Supporting Information

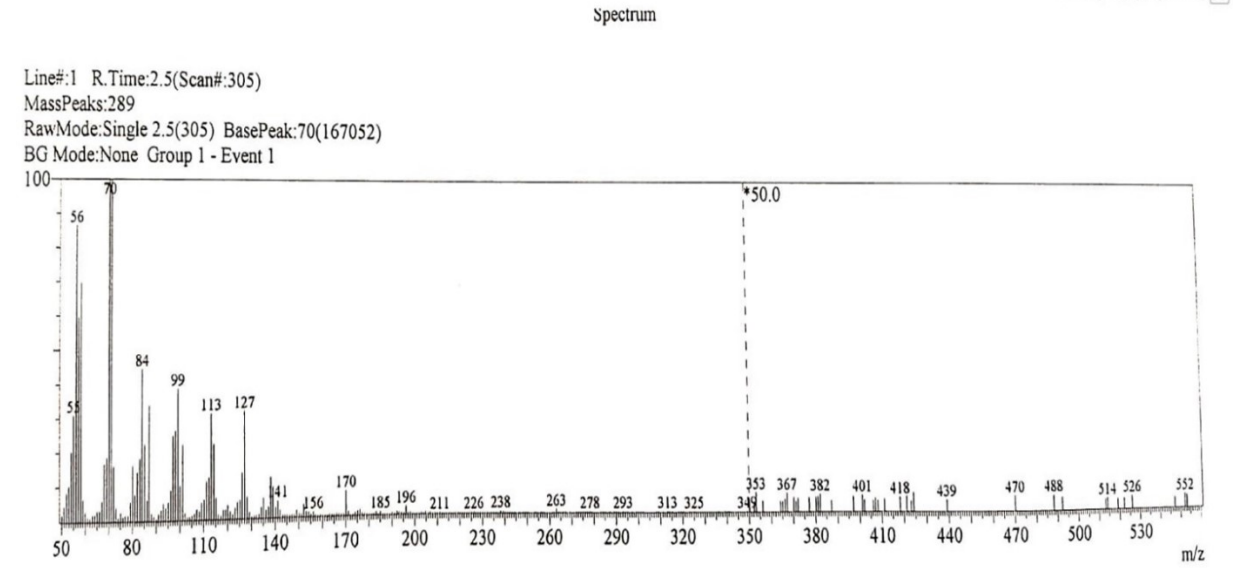

Figure S1 MS spectrum of the [Pd(BAPP)][PdCl4] complex.

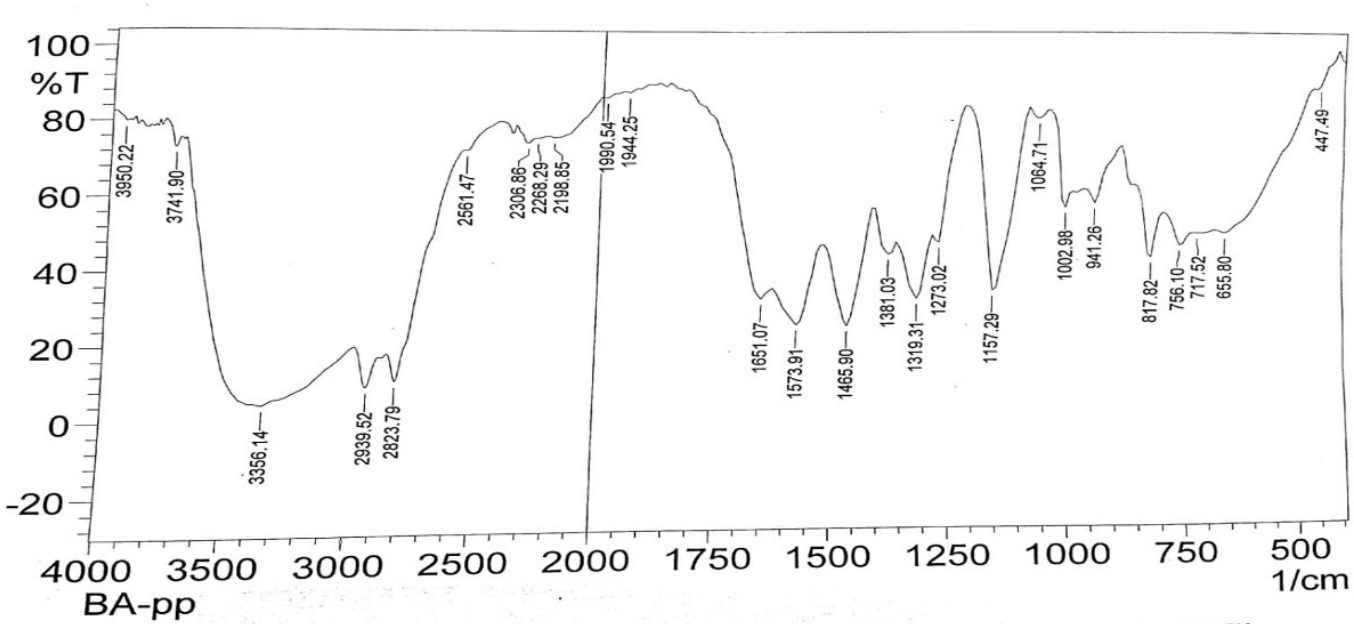

Figure S2 (A) IR spectrum of BAPP free ligand.

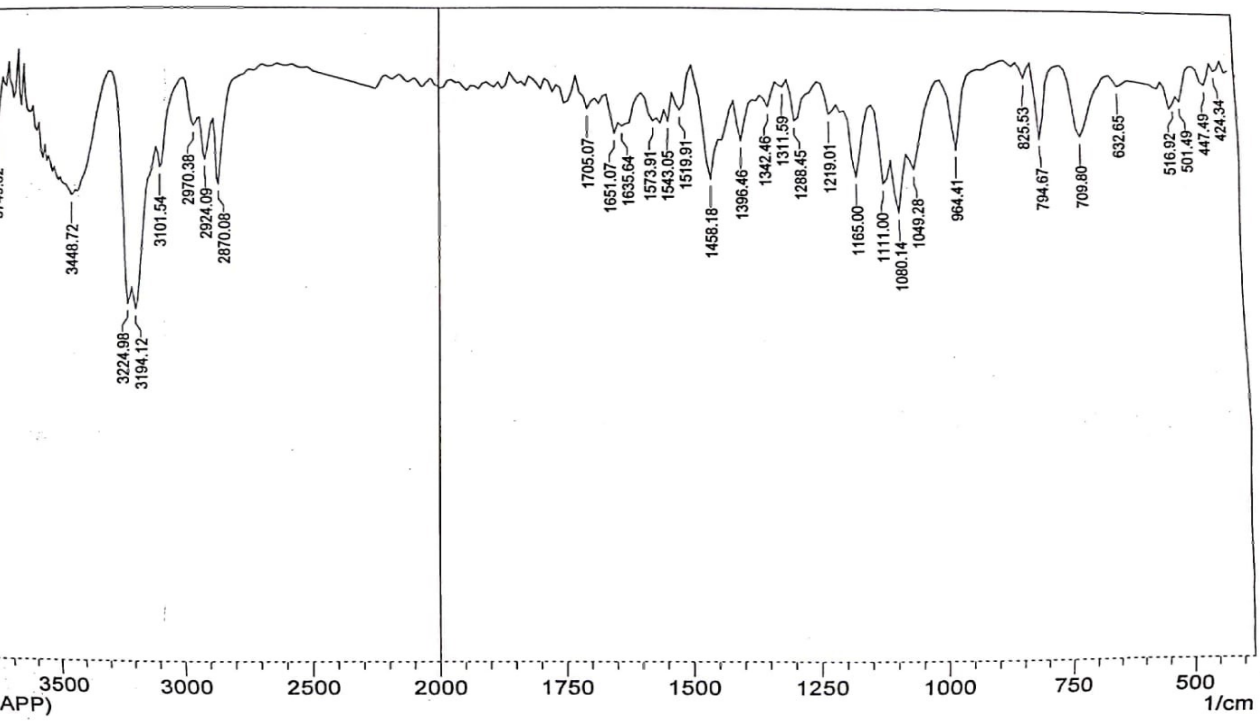

Figure S2 (B) IR spectrum of [Pd(BAPP)][$PdCl_4$] complex.

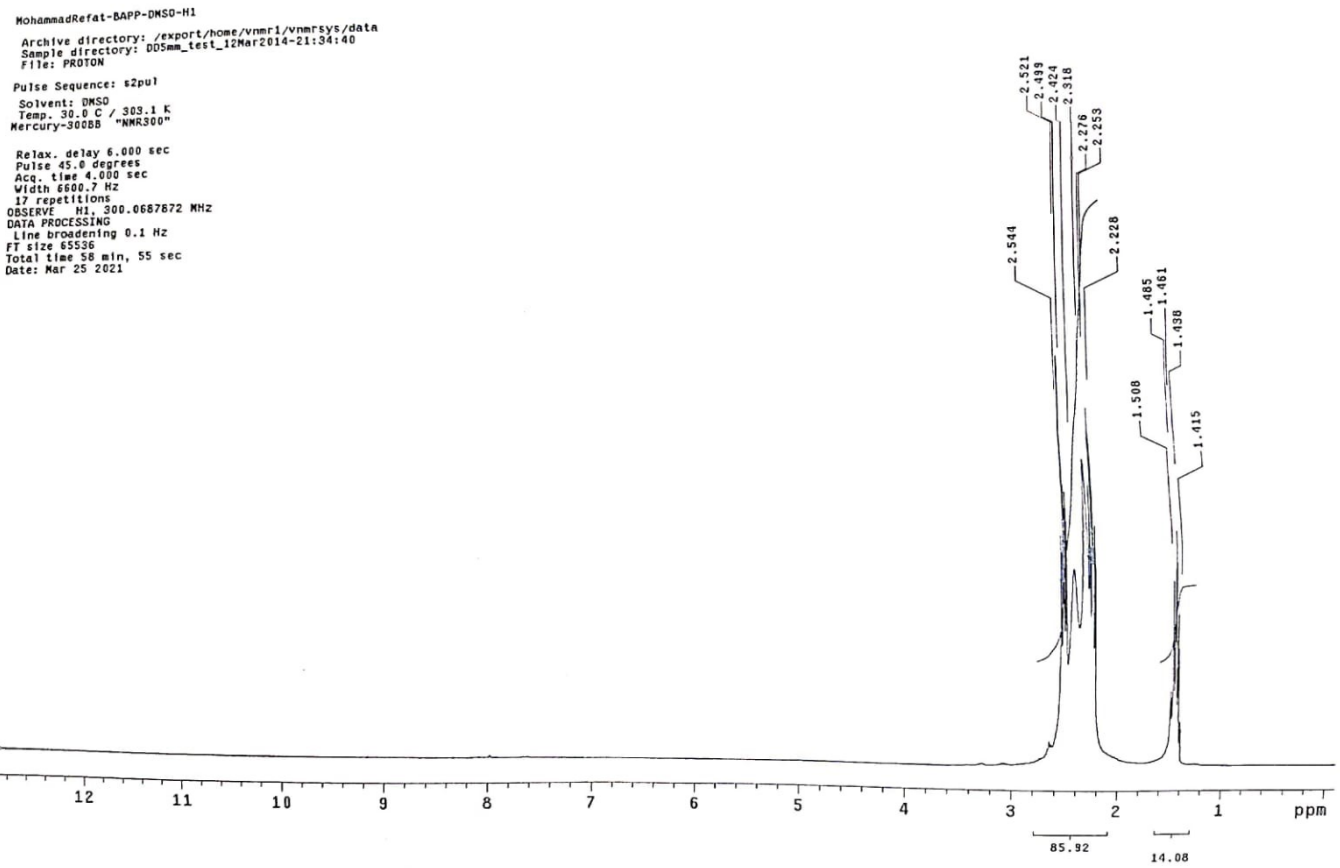

Figure S3 ^{1}H NMR spectrum of [Pd(BAPP)][$PdCl_4$] complex

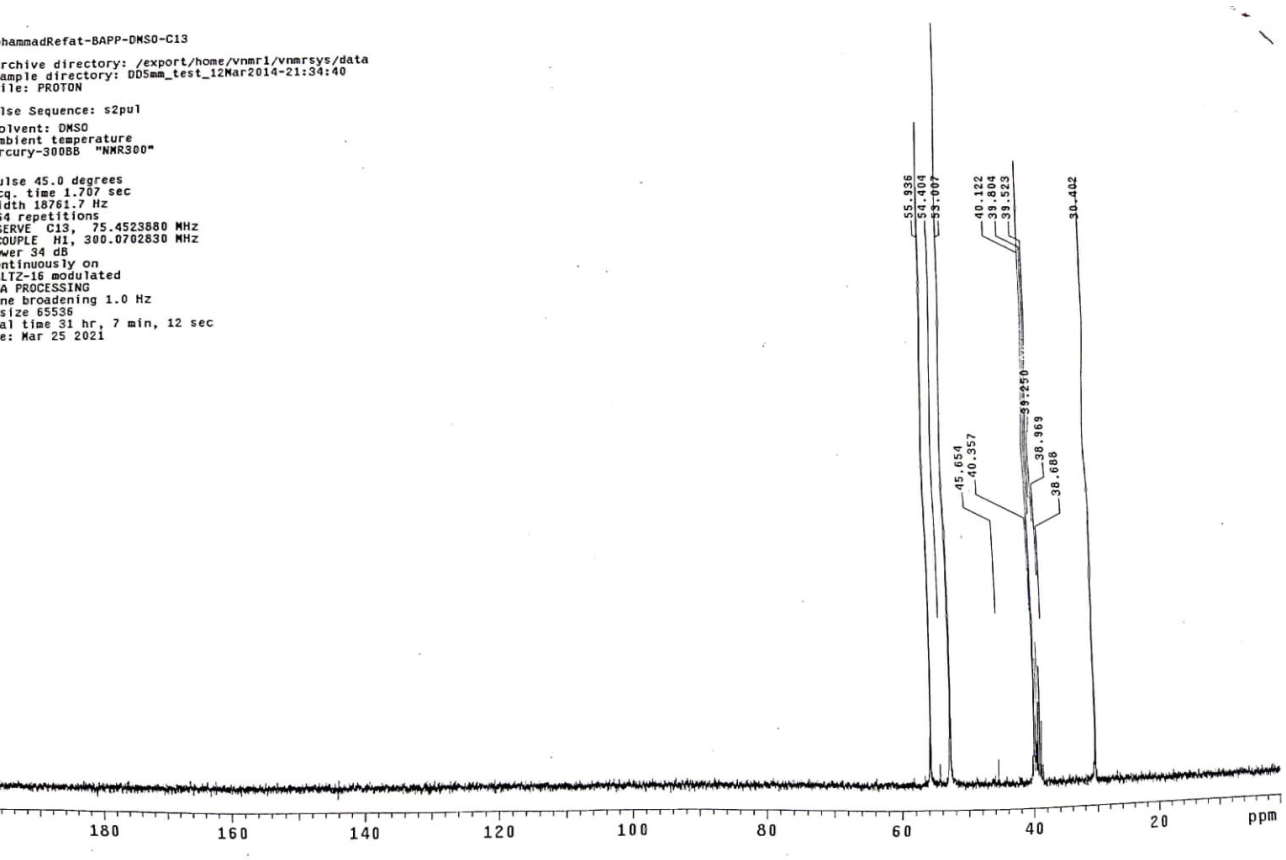

Figure S4 ^{13}C NMR spectrum of [Pd(BAPP)][$PdCl_4$] complex

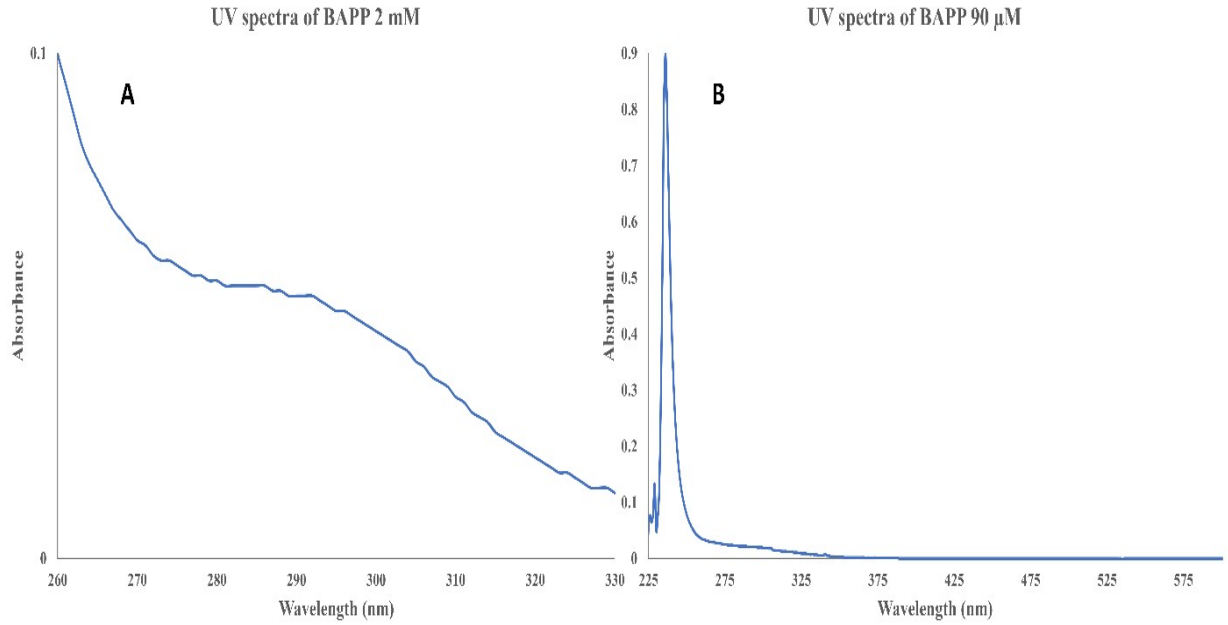

Figure S5 UV-absorption spectra of the concentrated **A** and diluted **B** BAPP free ligand in DMSO.

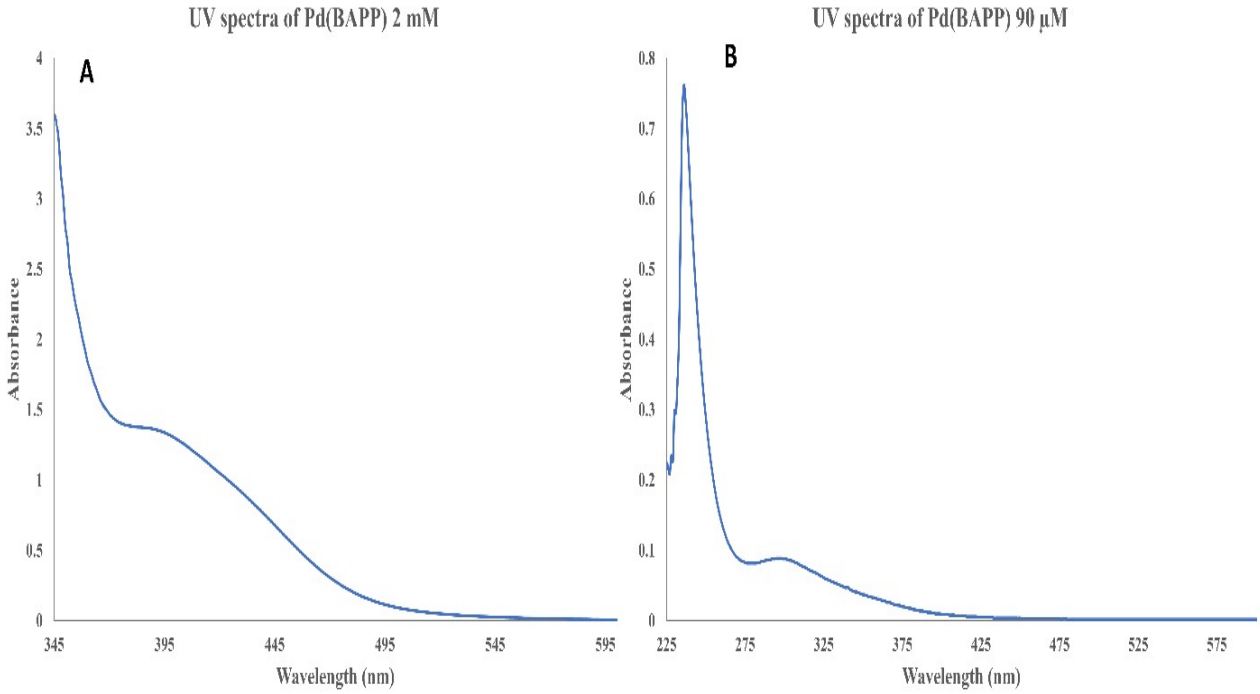

Figure S6 UV-absorption spectra of the concentrated (A) and diluted (B) [Pd(BAPP)][$PdCl_4$] complex in DMSO

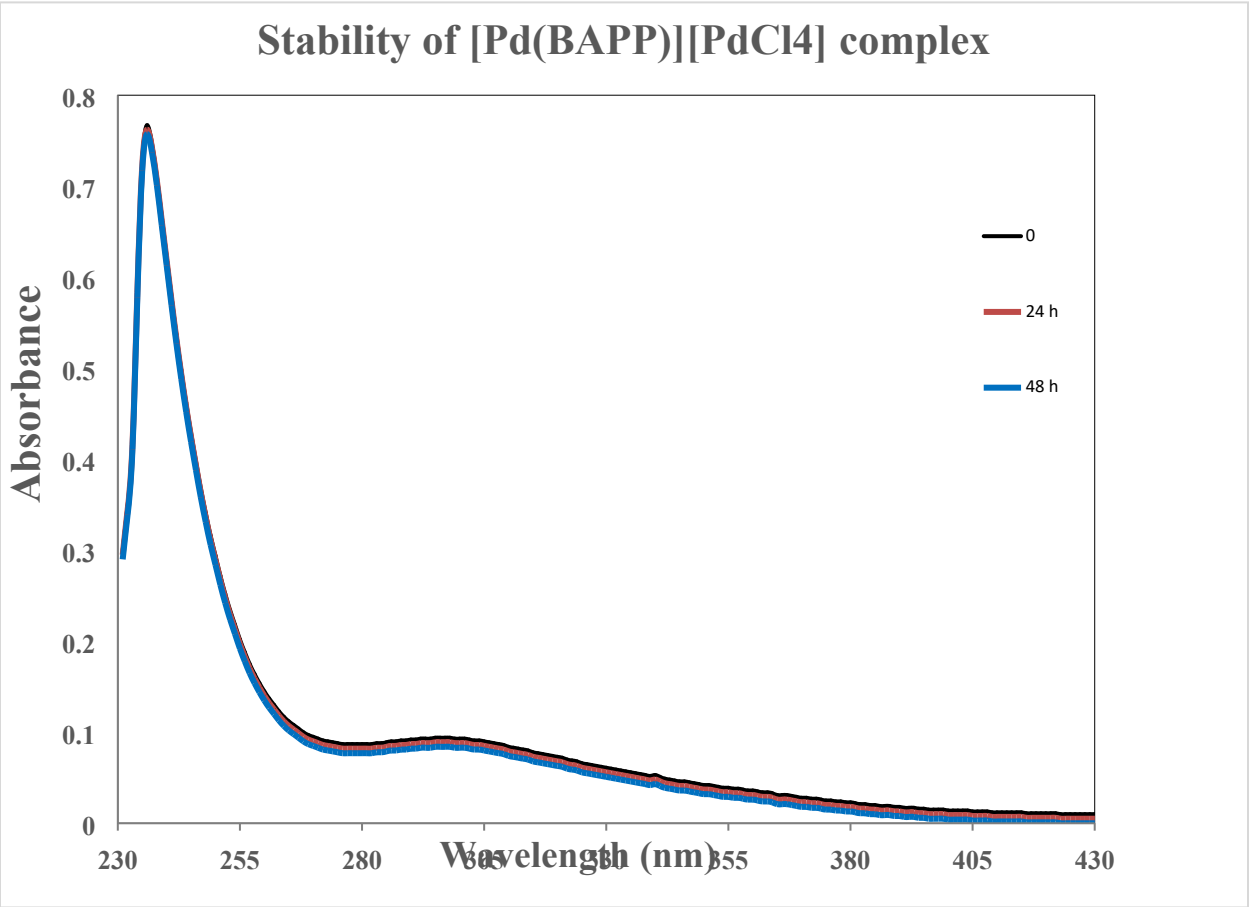

Figure S7 UV-absorption spectrum of the [Pd(BAPP)][$PdCl_4$] complex at different time 0, 24 and 48 h in DMSO

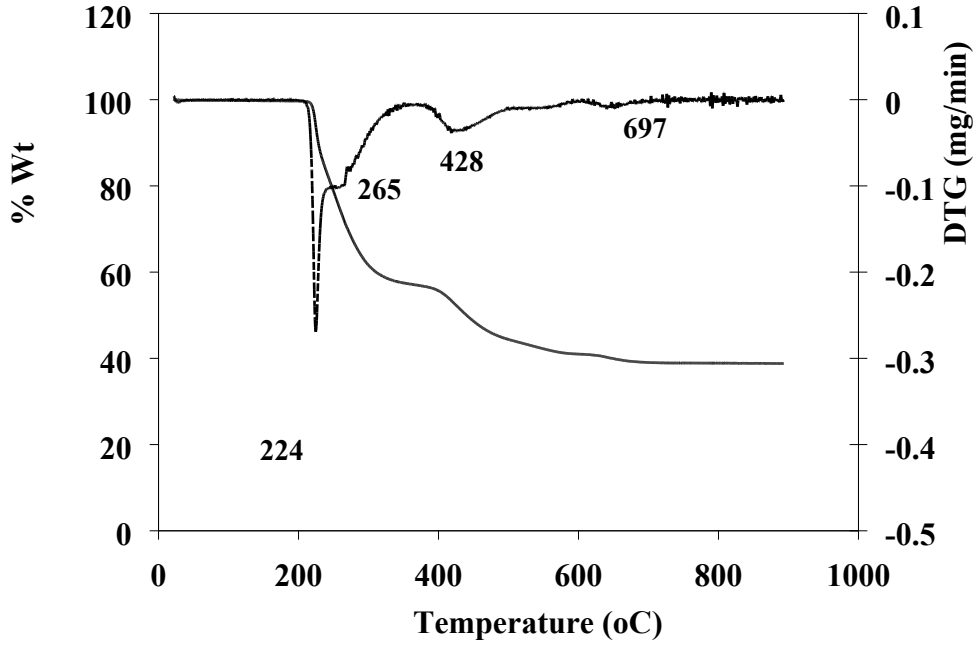

Figure S8 TG and DTG spectra of the [Pd(BAPP)][$PdCl_4$] complex.

Table S1. X-ray diffraction data for [Pd(BAPP)][$PdCl_4$]

a) Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Pd(BAPP)][PdCl4]. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5000	5000	0	30(1)
Cl(22)	7437(1)	2825(1)	58(1)	44(1)
Cl(23)	6212(1)	6121(1)	955(1)	42(1)
Pd(2)	3333(1)	2966(1)	2557(1)	29(1)
N(8)	1086(4)	4444(4)	3029(2)	35(1)
N(9)	1531(4)	2363(4)	2014(2)	33(1)
N(13)	4858(4)	3948(5)	3056(2)	44(1)
N(14)	5411(4)	1240(4)	2092(2)	42(1)
C(10)	1056(6)	5631(6)	3641(3)	50(1)
C(11)	2391(7)	6379(6)	3271(3)	59(1)
C(12)	4111(6)	5285(6)	3625(3)	58(1)
C(15)	2031(6)	1070(6)	1406(3)	52(1)
C(16)	3629(6)	-253(6)	1784(4)	54(1)
C(17)	5179(6)	184(6)	1463(3)	55(1)
C(18)	280(5)	3253(6)	3645(3)	43(1)
C(19)	481(5)	2016(6)	2987(3)	43(1)
C(20)	563(5)	3936(5)	1353(3)	40(1)
C(21)	189(5)	5221(5)	2009(3)	43(1)
Pd(3)	5000	0	5000	39(1)
Cl(24)	7232(1)	931(2)	4745(1)	61(1)
Cl(25)	3477(2)	2030(2)	5866(1)	60(1)

b) Selected bond lengths [Å] and angles [°] for [Pd(BAPP)][$PdCl_4$].

Pd(1)-Cl(23)	2.3008(11)
Pd(1)-Cl(22)	2.3128(11)
Pd(2)-N(8)	2.047(3)
Pd(2)-N(13)	2.054(3)
Pd(2)-N(9)	2.054(3)
Pd(2)-N(14)	2.058(3)

c) Bond lengths [Å] and angles [°] for [Pd(BAPP)][$PdCl_4$].

Pd(1)-Cl(23)#1	2.3008(11)	C(11)-H(11B)	0.97
Pd(1)-Cl(23)	2.3008(11)	C(12)-H(12A)	0.97
Pd(1)-Cl(22)#1	2.3128(11)	C(12)-H(12B)	0.97
Pd(1)-Cl(22)	2.3128(11)	C(15)-C(16)	1.511(6)
Pd(2)-N(8)	2.047(3)	C(15)-H(15A)	0.97
Pd(2)-N(13)	2.054(3)	C(15)-H(15B)	0.97
Pd(2)-N(9)	2.054(3)	C(16)-C(17)	1.502(6)

Pd(2)-N(14)	2.058(3)	C(16)-H(16A)	0.97
N(8)-C(10)	1.476(5)	C(16)-H(16B)	0.97
N(8)-C(21)	1.498(4)	C(17)-H(17A)	0.97
N(8)-C(18)	1.502(5)	C(17)-H(17B)	0.97
N(9)-C(15)	1.481(5)	C(18)-C(19)	1.519(6)
N(9)-C(20)	1.486(5)	C(18)-H(18A)	0.97
N(9)-C(19)	1.494(4)	C(18)-H(18B)	0.97
N(13)-C(12)	1.483(6)	C(19)-H(19A)	0.97
N(13)-H(13A)	0.89	C(19)-H(19B)	0.97
N(13)-H(13B)	0.89	C(20)-C(21)	1.528(6)
N(14)-C(17)	1.473(6)	C(20)-H(20A)	0.97
N(14)-H(14A)	0.89	C(20)-H(20B)	0.97
N(14)-H(14B)	0.89	C(21)-H(21A)	0.97
C(10)-C(11)	1.502(6)	C(21)-H(21B)	0.97
C(10)-H(10A)	0.97	Pd(3)-Cl(25)#2	2.3066(13)
C(10)-H(10B)	0.97	Pd(3)-Cl(25)	2.3066(13)
C(11)-C(12)	1.512(7)	Pd(3)-Cl(24)#2	2.3102(12)
C(11)-H(11A)	0.97	Pd(3)-Cl(24)	2.3102(12)
Cl(23)#1-Pd(1)-Cl(23)	180.00(5)	N(13)-C(12)-H(12B)	108.8
Cl(23)#1-Pd(1)-Cl(22)#1	89.73(4)	C(11)-C(12)-H(12B)	108.8
Cl(23)-Pd(1)-Cl(22)#1	90.27(4)	H(12A)-C(12)-H(12B)	107.6
Cl(23)#1-Pd(1)-Cl(22)	90.27(4)	N(9)-C(15)-C(16)	112.5(3)
Cl(23)-Pd(1)-Cl(22)	89.73(4)	N(9)-C(15)-H(15A)	109.1
Cl(22)#1-Pd(1)-Cl(22)	180	C(16)-C(15)-H(15A)	109.1
N(8)-Pd(2)-N(13)	98.61(14)	N(9)-C(15)-H(15B)	109.1
N(8)-Pd(2)-N(9)	73.44(13)	C(16)-C(15)-H(15B)	109.1
N(13)-Pd(2)-N(9)	170.55(14)	H(15A)-C(15)-H(15B)	107.8
N(8)-Pd(2)-N(14)	171.44(14)	C(17)-C(16)-C(15)	114.8(4)
N(13)-Pd(2)-N(14)	89.30(14)	C(17)-C(16)-H(16A)	108.6
N(9)-Pd(2)-N(14)	98.96(14)	C(15)-C(16)-H(16A)	108.6
C(10)-N(8)-C(21)	112.3(3)	C(17)-C(16)-H(16B)	108.6
C(10)-N(8)-C(18)	112.1(3)	C(15)-C(16)-H(16B)	108.6
C(21)-N(8)-C(18)	106.7(3)	H(16A)-C(16)-H(16B)	107.6
C(10)-N(8)-Pd(2)	119.1(3)	N(14)-C(17)-C(16)	113.5(3)
C(21)-N(8)-Pd(2)	103.4(2)	N(14)-C(17)-H(17A)	108.9
C(18)-N(8)-Pd(2)	102.0(2)	C(16)-C(17)-H(17A)	108.9
C(15)-N(9)-C(20)	111.4(3)	N(14)-C(17)-H(17B)	108.9
C(15)-N(9)-C(19)	112.0(3)	C(16)-C(17)-H(17B)	108.9
C(20)-N(9)-C(19)	107.6(3)	H(17A)-C(17)-H(17B)	107.7
C(15)-N(9)-Pd(2)	119.5(3)	N(8)-C(18)-C(19)	108.3(3)
C(20)-N(9)-Pd(2)	101.0(2)	N(8)-C(18)-H(18A)	110

C(19)-N(9)-Pd(2)	104.2(2)	C(19)-C(18)-H(18A)	110
C(12)-N(13)-Pd(2)	119.2(3)	N(8)-C(18)-H(18B)	110
C(12)-N(13)-H(13A)	107.5	C(19)-C(18)-H(18B)	110
Pd(2)-N(13)-H(13A)	107.5	H(18A)-C(18)-H(18B)	108.4
C(12)-N(13)-H(13B)	107.5	N(9)-C(19)-C(18)	107.8(3)
Pd(2)-N(13)-H(13B)	107.5	N(9)-C(19)-H(19A)	110.1
H(13A)-N(13)-H(13B)	107	C(18)-C(19)-H(19A)	110.1
C(17)-N(14)-Pd(2)	118.3(3)	N(9)-C(19)-H(19B)	110.1
C(17)-N(14)-H(14A)	107.7	C(18)-C(19)-H(19B)	110.1
Pd(2)-N(14)-H(14A)	107.7	H(19A)-C(19)-H(19B)	108.5
C(17)-N(14)-H(14B)	107.7	N(9)-C(20)-C(21)	108.2(3)
Pd(2)-N(14)-H(14B)	107.7	N(9)-C(20)-H(20A)	110.1
H(14A)-N(14)-H(14B)	107.1	C(21)-C(20)-H(20A)	110.1
N(8)-C(10)-C(11)	112.9(3)	N(9)-C(20)-H(20B)	110.1
N(8)-C(10)-H(10A)	109	C(21)-C(20)-H(20B)	110.1
C(11)-C(10)-H(10A)	109	H(20A)-C(20)-H(20B)	108.4
N(8)-C(10)-H(10B)	109	N(8)-C(21)-C(20)	107.7(3)
C(11)-C(10)-H(10B)	109	N(8)-C(21)-H(21A)	110.2
H(10A)-C(10)-H(10B)	107.8	C(20)-C(21)-H(21A)	110.2
C(10)-C(11)-C(12)	113.7(4)	N(8)-C(21)-H(21B)	110.2
C(10)-C(11)-H(11A)	108.8	C(20)-C(21)-H(21B)	110.2
C(12)-C(11)-H(11A)	108.8	H(21A)-C(21)-H(21B)	108.5
C(10)-C(11)-H(11B)	108.8	Cl(25)#2-Pd(3)-Cl(25)	180.00(5)
C(12)-C(11)-H(11B)	108.8	Cl(25)#2-Pd(3)-Cl(24)#2	90.77(5)
H(11A)-C(11)-H(11B)	107.7	Cl(25)-Pd(3)-Cl(24)#2	89.23(5)
N(13)-C(12)-C(11)	114.0(4)	Cl(25)#2-Pd(3)-Cl(24)	89.23(5)
N(13)-C(12)-H(12A)	108.8	Cl(25)-Pd(3)-Cl(24)	90.77(5)
C(11)-C(12)-H(12A)	108.8	Cl(24)#2-Pd(3)-Cl(24)	180

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 -x+1,-y,-z+1

d) Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [Pd(BAPP)][$PdCl_4$]. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	29(1)	31(1)	29(1)	-6(1)	0(1)	-11(1)
Cl(22)	34(1)	40(1)	56(1)	-11(1)	-1(1)	-8(1)
Cl(23)	40(1)	45(1)	46(1)	-16(1)	-5(1)	-16(1)
Pd(2)	28(1)	33(1)	26(1)	-5(1)	-3(1)	-12(1)
N(8)	33(2)	36(2)	33(2)	-8(1)	0(1)	-10(2)
N(9)	33(2)	37(2)	31(2)	-8(1)	-6(1)	-13(2)
N(13)	46(2)	52(3)	38(2)	2(2)	-12(2)	-28(2)
N(14)	40(2)	44(2)	35(2)	-1(2)	0(1)	-10(2)
C(10)	62(3)	45(3)	45(2)	-21(2)	3(2)	-15(3)
C(11)	90(4)	45(3)	51(3)	-20(2)	3(2)	-31(3)

C(12)	85(4)	69(4)	41(2)	-14(2)	-7(2)	-49(3)
C(15)	63(3)	55(4)	50(3)	-24(2)	-6(2)	-26(3)
C(16)	72(3)	35(3)	62(3)	-20(2)	10(2)	-25(3)
C(17)	61(3)	42(3)	57(3)	-18(2)	8(2)	-11(3)
C(18)	37(2)	57(3)	37(2)	-9(2)	8(2)	-21(2)
C(19)	41(3)	53(3)	41(2)	-5(2)	4(2)	-28(2)
C(20)	32(2)	51(3)	33(2)	-4(2)	-8(2)	-10(2)
C(21)	34(2)	46(3)	42(2)	0(2)	-6(2)	-8(2)
Pd(3)	37(1)	44(1)	32(1)	3(1)	-7(1)	-16(1)
Cl(24)	47(1)	68(1)	65(1)	12(1)	-14(1)	-31(1)
Cl(25)	62(1)	55(1)	55(1)	-10(1)	-5(1)	-9(1)

e) Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for [Pd(BAPP)][$PdCl_4$].

	x	y	z	U(eq)
H(13A)	5596	3156	3481	52
H(13B)	5425	4296	2484	52
H(14A)	6090	1738	1715	51
H(14B)	5935	616	2678	51
H(10A)	1196	5105	4389	60
H(10B)	-23	6473	3579	60
H(11A)	2108	7352	3541	71
H(11B)	2412	6683	2498	71
H(12A)	4840	5923	3517	69
H(12B)	4047	4833	4384	69
H(15A)	2173	1530	657	62
H(15B)	1147	612	1477	62
H(16A)	3555	-563	2556	65
H(16B)	3729	-1183	1504	65
H(17A)	6137	-795	1542	66
H(17B)	5134	719	716	66
H(18A)	-893	3801	3784	52
H(18B)	804	2727	4323	52
H(19A)	1012	940	3398	52
H(19B)	-601	2084	2786	52
H(20A)	-468	3883	1154	48
H(20B)	1201	4198	707	48
H(21A)	567	6097	1618	52
H(21B)	-1001	5653	2157	52

f) Torsion angles [°] for [Pd(BAPP)][PdCl4].

C(21)-N(8)-C(10)-C(11)	-83.1(4)
C(18)-N(8)-C(10)-C(11)	156.8(4)
Pd(2)-N(8)-C(10)-C(11)	37.9(5)
N(8)-C(10)-C(11)-C(12)	-75.7(5)
Pd(2)-N(13)-C(12)-C(11)	-32.4(5)

C(10)-C(11)-C(12)-N(13)	72.7(5)
C(20)-N(9)-C(15)-C(16)	151.3(4)
C(19)-N(9)-C(15)-C(16)	-88.2(4)
Pd(2)-N(9)-C(15)-C(16)	34.1(5)
N(9)-C(15)-C(16)-C(17)	-73.8(5)
Pd(2)-N(14)-C(17)-C(16)	-36.2(5)
C(15)-C(16)-C(17)-N(14)	75.7(5)
C(10)-N(8)-C(18)-C(19)	-175.9(3)
C(21)-N(8)-C(18)-C(19)	60.7(4)
Pd(2)-N(8)-C(18)-C(19)	-47.4(3)
C(15)-N(9)-C(19)-C(18)	170.7(3)
C(20)-N(9)-C(19)-C(18)	-66.6(4)
Pd(2)-N(9)-C(19)-C(18)	40.1(4)
N(8)-C(18)-C(19)-N(9)	4.7(4)
C(15)-N(9)-C(20)-C(21)	-176.5(3)
C(19)-N(9)-C(20)-C(21)	60.4(4)
Pd(2)-N(9)-C(20)-C(21)	-48.6(3)
C(10)-N(8)-C(21)-C(20)	169.9(3)
C(18)-N(8)-C(21)-C(20)	-66.8(4)
Pd(2)-N(8)-C(21)-C(20)	40.2(3)
N(9)-C(20)-C(21)-N(8)	5.7(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 -x+1,-y,-z+1

g) Hydrogen bonds for [Pd(BAPP)][$PdCl_4$] [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(13)-H(13A)...Cl(24)	0.89	2.39	3.268(3)	171.6
N(13)-H(13B)...Cl(23)	0.89	2.45	3.300(3)	160.2
N(14)-H(14A)...Cl(22)	0.89	2.47	3.294(3)	154.6
N(14)-H(14B)...Cl(25)#2	0.89	2.60	3.395(3)	149.0
C(10)-H(10B)...Cl(25)#3	0.97	2.88	3.783(5)	155.8
C(12)-H(12B)...Cl(25)	0.97	2.95	3.747(5)	140.5
C(16)-H(16B)...Cl(23)#4	0.97	2.80	3.596(5)	139.4
C(19)-H(19A)...Cl(24)#2	0.97	2.83	3.676(4)	146.1
C(20)-H(20A)...Cl(22)#5	0.97	2.94	3.846(4)	156.2
C(20)-H(20A)...Cl(23)#5	0.97	2.86	3.592(4)	133.1
C(20)-H(20B)...Cl(23)#1	0.97	2.89	3.816(4)	160.7
C(21)-H(21A)...Cl(22)#1	0.97	2.80	3.658(4)	147.6
C(21)-H(21B)...Cl(23)#5	0.97	2.86	3.573(4)	131.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 -x+1,-y,-z+1 #3 -x,-y+1,-z+1
#4 x,y-1,z #5 x-1,y,z

Table S2. Important DFT optimized bond lengths (Å) of BAPP and the Pd(II) complex

Type of bond	Bond length (Å)	
	BAPP	Pd(II) complex
N1- - - - N2	2.885	2.500
N1- - - - N3	4.390	3.215
N2- - - - N4	4.459	3.049
N3- - - - N4	11.413	3.085

Table S3 Antimicrobial activity of the complex and the free ligand

Compounds	Microbial species					
	Bacteria				Fungus	
	P. aeruginosa	E. coli	B. subtilis	S. aureus	A. flavus	C. albicans
BAPP	21	20	20	21	16	13
Pd(BAPP) complex	12	14	12	13	13	20
Control (DMSO)	0	0	0	0	0	0
Standard Ampicilline Amphotericin B	17 -	22 -	20 -	18 -	- 17	- 19

Table S4 Some selected pharmacokinetics data calculated for BAPP and [Pd(BAPP)][$PdCl_4$] complex:

ADME FACTOR[a]	BAPP	complex
Physicochemical Properties		
Formula	$C_{10}H_{24}N_4$	$C_{10}H_{24}Cl_4N_4Pd_2$
Molecular weight	200.32 g/mol	554.98 g/mol
Num. heavy atoms	14	20
Fraction Csp3	1.00	1.00
Molar Refractivity	67.11	98.35
TPSA	58.52 Å²	58.52 Å²
Lipophilicity		

Log $P_{o/w}$ (iLOGP)	2.23	0.00
Log $P_{o/w}$ (XLOGP3)	-1.43	3.10
Log $P_{o/w}$ (WLOGP)	-1.46	0.54
Log $P_{o/w}$ (MLOGP)	-0.21	0.90
Log $P_{o/w}$ (SILICOS-IT)	-0.01	-2.46
Consensus Log $P_{o/w}$	-0.18	0.42
Water Solubility		
Log *S* (ESOL)	0.21	-5.23
Class	Highly soluble	Moderately soluble
Log *S* (Ali)	0.70	-4.00
Class	Highly soluble	Soluble
Log *S* (SILICOS-IT)	-1.38	-3.22
Class	Soluble	Soluble
Pharmacokinetics		
GI absorption	High	High
BBB permeant	No	No
P-gp substrate	Yes	Yes
CYP1A2 inhibitor	No	No
CYP2C19 inhibitor	No	No
CYP2C9 inhibitor	No	No
CYP2D6 inhibitor	No	No
CYP3A4 inhibitor	No	No
Log K_p (skin permeation)	-8.54 cm/s	-7.48 cm/s
Medicinal Chemistry		
PAINS	0 alert	0 alert
Brenk	0 alert	0 alert
Synthetic accessibility	1.88	5.18

(TPSA: Topological Polar Surface Area), Consensus $LogP_{o/w}$: Average of all five predictions, GI absorption: Gastrointestinal absorption, P-gp substrate: P-glycoprotein substrate, CYP1A2 inhibitor: Cytochrome P450 1A2 inhibitor, CYP2C19 inhibitor: Cytochrome P450 2C19

inhibitor, CYP2C9 inhibitor: Cytochrome P450 2C9 inhibitor), CYP2D6 inhibitor: Cytochrome P450 2D6 inhibitor, CYP3A4 inhibitor: Cytochrome P450 3A4 inhibitor, PAINS: Pan Assay Interference Structures, Brenk: Structural Alert, Synthetic accessibility score: from 1 (very easy) to 10 (very difficult).