Supporting Information

Palladium(II) and platinum(II) complexes with ONN donor pincer ligand: Synthesis, characterization and in vitro cytotoxicity study

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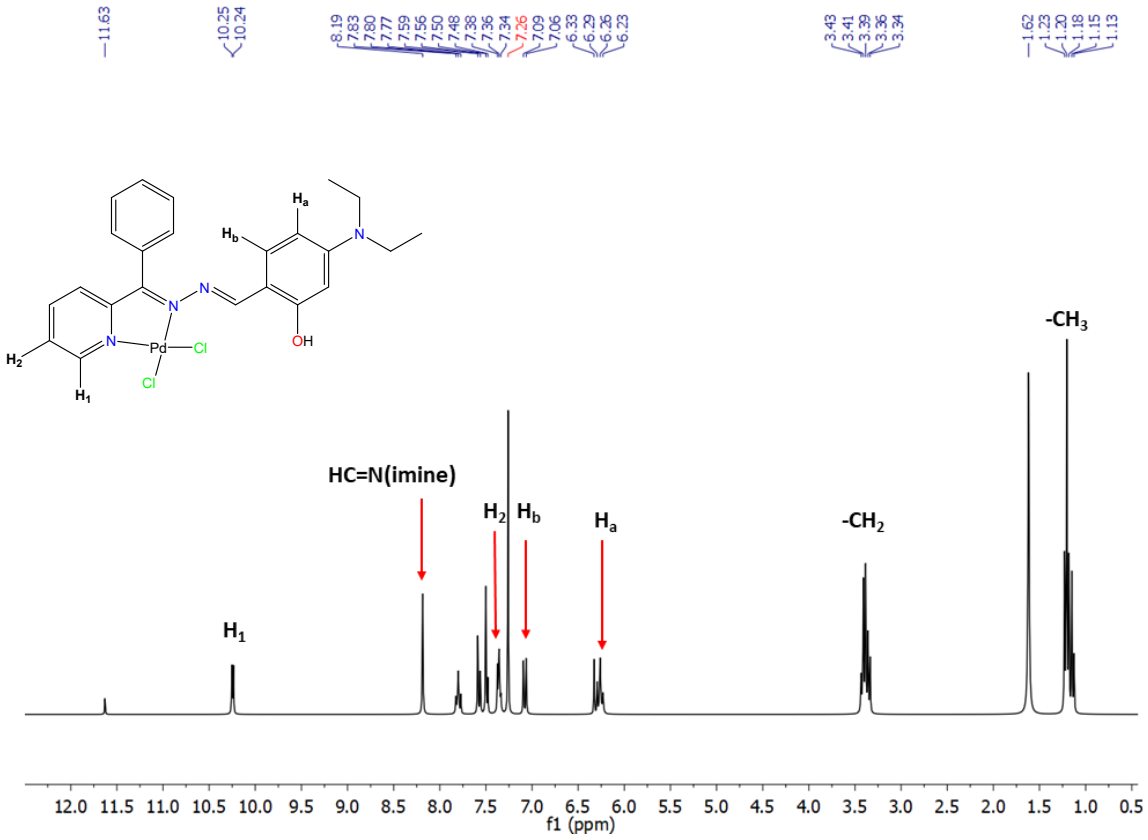


Figure S1: ^{1}H-NMR spectrum of [Pd(HL)Cl$_2$] (**C1**) in CDCl$_3$

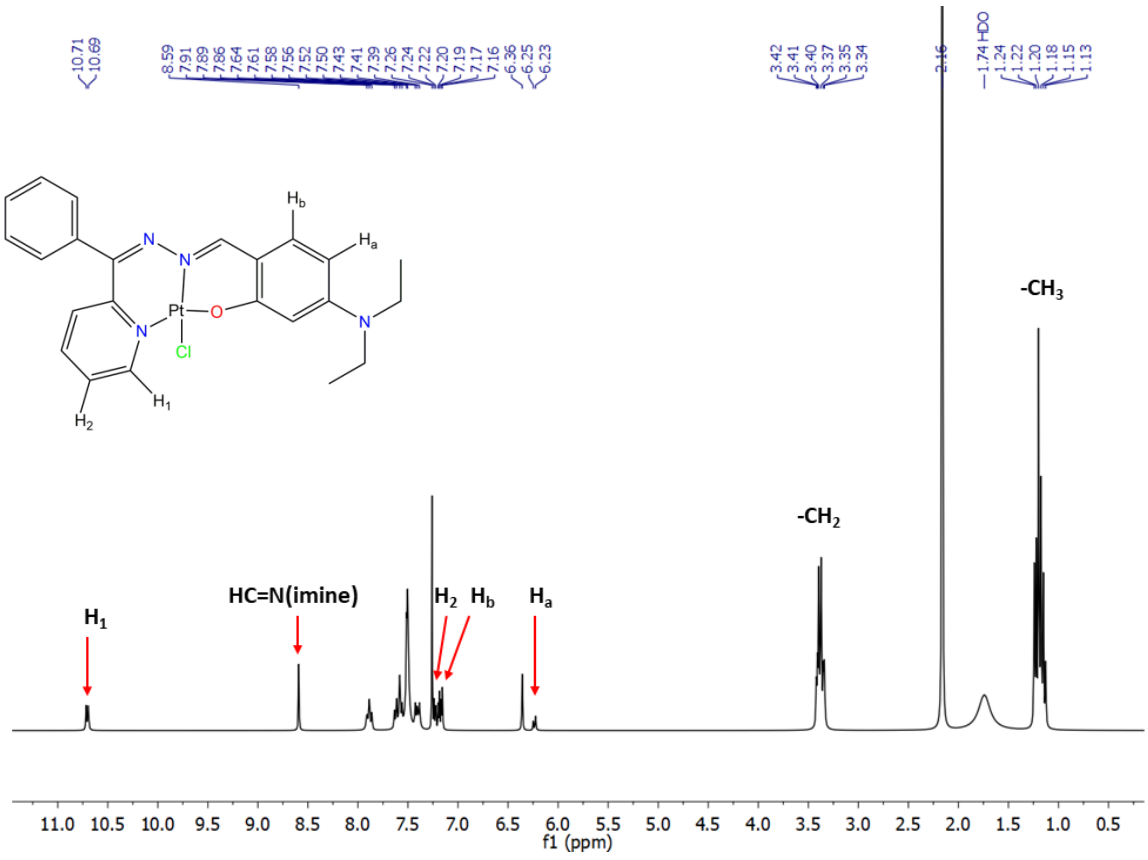


Figure S2: ^{1}H-NMR spectrum of [Pt(L)Cl] (**C2**) in CDCl$_3$

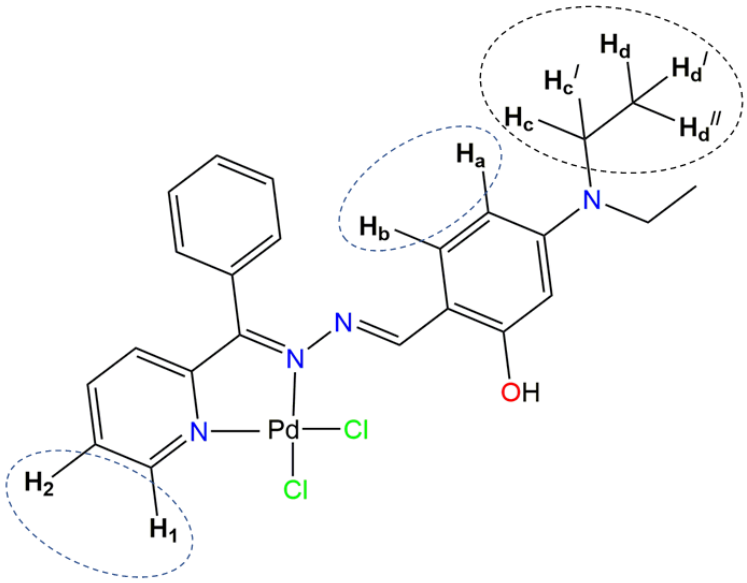


Figure S3: Coupling between H1 and H4, between H_a and H_b and diastereotopic hydrogens (H_c, $H_c^{/}$, H_d, $H_d^{/}$ and $H_d^{//}$) in **C1**

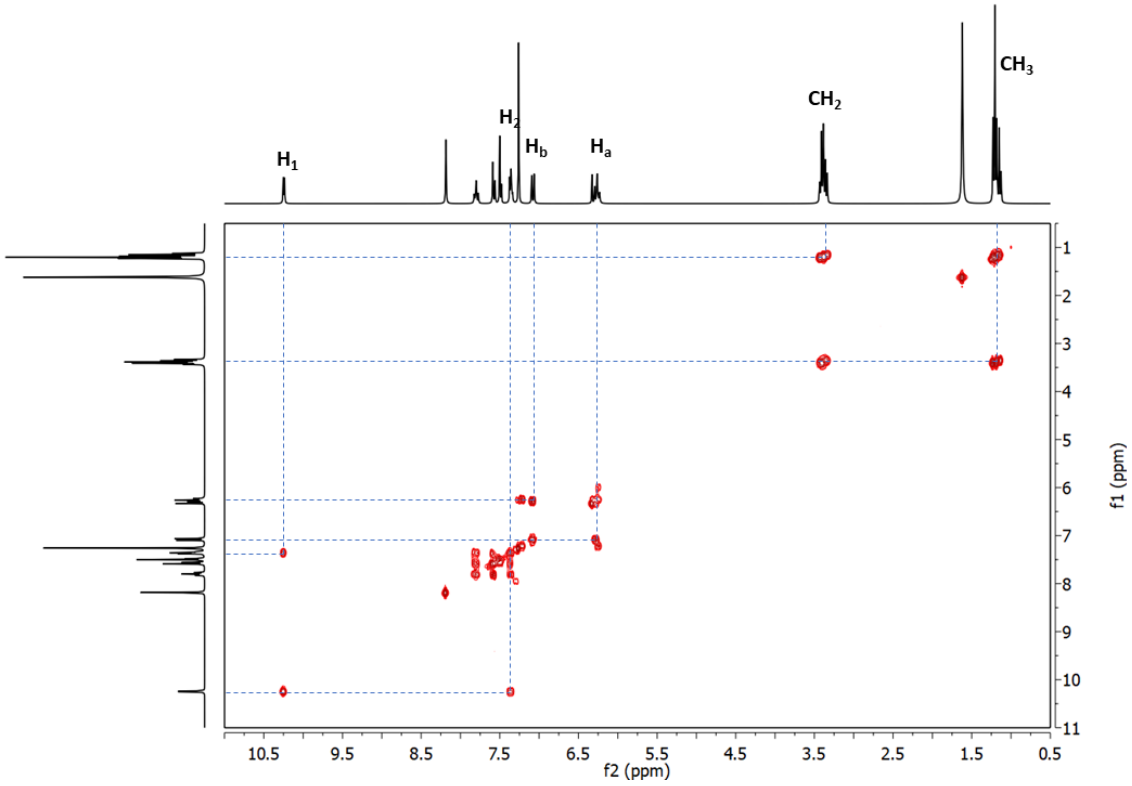


Figure S4: ^{1}H-^{1}H-2D COSY NMR spectrum of **C1** in $CDCl_3$

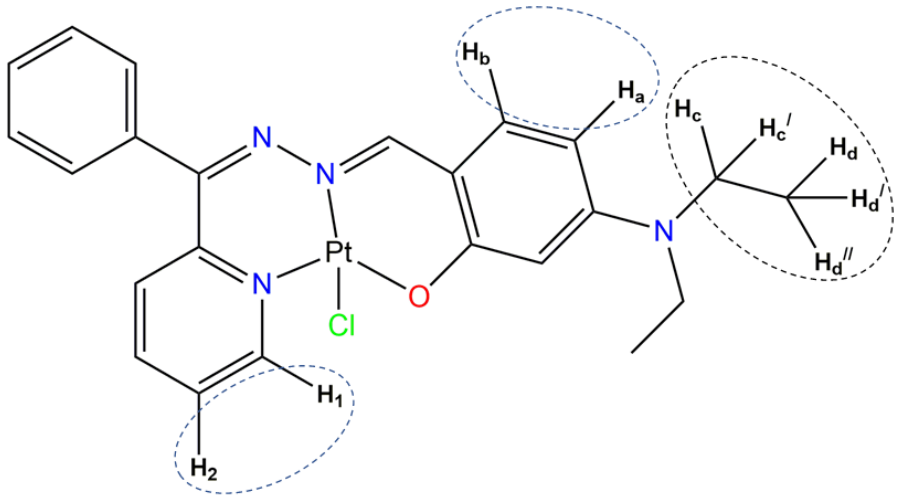


Figure S5: Coupling between H1 and H4, between H_a and H_b and diastereotopic hydrogens (H_c, $H_c^{/}$, H_d, $H_d^{/}$ and $H_d^{//}$) in **C2**

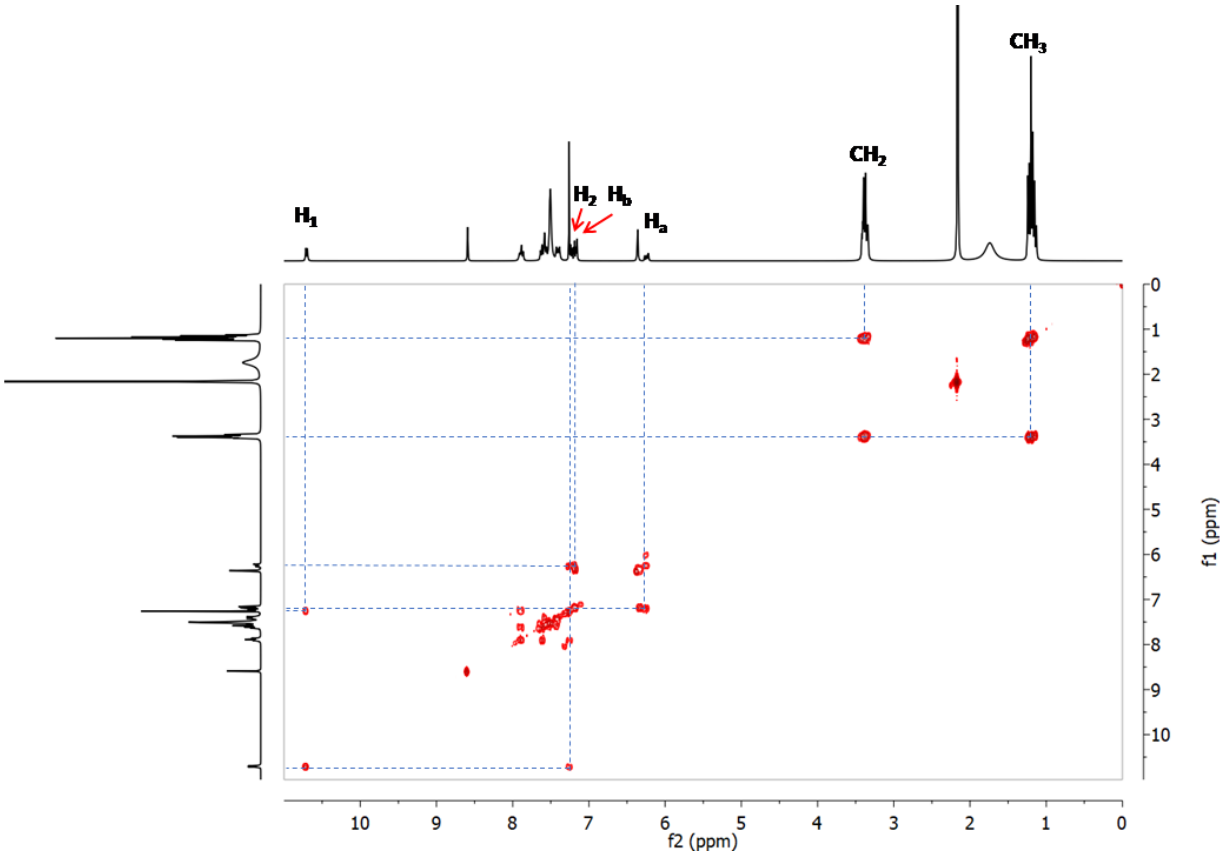


Figure S6: ^{1}H-^{1}H-2D COSY NMR spectrum of **C2** in $CDCl_3$

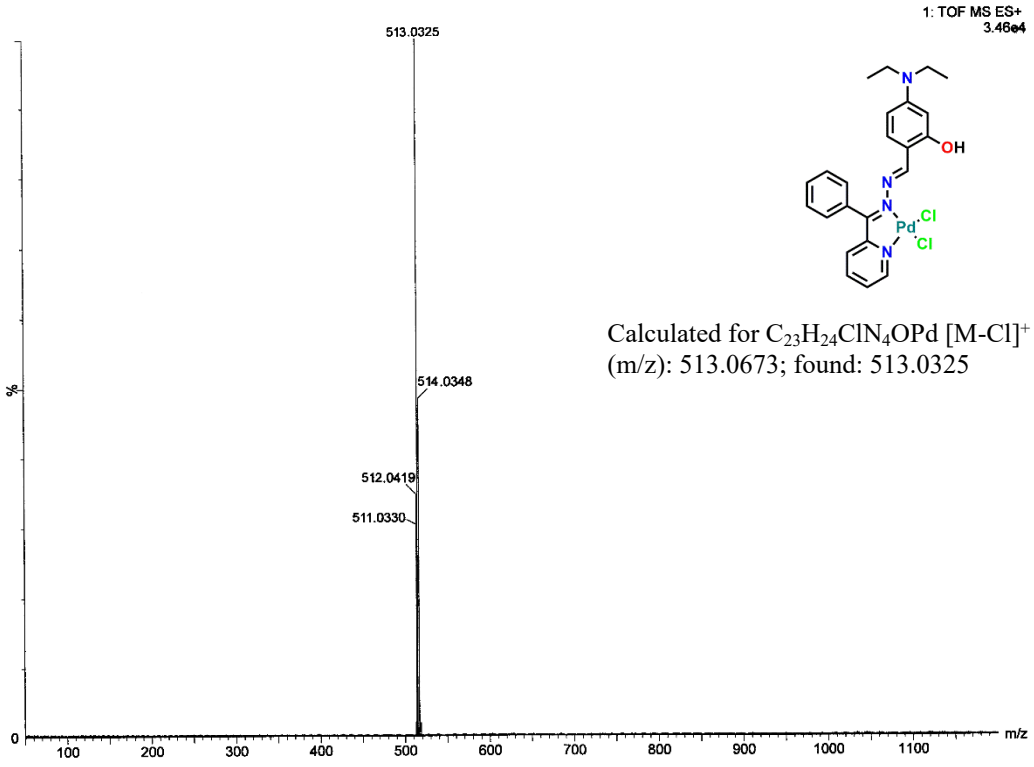


Figure S7: HRMS of $[Pd(HL)Cl_2]$ (**C1**) in acetonitrie

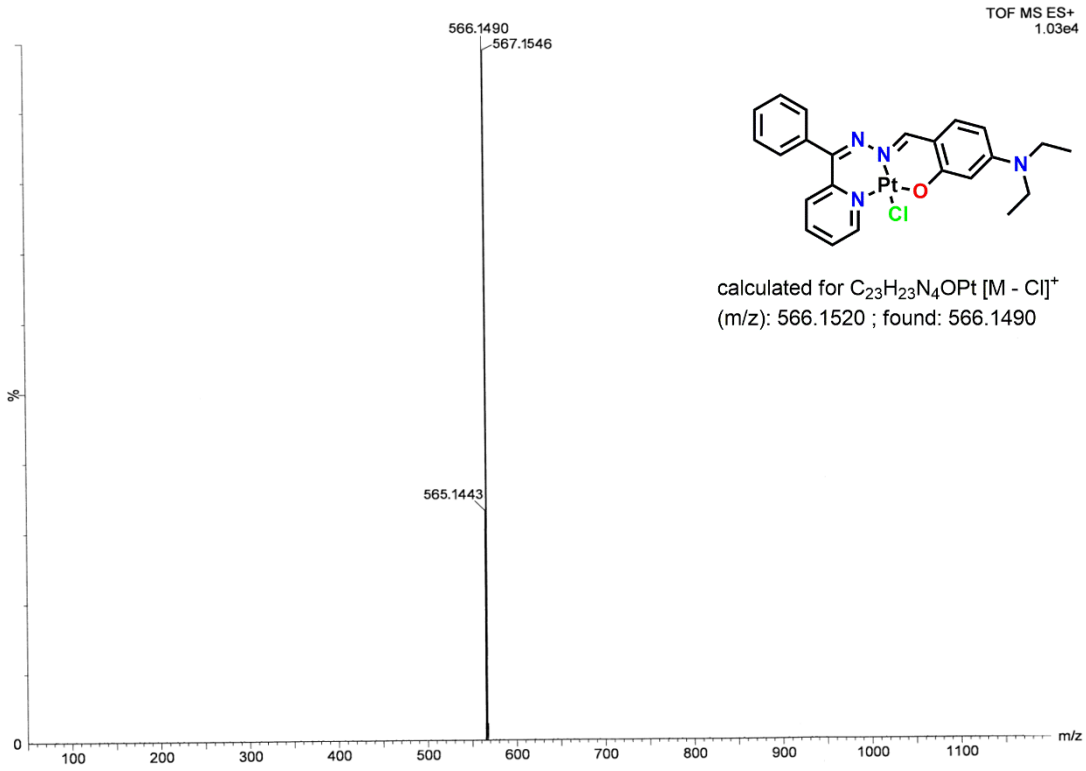


Figure S8: HRMS of [Pt(L)Cl] (**C2**) in acetonitrile

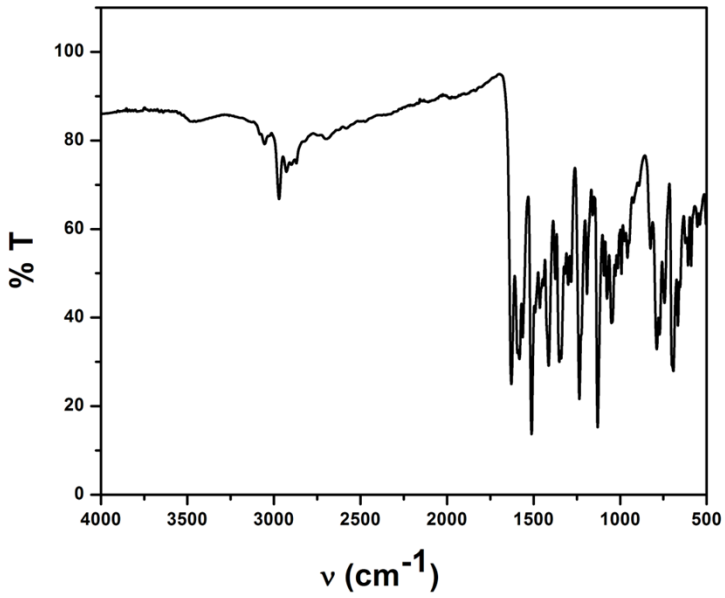


Figure S9: IR spectrum of free HL ligand

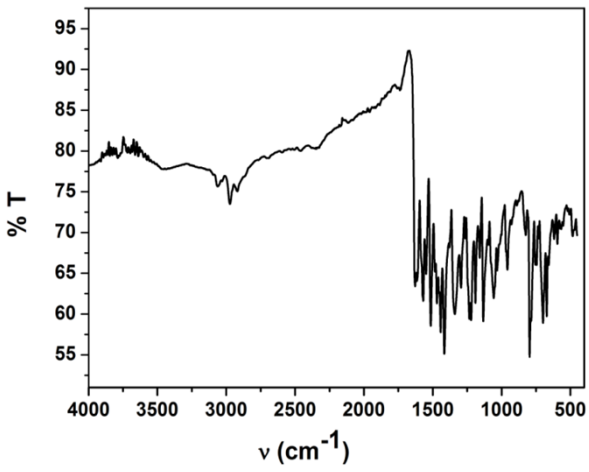


Figure S10: IR spectrum of **C1** complex

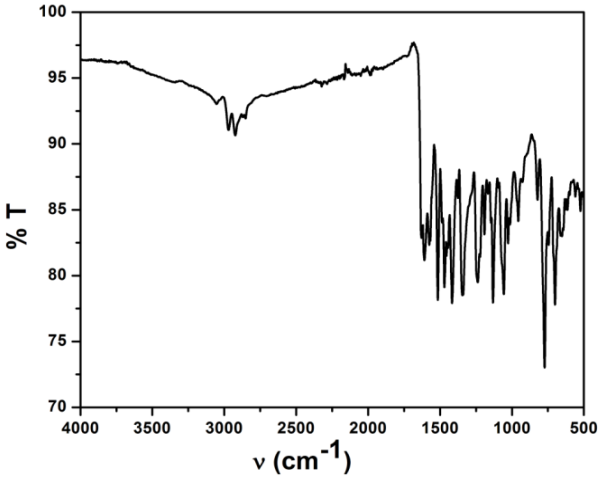


Figure S11: IR spectrum of **C2** complex

Table S1. Crystallographic data and refinement parameters of $[Pd(HL)Cl_2]$ (**C1**) and [Pt(L)Cl] (**C2**)

Complex	$[Pd(HL)Cl_2]$ (**C1**)	[Pt(L)Cl] (**C2**)
Formula	$C_{23}H_{24}Cl_2N_4OPd$	$C_{23}H_{23}ClN_4OPt$
Formula Weight	549.76	601.99
Crystal System	*Triclinic*	*Triclinic*
Space group	*P -1*	*P -1*
a, b, c [Å]	9.2645(16), 10.3915(18), 24.989(4)	8.3273(7), 10.4097(8), 13.1711(11)
α	80.629(4)	76.354(3)
β	84.019(4)	79.382(3)
γ	79.944(4)	79.593(3)
V [$Å^3$]	2330.1(7)	1079.20(15)
Z	4	2
D(calc) [g/cm^3]	1.567	1.853
Mu(MoKa) [/mm]	1.048	6.647
F(000)	1112	584
Temperature (K)	293(2)	293(2)
Radiation [Å]	0.71073	0.71073
θ(Min-Max) [°]	2.012 - 25.000	2.034 - 25.499
Dataset (h; k; l)	-11 to 11, -12 to 12, -29 to 29	-10 to 10, -12 to 12, -15 to 15
R, wR_2	0.0983 , 0.1925	0.0462, 0.1083
Goodness of fit(S)	1.071	1.031
CCDC No.	2123838	2123839

Table S2. Selected X-ray and calculated bond distances (Å) and angles (°) of **C1** and **C2**

C1			**C2**		
Bonds(Å)	X-ray	Calc.	Bonds(Å)	X-ray	Calc.
Pd1-N2	2.065(8)	2.028	Pt1-N2	1.971(6)	2.021
Pd1-N1	2.067(8)	2.044	Pt1-N1	2.014(6)	2.055
Pd1-Cl1	2.270(3)	2.263	Pt1-O1	1.989(5)	2.014
Pd1-Cl2	2.290(3)	2.294	Pt1-Cl1	2.329(2)	2.381
N2-N3	1.363(12)	1.396	N2-N3	1.394(9)	1.352
O1-C15	1.348(14)	1.347	O1-C15	1.296(10)	1.298
Angles (°)					
Cl1-Pd1-Cl2	89.33(11)	89.73039	O1-Pt1-N1	172.4(2)	174.348
N2-Pd1-N1	81.3(3)	80.74118	O1-Pt1-N2	92.5(2)	92.304
N2-Pd1-Cl1	95.5(2)	95.21670	O1-Pt1-Cl1	82.41(18)	83.269
N2-Pd1-Cl2	174.9(2)	175.03813	N2-Pt1-N1	91.9(2)	90.964
N1-Pd1-Cl1	176.9(2)	175.05901	N2-Pt1-Cl1	170.6(2)	173.729
N1-Pd1-Cl2	93.8(2)	94.33672	N1-Pt1-Cl1	94.04(18)	93.812

Table S3. Energy and % of composition of some selected molecular orbitals of $[Pd(HL)Cl_2]$ (**C1**)

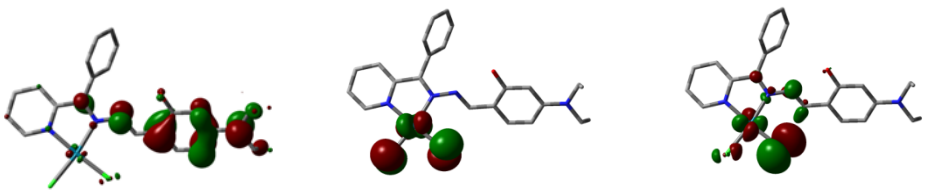
MO	Energy	% of composition		
		Pd	HL	Cl
LUMO+5	-0.58	01	99	0
LUMO+4	-0.87	01	99	0
LUMO+3	-1.00	04	94	02
LUMO+2	-1.54	02	97	01
LUMO+1	-2.01	47	23	30
LUMO	-2.85	05	94	01
HOMO	-5.44	01	97	02
HOMO-1	-5.90	29	03	68
HOMO-2	-6.04	14	13	73
HOMO-3	-6.17	28	21	51
HOMO-4	-6.20	06	84	10
HOMO-5	-6.23	15	04	81
HOMO-6	-6.45	84	04	12
HOMO-7	-7.14	08	80	12
HOMO-8	-7.30	03	89	08
HOMO-9	-7.47	03	95	02
HOMO-10	-7.57	05	77	18

Table S4. Energy and composition of some selected molecular orbitals of [Pt(L)Cl] (**C2**)

MO	Energy	% of composition		
		Pt	L	Cl
LUMO+5	-0.24	03	97	00
LUMO+4	-0.47	02	98	00
LUMO+3	-0.64	54	34	12
LUMO+2	-0.99	03	97	00
LUMO+1	-1.42	02	98	00
LUMO	-2.36	04	96	00
HOMO	-5.21	17	72	11
HOMO-1	-5.42	15	84	01
HOMO-2	-5.98	25	30	45
HOMO-3	-6.07	25	08	67
HOMO-4	-6.25	86	05	09
HOMO-5	-6.70	06	89	05
HOMO-6	-6.83	53	46	01
HOMO-7	-7.01	01	93	06
HOMO-8	-7.20	29	58	13
HOMO-9	-7.24	10	63	27
HOMO-10	-7.31	07	79	14

Table S5: Vertical electronic transition calculated by TDDFT/CPCM method of **C1** and **C2**

Compd.	λ (nm)	E (eV)	Osc. Strength (f)	Key excitations	Character	$\lambda_{expt.}$ (nm) (ε, $M^{-1}cm^{-1}$)
C1	533.0	2.3261	0.3738	(59%)HOMO→LUMO+1 (27%)HOMO→LUMO	LMCT/ILCT	496 (13860)
	469.6	2.6402	0.0289	(51%)HOMO-4→LUMO+1 (37%)HOMO-2→LUMO+1	LMCT/XMCT	453 (sh.)
	375.4	3.3024	0.1254	(73%)HOMO-3→LUMO	MLCT/XLCT	
	346.6	3.5775	0.1549	(67%)HOMO→LUMO+2	ILCT	354 (sh.)
	316.9	3.9119	0.3436	(49%)HOMO-9→LUMO	ILCT	325 (12100)
	269.6	4.5982	0.1055	(68%)HOMO→LUMO+5	ILCT	267 (7478)
C2	492.1	2.5196	0.6759	(96%)HOMO→LUMO	ILCT/MLCT	505 (16277)
	454.2	2.7298	0.0352	(97%)HOMO-1→LUMO	ILCT/MLCT	432 (9778)
	360.7	3.4376	0.1339	(59%)HOMO→LUMO+1	ILCT/MLCT	
	340.2	3.6441	0.2962	(67%)HOMO-5→LUMO	ILCT	348 (14258)
	277.8	4.4636	0.1107	(86%)HOMO-7→LUMO	ILCT	270 (9068)



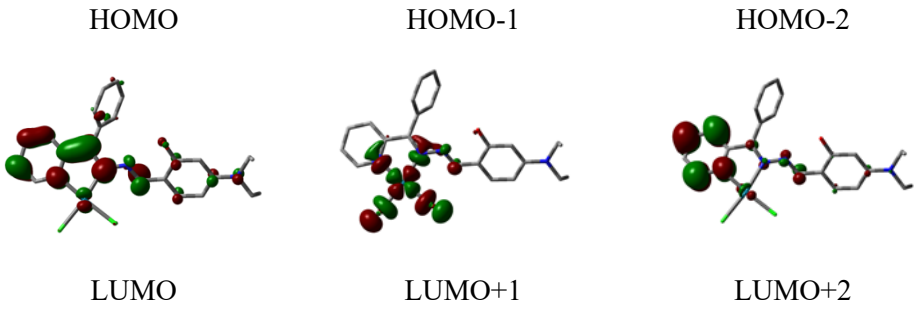


Figure S12: Contour plots of some selected molecular orbital of **C1**

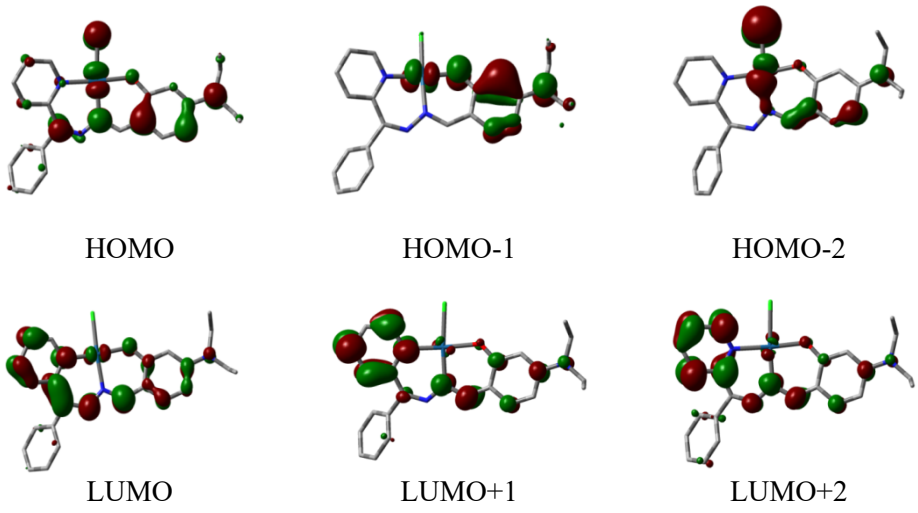


Figure S13: Contour plots of some selected molecular orbital of **C2**