Organometallic Palladium Complexes with a Water-Soluble Iminophosphorane Ligand as Potential Anticancer Agents

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Supporting Information

1. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra for compounds 2 and 3.

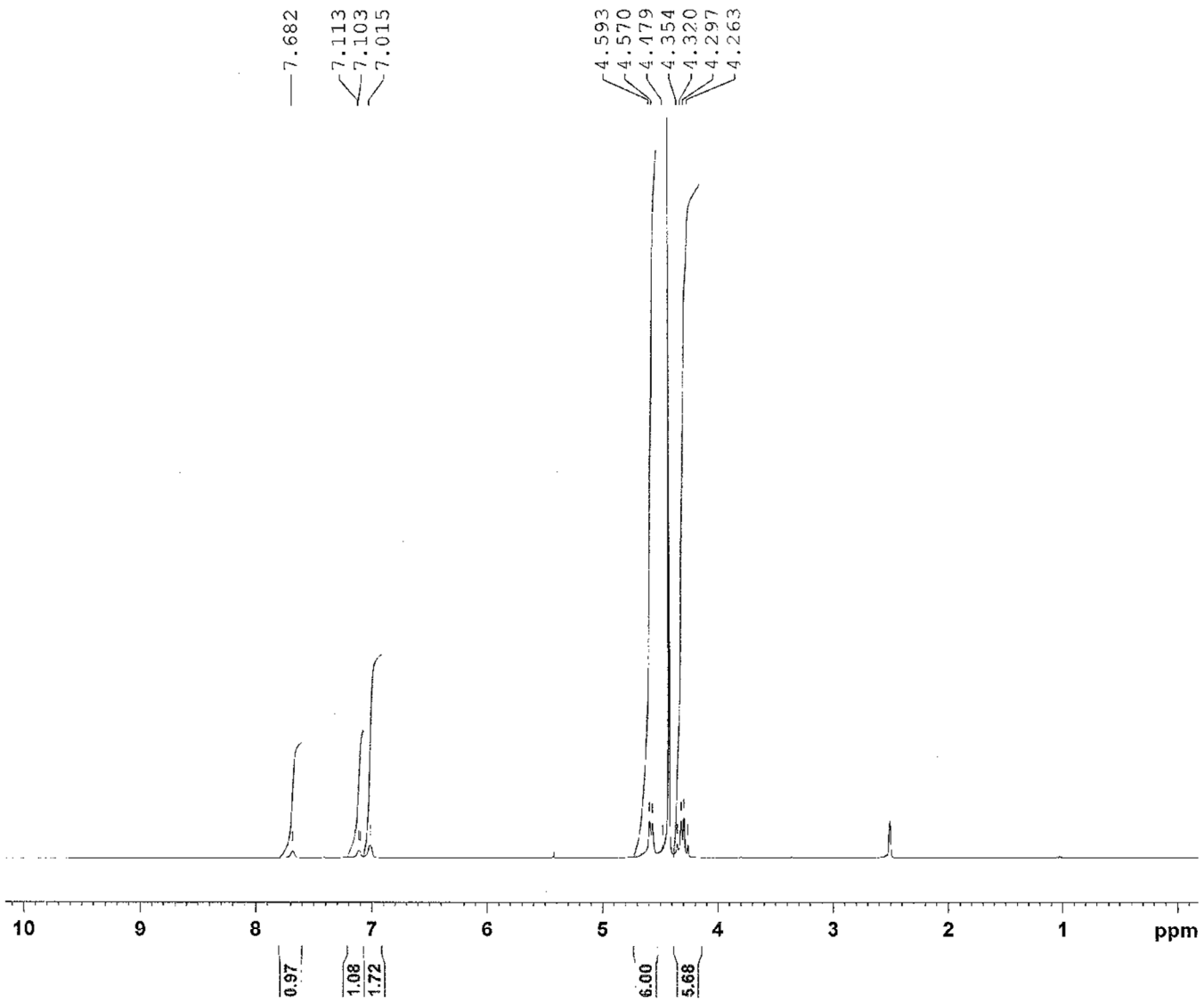

Figure S1. ^{1}H NMR spectra for compound **2**.

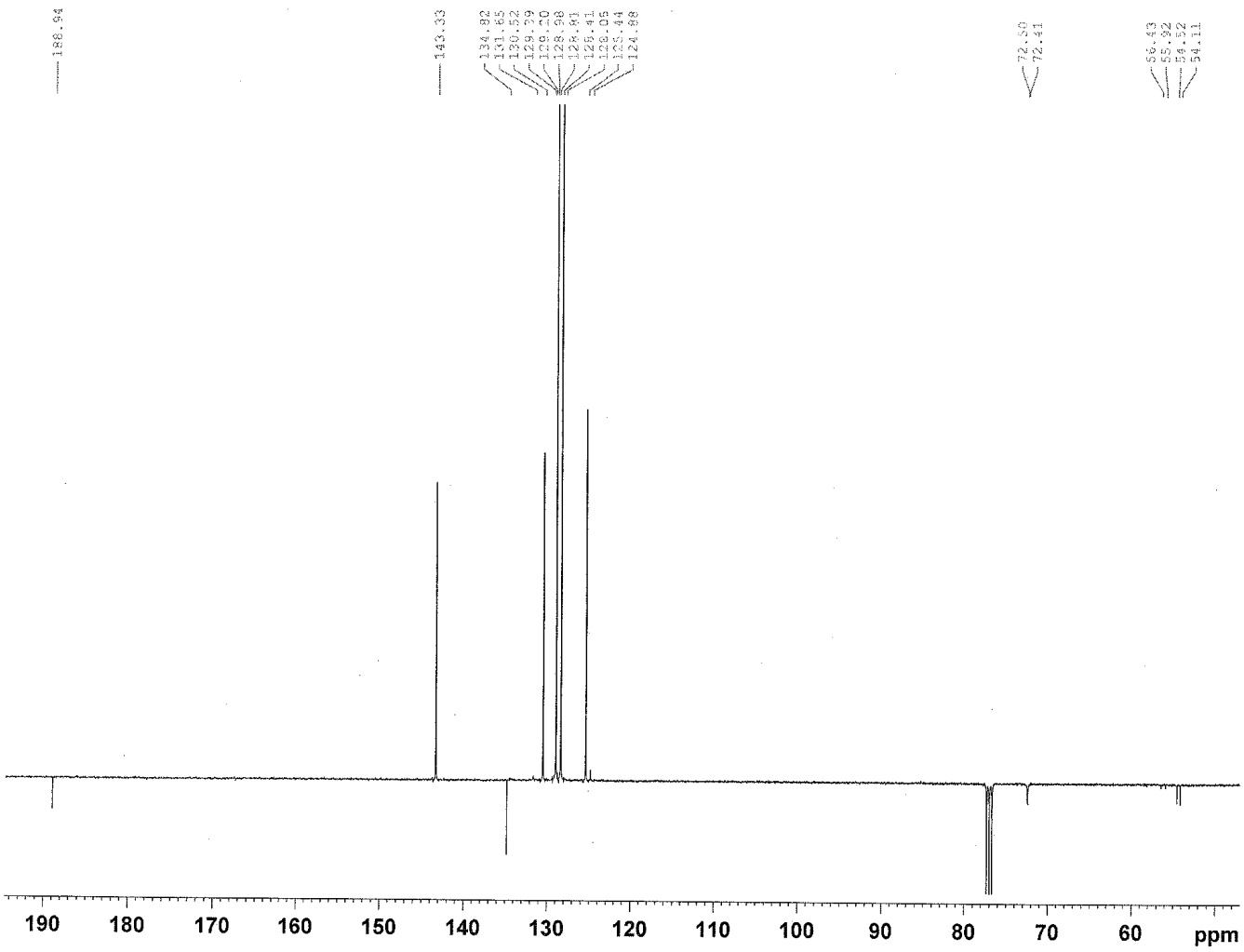

Figure S2. $^{13}C\{^{1}H\}$ NMR spectra for compound **2**.

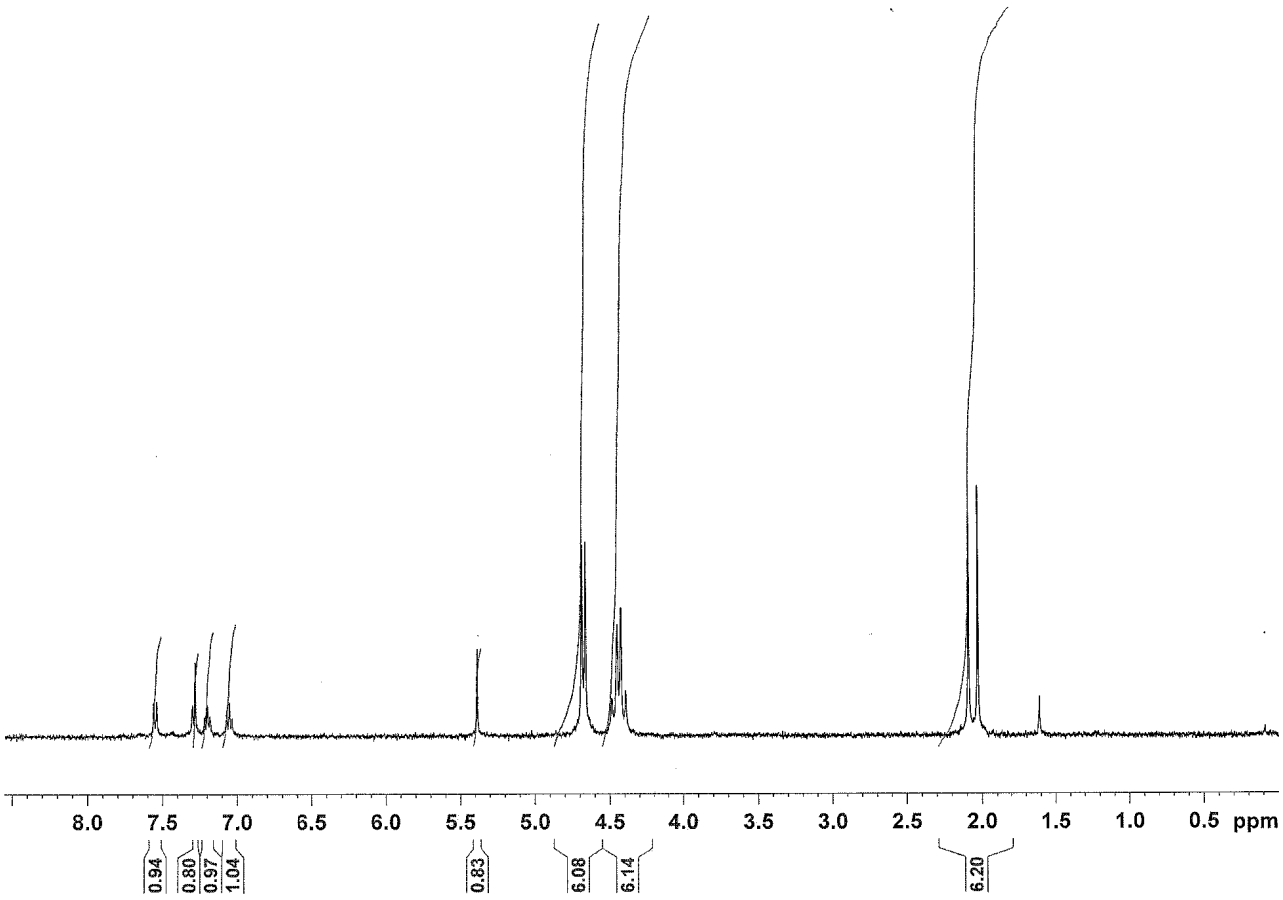

Figure S3. ^{1}H NMR spectra for compound **3**.

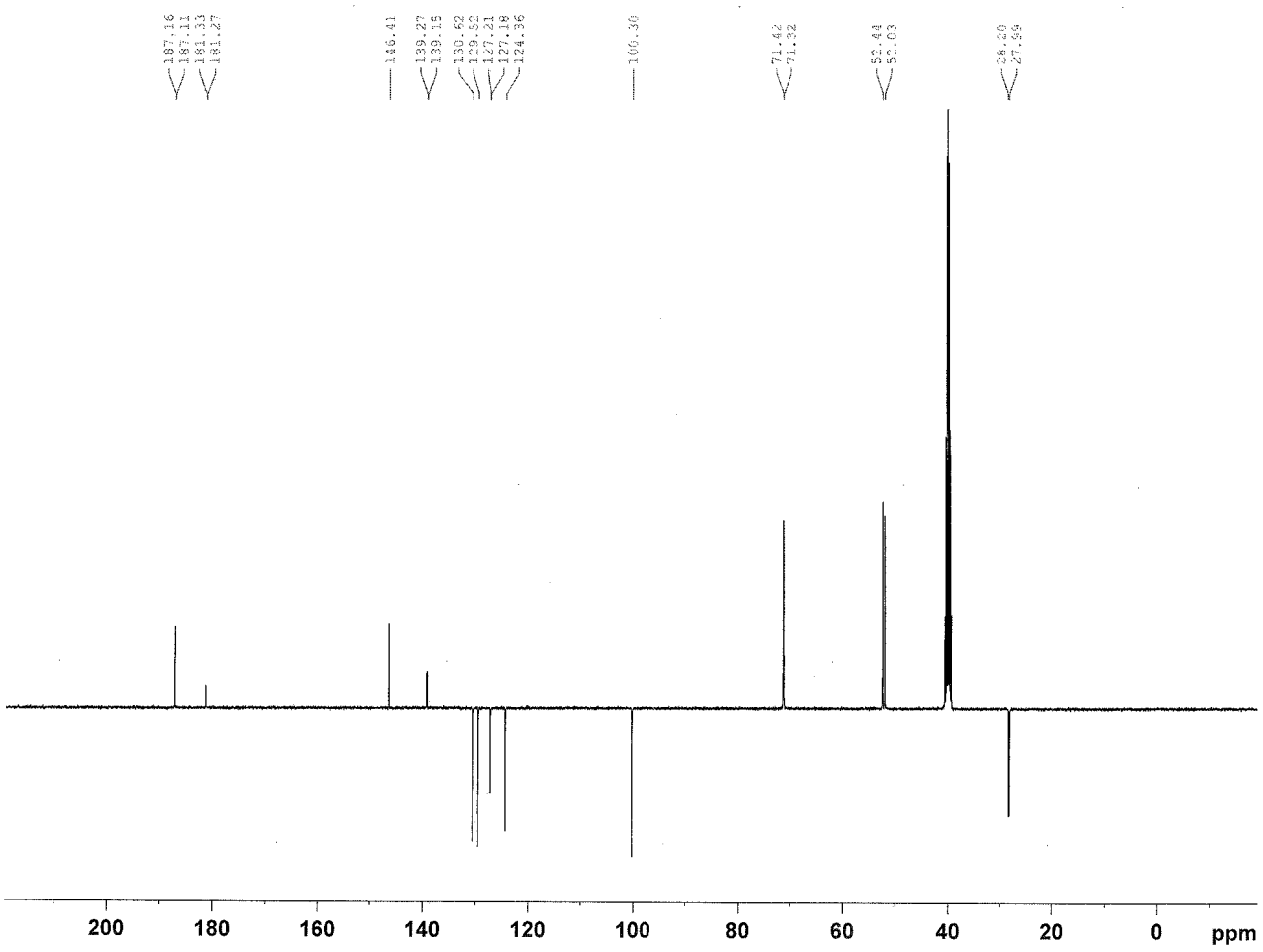

Figure S4. $^{13}C\{^{1}H\}$ NMR spectra for compound **3**.

2. Stability of ligand 1 and compounds 2-8 in d^6-DMSO solution and mixtures d^6-DMSO:D_2O (50:50) overtime assessed by $^{31}P\{^1H\}$ NMR spectroscopy.

Table S1. Stability of compounds **2-8** in d^6-DMSO solution and mixtures d^6-DMSO:D_2O (50:50) overtime assessed by $^{31}P\{^1H\}$ NMR spectroscopy.

	d^6-DMSO						d^6-DMSO/D_2O				
	1 day	4 days	1 week	2 weeks	Half life (50%)		1	4	1 week	2 weeks	Half life (50%)
1											
2	>99%	>99%	>99%		**months**	**2**	88%	75%		50%	**2 weeks**
3	>99%		>99%	>99%	**months**	**3**	>99%	>99%	>99%		**months**
4			>99%	>99%	**months**	**4**	>99%		>99%		**months**
5		43%	0%		**~4 days**	**5**	83%	45%	0%		**~4 days**
6		94%		93%	**months**	**6**	92%	86%			**~1 month**
7	>95%	90%			**~1 month**	**7**	85%	65%	50%		**~1 week**
8	64%	23%	0%		**2 days**	**8**	90%	75%	65%		**~2 weeks**

Half life of ligand **1** (assessed by $^{31}P\{^1H\}$ NMR spectroscopy**)** was: months in d^6-DMSO; 2 weeks in d^6-DMSO:D_2O (50:50) and 2 days in D_2O.

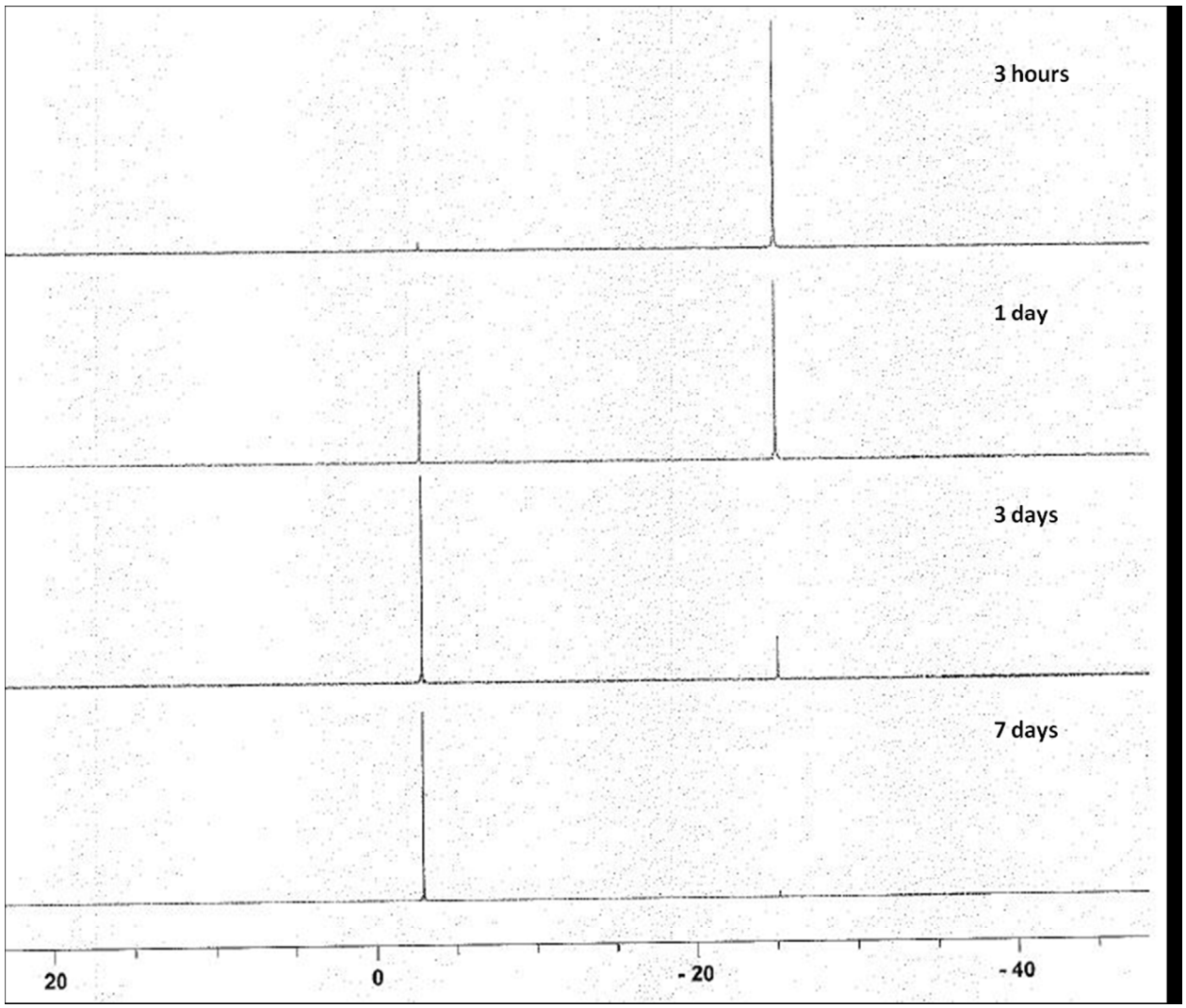

Figure S5. Selected $^{31}P\{^{1}H\}$ NMR spectra showing the decomposition of ligand **1** in D_2O (δ-25.1 (s)) overtime. The peak at -3.4 ppm corresponds to TPA=O in D_2O.

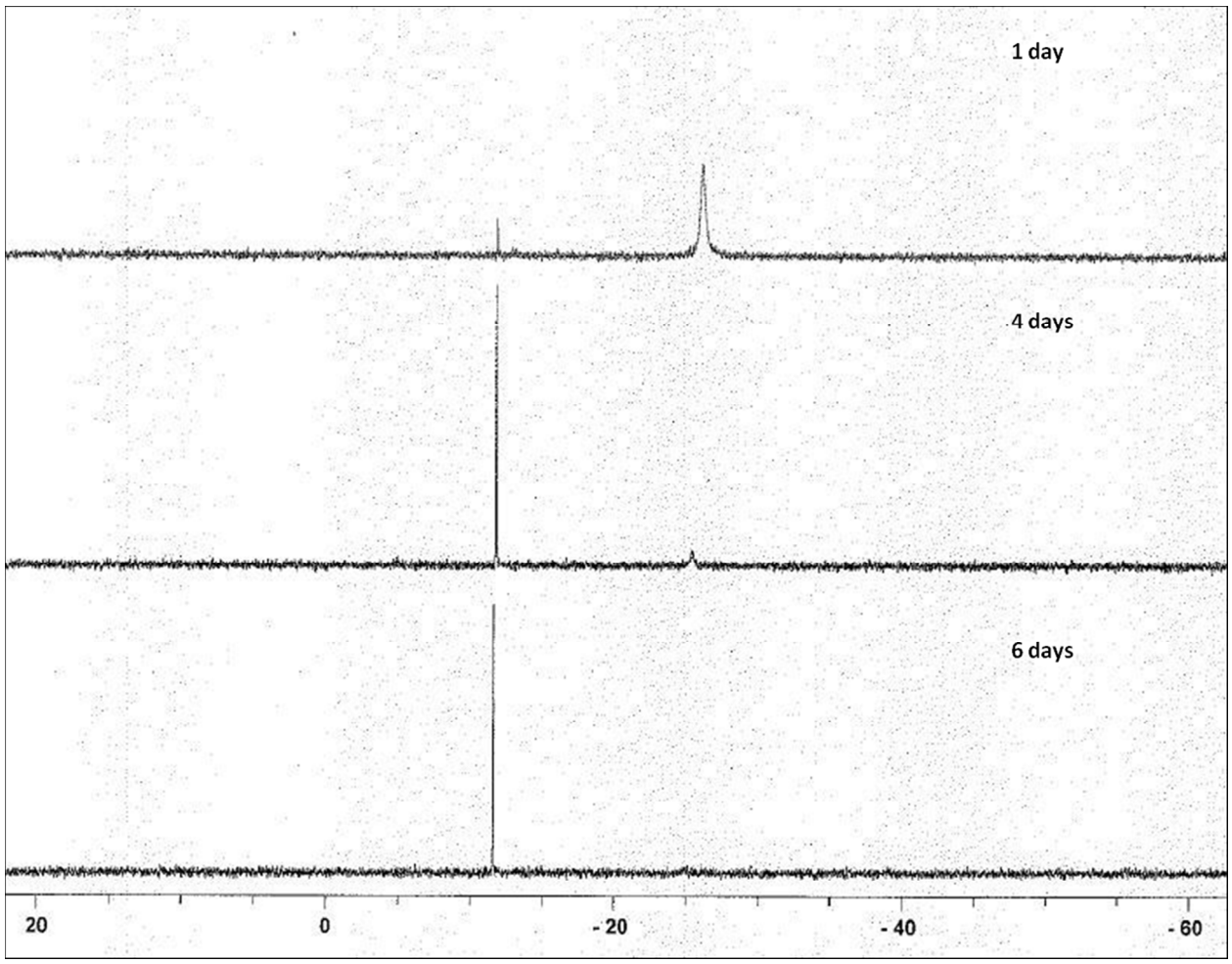

Figure S6. Selected $^{31}P\{^{1}H\}$ NMR spectra showing the decomposition of compound **5** in d^6-DMSO:D_2O (50:50) (δ -27.0 (s)) overtime. The peak at -12.0 ppm corresponds to TPA=O in d^6-DMSO:D_2O (50:50).

3. Crystal data and structure refinement for complex 3.

Table S2. Crystal data and structure refinement for complex **3**.

formula	$C_{18}H_{24}N_4O_3PPd$
Fw	481.78
T [K]	293(2) K
λ ($Mo_{K\alpha}$)[Å]	0.71073
crystal system	monoclinic,
Space group	P2(1)/c
a [Å]	9.5820(19)
b [Å]	20.496(4)
c [Å]	10.647(2)
α [°]	90 deg
β [°]	106.92(3)
χ [°]	90 deg.
V [Å]^3	2000.5(7)
Z	4
D_{calcd} (g cm^{-3})	1.600
μ (mm^{-1})	1.033
R(Fo)[a]	0.0376 [for 3411 data with $F_o^2 > 2\sigma(F_o^2)$]
$R_w(F_o^2)$[b]	0.0968

[a] $R(F_o)$ (= $R1$) = $\Sigma \mid |F_o| - |F_c| \mid / \Sigma |F_o|$. [b] $R_w(F_o^2)$ (= $wR2$) = $\{ \Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2] \}^{1/2}$