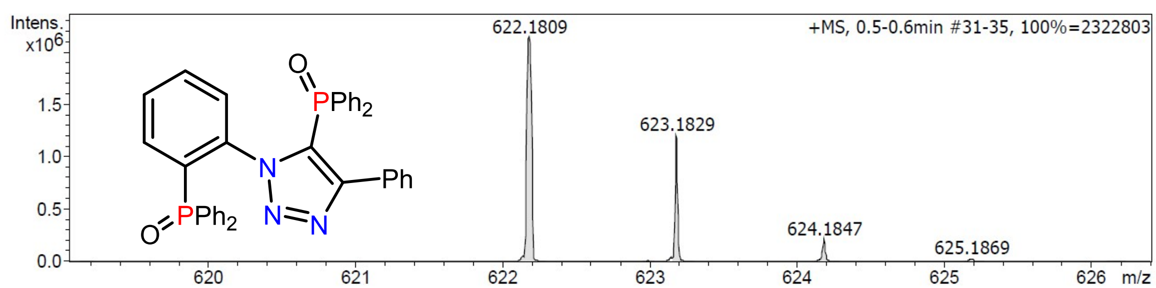


Fig. S10 ^{1}H NMR spectrum of **2a** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
622.1809	1	C38H30N3O2P2	622.1808	-0.2	66.8	1	100.00	26.5	even	ok

Fig. S11 EI mass spectrum of **2a**

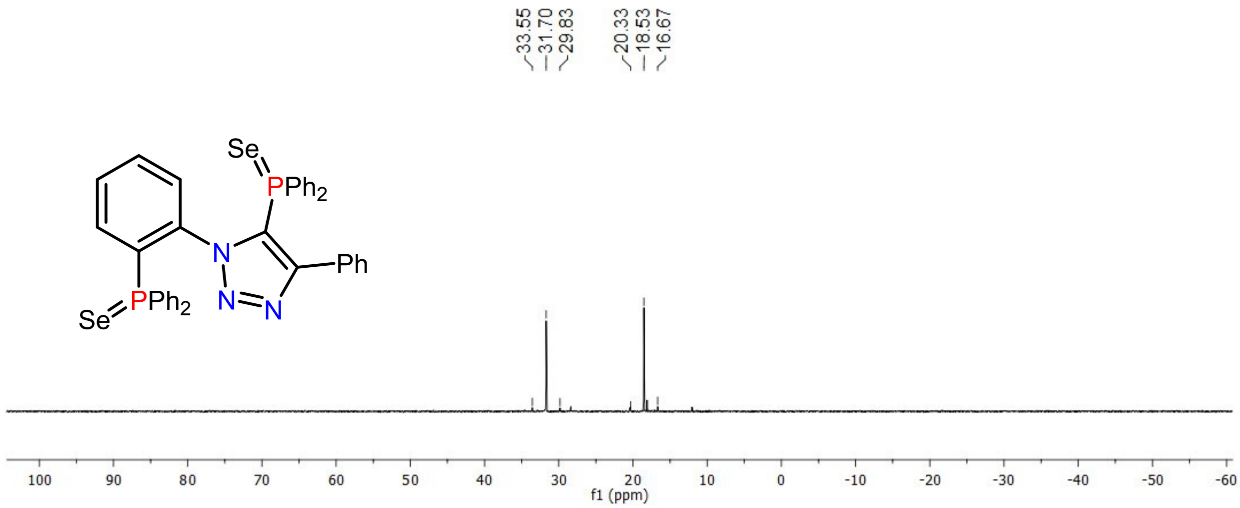


Fig. S12 $^{31}P\{^{1}H\}$ NMR spectrum of **2b** in $CDCl_3$ (162 MHz)

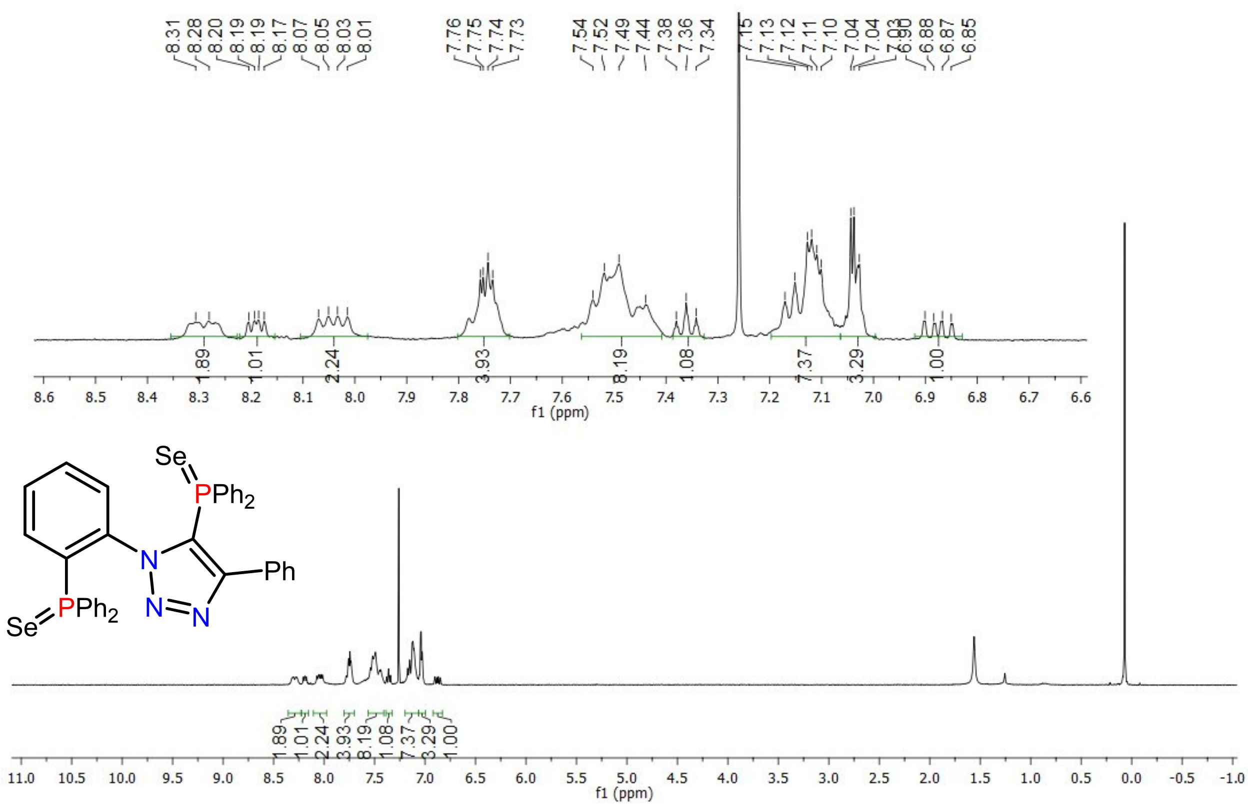
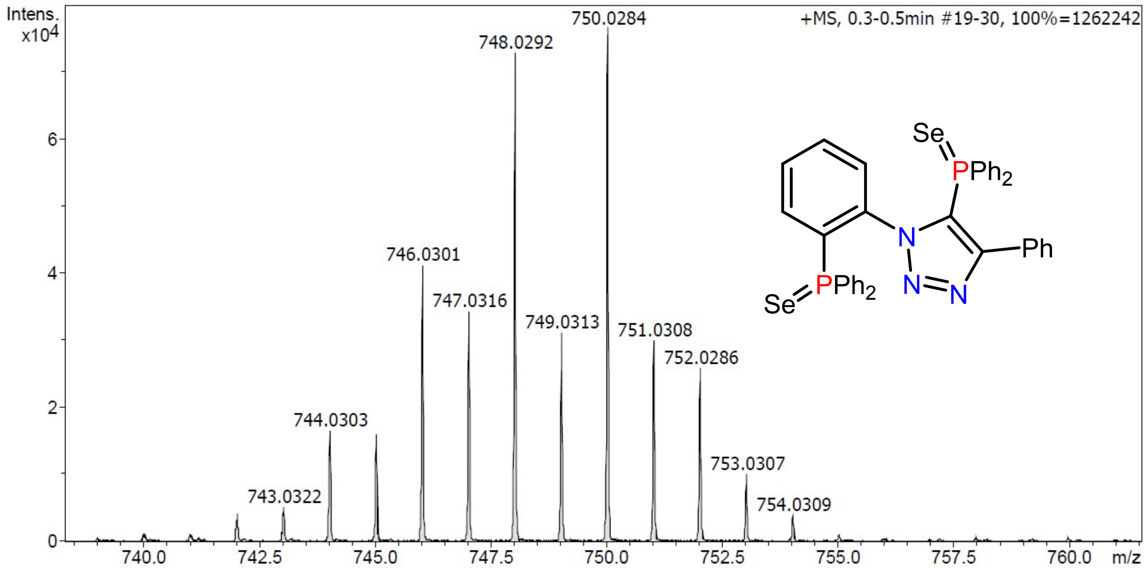


Fig. S13 ^{1}H NMR spectrum of **2b** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
750.0284	1	C38H30N3P2Se2	750.0248	4.8	8.1	1	100.00	26.5	even	ok

Fig. S14 EI mass spectrum of **2b**

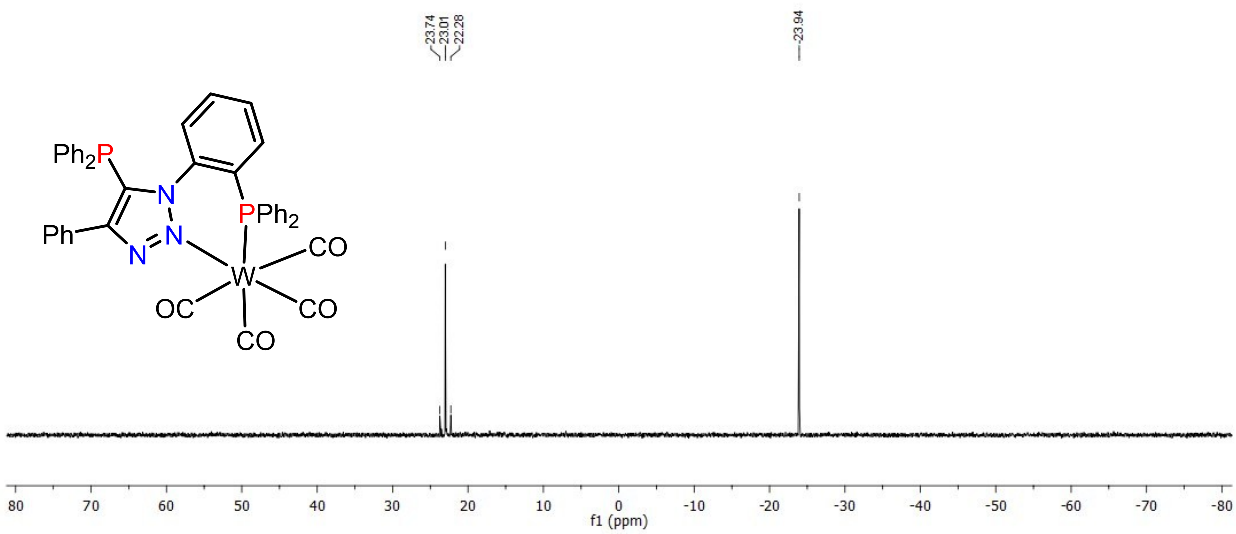


Fig. S15 $^{31}P\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$ (162 MHz)

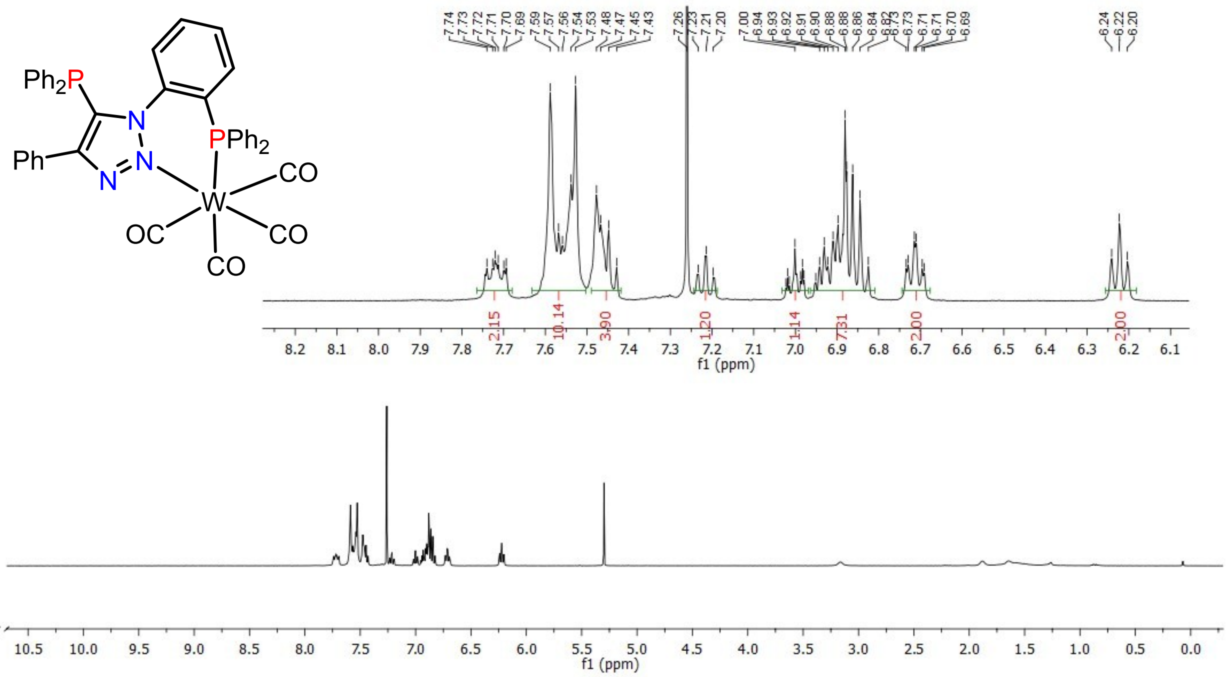
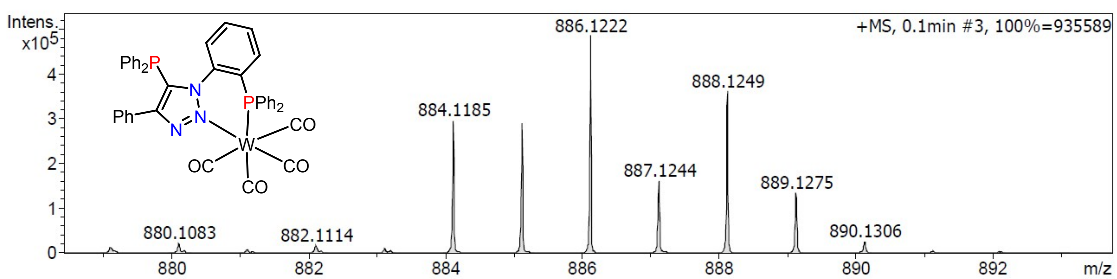


Fig. S16. ^{1}H NMR spectrum of **4** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
886.1222	1	C42H30N3O4P2W	886.1222	-0.0	53.0	1	100.00	32.5	even	ok

Fig. S17 EI mass spectrum of **4**

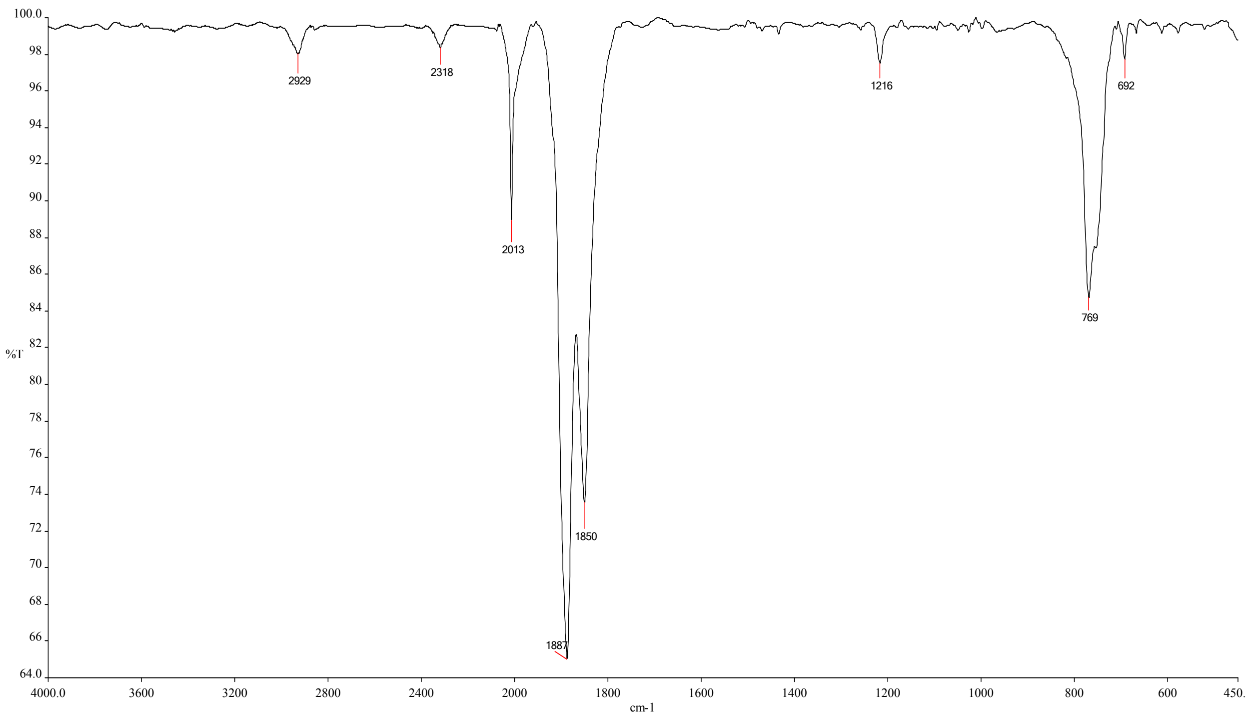


Fig. S18 IR spectrum of **4**

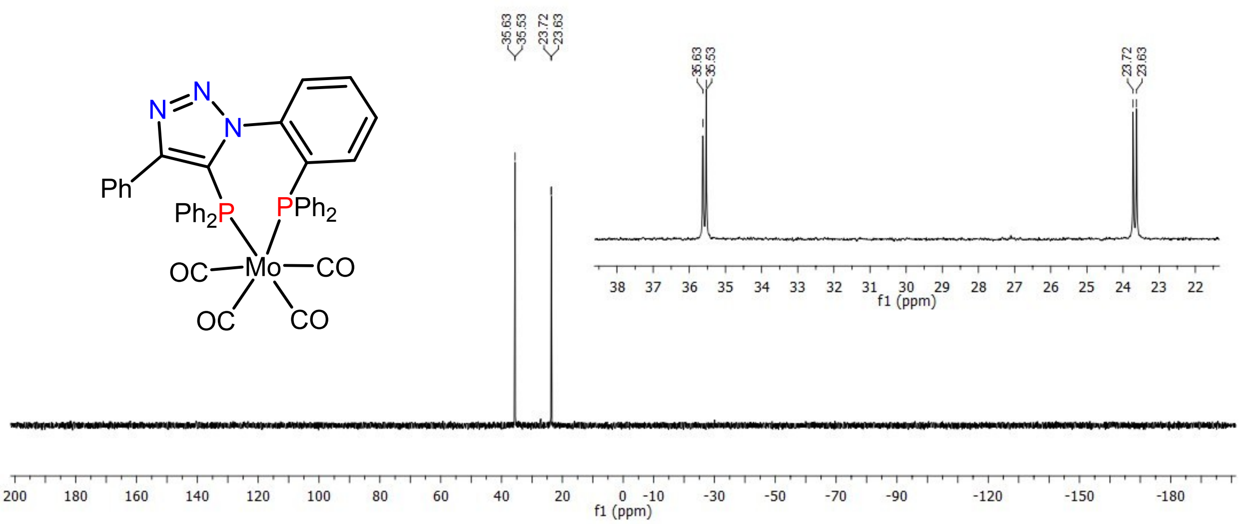


Fig. S19 $^{31}P\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$ (202 MHz)

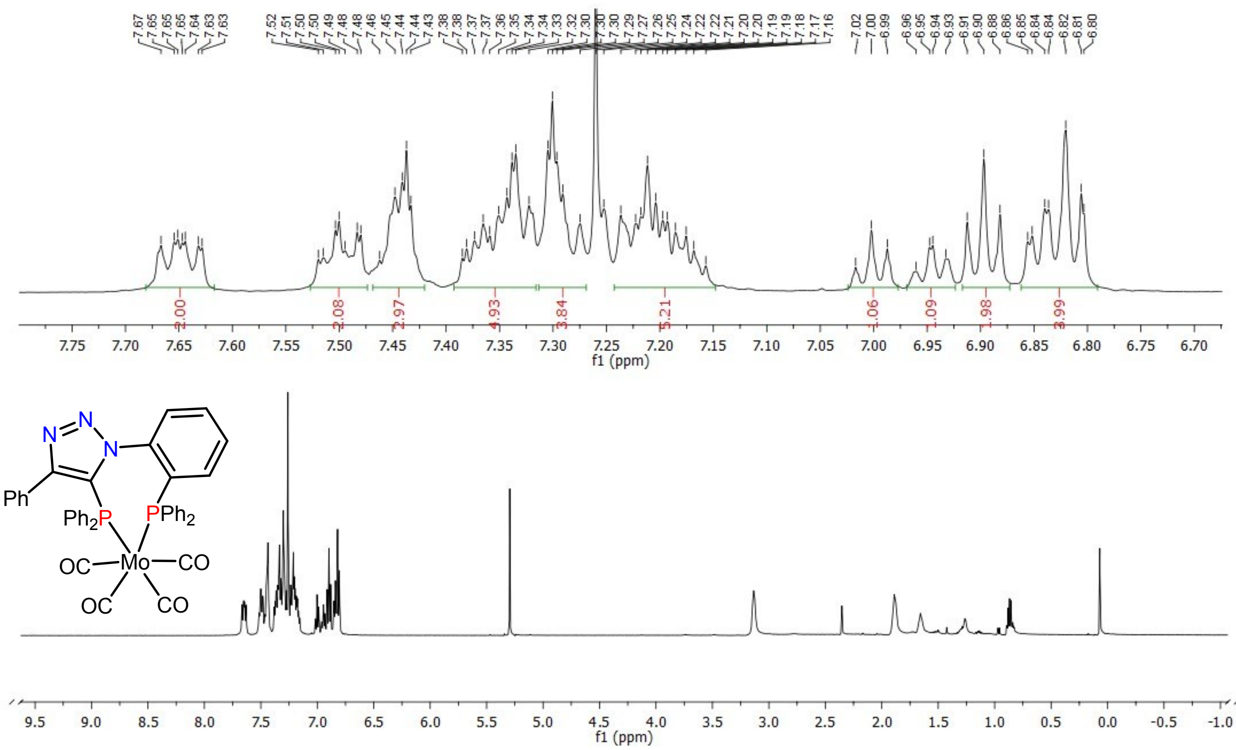
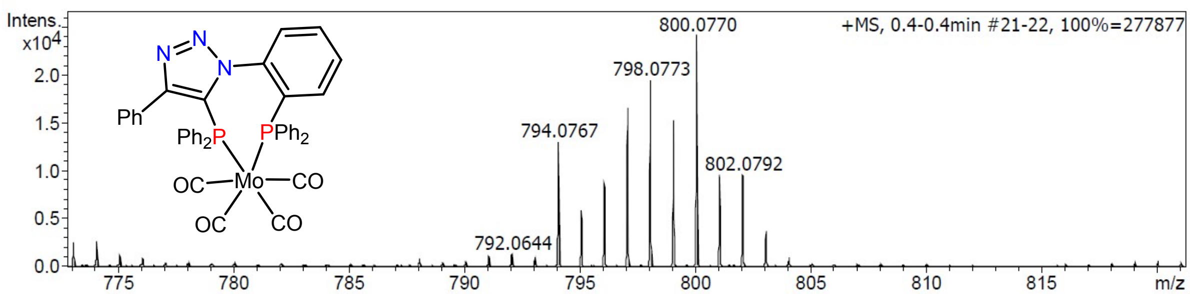


Fig. S20 ^{1}H NMR spectrum of **5** in $CDCl_3$ (500 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
800.0770	1	C42H30MoN3O4P2	800.0770	-1.3	20.7	1	100.00	32.5	even	ok

Fig. S21 EI mass spectrum of **5**

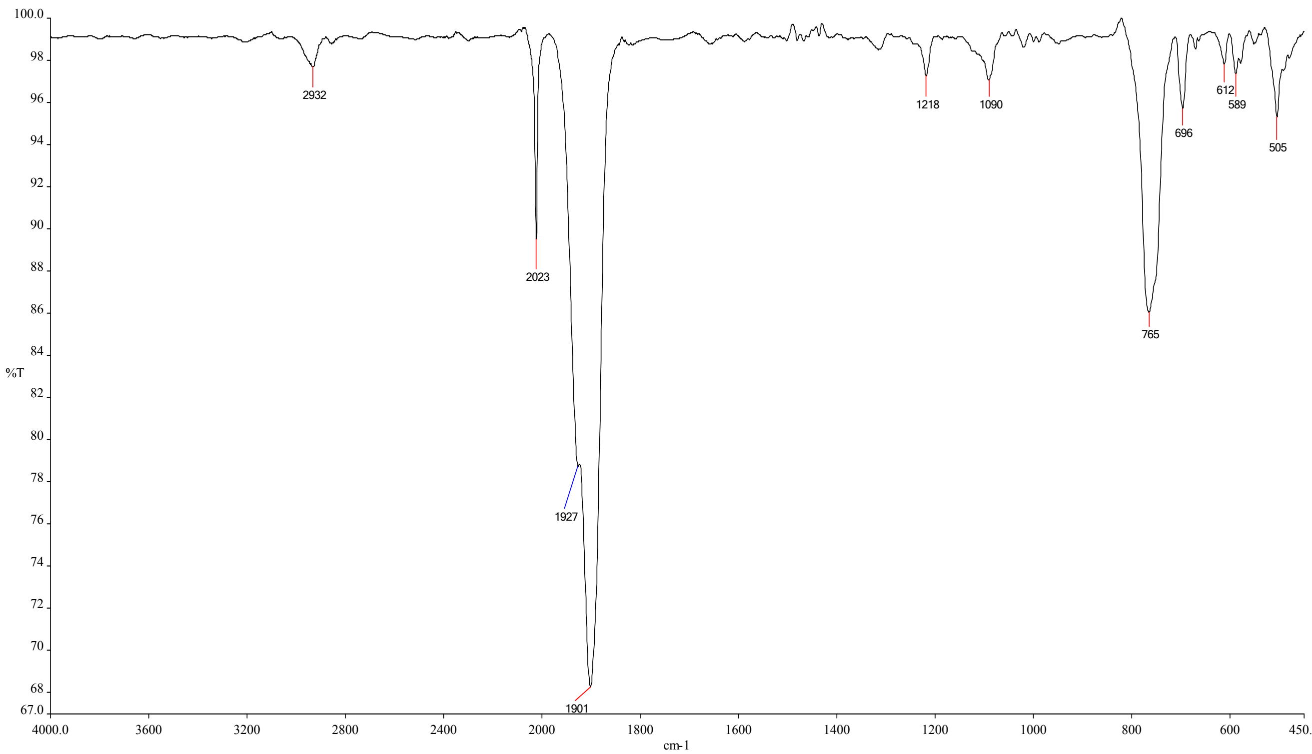


Fig. S22 IR spectrum of **5**

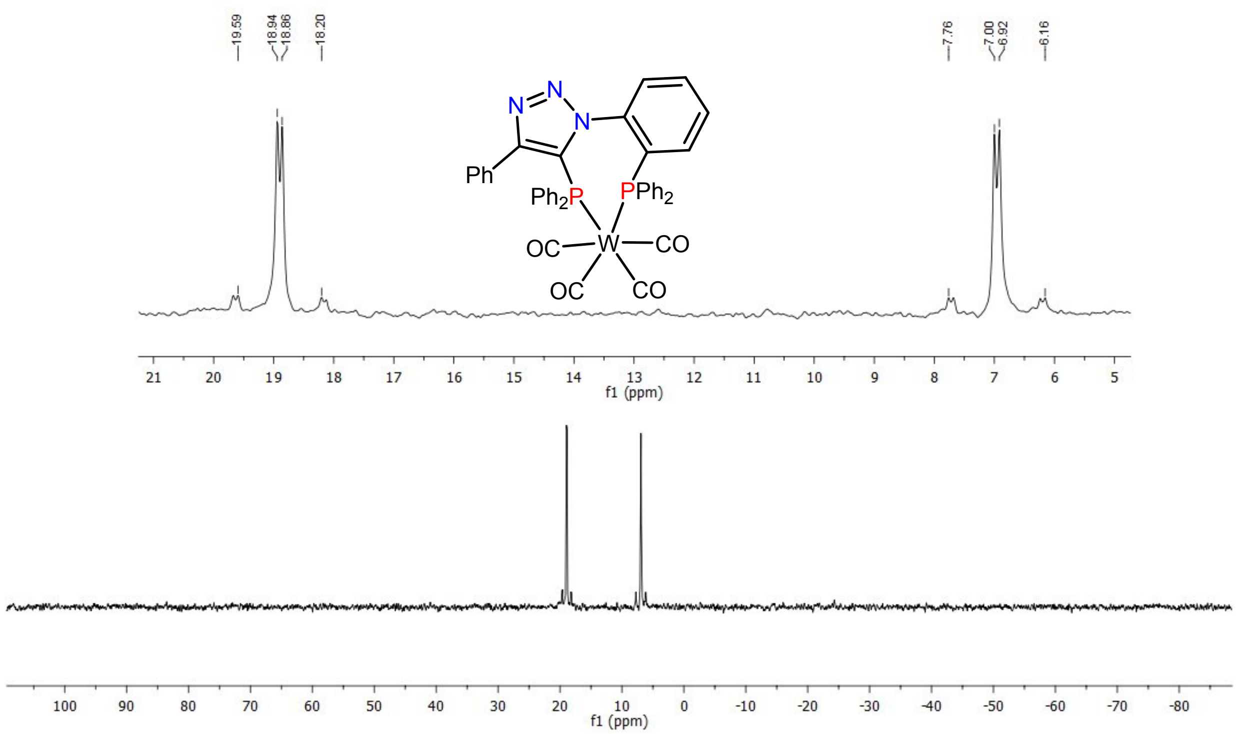


Fig. S23 $^{31}P\{^{1}H\}$ NMR spectrum of **6** in $CDCl_3$ (162 MHz)

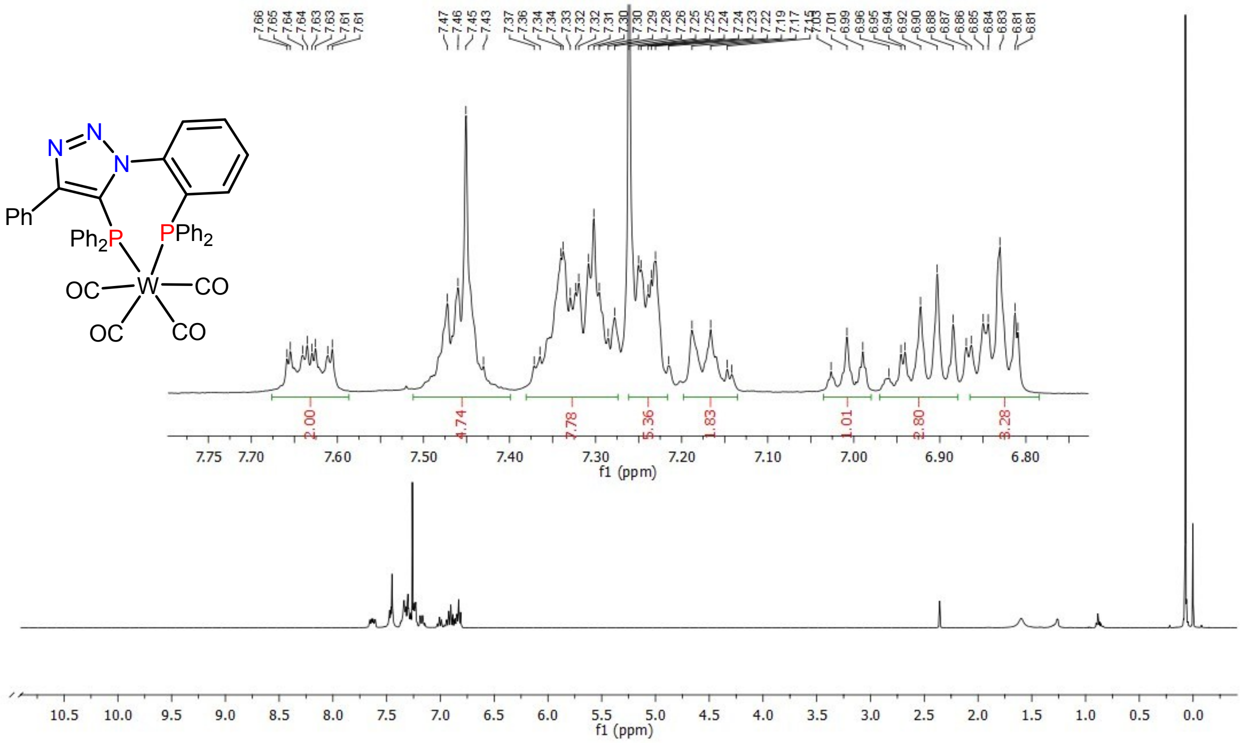
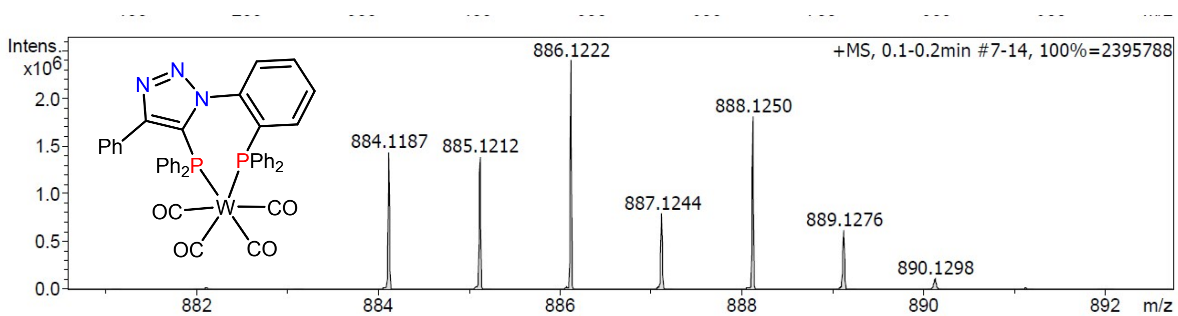


Fig. S24 ^{1}H NMR spectrum of **6** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
886.1222	1	C42H30N3O4P2W	886.1222	0.0	60.0	1	100.00	32.5	even	ok

Fig. S25 EI mass spectrum of **6**

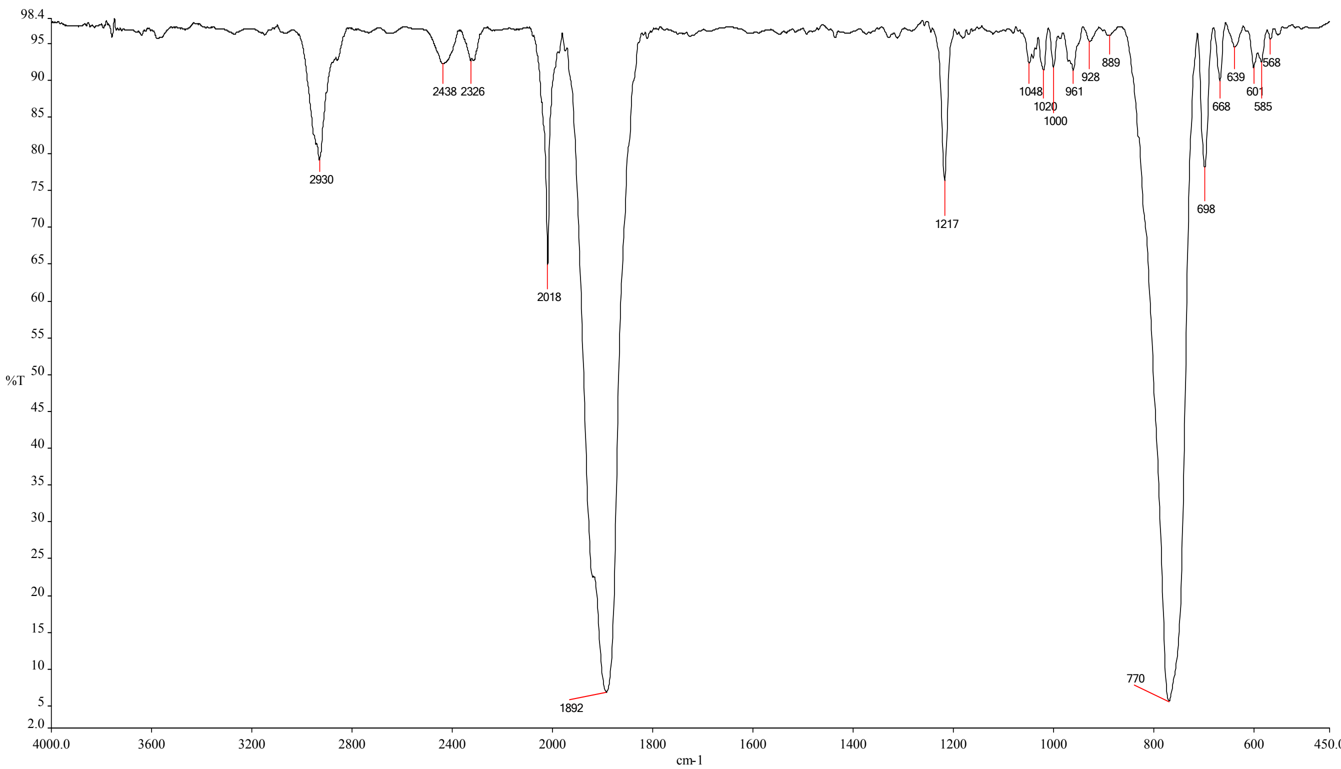


Fig. S26 IR spectrum of **6**

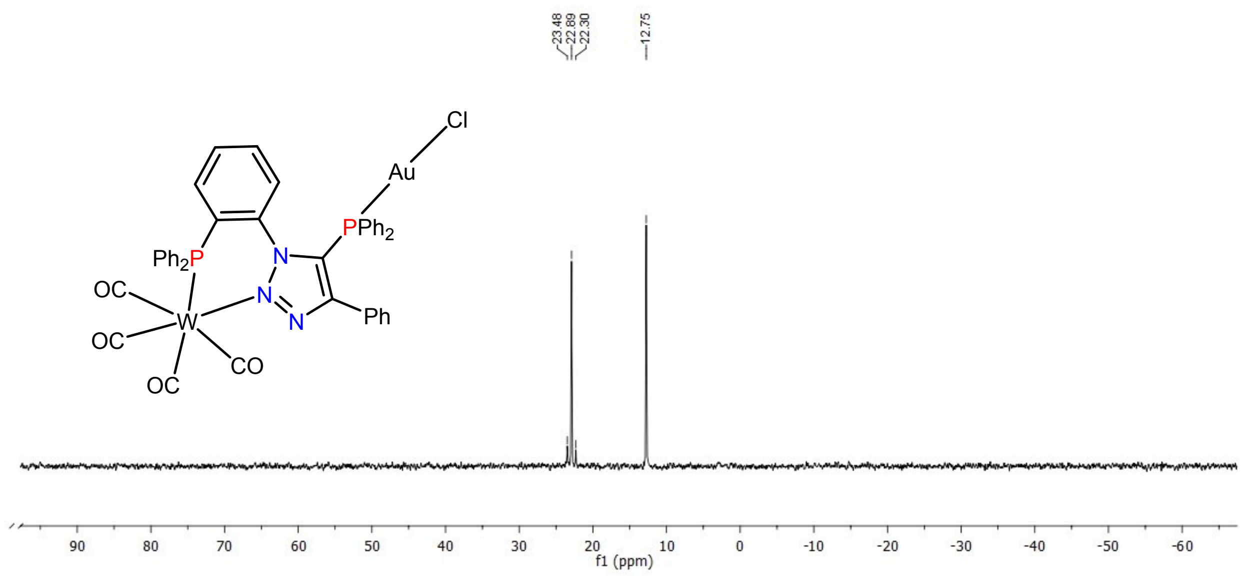


Fig. S27 $^{31}P\{^1H\}$ NMR spectrum of **7** in $CDCl_3$ (2022 MHz)

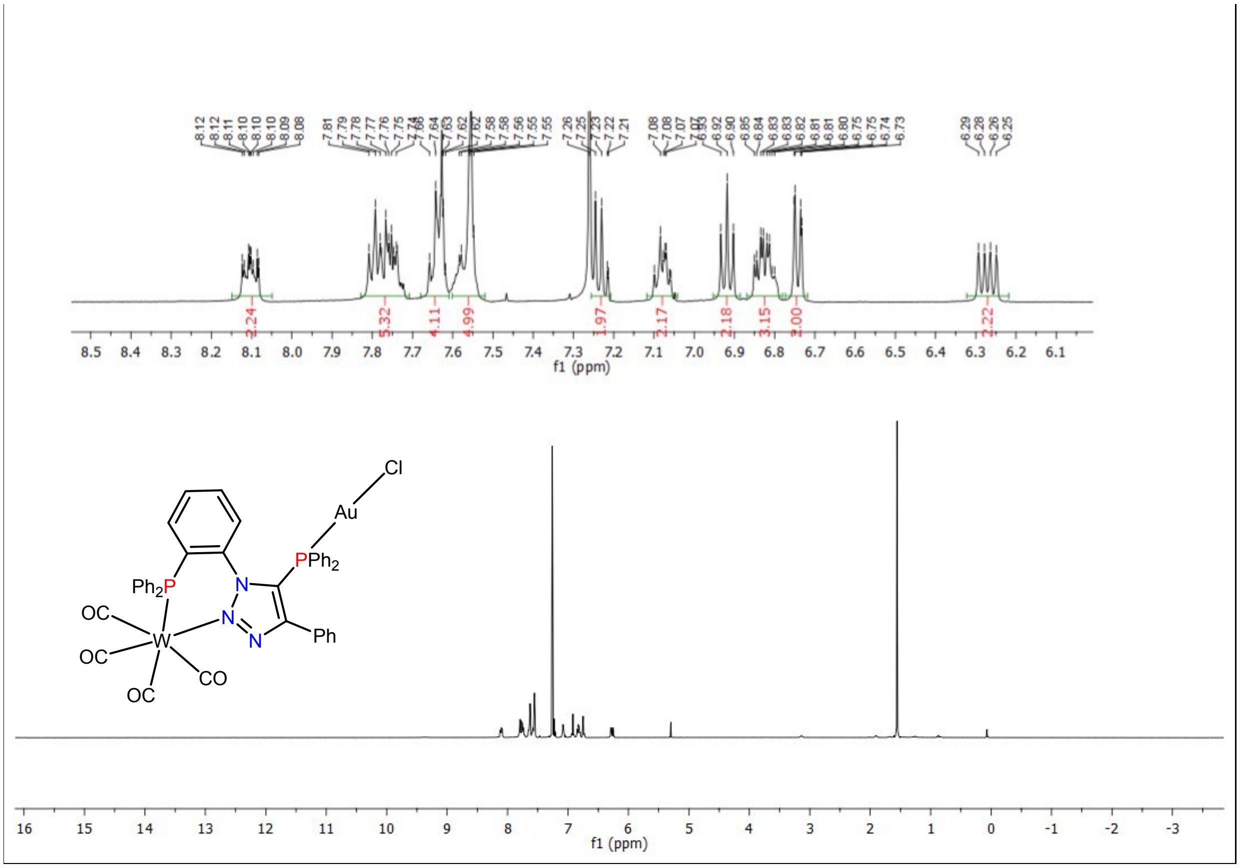


Fig. S28 ^{1}H NMR spectrum of **7** in $CDCl_3$ (500 MHz)

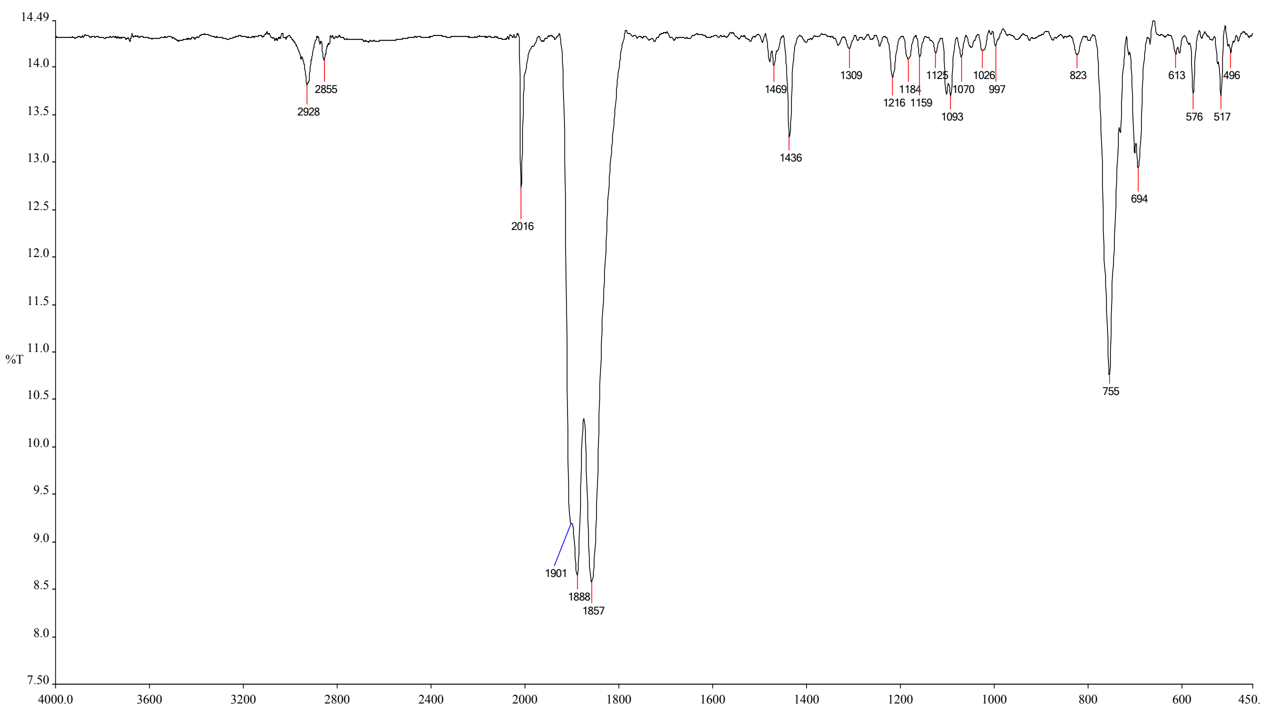


Fig. S29 IR spectrum of **7**

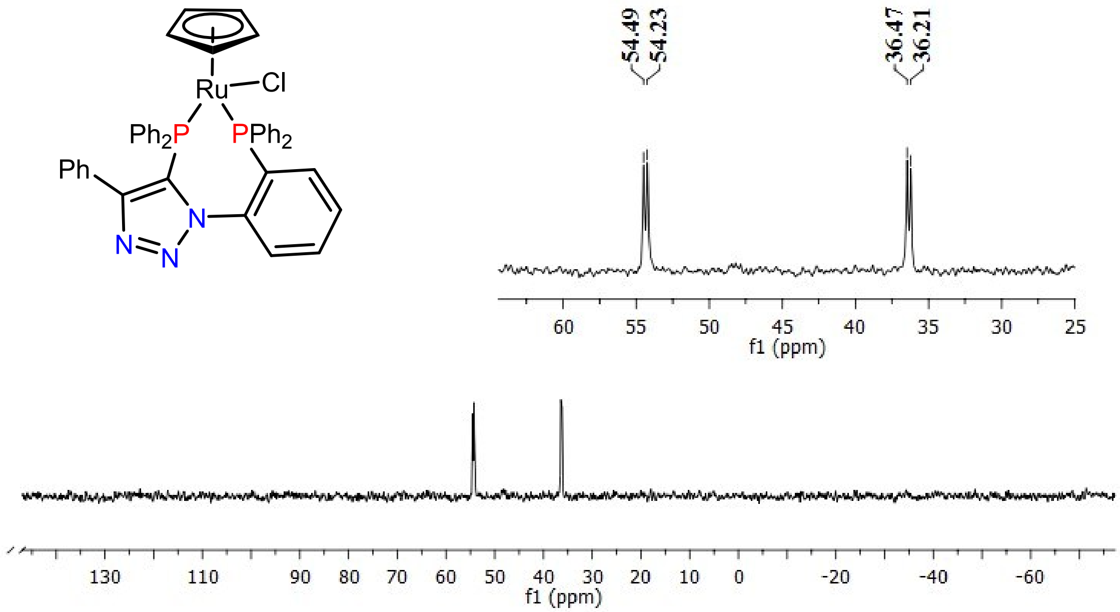


Fig. S30 $^{31}P\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$ (202 MHz)

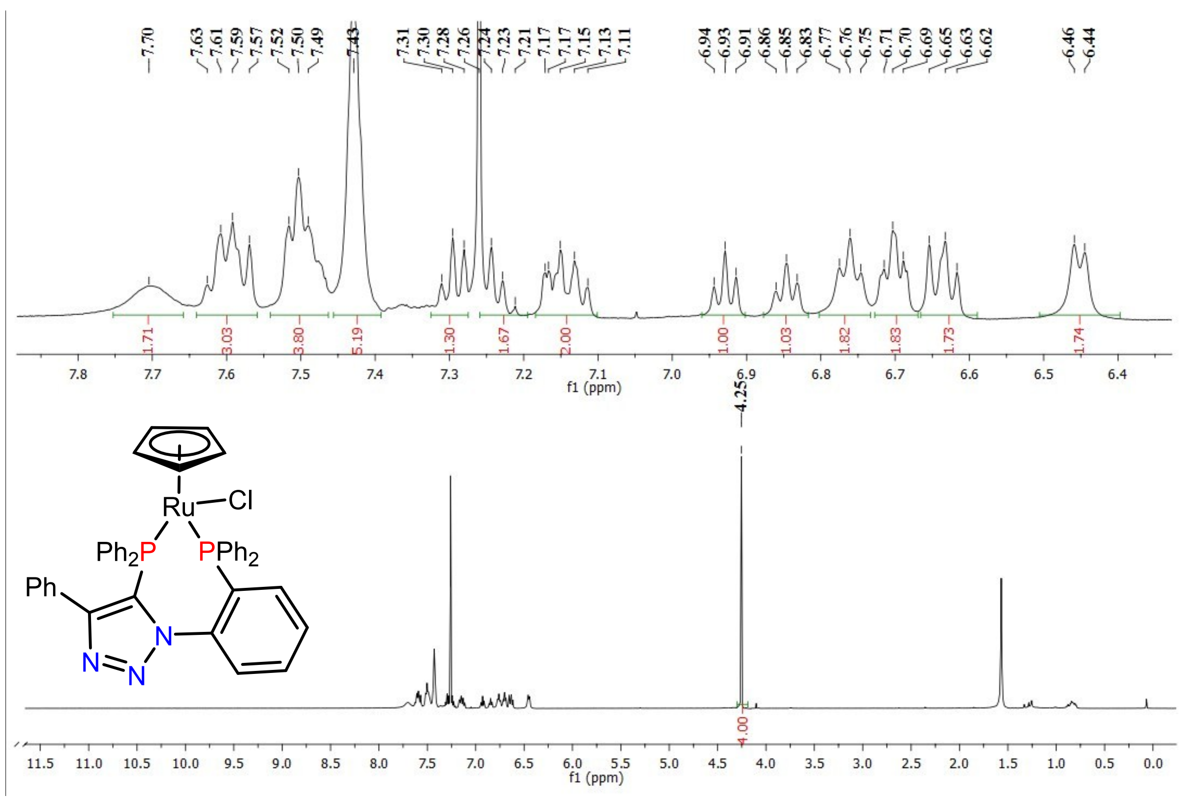
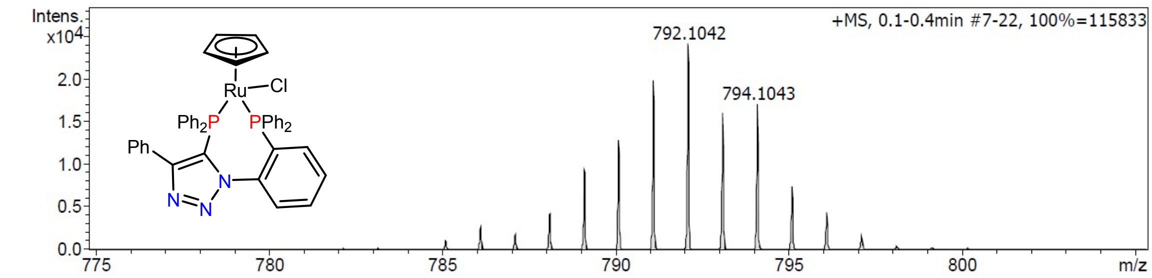


Fig. S31 ^{1}H NMR spectrum of **8** in $CDCl_3$ (500 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
792.1042	1	C43H35ClN3P2Ru	792.1041	0.1	84.7	1	100.00	29.0	odd	-

Fig. S32 EI mass spectrum of **8**

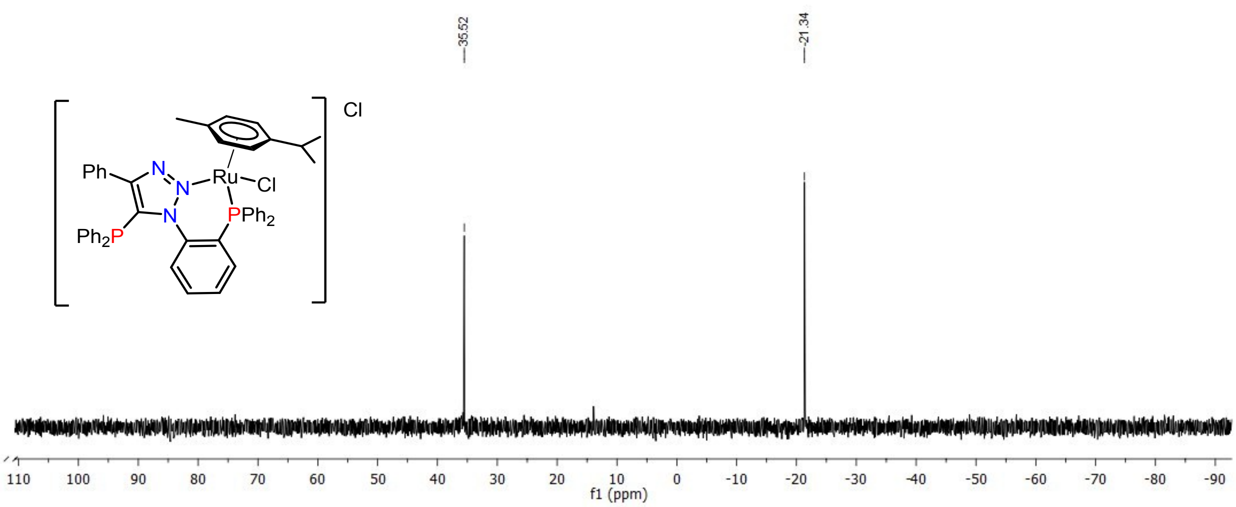


Fig. S33 $^{31}P\{^{1}H\}$ NMR spectrum of **9** in $CDCl_3$ (202 MHz)

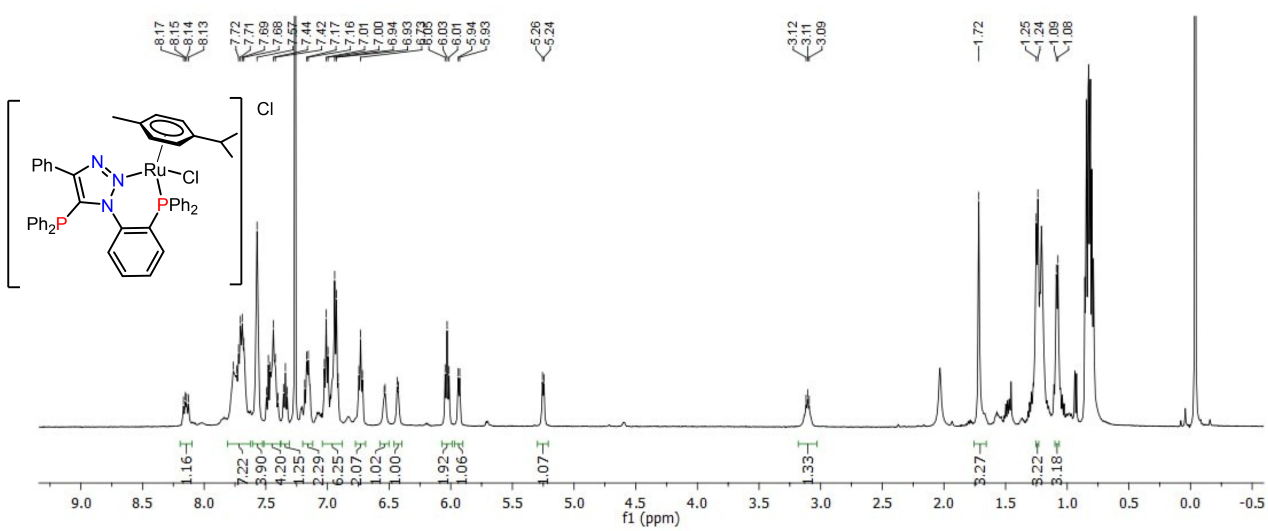
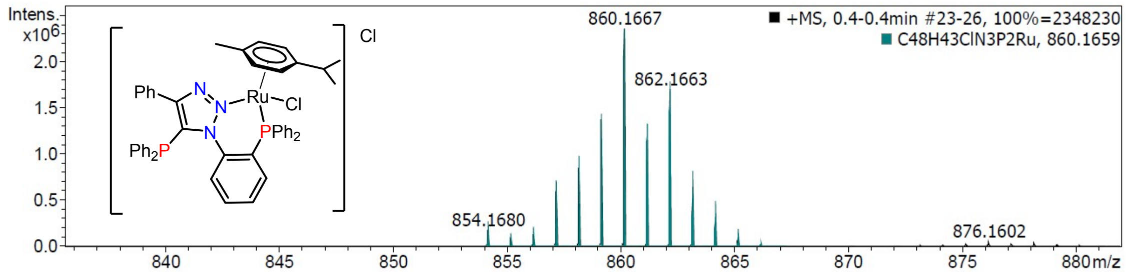


Fig. S34 ^{1}H NMR spectrum of **9** in $CDCl_3$ (500 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
860.1667	1	C48H43ClN3P2Ru	860.1669	-0.2	46.9	1	100.00	30.0	odd	-

Fig. S35 EI mass spectrum of **9**

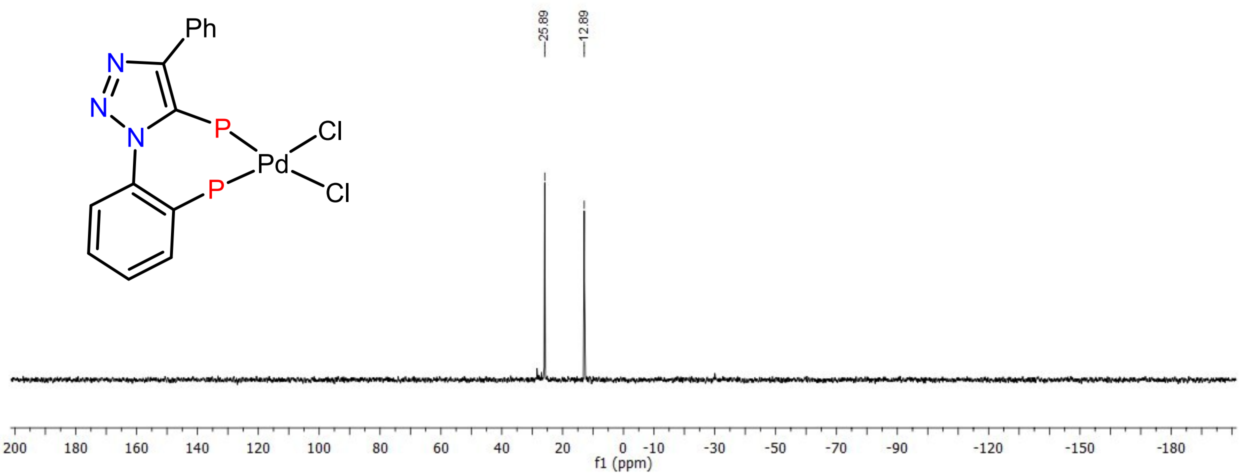


Fig. S36 $^{31}P\{^1H\}$ NMR spectrum of **10** in $CDCl_3$ (202 MHz)

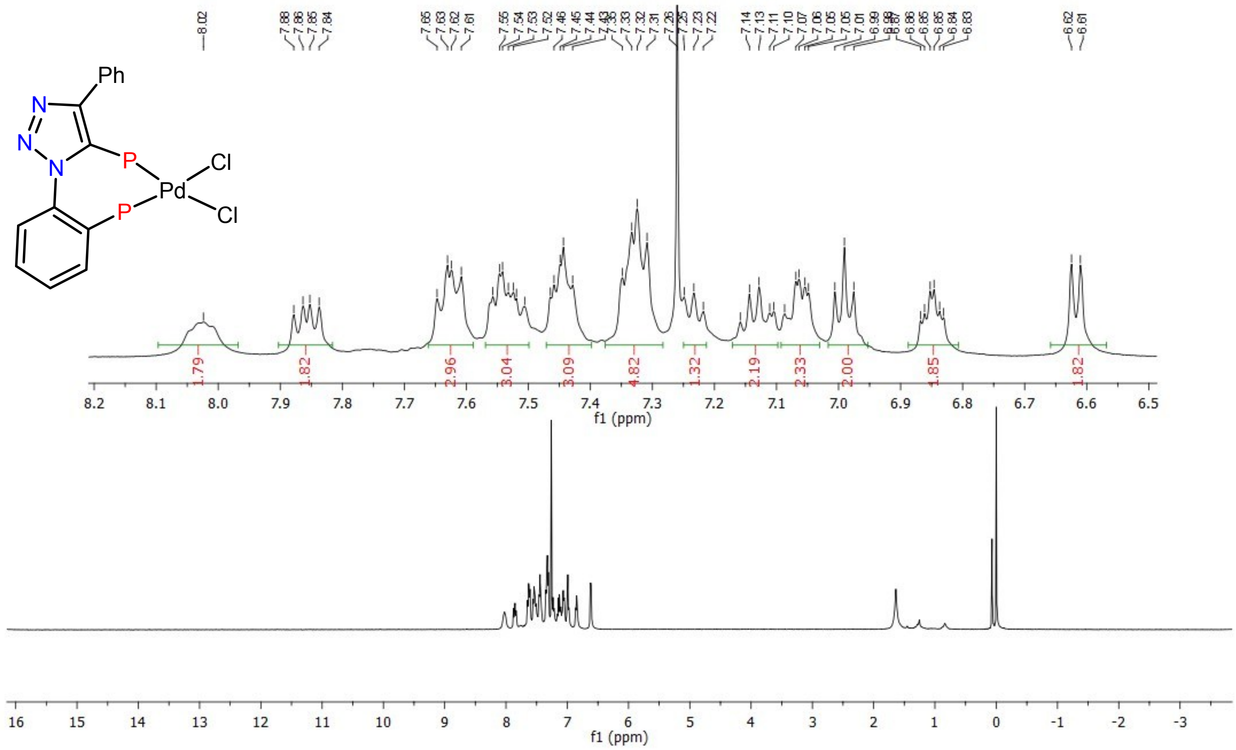
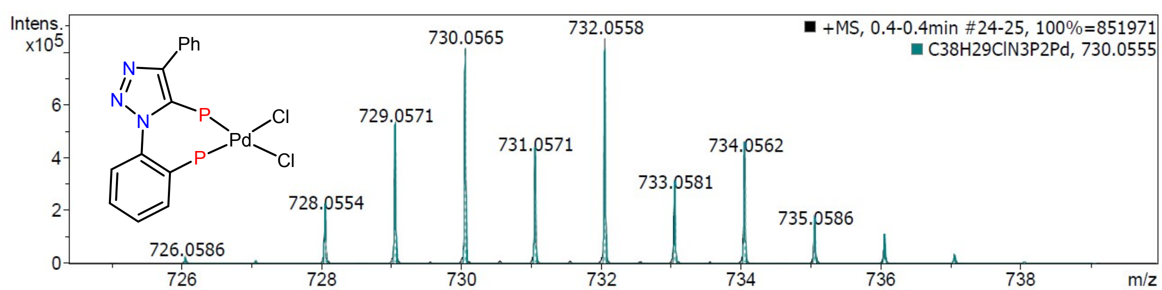


Fig. S37 ^{1}H NMR spectrum of **10** in $CDCl_3$ (500 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
730.0565	1	C38H29ClN3P2Pd	730.0565	-1.4	49.4	1	100.00	26.5	even	ok

Fig. S38 EI mass spectrum of **10**

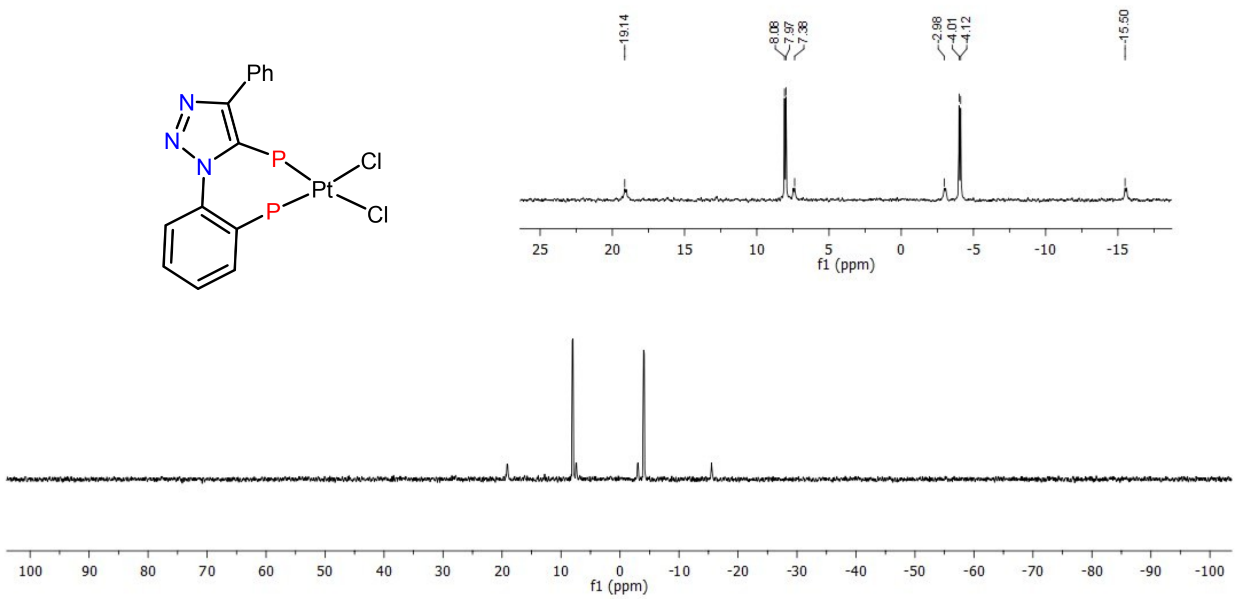


Fig. S39 $^{31}P\{^{1}H\}$ NMR spectrum of **11** in $CDCl_3$ (202 MHz)

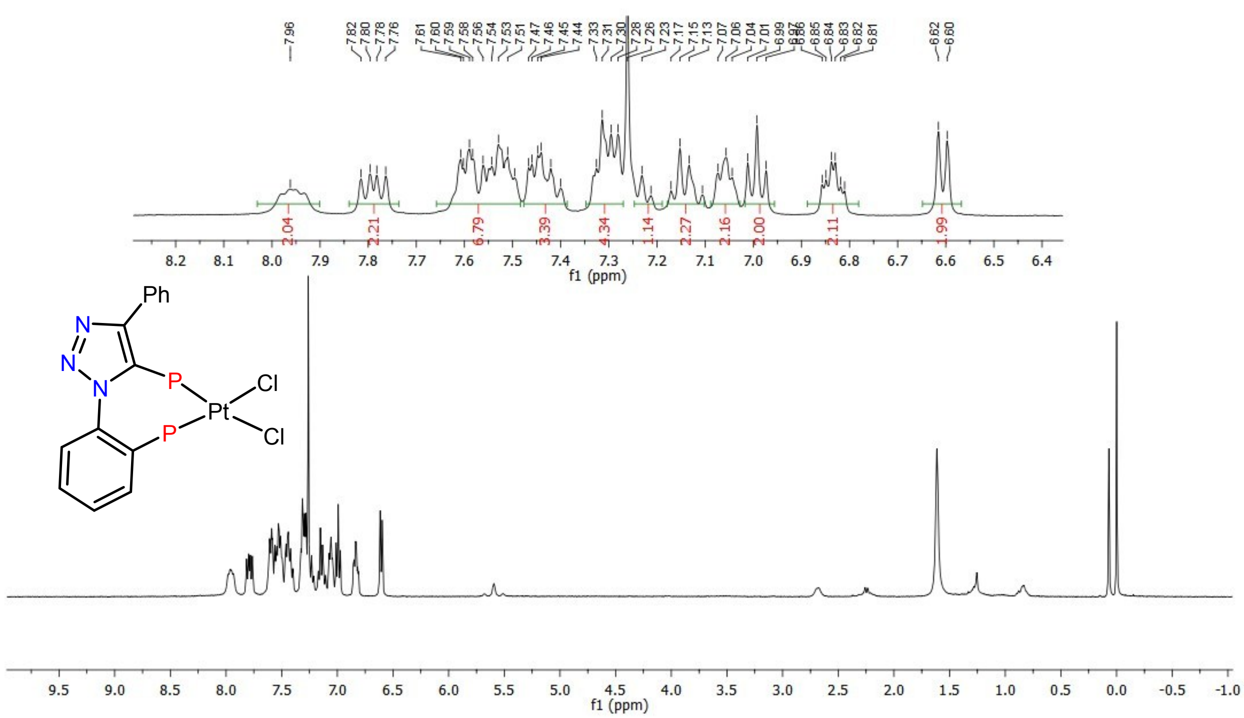
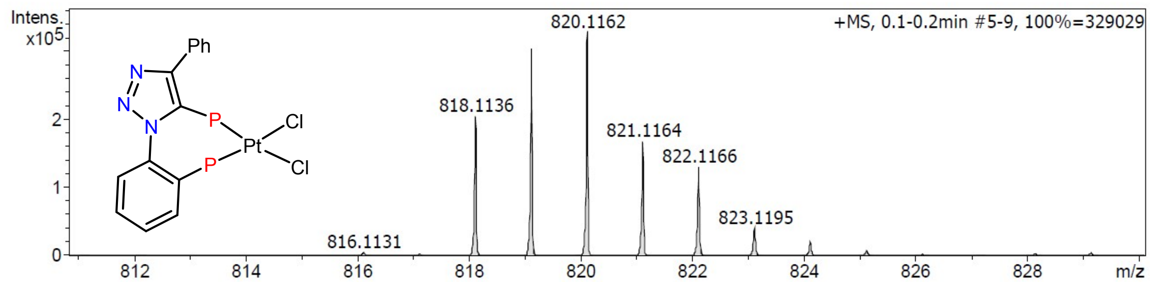


Fig. S40 ^{1}H NMR spectrum of **11** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
820.1162	1	C38H29ClN3P2Pt	819.1171	-0.9	22.4	1	100.00	26.5	even	-

Fig. S41 EI mass spectrum of **11**

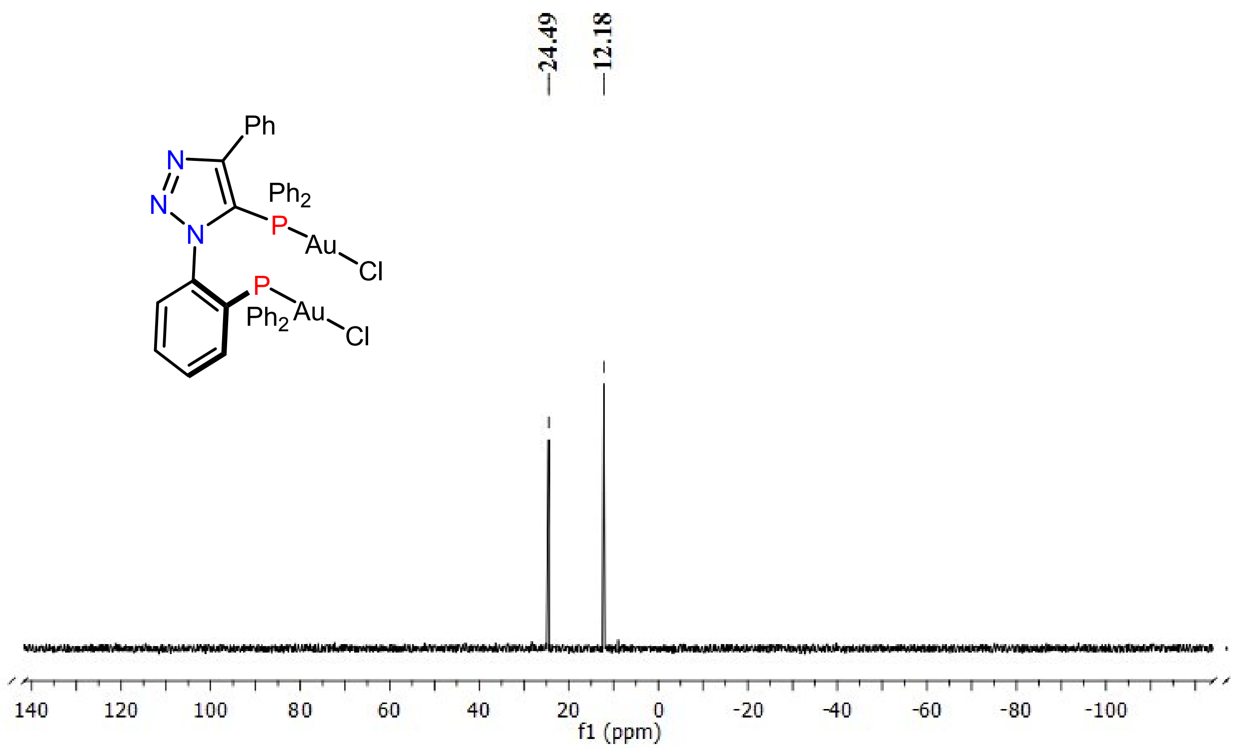


Fig. S42 $^{31}P\{^{1}H\}$ NMR spectrum of **12** in $CDCl_3$ (202 MHz)

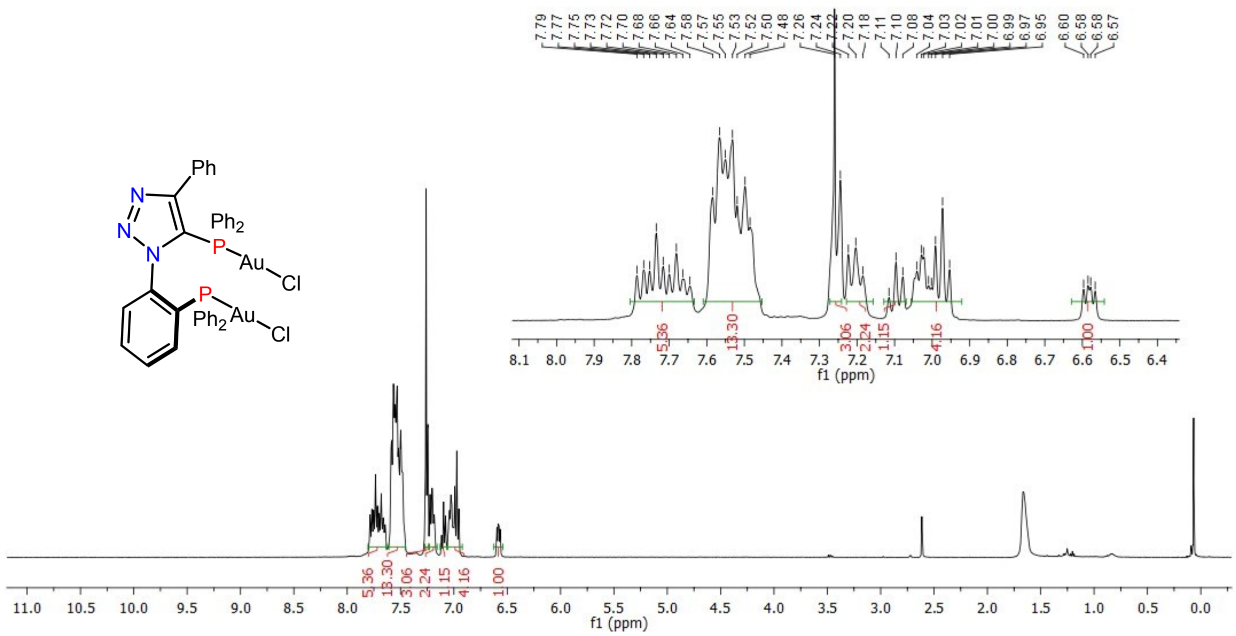
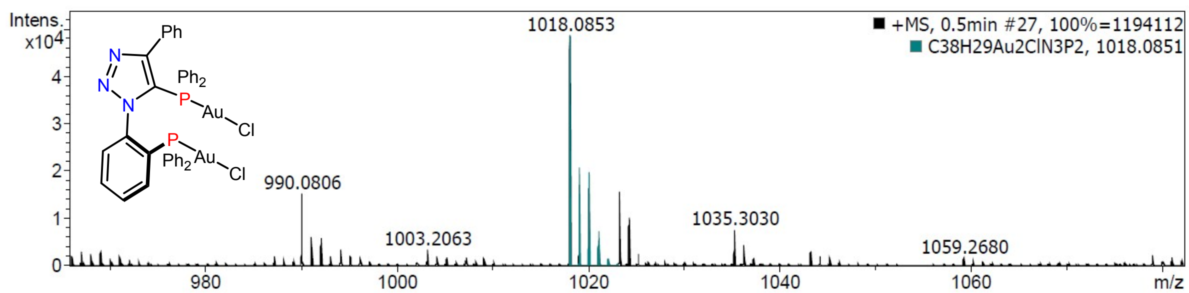


Fig. S43 ^{1}H NMR spectrum of **12** in $CDCl_3$ (400 MHz)



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e¯ Conf	N-Rule
1018.0853	1	C38H29Au2ClN3P2	1018.0851	0.2	46.5	1	100.00	25.5	even	ok

Fig. S44 EI mass spectrum of **12**

(5) NMR spectra of a-i and k

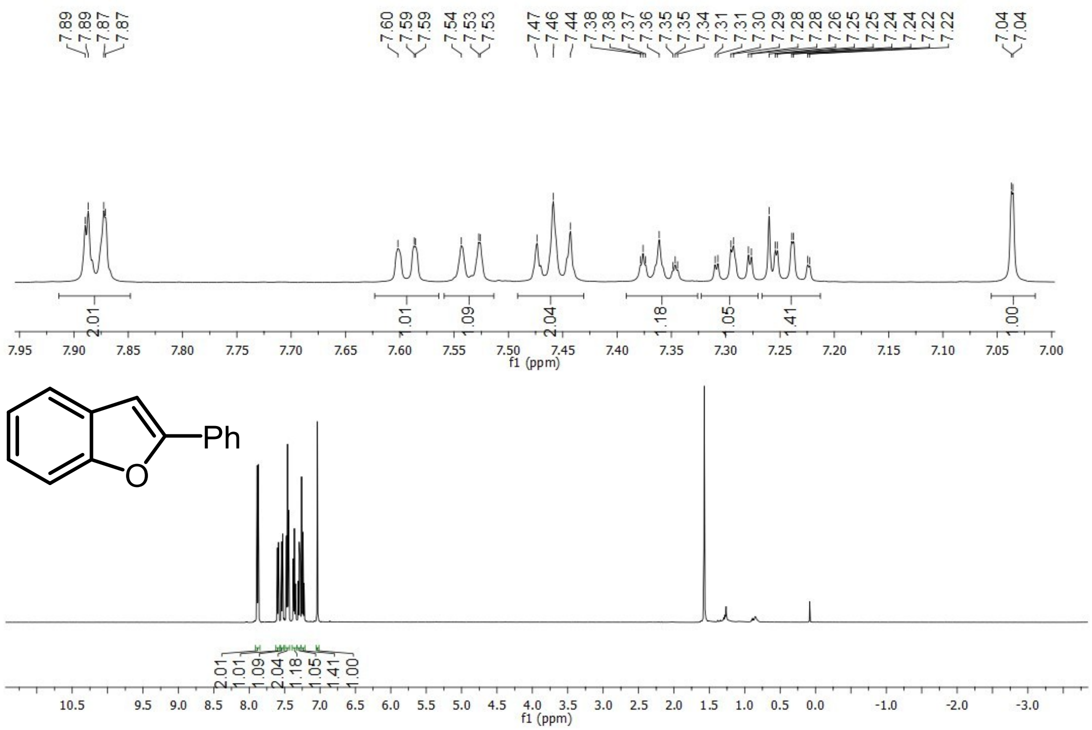


Fig. S45 ^{1}H NMR spectrum of **a** in $CDCl_3$ (500 MHz)

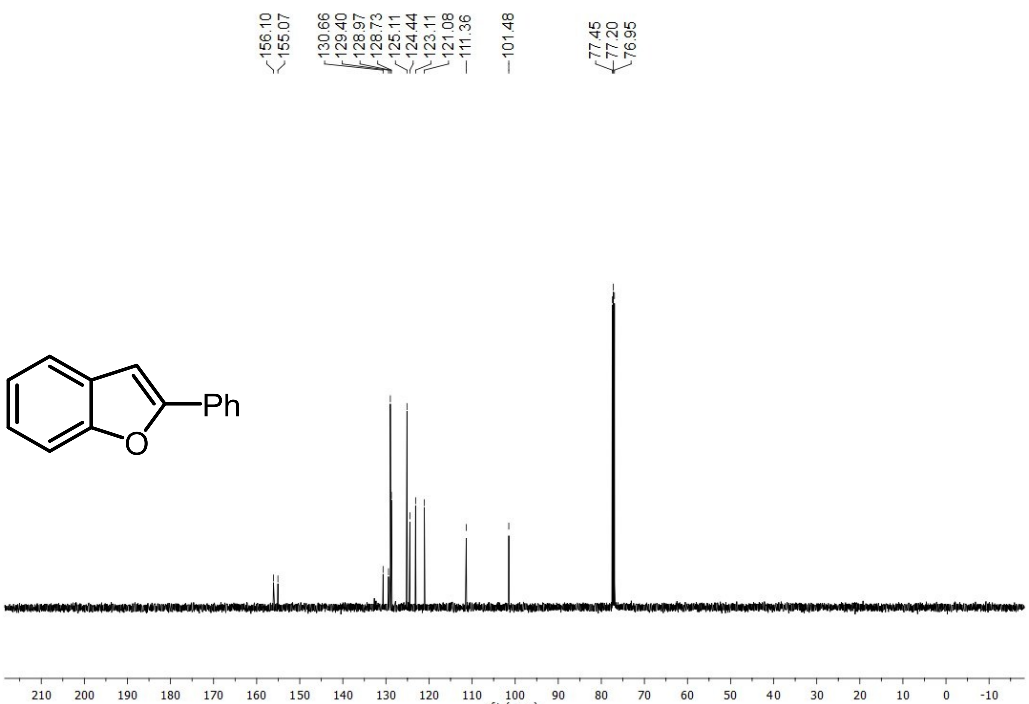


Fig. S46 ^{13}C NMR spectrum of **a** in $CDCl_3$ (126 MHz)

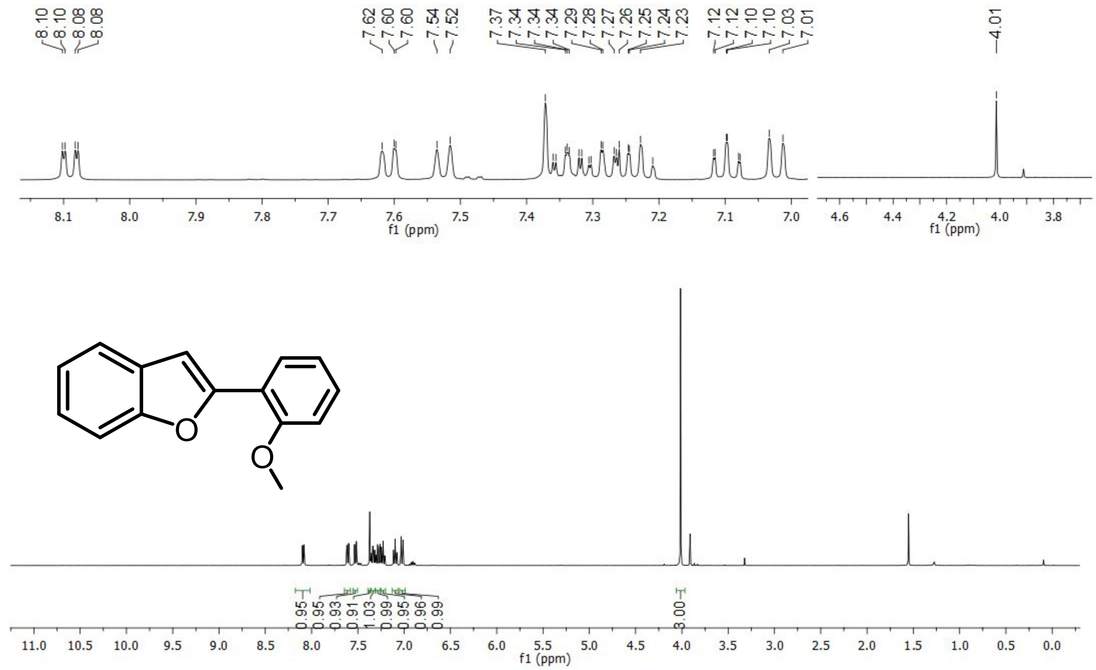


Fig. S47 ^{1}H NMR spectrum of **b** in $CDCl_3$ (400 MHz)

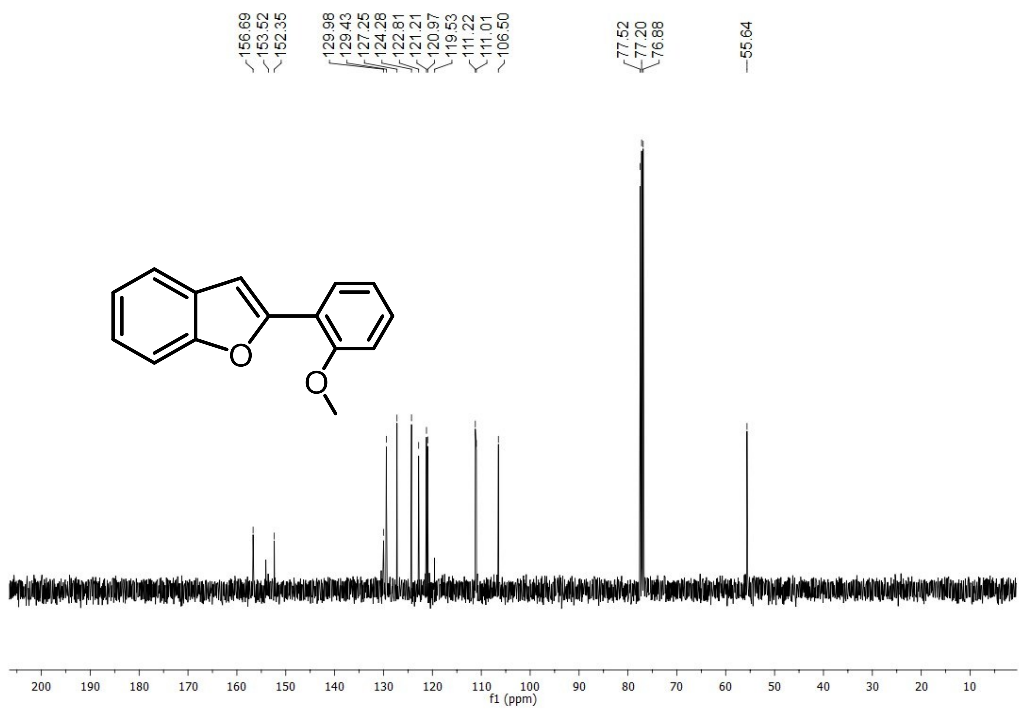


Fig. S48 ^{13}C NMR spectrum of **b** in $CDCl_3$ (100 MHz)

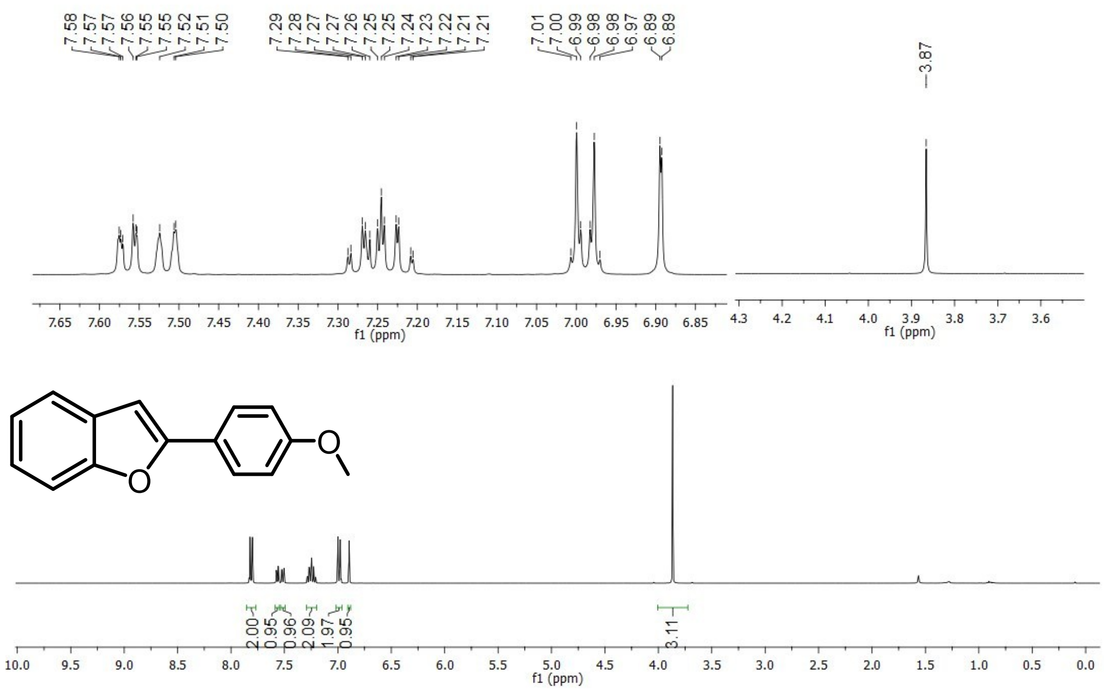


Fig. S49 ^{1}H NMR spectrum of **c** in $CDCl_3$ (400 MHz)

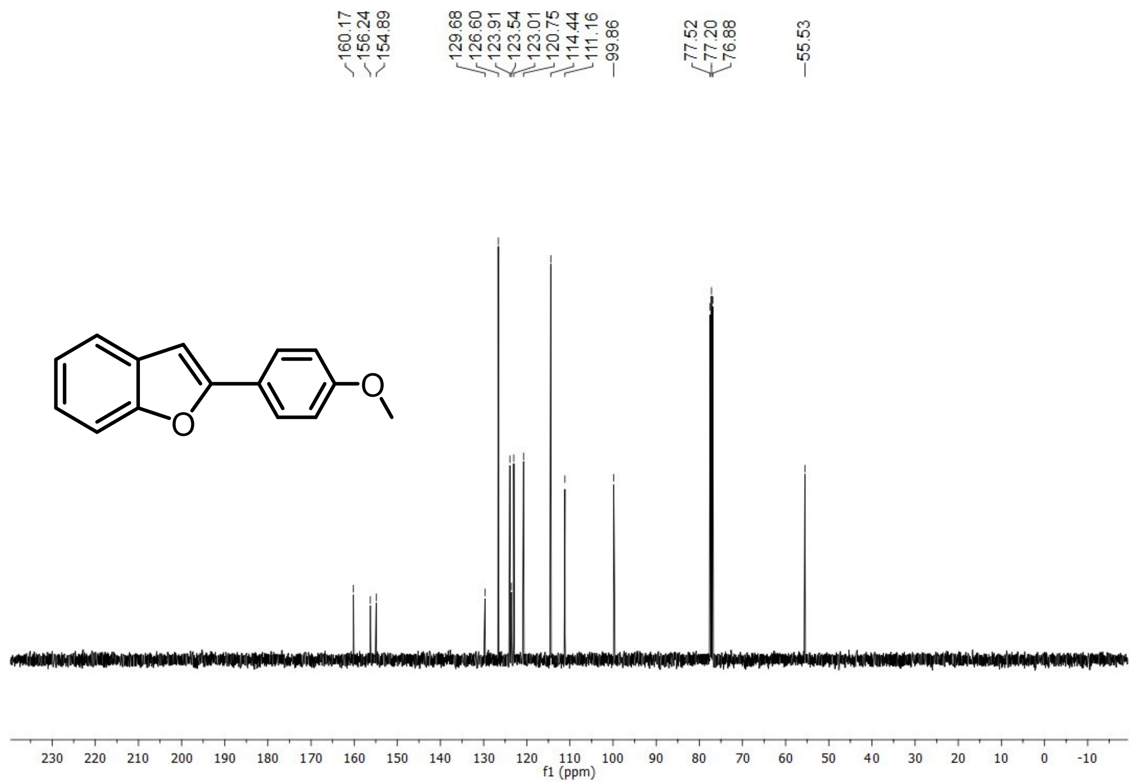


Fig. S50 ^{13}C NMR spectrum of **c** in $CDCl_3$ (100 MHz)

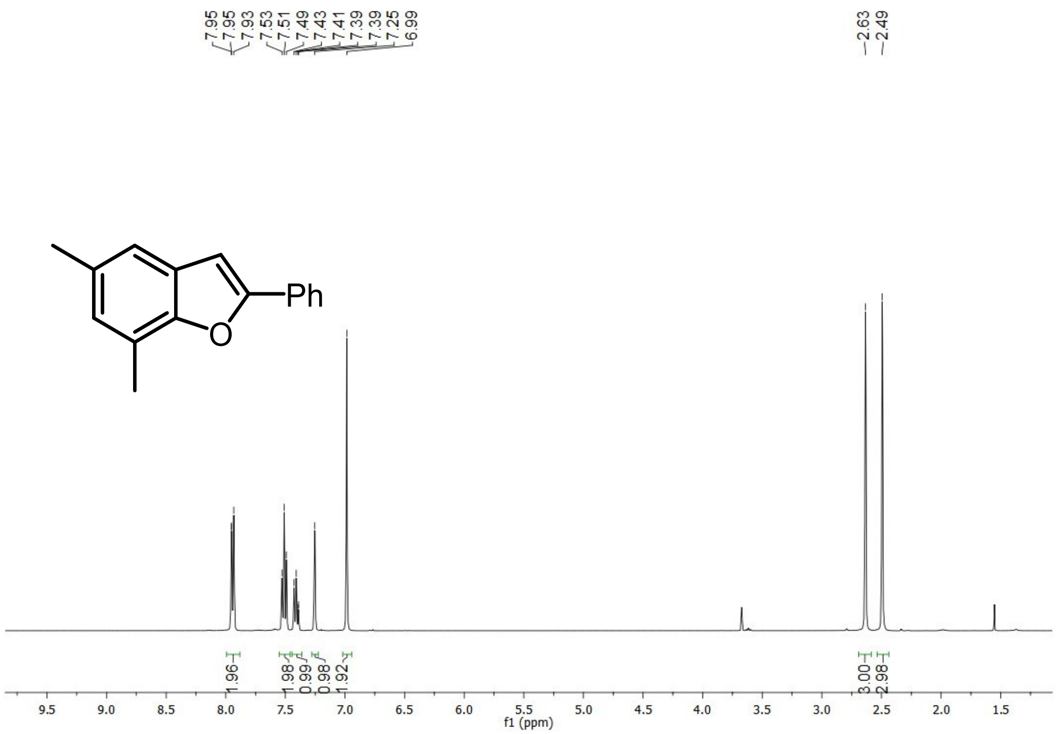


Fig. S51 ^{1}H NMR spectrum of **d** in $CDCl_3$ (400 MHz)

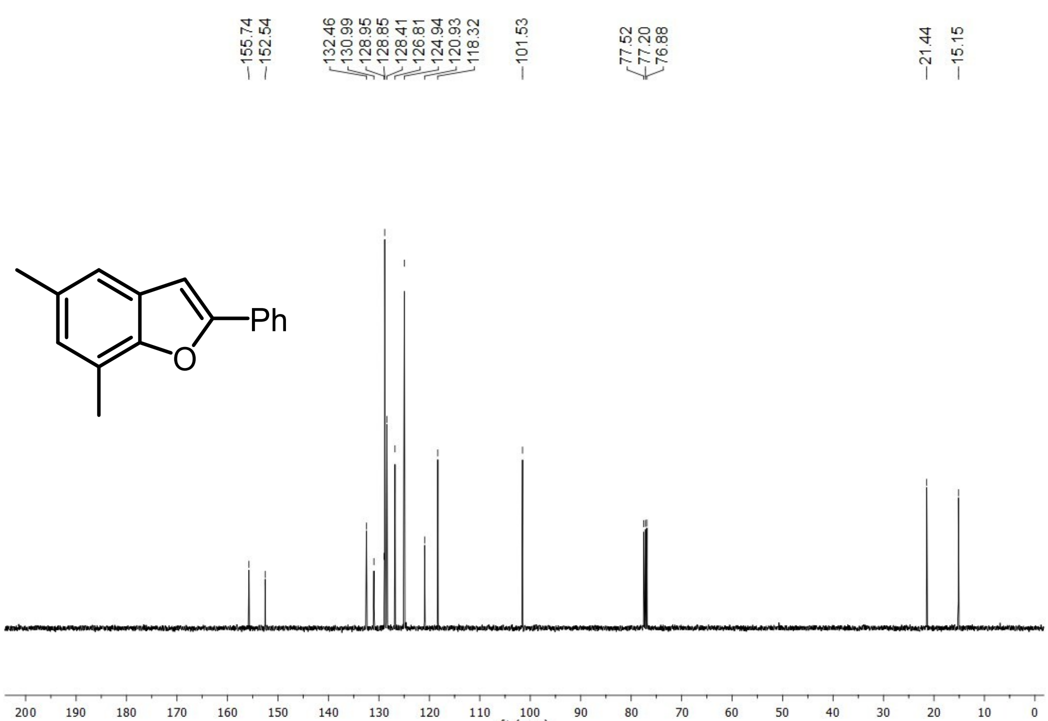


Fig. S52 ^{13}C NMR spectrum of **d** in $CDCl_3$ (100 MHz)

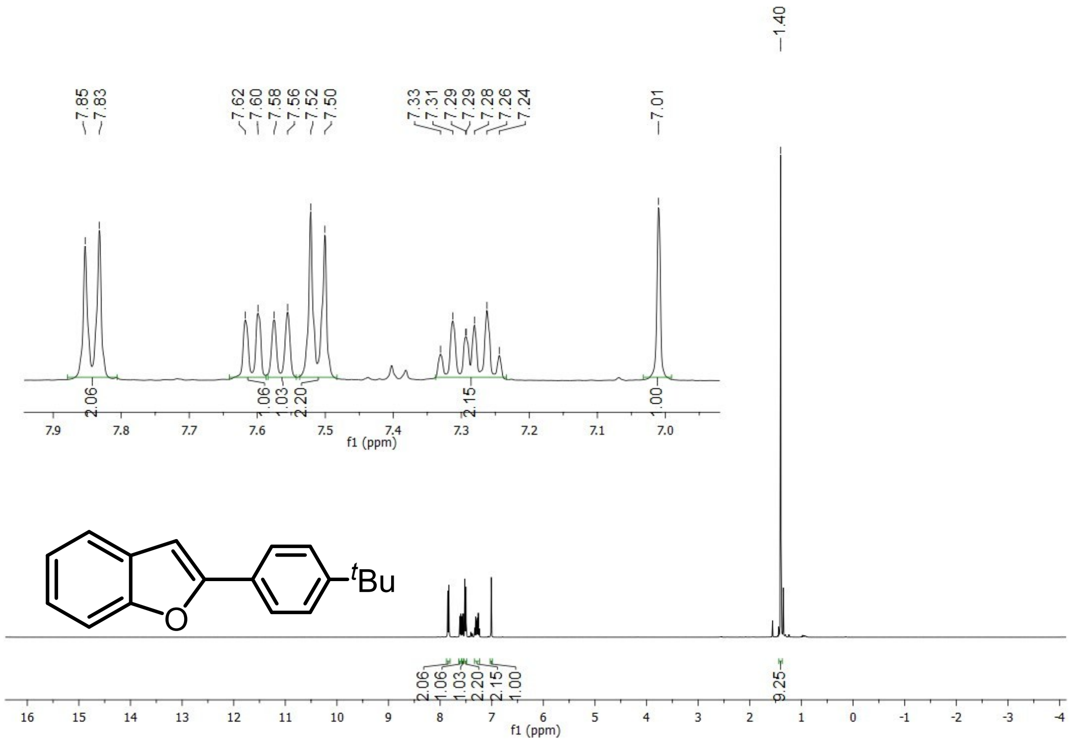


Fig. S53 ^{1}H NMR spectrum of **e** in $CDCl_3$ (400 MHz)

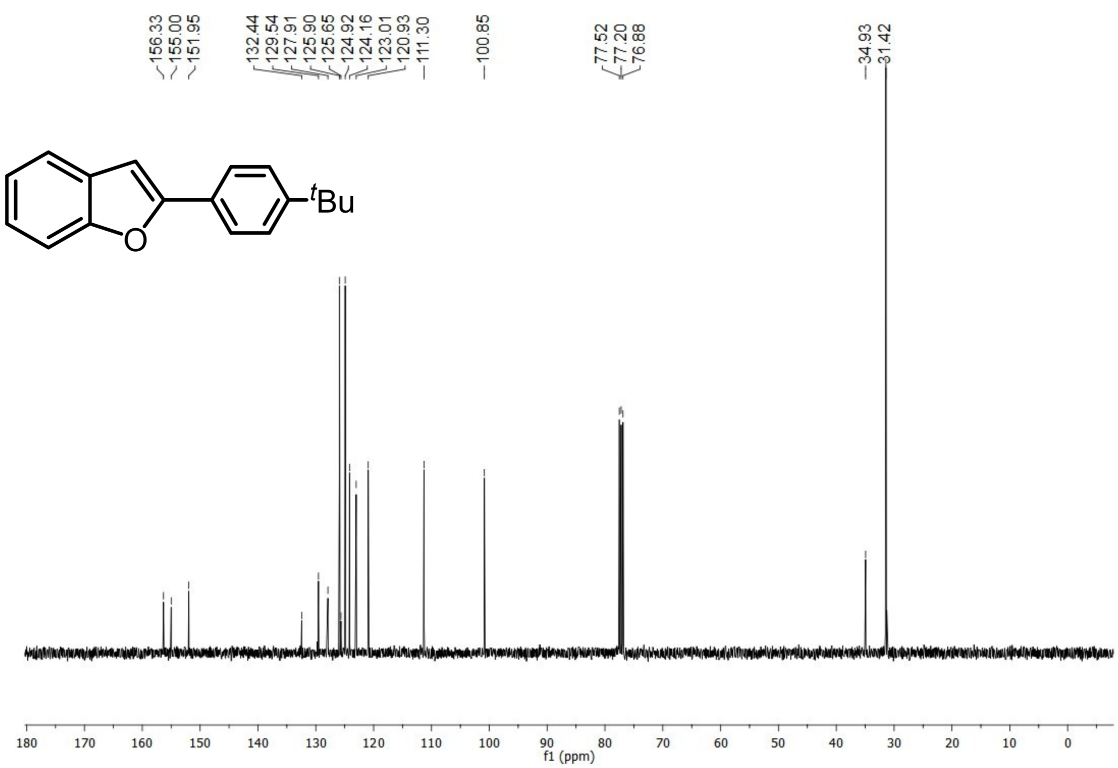


Fig. S54 ^{13}C NMR spectrum of **e** in $CDCl_3$ (100 MHz)

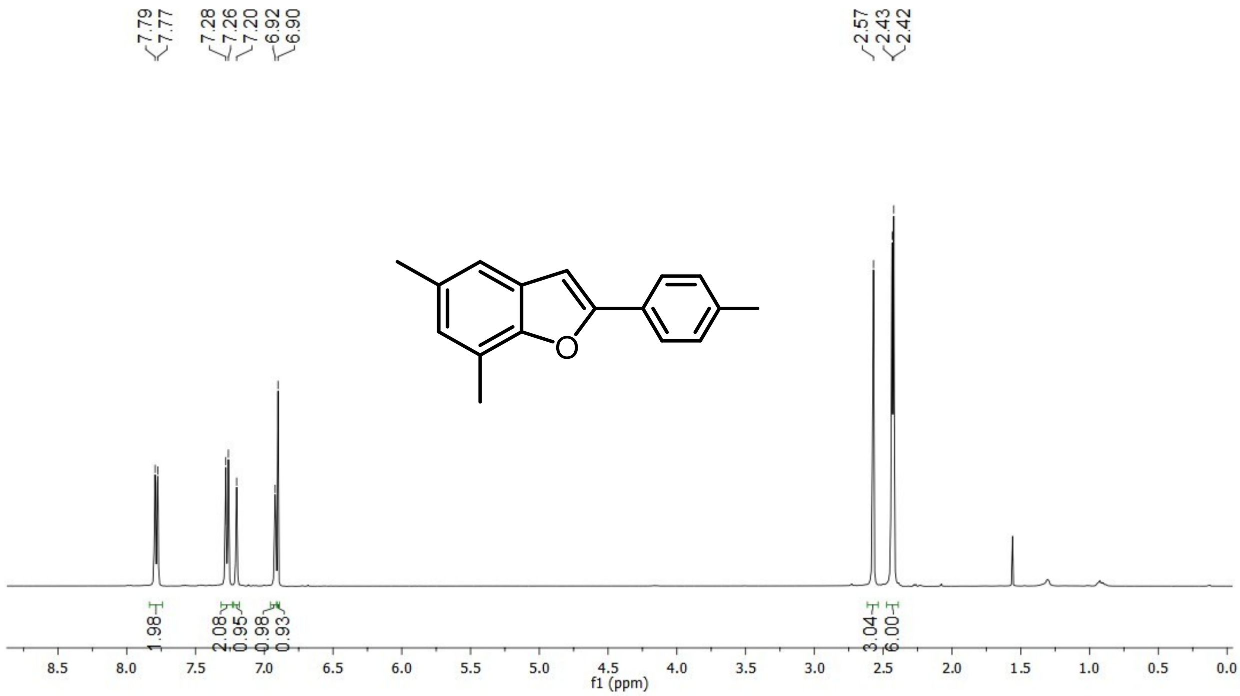


Fig. S55 ^{1}H NMR spectrum of **f** in $CDCl_3$ (400 MHz)

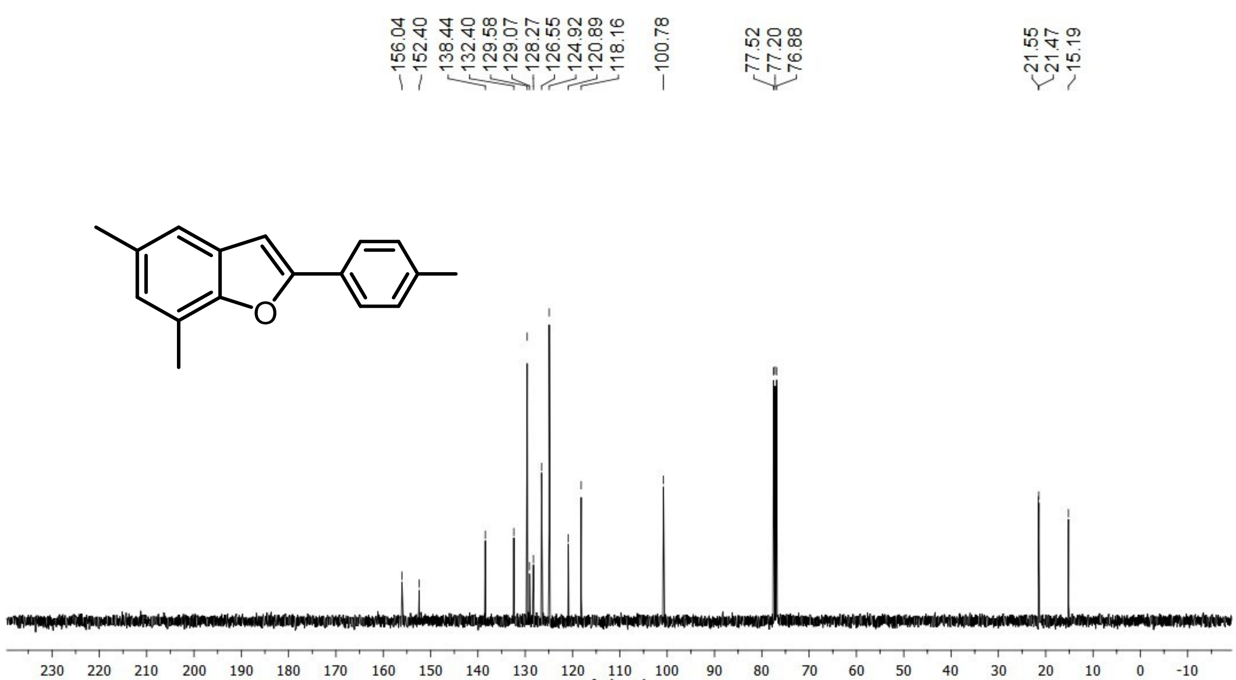


Fig. S56 ^{13}C NMR spectrum of **f** in $CDCl_3$ (100 MHz)

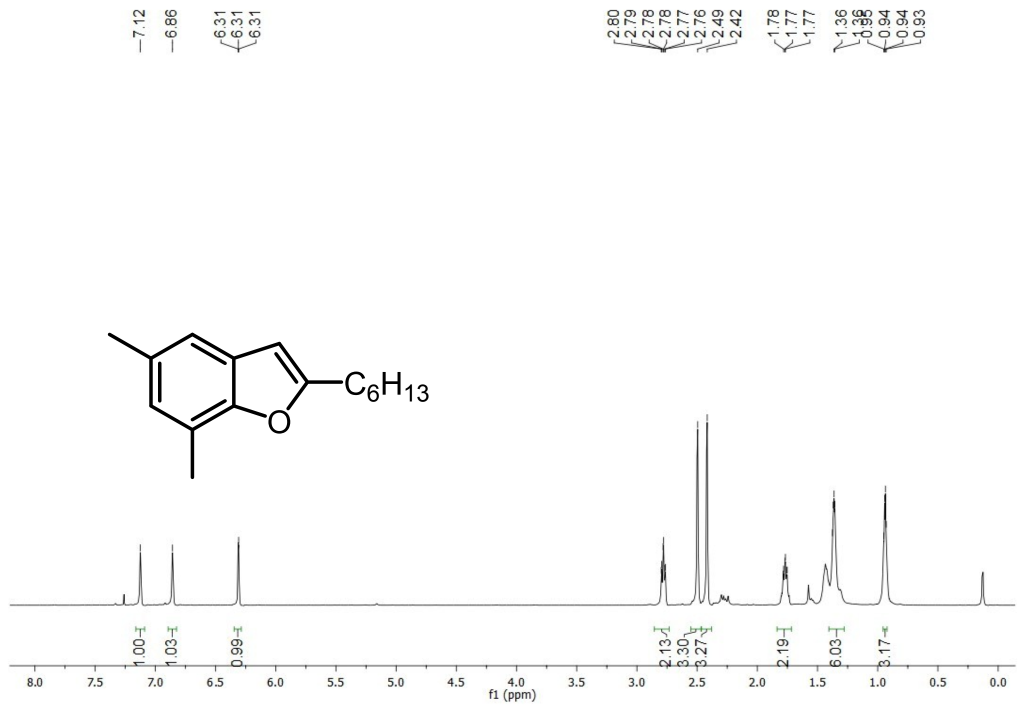


Fig. S57 ^{1}H NMR spectrum of **g** in $CDCl_3$ (500 MHz)

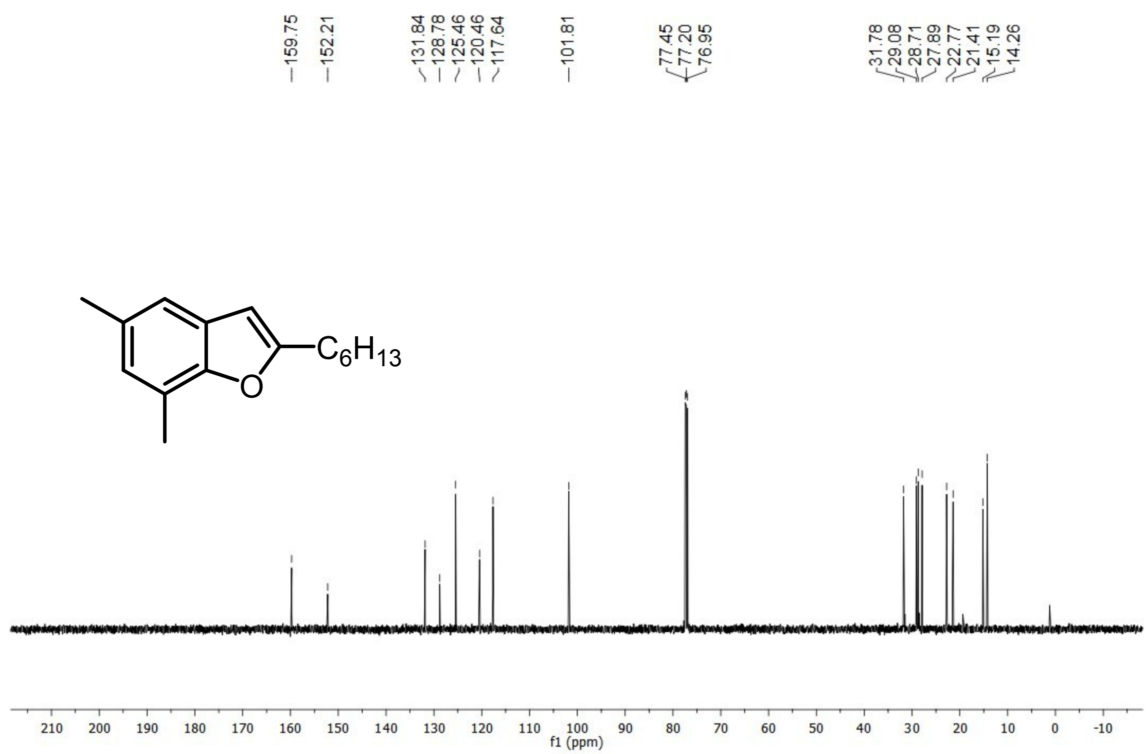


Fig. S58 ^{13}C NMR spectrum of **g** in $CDCl_3$ (126 MHz)

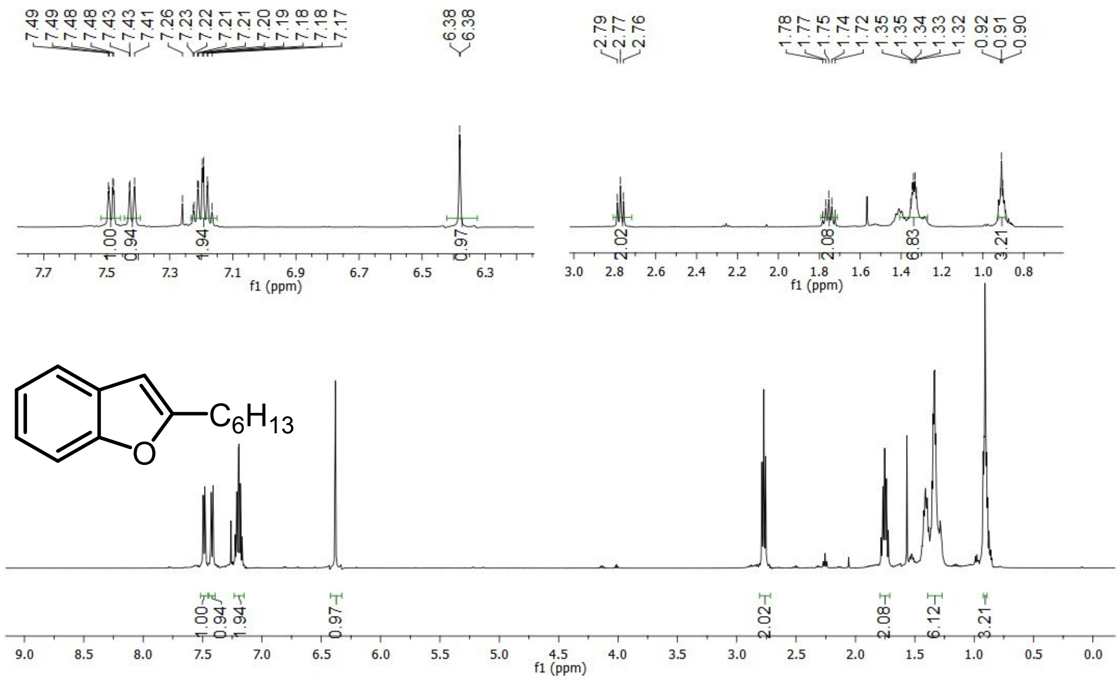


Fig. S59 ^{1}H NMR spectrum of **h** in $CDCl_3$ (500 MHz)

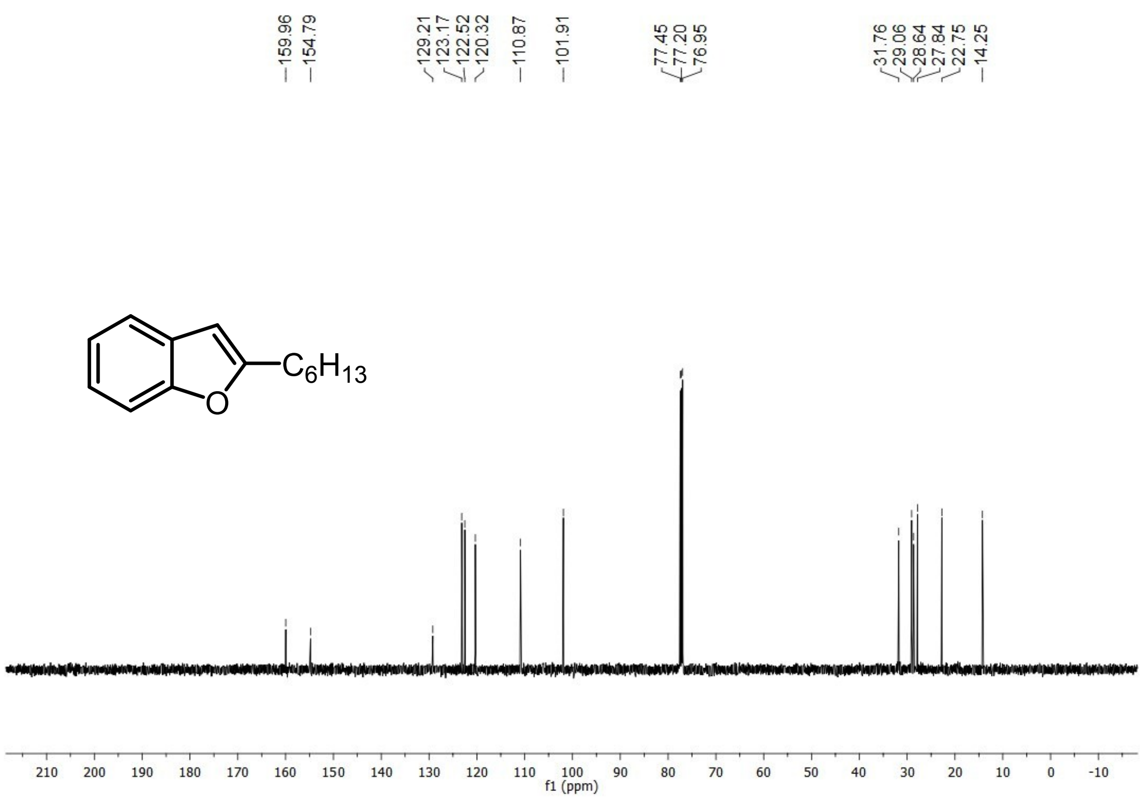


Fig. S60 ^{13}C NMR spectrum of **h** in $CDCl_3$ (126 MHz)

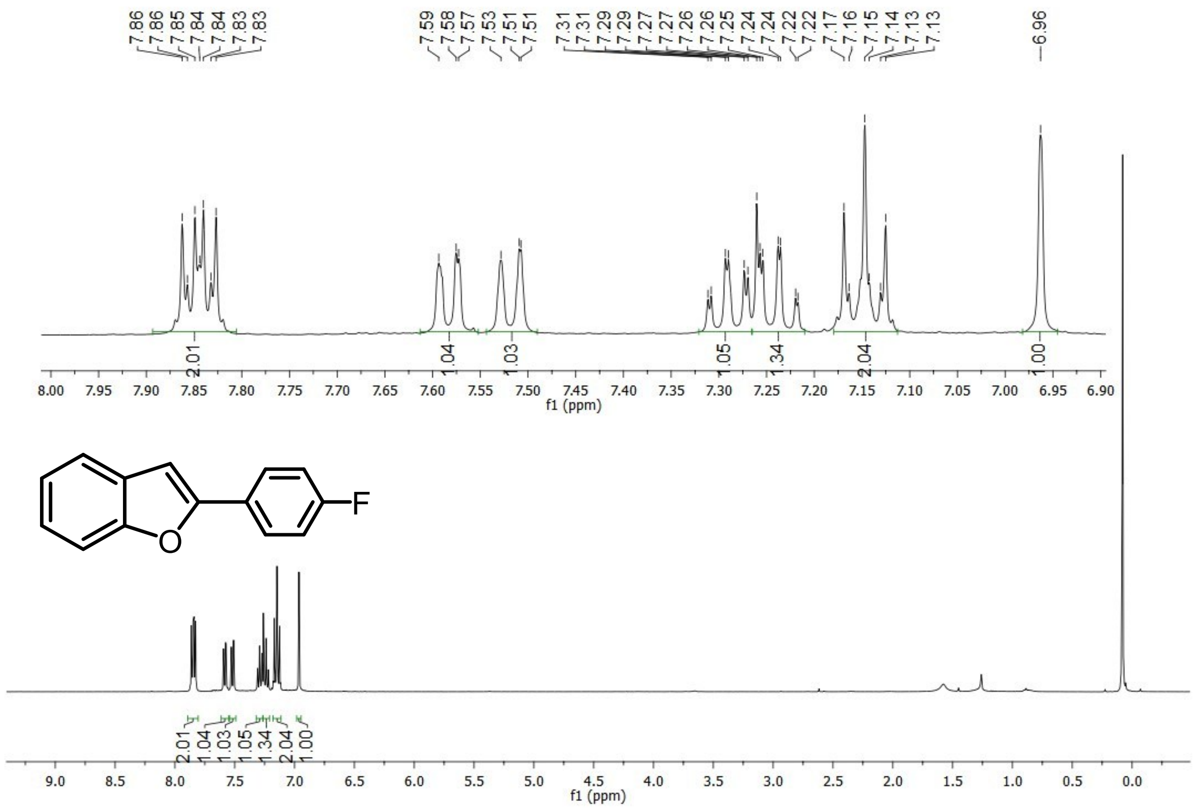


Fig. S61 ^{1}H NMR spectrum of **i** in $CDCl_3$ (400 MHz)

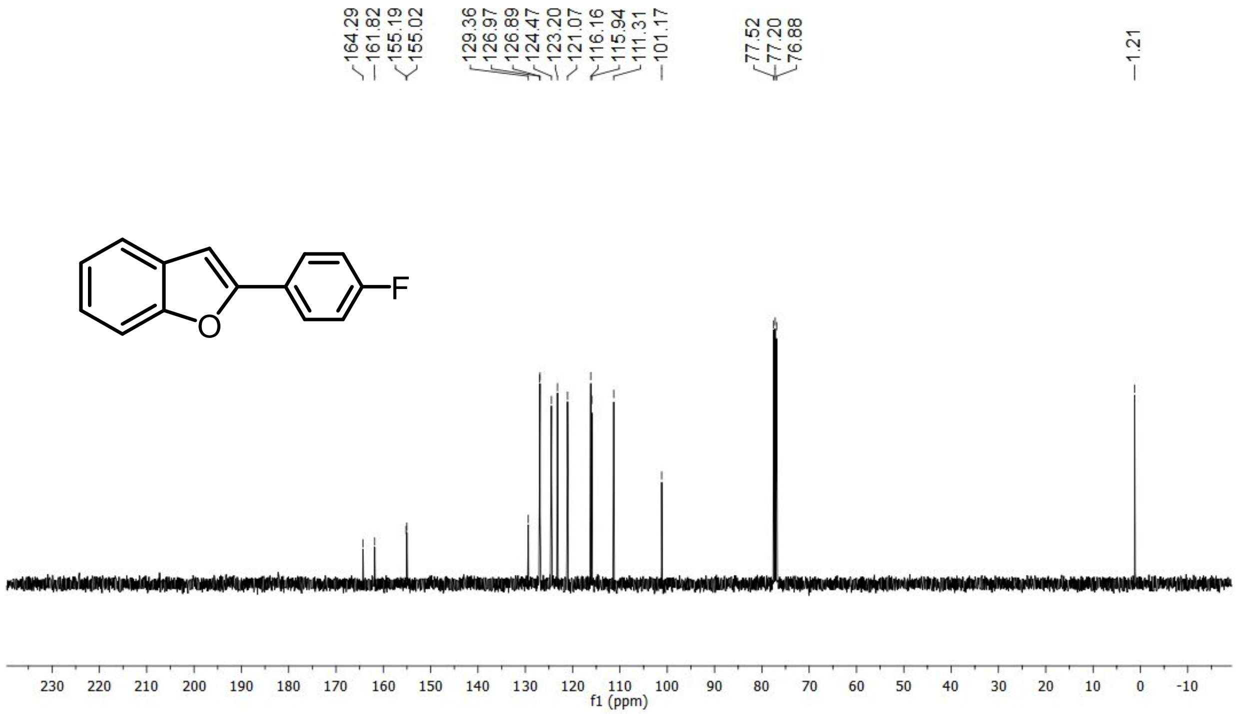


Fig. S62 ^{13}C NMR spectrum of **i** in $CDCl_3$ (100 MHz)

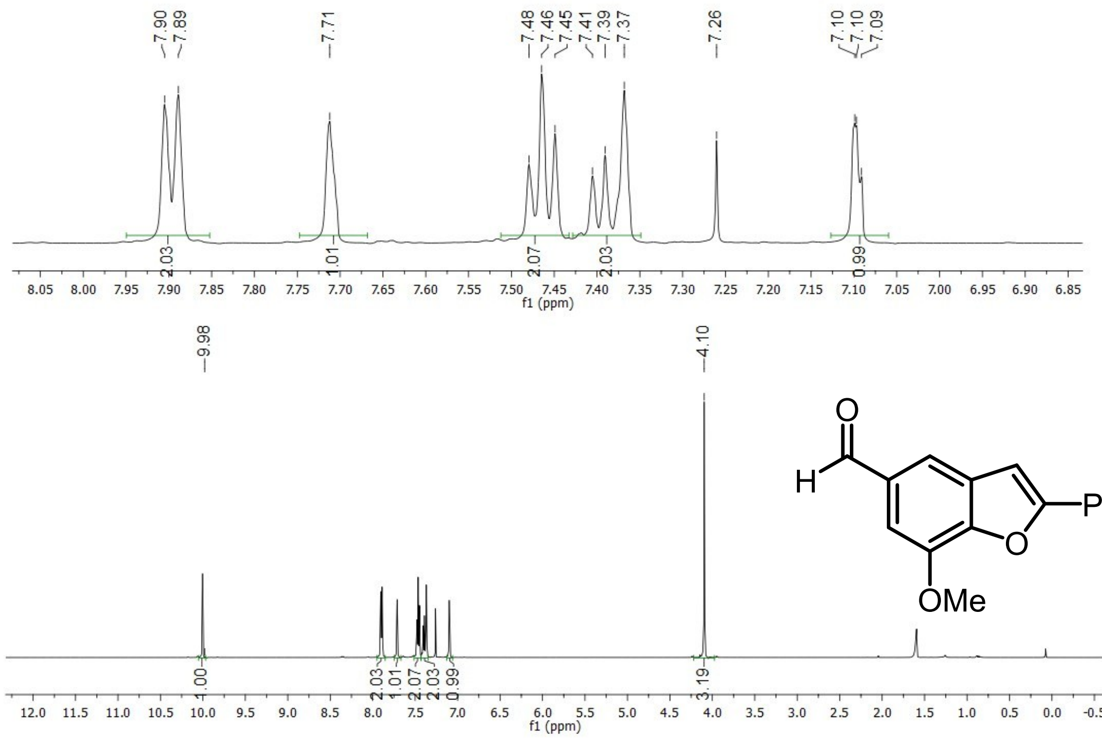


Fig. S63 ^{1}H NMR spectrum of **k** in $CDCl_3$ (400 MHz)

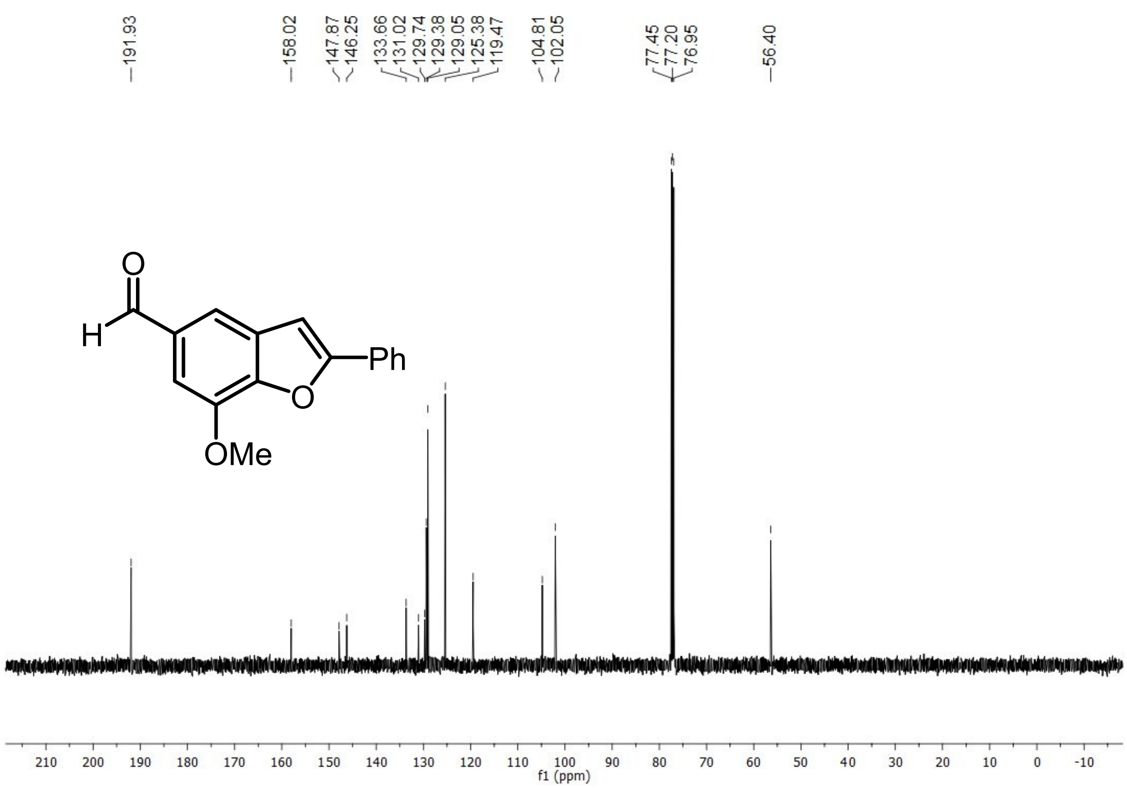


Fig. S64 ^{13}C NMR spectrum of **k** in $CDCl_3$ (100 MHz)

(6). Cartesian coordinates of optimized geometries of 3-6

Total electronic energies and Gibbs free energies (in a.u) and Cartesian coordinates of optimized geometries of 3-6 at the M06/6-31G, lanl2dz (Mo, W) level of theory.**

3			
Zero-point correction=	0.601737		
Thermal correction to Energy=	0.647798		
Thermal correction to Enthalpy=	0.648743		
Thermal correction to Gibbs Free Energy=	0.520580		
Sum of electronic and zero-point Energies=	-2831.257341		
Sum of electronic and thermal Energies=	-2831.211280		
Sum of electronic and thermal Enthalpies=	-2831.210335		
Sum of electronic and thermal Free Energies=	-2831.338498		
P	11.437326000	7.908129000	9.578342000
P	15.302934000	9.703889000	6.891941000
O	15.198479000	13.491865000	8.257261000
N	13.697080000	9.506659000	9.490891000
C	14.106870000	7.965196000	10.965563000
N	15.234388000	8.689890000	10.744364000
O	18.573693000	8.149394000	9.351991000
C	14.164473000	6.823744000	11.882645000
C	13.090431000	8.466418000	10.151994000
O	17.975992000	11.989129000	11.375772000
C	14.864418000	7.917924000	6.858080000
N	14.991432000	9.611862000	9.866300000
C	15.805128000	6.977284000	7.282379000
H	16.758924000	7.311092000	7.685845000
C	13.629302000	7.473524000	6.366194000
H	12.877974000	8.196626000	6.049406000

C	13.361375000	6.113351000	6.263810000
H	12.399404000	5.778351000	5.882714000
C	15.604129000	10.119562000	5.132319000
C	11.360391000	11.927453000	7.961191000
H	10.481247000	12.496699000	8.249988000
C	11.872501000	12.022618000	6.674650000
H	11.390654000	12.664466000	5.941415000
C	14.319540000	5.182316000	6.660162000
H	14.107117000	4.118279000	6.579324000
C	11.983897000	11.101948000	8.890411000
H	11.604344000	11.019311000	9.906912000
C	15.319217000	9.252237000	4.074710000
H	14.904409000	8.266066000	4.272327000
C	13.660125000	10.477314000	7.231933000
C	13.096005000	6.465790000	12.708135000
H	12.184118000	7.060166000	12.705165000
C	11.475193000	6.132489000	10.050236000
C	13.111314000	10.378966000	8.520794000
C	13.014292000	11.309071000	6.317886000
H	13.420007000	11.409946000	5.313107000
C	15.534711000	5.614226000	7.180564000
H	16.278861000	4.892018000	7.507804000
C	13.190733000	5.350880000	13.531893000
H	12.348461000	5.076905000	14.163038000
C	10.438451000	5.514907000	10.751912000
H	9.609715000	6.107711000	11.136411000
C	10.309723000	8.652634000	10.826715000
C	17.878707000	9.044598000	9.121954000
C	16.154344000	11.376804000	4.856388000
H	16.393645000	12.050750000	5.678230000
C	16.110902000	10.896076000	2.496804000

H	16.312762000	11.194784000	1.470735000
C	11.533733000	3.376100000	10.524168000
H	11.559362000	2.305985000	10.715933000
C	12.532038000	5.351551000	9.571681000
H	13.351504000	5.817666000	9.024353000
C	8.941342000	8.612577000	10.533755000
H	8.603625000	8.141485000	9.609858000
C	10.729779000	9.294519000	11.996095000
H	11.792328000	9.355213000	12.231259000
C	16.397477000	11.765813000	3.545107000
H	16.824658000	12.745222000	3.344717000
C	15.576078000	9.640158000	2.763434000
H	15.358956000	8.954590000	1.947526000
C	15.711686000	12.473886000	8.458332000
C	15.339245000	6.063703000	11.916223000
H	16.172288000	6.352552000	11.278052000
C	12.567756000	3.986391000	9.819031000
H	13.411237000	3.400037000	9.458868000
C	14.354859000	4.589231000	13.547698000
H	14.424769000	3.715191000	14.191164000
C	17.520638000	11.518575000	10.420689000
C	9.800289000	9.868490000	12.858818000
H	10.141910000	10.368920000	13.761929000
C	8.441141000	9.799669000	12.569818000
H	7.716770000	10.245244000	13.247377000
C	15.431591000	4.952770000	12.743700000
H	16.346674000	4.365360000	12.757811000
C	10.468094000	4.142703000	10.983354000
H	9.656787000	3.673300000	11.535548000
C	8.012082000	9.167851000	11.406349000
H	6.951673000	9.120817000	11.169539000

O	19.031318000	11.831659000	6.960681000
C	18.186103000	11.421128000	7.647190000
Mo	16.716673000	10.707627000	8.764840000

4

Zero-point correction= 0.601087

Thermal correction to Energy= 0.647064

Thermal correction to Enthalpy= 0.648008

Thermal correction to Gibbs Free Energy= 0.521132

Sum of electronic and zero-point Energies= -2831.269011

Sum of electronic and thermal Energies= -2831.223035

Sum of electronic and thermal Enthalpies= -2831.222090

Sum of electronic and thermal Free Energies= -2831.348967

Mo	8.978970000	3.742515000	10.537012000
P	8.853286000	4.706306000	8.167555000
P	9.354590000	6.168497000	11.362845000
O	9.265549000	2.513760000	13.445419000
O	12.054652000	2.936796000	10.107809000
N	8.950755000	7.492448000	8.505872000
O	5.862776000	4.292693000	11.106142000
N	9.579441000	8.625708000	8.111397000
N	10.598045000	8.280851000	7.401275000
O	8.123911000	0.888892000	9.476648000
C	6.231787000	3.964171000	7.640463000
H	6.476832000	3.110456000	8.271642000
C	7.186463000	4.959795000	7.418732000
C	6.763725000	8.371635000	8.960146000
H	6.766618000	8.721163000	7.931208000
C	13.338804000	6.293568000	4.759152000
H	13.692242000	6.736350000	3.830569000

C	7.948071000	7.212849000	10.751198000
C	6.870291000	7.513194000	11.588953000
H	6.899662000	7.203464000	12.630632000
C	13.962771000	5.159503000	5.272491000
H	14.802345000	4.712436000	4.744908000
C	4.973953000	4.048737000	7.054459000
H	4.240748000	3.267192000	7.237737000
C	10.109699000	7.262351000	13.884549000
H	10.849177000	7.851161000	13.347487000
C	12.263705000	6.862740000	5.429564000
H	11.771887000	7.752435000	5.042275000
C	7.859528000	7.646856000	9.417022000
C	9.652657000	3.773946000	6.794602000
C	10.666896000	6.919018000	7.315719000
C	10.023701000	7.377741000	15.268919000
H	10.694573000	8.055370000	15.791861000
C	9.264485000	6.390985000	13.191833000
C	9.091479000	6.631760000	15.979875000
H	9.028179000	6.722750000	17.061616000
C	6.864946000	6.034984000	6.586052000
H	7.600379000	6.815215000	6.391034000
C	9.580263000	6.382316000	7.999611000
C	5.760133000	8.213153000	11.129267000
H	4.942155000	8.425754000	11.812920000
C	5.704764000	8.649560000	9.812361000
H	4.846935000	9.208734000	9.448890000
C	10.821809000	7.174866000	10.911760000
C	10.777687000	8.574046000	10.909228000
H	9.847769000	9.089700000	11.147250000
C	8.338586000	5.634125000	13.921146000
H	7.683461000	4.934438000	13.404460000

C	10.835219000	2.322057000	4.720907000
H	11.302437000	1.761989000	3.914166000
C	13.515921000	4.604990000	6.468498000
H	14.001135000	3.724168000	6.883138000
C	10.236078000	2.532060000	7.044436000
H	10.239812000	2.128392000	8.053604000
C	4.655015000	5.132344000	6.243167000
H	3.668040000	5.205043000	5.792356000
C	9.158152000	2.981359000	12.390962000
C	12.022469000	6.533203000	10.603163000
H	12.074035000	5.446865000	10.607252000
C	8.245382000	5.759689000	15.301456000
H	7.518290000	5.163543000	15.847332000
C	10.244118000	3.556905000	4.459500000
H	10.247142000	3.962059000	3.450356000
C	9.645279000	4.271395000	5.486549000
H	9.182453000	5.232703000	5.268745000
C	12.441353000	5.173935000	7.139729000
H	12.102423000	4.750304000	8.083574000
C	5.603328000	6.122832000	6.007417000
H	5.361933000	6.970024000	5.369001000
C	8.458340000	1.929306000	9.869241000
C	11.794648000	6.297000000	6.618439000
C	10.955178000	3.270921000	10.257445000
C	11.910634000	9.311985000	10.590265000
H	11.858820000	10.397648000	10.575302000
C	13.097673000	8.662028000	10.266321000
H	13.978579000	9.240815000	9.999237000
C	6.981122000	4.114341000	10.877175000
C	10.822698000	1.807214000	6.010477000
H	11.272899000	0.839993000	6.220112000

C	13.154543000	7.273066000	10.276943000
H	14.077510000	6.758645000	10.019972000

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Zero-point correction= 0.601806

Thermal correction to Energy= 0.647836

Thermal correction to Enthalpy= 0.648780

Thermal correction to Gibbs Free Energy= 0.519964

Sum of electronic and zero-point Energies= -2831.535655

Sum of electronic and thermal Energies= -2831.489625

Sum of electronic and thermal Enthalpies= -2831.488680

Sum of electronic and thermal Free Energies= -2831.617497

W	16.706960000	10.671880000	8.780968000
P	11.426449000	7.925961000	9.586146000
P	15.303786000	9.708517000	6.898078000
O	15.177707000	13.441928000	8.293440000
N	13.704248000	9.497713000	9.489550000
C	14.107494000	7.939933000	10.950598000
N	15.244181000	8.644394000	10.720558000
O	18.555969000	8.108311000	9.316586000
C	14.158235000	6.791672000	11.859398000
C	13.089462000	8.463164000	10.152401000
O	17.931456000	11.898067000	11.428978000
C	14.862789000	7.924011000	6.845721000
N	15.007388000	9.574935000	9.847453000
C	15.800678000	6.974136000	7.255899000
H	16.758710000	7.296520000	7.658311000
C	13.624218000	7.491519000	6.352083000
H	12.875347000	8.221439000	6.045397000
C	13.348112000	6.133881000	6.237560000
H	12.383144000	5.808202000	5.856047000

C	15.629077000	10.142454000	5.149039000
C	11.376894000	11.943406000	7.984861000
H	10.502505000	12.516571000	8.280152000
C	11.886369000	12.045448000	6.697868000
H	11.407580000	12.697260000	5.971509000
C	14.301734000	5.193659000	6.622818000
H	14.082808000	4.131662000	6.533028000
C	11.997509000	11.107719000	8.907229000
H	11.621203000	11.022511000	9.924678000
C	15.363848000	9.277602000	4.084448000
H	14.952174000	8.288382000	4.272671000
C	13.663442000	10.484293000	7.238704000
C	13.092130000	6.440314000	12.690577000
H	12.187003000	7.044815000	12.698756000
C	11.453005000	6.145725000	10.040675000
C	13.118979000	10.380335000	8.528843000
C	13.022793000	11.327357000	6.332455000
H	13.428493000	11.434161000	5.328312000
C	15.521415000	5.613826000	7.142286000
H	16.262982000	4.884513000	7.459321000
C	13.181264000	5.319413000	13.506790000
H	12.341013000	5.050480000	14.142752000
C	10.417909000	5.530195000	10.746537000
H	9.597818000	6.126205000	11.144407000
C	10.312597000	8.669256000	10.846939000
C	17.863961000	9.014072000	9.108202000
C	16.174979000	11.404696000	4.887761000
H	16.397982000	12.076890000	5.715426000
C	16.168784000	10.932584000	2.525758000
H	16.383956000	11.236880000	1.504048000
C	11.494471000	3.385191000	10.490216000

H	11.513717000	2.313337000	10.672702000
C	12.498845000	5.360798000	9.544591000
H	13.316659000	5.825309000	8.993247000
C	8.942194000	8.639665000	10.562363000
H	8.595430000	8.175770000	9.638180000
C	10.744478000	9.302069000	12.016934000
H	11.808863000	9.354353000	12.245716000
C	16.434895000	11.799783000	3.581569000
H	16.859253000	12.782374000	3.391294000
C	15.637154000	9.672539000	2.778712000
H	15.435872000	8.989295000	1.956877000
C	15.702496000	12.426983000	8.494979000
C	15.324769000	6.018411000	11.878125000
H	16.155847000	6.302603000	11.235230000
C	12.526556000	3.993465000	9.780356000
H	13.361919000	3.403675000	9.407210000
C	14.336846000	4.544708000	13.508027000
H	14.402129000	3.665900000	14.145451000
C	17.488461000	11.447027000	10.456171000
C	9.824194000	9.878002000	12.888296000
H	10.174856000	10.371330000	13.791836000
C	8.462898000	9.819831000	12.607405000
H	7.745796000	10.266922000	13.291657000
C	15.411167000	4.901229000	12.697631000
H	16.319663000	4.303570000	12.700758000
C	10.438819000	4.155743000	10.965465000
H	9.629022000	3.687765000	11.521041000
C	8.022207000	9.196714000	11.443559000
H	6.960050000	9.157920000	11.213242000
O	19.019617000	11.830565000	6.994698000
C	18.175916000	11.405586000	7.677943000

6
Zero-point correction= 0.602149 Thermal correction to Energy= 0.647750 Thermal correction to Enthalpy= 0.648694 Thermal correction to Gibbs Free Energy= 0.522955 Sum of electronic and zero-point Energies= -2831.548543 Sum of electronic and thermal Energies= -2831.502941 Sum of electronic and thermal Enthalpies= -2831.501997 Sum of electronic and thermal Free Energies= -2831.627736 W 1.834967000 3.734001000 10.479670000 P 1.732798000 4.726034000 8.134981000 P 2.197840000 6.135025000 11.325713000 C -2.128458000 4.044549000 6.972915000 H -2.858890000 3.258304000 7.146653000 C -0.878396000 3.968009000 7.576406000 H -0.637177000 3.115631000 8.210420000 C -0.152790000 4.098990000 10.819283000 O 4.906507000 2.992685000 9.978985000 C 3.705772000 7.084261000 10.891260000 O -1.273628000 4.284659000 11.040207000 N 3.397632000 8.332841000 7.350284000 C 4.923439000 6.401774000 10.814410000 H 4.957324000 5.327100000 10.978852000 C 0.072730000 4.969751000 7.367638000 N 1.776294000 7.510933000 8.469218000 N 2.365589000 8.657044000 8.051322000 O 2.148908000 2.468581000 13.363986000 C 3.686876000 8.468390000 10.699139000

H	2.749623000	9.018848000	10.764329000
C	3.800747000	3.294268000	10.166995000
C	4.860875000	9.150113000	10.398378000
H	4.827307000	10.222177000	10.221531000
C	0.694191000	7.643856000	9.392157000
O	0.997033000	0.898459000	9.369401000
C	-2.442775000	5.125252000	6.156271000
H	-3.423658000	5.191147000	5.691383000
C	2.915257000	7.293085000	13.819603000
H	3.620137000	7.906637000	13.263133000
C	-1.497540000	6.121647000	5.933130000
H	-1.735189000	6.966658000	5.290535000
C	3.514768000	6.972997000	7.296246000
C	4.672001000	6.367334000	6.636024000
C	5.155382000	6.918979000	5.446294000
H	4.654093000	7.789809000	5.029172000
C	6.255847000	6.357759000	4.811597000
H	6.622180000	6.788823000	3.882496000
C	1.937044000	6.658647000	15.932013000
H	1.873866000	6.769808000	17.011898000
C	-0.271026000	7.483069000	11.572183000
H	-0.230822000	7.161609000	12.609731000
C	5.328405000	5.268791000	7.196831000
H	4.984170000	4.862794000	8.146733000
C	2.112333000	6.363331000	13.152658000
C	-0.243662000	6.042648000	6.529503000
H	0.487718000	6.829186000	6.344276000
C	6.097060000	7.086873000	10.522362000
H	7.035061000	6.541551000	10.451695000
C	1.222607000	5.582185000	13.899461000
H	0.593888000	4.848615000	13.397808000

C	2.828311000	7.435475000	15.200925000
H	3.464954000	8.158081000	15.706064000
C	0.801576000	7.198349000	10.721681000
C	6.064664000	8.460422000	10.303356000
H	6.978787000	8.994261000	10.055028000
C	-0.412967000	8.362029000	8.952502000
H	-0.423909000	8.717957000	7.925931000
C	2.442762000	6.413322000	7.986224000
C	1.130080000	5.732995000	15.277518000
H	0.434010000	5.116101000	15.840413000
C	2.028599000	2.947649000	12.313489000
C	3.209370000	3.640675000	4.442856000
H	3.232889000	4.064307000	3.441588000
C	6.425092000	4.705230000	6.557643000
H	6.916183000	3.841615000	7.000882000
C	2.580617000	4.331913000	5.467708000
H	2.114176000	5.292229000	5.253904000
C	-1.391722000	8.177345000	11.130440000
H	-2.204445000	8.375471000	11.824490000
C	1.324779000	1.935194000	9.783626000
C	3.805753000	2.406884000	4.696521000
H	4.298217000	1.865878000	3.891788000
C	6.887166000	5.244274000	5.360211000
H	7.745413000	4.802134000	4.859087000
C	3.146463000	2.569014000	7.007651000
H	3.125226000	2.142902000	8.006590000
C	-1.465009000	8.623918000	9.817956000
H	-2.331976000	9.177408000	9.467751000
C	2.562986000	3.812707000	6.767343000
C	3.764180000	1.868229000	5.975491000
H	4.215417000	0.900216000	6.178875000

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