

# **Water soluble binary and ternary palladium(II) complexes containing amino acids and intercalating ligands: Synthesis, characterization, biomolecular interactions and cytotoxicities**

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## Supplementary Material

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 1810954 for the complex **1** and 1810955 for the complex **4**. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: [deposit@ccdc.cam.ac.uk](mailto:deposit@ccdc.cam.ac.uk) or www: <http://www.ccdc.cam.ac.uk>).

**Table S1** Selected bond lengths (Å) and bond angles (°) for the complexes **1** and **4**

<b>Complex 1</b>			
Pd1-N2	2.041(2)	Pd1-N1	2.043(2)
N2-Pd1-N1	81.04(9)	N2-Pd1-N1 <sup>i</sup>	165.53(9)
N1-Pd1-N1 <sup>i</sup>	101.15(14)		
<b>Complex 4</b>			
N1-Pd1	2.024(5)	N2-Pd1	2.034(5)
O1-Pd1	1.989(4)	Pd1-N3	2.036(5)
O1-Pd1-N1	176.79(18)	O1-Pd1-N2	95.32(18)
N1-Pd1-N2	81.80(19)	O1-Pd1-N3	82.50(18)
N1-Pd1-N3	100.42(19)	N2-Pd1-N3	177.15(19)

Symmetry code: (i)  $-x+1, y, -z+1/2$  for the complex **1**.

**Table S2** Hydrogen-bond parameters for the complexes **1** and **4**

D-H···A	D-H	H···A	D···A	D-H···A
<b>Complex 1</b>				
C1—H1···O2 <sup>iii</sup>	0.93	2.57	3.082 (10)	115
C2—H2···O2 <sup>iii</sup>	0.93	2.43	3.011 (9)	121
<b>Complex 4</b>				
C1—H1···O2 <sup>i</sup>	0.93	2.57	3.165 (8)	122
C1—H1···O6 <sup>ii</sup>	0.93	2.52	3.203 (11)	130
C9—H9···O6 <sup>iii</sup>	0.93	2.51	3.238 (10)	135
O3—H3C···O5	0.82	2.31	3.084 (12)	156
N3—H3A···O2 <sup>i</sup>	0.91	2.02	2.881 (6)	159
N3—H3B···O5 <sup>ii</sup>	0.85	2.39	3.122 (9)	144
N3—H3B···O6 <sup>ii</sup>	0.85	2.28	3.104 (9)	161
O4—H4B···O7 <sup>iv</sup>	0.84 (2)	2.02 (5)	2.834 (13)	162

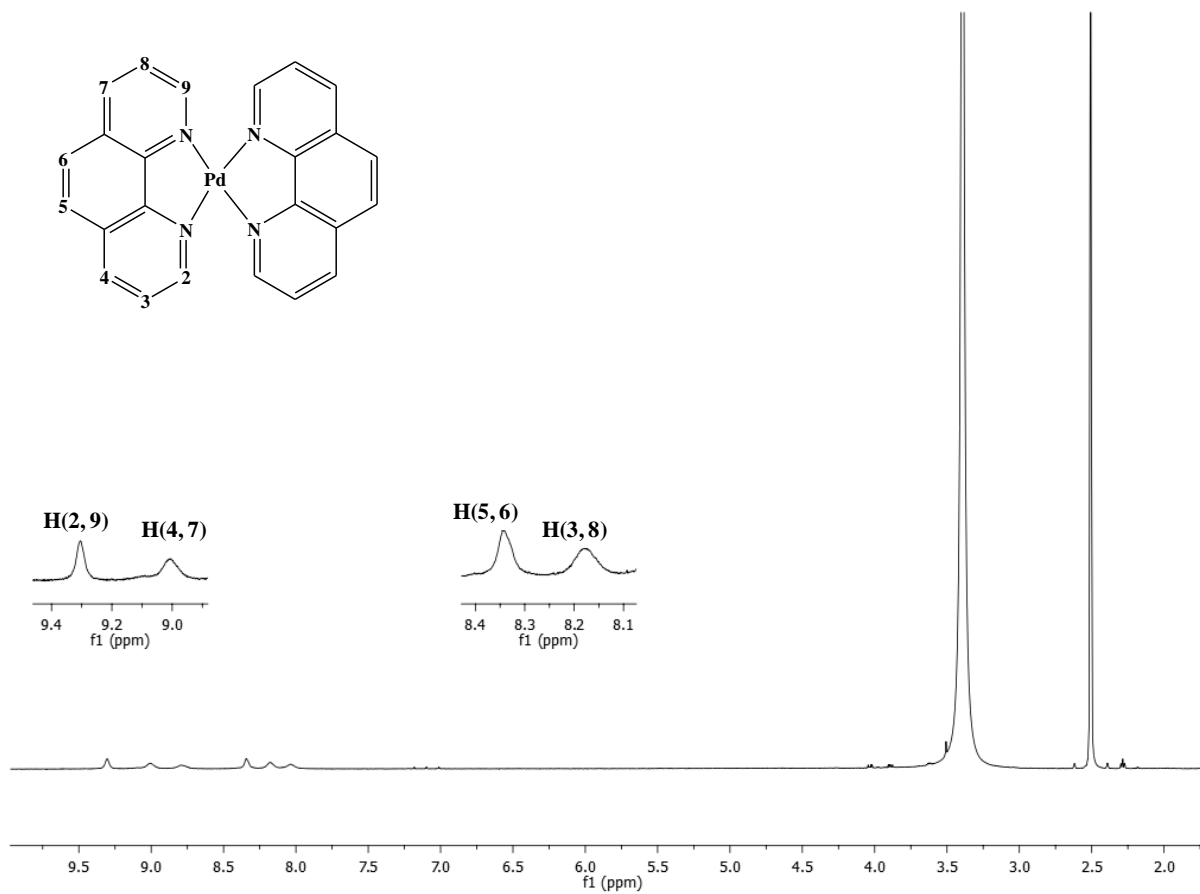
Symmetry codes: (iii)  $-x+1, -y, -z+1$  for **1**; (i)  $x+1/2, -y+1/2, z+1/2$ ; (ii)  $x-1/2, -y+1/2, z-1/2$ ; (iii)  $x-1/2, -y+1/2, z-3/2$ ; (iv)  $x, y, z-1$  for **4**.

**Table S3**  $\pi \cdots \pi$  interactions distances for the complexes **1** and **4** (Å)

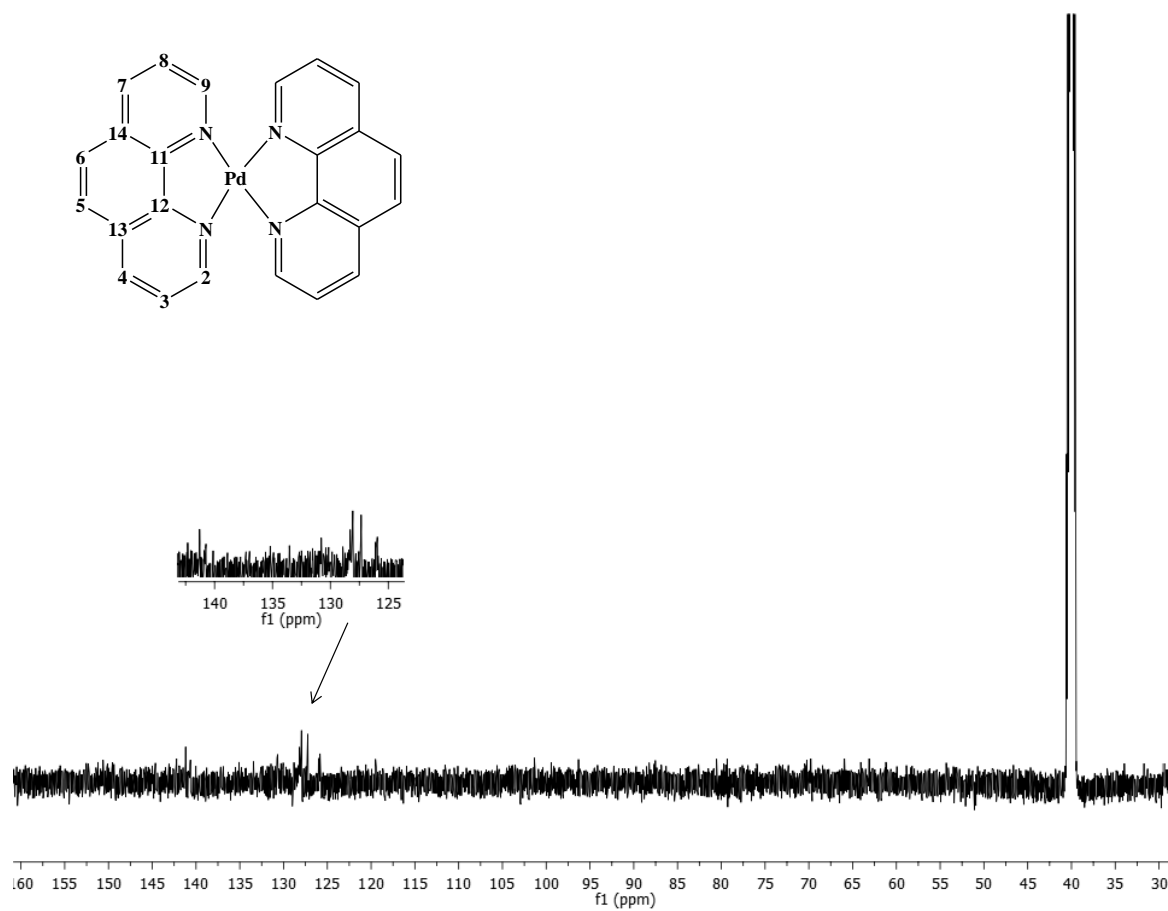
Cg(I)	Cg(J)	Cg-Cg	Perpendicular distance
<b>Complex 1</b>			
Cg(3)	Cg(4) <sup>i</sup>	3.7289 (18)	3.4561 (11)
Cg(4)	Cg(5) <sup>i</sup>	3.8374 (17)	3.3531 (11)
Cg(4)	Cg(5) <sup>ii</sup>	3.6678 (17)	3.3457 (11)
Cg(5)	Cg(5) <sup>i</sup>	3.6293 (18)	3.4207 (11)
Cg(5)	Cg(5) <sup>ii</sup>	3.9389 (18)	3.4009 (11)
<b>Complex 4</b>			
Cg(3)	Cg(4) <sup>i</sup>	3.671 (4)	3.470 (3)
Cg(4)	Cg(5) <sup>i</sup>	3.734 (4)	3.457 (3)
Cg(4)	Cg(6) <sup>ii</sup>	3.715 (4)	3.415 (4)

Symmetry codes: (i)  $1/2-x, 1/2-y, -z$ ; (ii)  $1/2-x, 1/2-y, 1-z$ ; Cg(3)=N1/C1/C2/C3/C4/C12; Cg(2)=N2/C7/C8/C9/C10/C11; Cg(5)=C4/C5/C6/C7/C11/C12 for **1**; (i)  $1-x, 1-y, -z$ ; (ii)  $1/2+x, 1/2-y, -1/2+z$ ; Cg(3)=N1/C1/C2/C3/C4/C12; Cg(4)=N2/C7/C8/C9/C10/C11; Cg(5)=C4/C5/C6/C7/C11/C12; Cg(6)=C16-C21 for **4**.

a)



b)



**Fig. S1 a)** <sup>1</sup>H NMR spectra and **b)** <sup>13</sup>C NMR spectra of the complex **1**

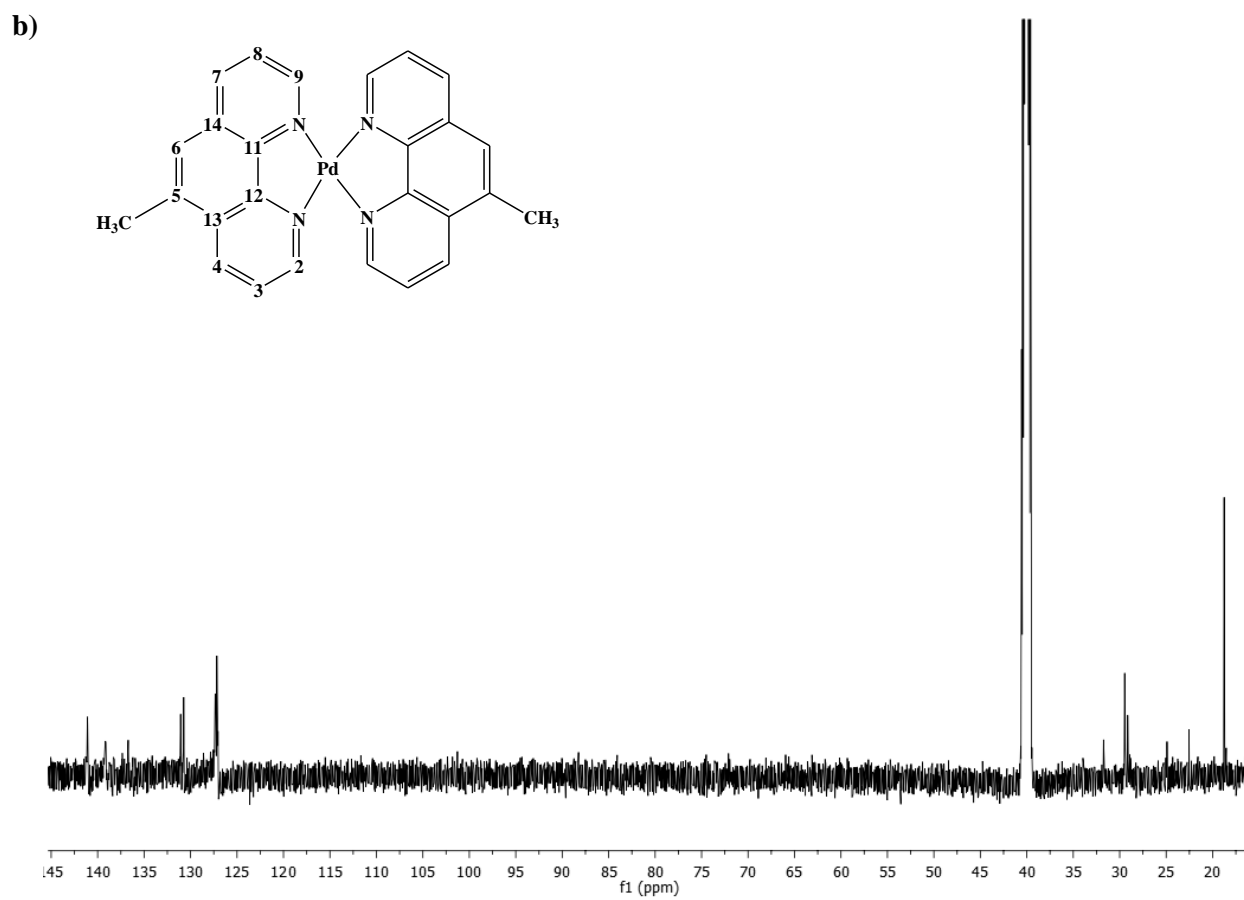
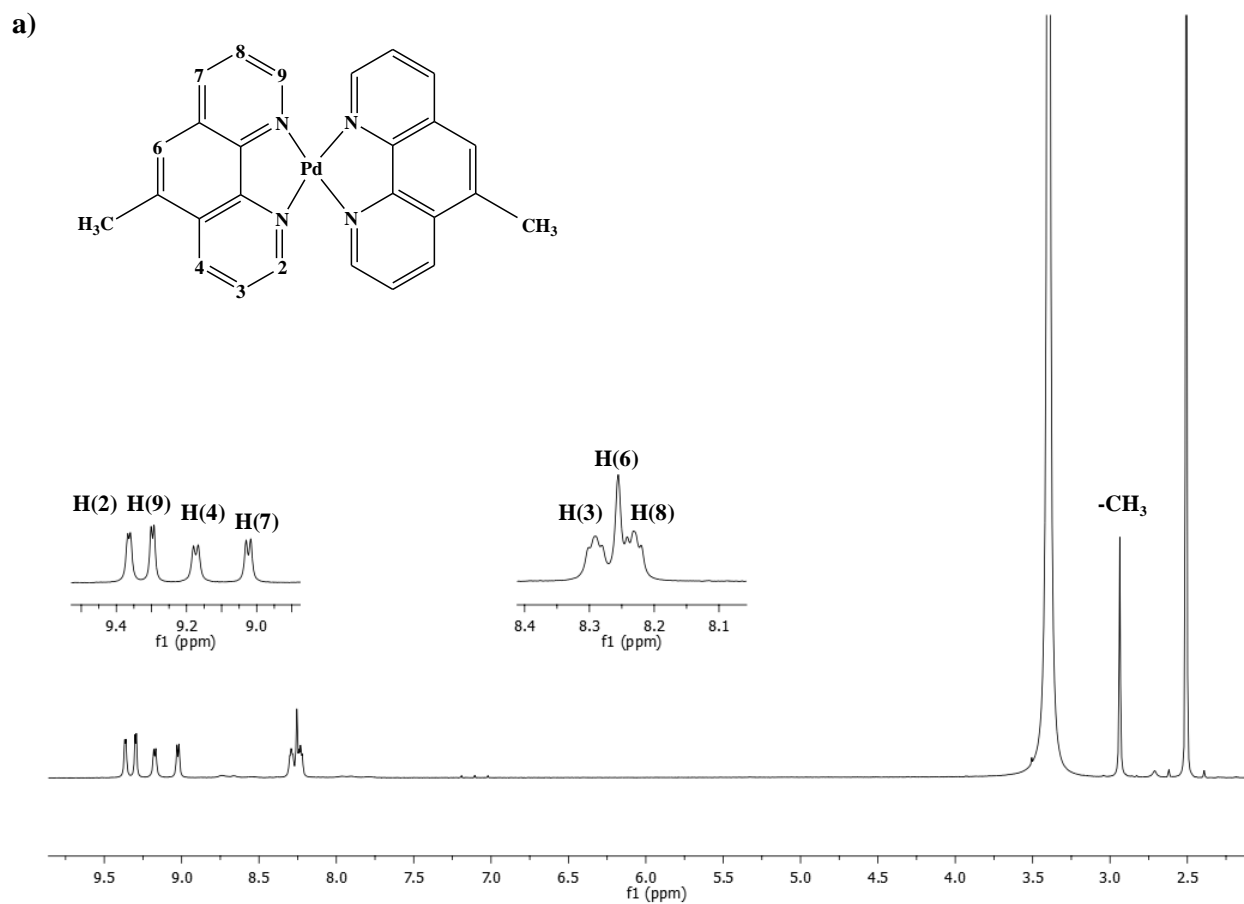
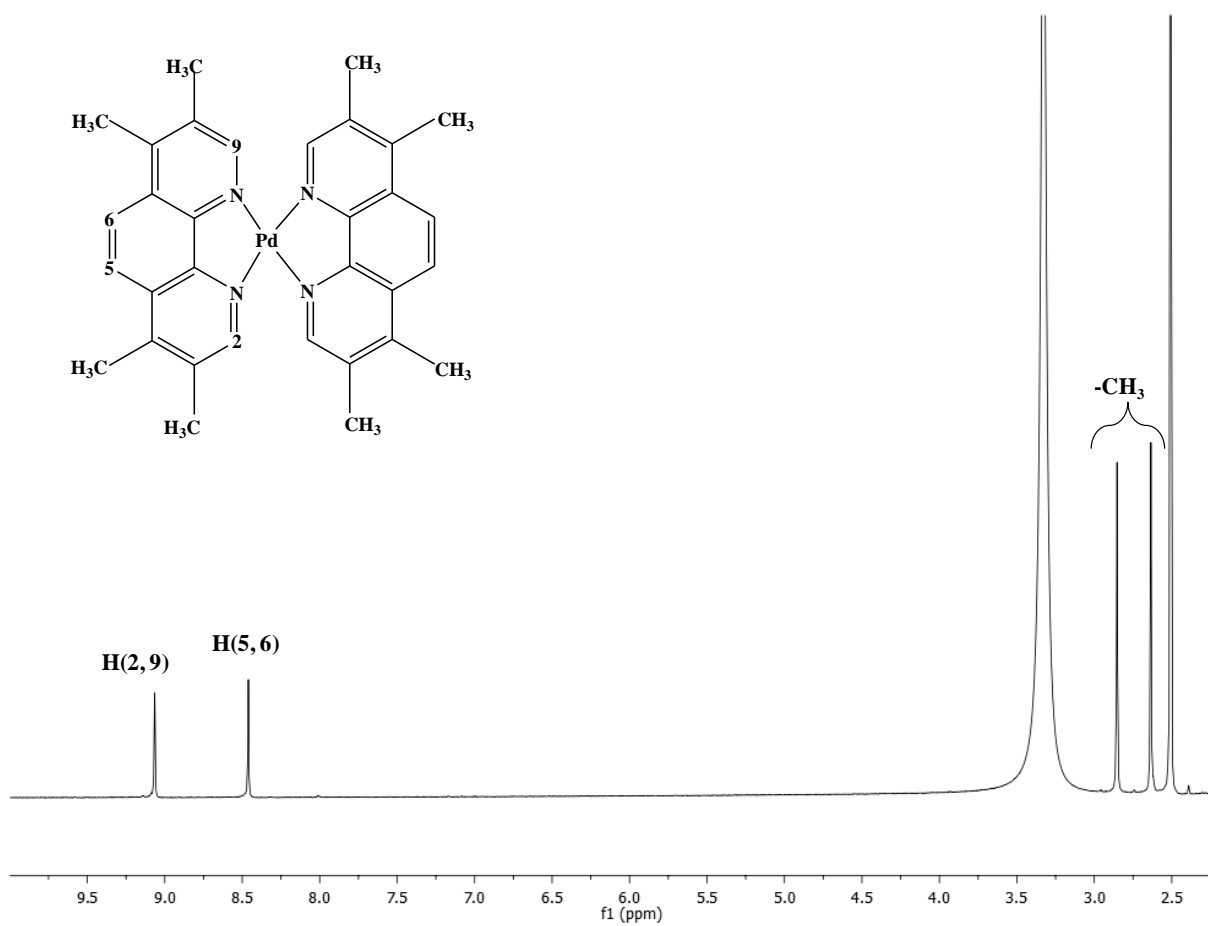


Fig. S2 a) <sup>1</sup>H NMR spectra and b) <sup>13</sup>C NMR spectra of the complex 2

a)



b)

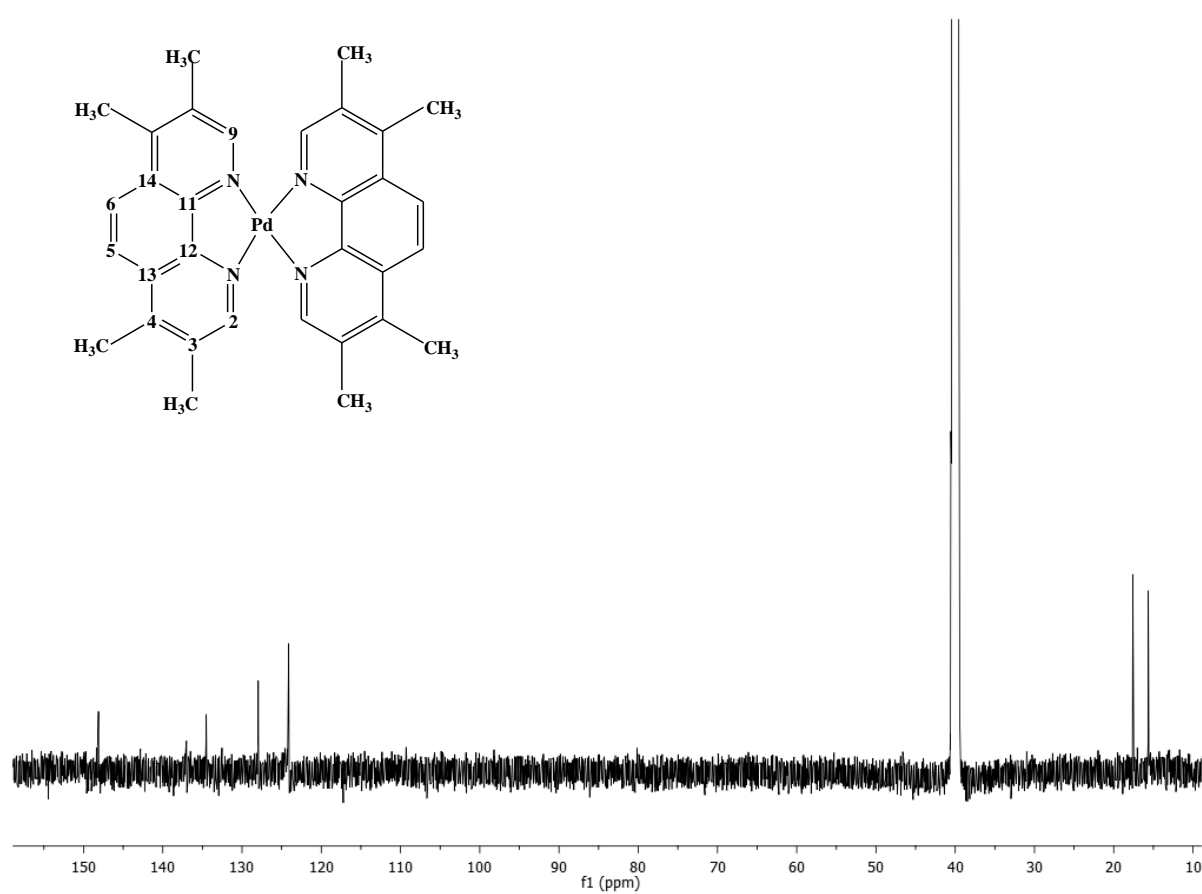
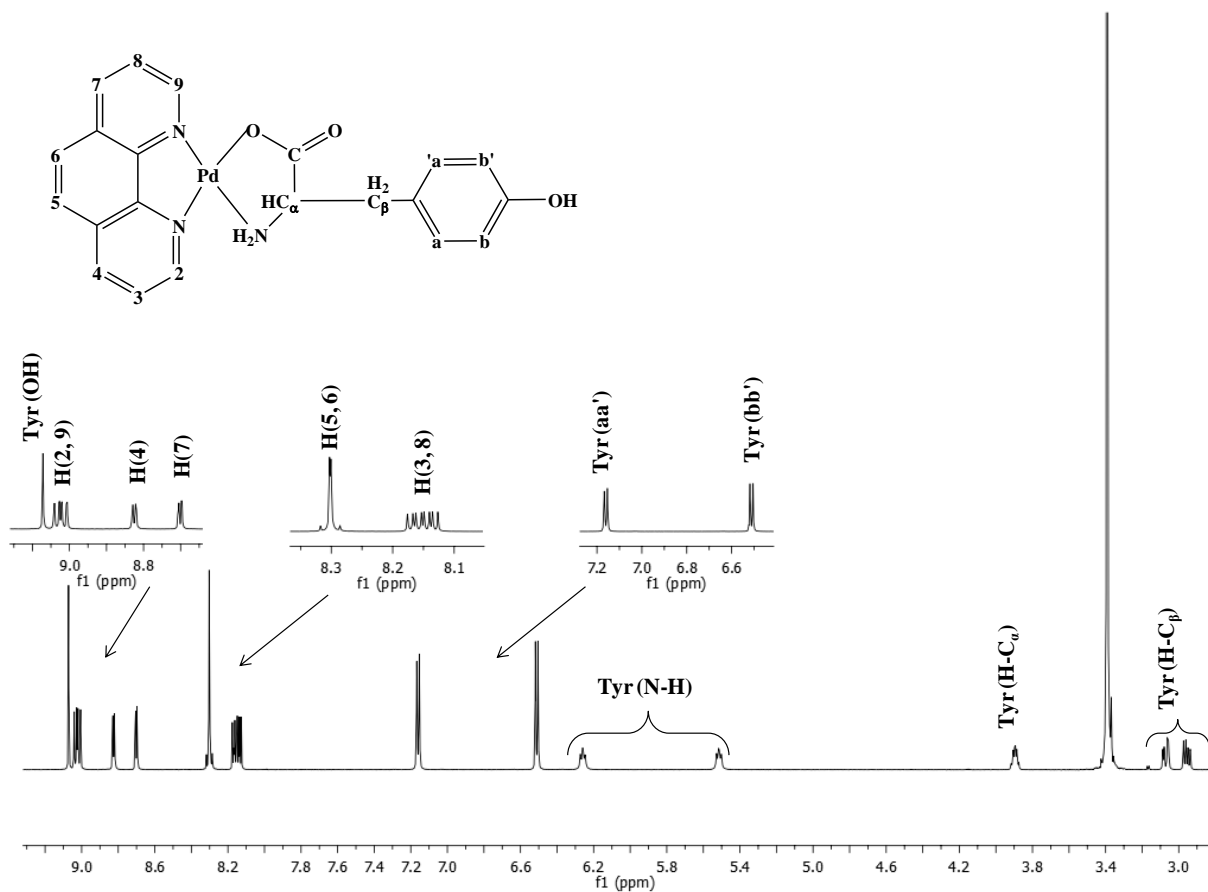


Fig. S3 a) <sup>1</sup>H NMR spectra and b) <sup>13</sup>C NMR spectra of the complex **3**

a)



b)

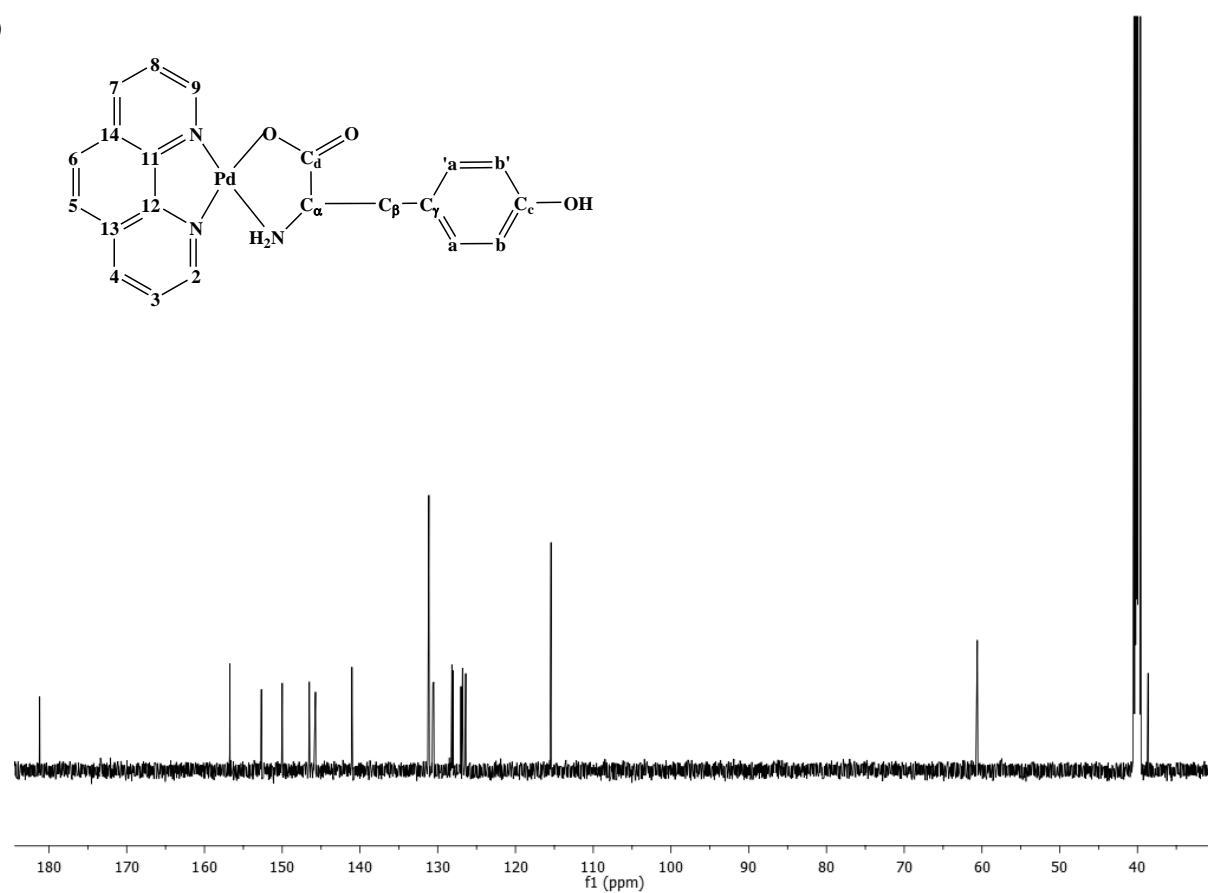
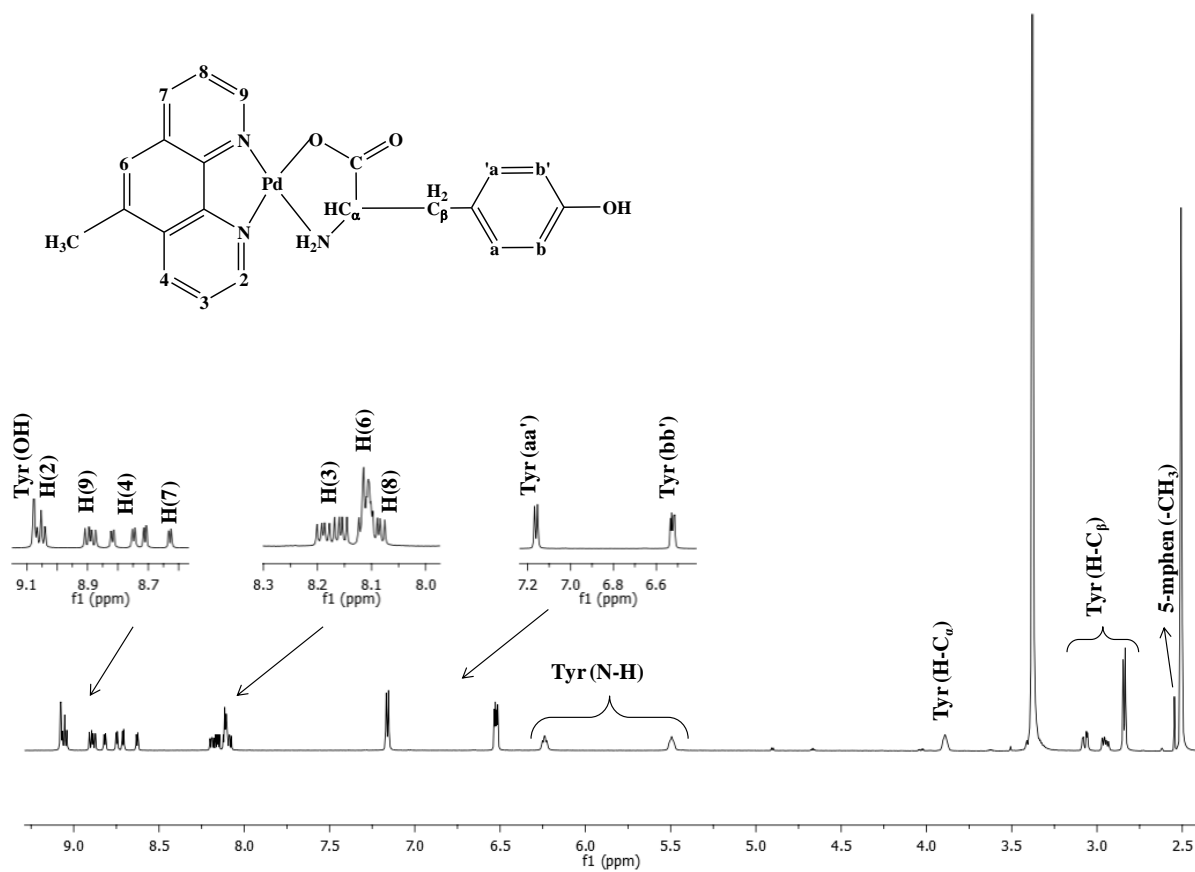


Fig. S4 a) <sup>1</sup>H NMR spectra and b) <sup>13</sup>C NMR spectra of the complex 4

a)



b)

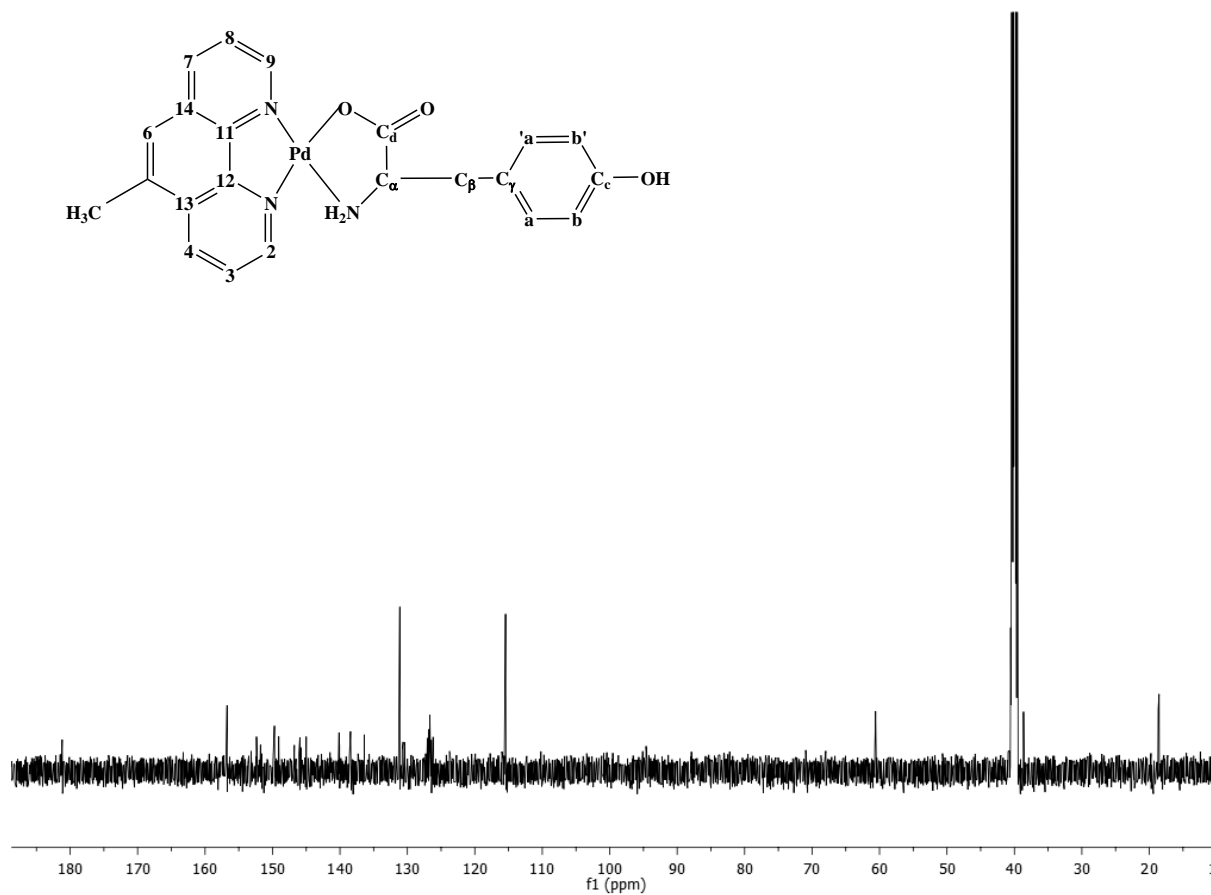
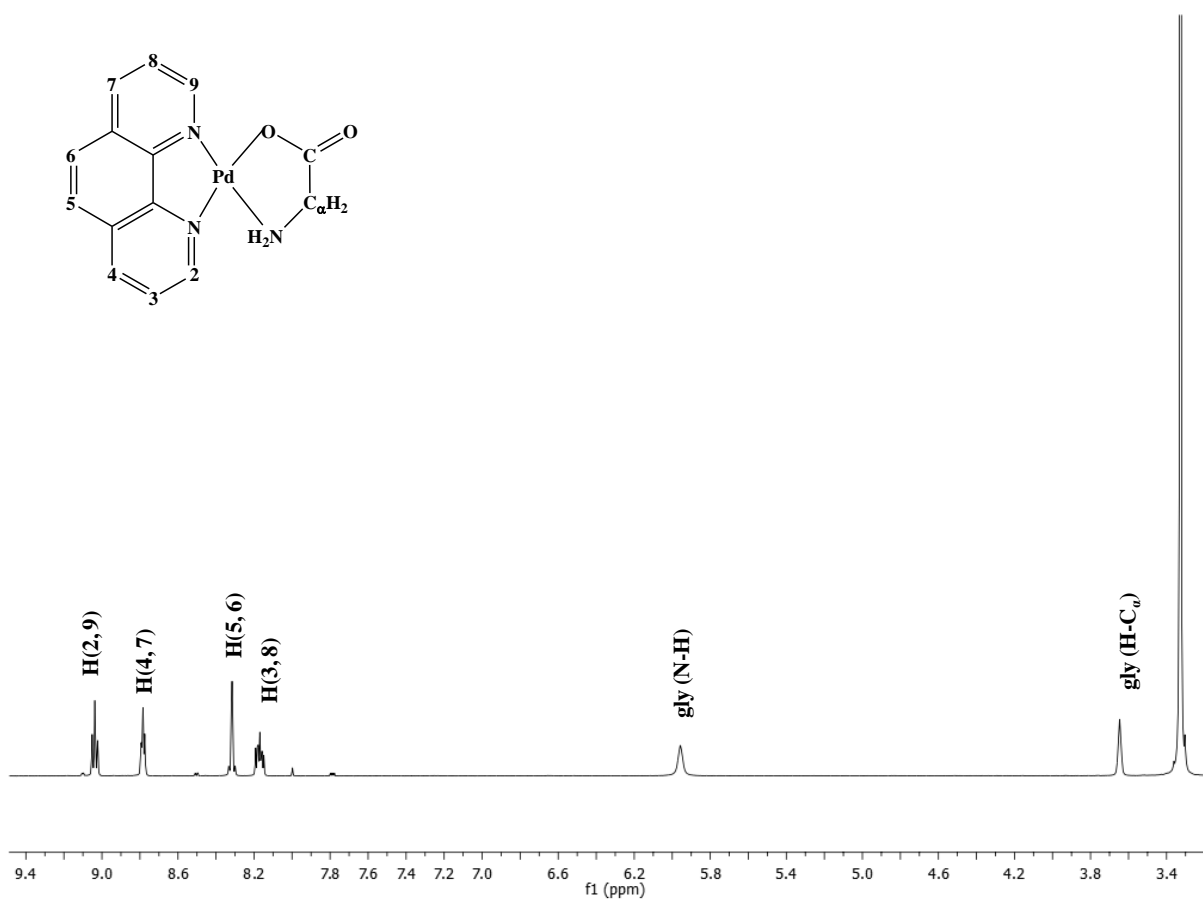


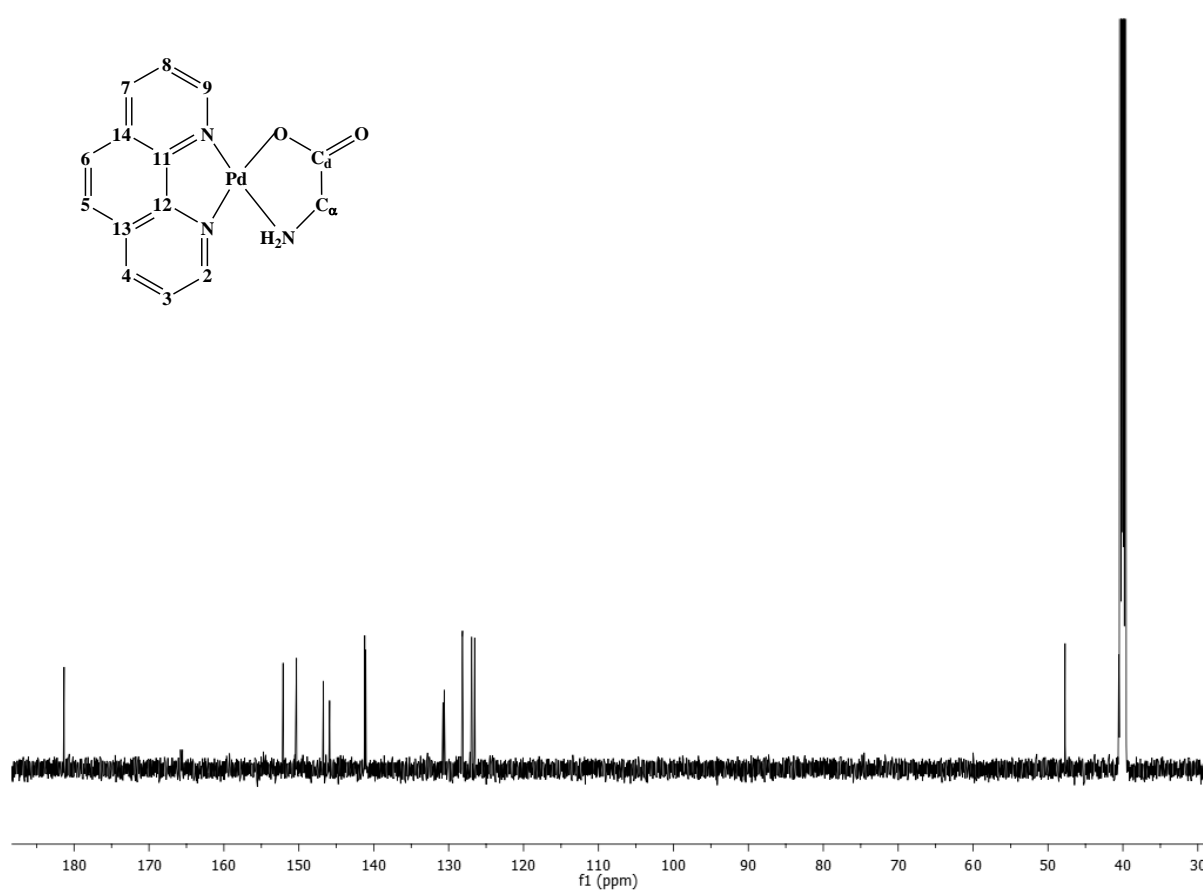
Fig. S5 a)  $^1\text{H}$  NMR spectra and b)  $^{13}\text{C}$  NMR spectra of the complex 5



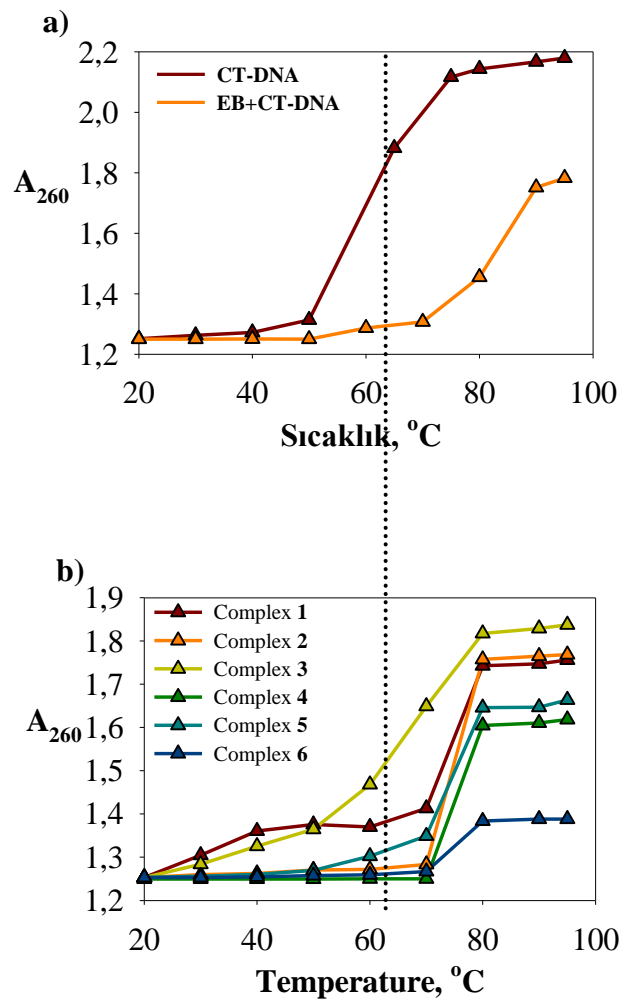
a)



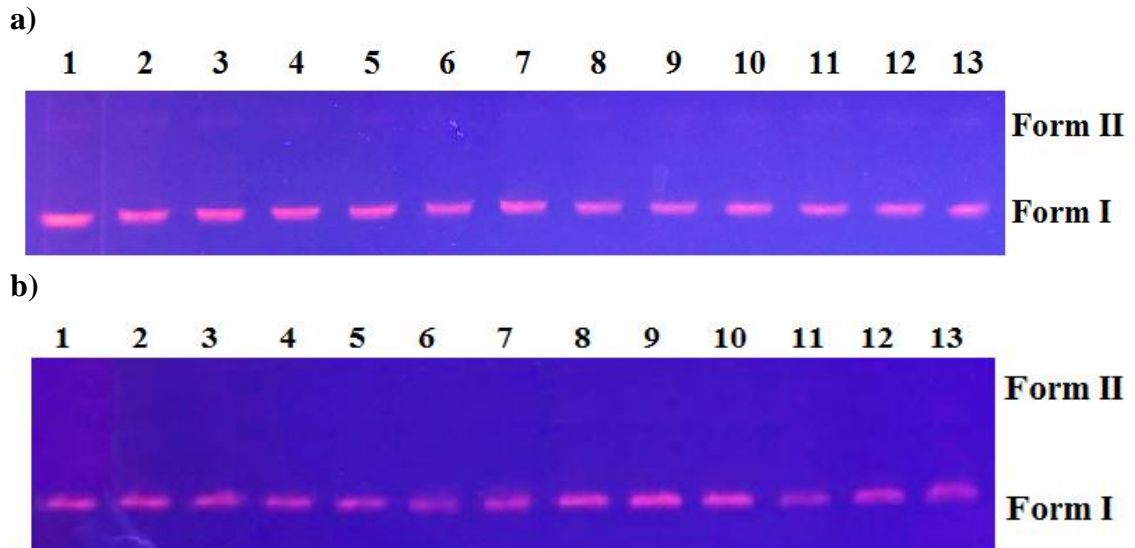
b)



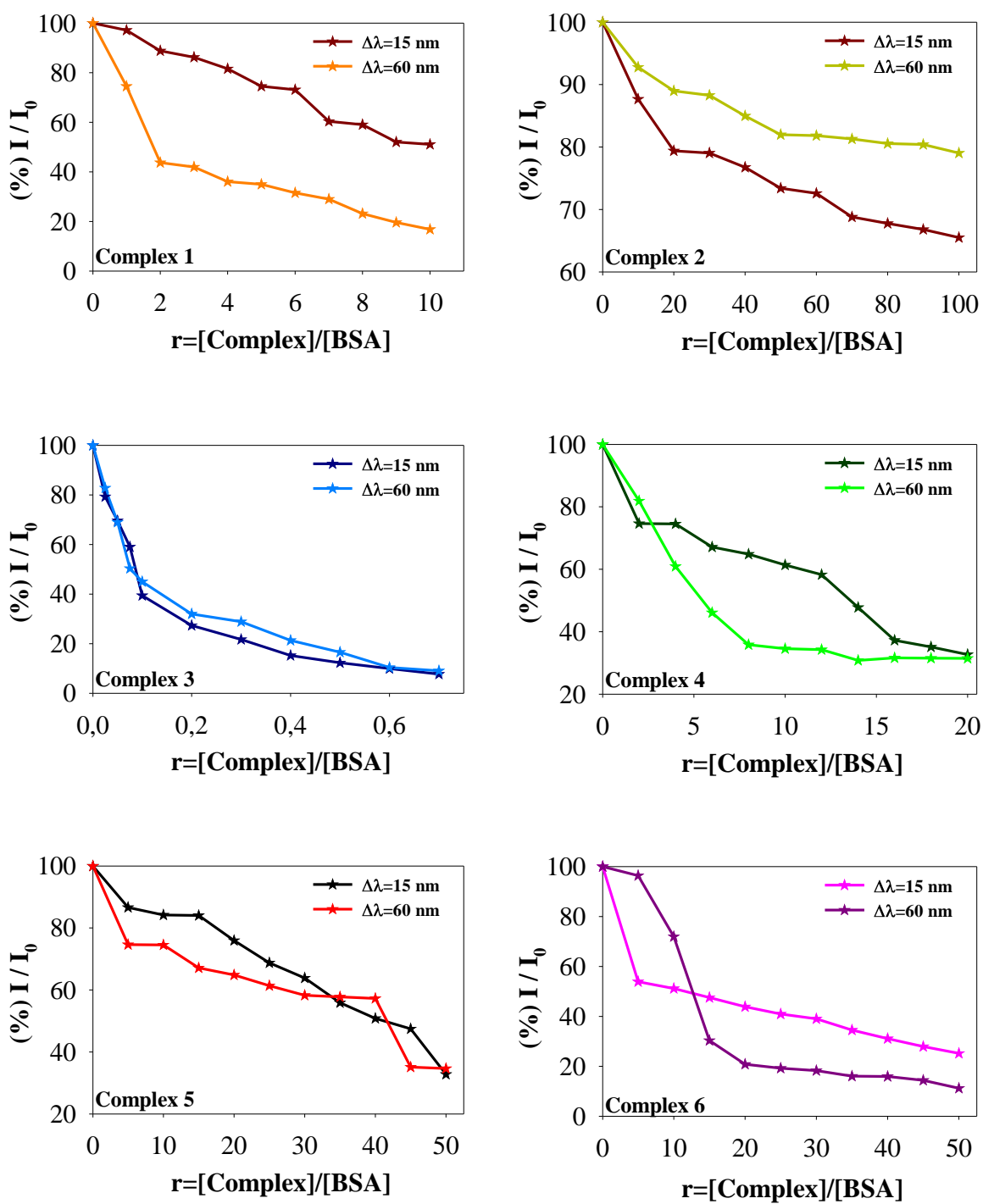
**Fig. S6 a)**  $^1\text{H}$  NMR spectra and **b)**  $^{13}\text{C}$  NMR spectra of the complex **6**



**Fig. S7** Thermal denaturation curves of **a)** CT-DNA and EB+CT-DNA, **b)** CT-DNA+the complexes **1-6** systems



**Fig. S8** Agarose gel electrophoresis diagrams. Cleavage of pUC19 plasmid DNA induced by the complexes 1-6: **Fig. S8a** **Line 1:** Control pUC19 plasmid DNA + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 2:** pUC19 plasmid DNA + the complex 1 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 3:** pUC19 plasmid DNA + the complex 1 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 4:** pUC19 plasmid DNA + the complex 2 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 5:** pUC19 plasmid DNA + the complex 2 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 6:** pUC19 plasmid DNA + the complex 3 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 7:** pUC19 plasmid DNA + the complex 3 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 8:** pUC19 plasmid DNA + the complex 4 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 9:** pUC19 plasmid DNA + the complex 4 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 10:** pUC19 plasmid DNA + the complex 5 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 11:** pUC19 plasmid DNA + the complex 5 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 12:** pUC19 plasmid DNA + the complex 6 (1 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 13:** pUC19 plasmid DNA + the complex 6 (500 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM). **Fig. S8b** **Line 1:** Control pUC19 plasmid DNA + DMSO (1 μM) **Line 2:** pUC19 plasmid DNA + the complex 1 (1 μM) + DMSO (1 μM) **Line 3:** pUC19 plasmid DNA + the complex 1 (100 μM) + H<sub>2</sub>O<sub>2</sub> (1 μM) **Line 4:** pUC19 plasmid DNA + the complex 2 (1 μM) + DMSO (1 μM) **Line 5:** pUC19 plasmid DNA + the complex 2 (100 μM) + DMSO (1 μM) **Line 6:** pUC19 plasmid DNA + the complex 3 (1 μM) + DMSO (1 μM) **Line 7:** pUC19 plasmid DNA + the complex 3 (100 μM) + DMSO (1 μM) **Line 8:** pUC19 plasmid DNA + the complex 4 (1 μM) + DMSO (1 μM) **Line 9:** pUC19 plasmid DNA + the complex 4 (100 μM) + DMSO (1 μM) **Line 10:** pUC19 plasmid DNA + the complex 5 (1 μM) + DMSO (1 μM) **Line 11:** pUC19 plasmid DNA + the complex 5 (100 μM) + DMSO (1 μM) **Line 12:** pUC19 plasmid DNA + the complex 6 (1 μM) + DMSO (1 μM) **Line 13:** pUC19 plasmid DNA + the complex 6 (100 μM) + DMSO (1 μM).



**Fig. S9** Effect of addition of the complexes 1-6 on the relative synchronous fluorescence intensity of BSA at  $\Delta\lambda = 15 \text{ nm}$  and  $\Delta\lambda = 60 \text{ nm}$ .