Crystal structure, electronic properties and cytotoxic activity of palladium chloride complexes with monosubstituted pyridines.

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SUPPLEMENTARY INFORMATION

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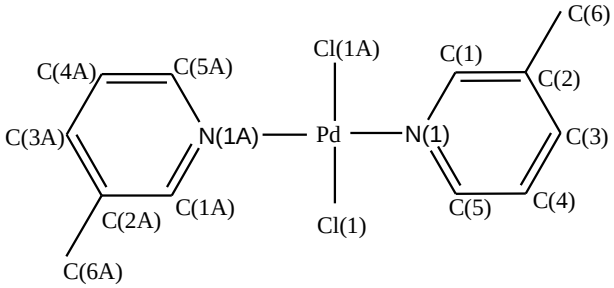
Table S1. Elemental analysis of compounds: $PdCl_2(Py)_2$ (complex I), $PdCl_2(2\text{-}MePy)_2$ (complex II), $PdCl_2(3\text{-}ClPy)_2$ (complex VIII).[a]

Complex	Results	%C	%H	%N	%Cl
$PdCl_2(Py)_2$	experimental theoretical	35,80 35,76	3,01 2,98	8,36 8,34	21,21 21,16
$PdCl_2(2\text{-}MePy)_2$	experimental theoretical	39,64 39,61	3,94 3,85	7,64 7,7	19,43 19,53
$PdCl_2(3\text{-}ClPy)_2$	experimental theoretical	29,76 29,67	1,95 1,97	6,85 6,92	35,19 35,11

[a]Data have been published in ref. 1.

A



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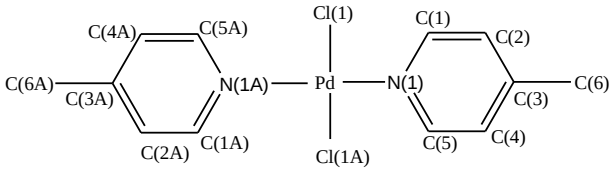

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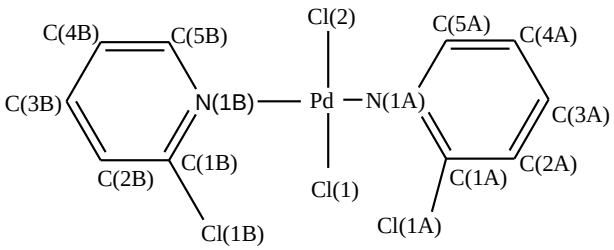

Figure S1. Structures of complexes III (A), IV (B) and V (C).

Table S2. Selected bond distances (Å) and angles (°) for complex III.

Pd-N(1A)	2.0191(11)	C(1)-C(2)	1.3907(18)
Pd-N(1)	2.0191(11)	C(2)-C(3)	1.3916(19)
Pd-Cl(1A)	2.3027(5)	C(2)-C(6)	1.5019(18)
Pd-Cl(1)	2.3027(5)	C(3)-C(4)	1.3883(19)
N(1)-C(1)	1.3448(17)	C(4)-C(5)	1.3857(18)
N(1)-C(5)	1.3477(17)		
N(1A)-Pd-N(1)	180.00	C(5)-N(1)-Pd	121.38(9)
N(1A)-Pd-Cl(1A)	89.47(3)	N(1)-C(1)-C(2)	123.04(12)
N(1)-Pd-Cl(1A)	90.53(3)	C(1)-C(2)-C(3)	117.27(12)
N(1A)-Pd-Cl(1)	90.53(3)	C(1)-C(2)-C(6)	119.76(12)
N(1)-Pd-Cl(1)	89.47(3)	C(3)-C(2)-C(6)	122.96(12)
Cl(1A)-Pd-Cl(1)	180.00	C(4)-C(3)-C(2)	119.95(12)
C(1)-N(1)-C(5)	119.21(11)	C(5)-C(4)-C(3)	119.29(12)
C(1)-N(1)-Pd	119.36(9)	N(1)-C(5)-C(4)	121.21(12)

Table S3. Selected bond distances (Å) and angles (°) for complex IV.

Pd-N(1)	2.0139(11)	C(1)-C(2)	1.377(2)
Pd-N(1A)	2.0139(11)	C(2)-C(3)	1.397(2)
Pd-Cl(1)	2.3054(3)	C(3)-C(4)	1.386(2)
Pd-Cl(1A)	2.3054(3)	C(3)-C(6)	1.495(2)
N(1)-C(5)	1.3408(18)	C(4)-C(5)	1.3813(19)
N(1)-C(1)	1.3472(19)		
N(1)-Pd-N(1A)	180.00(6)	C(1)-N(1)-Pd	120.87(10)
N(1)-Pd-Cl(1)	89.48(3)	N(1)-C(1)-C(2)	122.27(14)
N(1A)-Pd-Cl(1)	90.52(3)	C(1)-C(2)-C(3)	119.99(14)
N(1)-Pd-Cl(1A)	90.52(3)	C(4)-C(3)-C(2)	116.79(13
N(1A)-Pd-Cl(1A)	89.48(3)	C(4)-C(3)-C(6)	121.82(14)
Cl(1)-Pd-Cl(1A)	180.0	C(2)-C(3)-C(6)	121.39(13)
C(5)-N(1)-C(1)	118.50(12)	C(5)-C(4)-C(3)	120.68(14)
C(5)-N(1)-Pd	120.62(9)	N(1)-C(5)-C(4)	121.76(13)

Table S4. Selected bond distances (Å) and angles (°) for complex V.

Pd-N(1B)	2.032(3)	C(4A)-C(5A)	1.375(5)
Pd-N(1A)	2.034(3)	N(1B)-C(1B)	1.338(4)
Pd-Cl(1)	2.3036(11)	N(1B)-C(5B)	1.360(5)
Pd-Cl(2)	2.3045(11)	C(1B)-C(2B)	1.388(5)
N(1A)-C(1A)	1.328(5)	C(1B)-Cl(1B)	1.726(4)
N(1A)-C(5A)	1.405(5)	C(2B)-C(3B)	1.387(6)
C(1A)-C(2A)	1.402(5)	C(3B)-C(4B)	1.381(6)
C(1A)-Cl(1A)	1.721(4)	C(4B)-C(5B)	1.379(5)
C(2A)-C(3A)	1.380(5)		
C(3A)-C(4A)	1.384(5)		
N(1B)-Pd-N(1A)	178.88(12)	C(2A)-C(3A)-C(4A)	120.5(3)
N(1B)-Pd-Cl(1)	89.32(9)	C(5A)-C(4A)-C(3A)	120.5(4)
N(1A)-Pd-Cl(1)	91.02(9)	C(4A)-C(5A)-N(1A)	119.5(4)
N(1B)-Pd-Cl(2)	89.93(9)	C(1B)-N(1B)-C(5B)	118.0(3)
N(1A)-Pd-Cl(2)	89.65(9)	C(1B)-N(1B)-Pd	122.3(2)
Cl(1)-Pd-Cl(2)	176.17(4)	C(5B)-N(1B)-Pd	119.7(2)
C(1A)-N(1A)-C(5A)	118.7(3)	N(1B)-C(1B)-C(2B)	123.1(4)
C(1A)-N(1A)-Pd	123.8(2)	N(1B)-C(1B)-Cl(1B)	116.8(3)
C(5A)-N(1A)-Pd	117.6(2)	C(2B)-C(1B)-Cl(1B)	120.1(3)
N(1A)-C(1A)-C(2A)	123.9(3)	C(3B)-C(2B)-C(1B)	118.6(4)
N(1A)-C(1A)-Cl(1A)	116.5(3)	C(4B)-C(3B)-C(2B)	118.7(3)
C(2A)-C(1A)-Cl(1A)	119.6(3)	C(5B)-C(4B)-C(3B)	119.8(4)
C(3A)-C(2A)-C(1A)	116.9(4)	N(1B)-C(5B)-C(4B)	121.8(4)

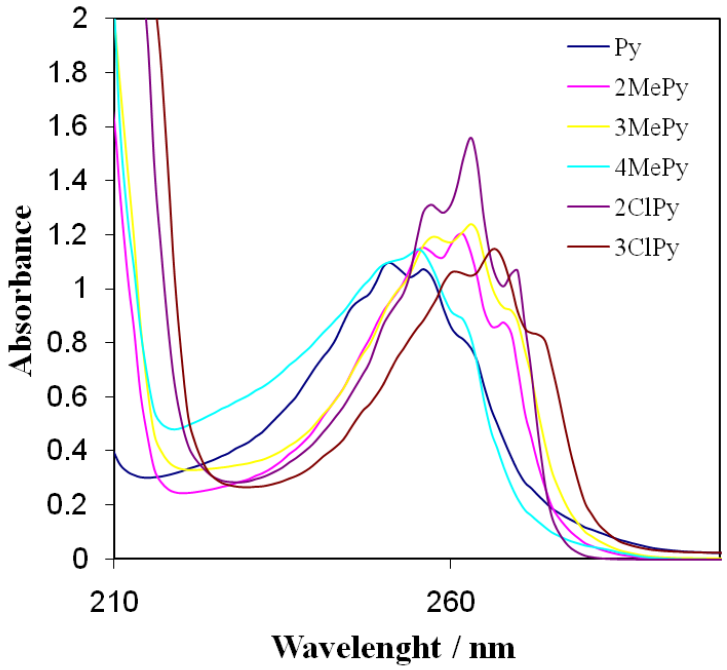

Figure S2. UV-Vis spectra of free XPy ligands.

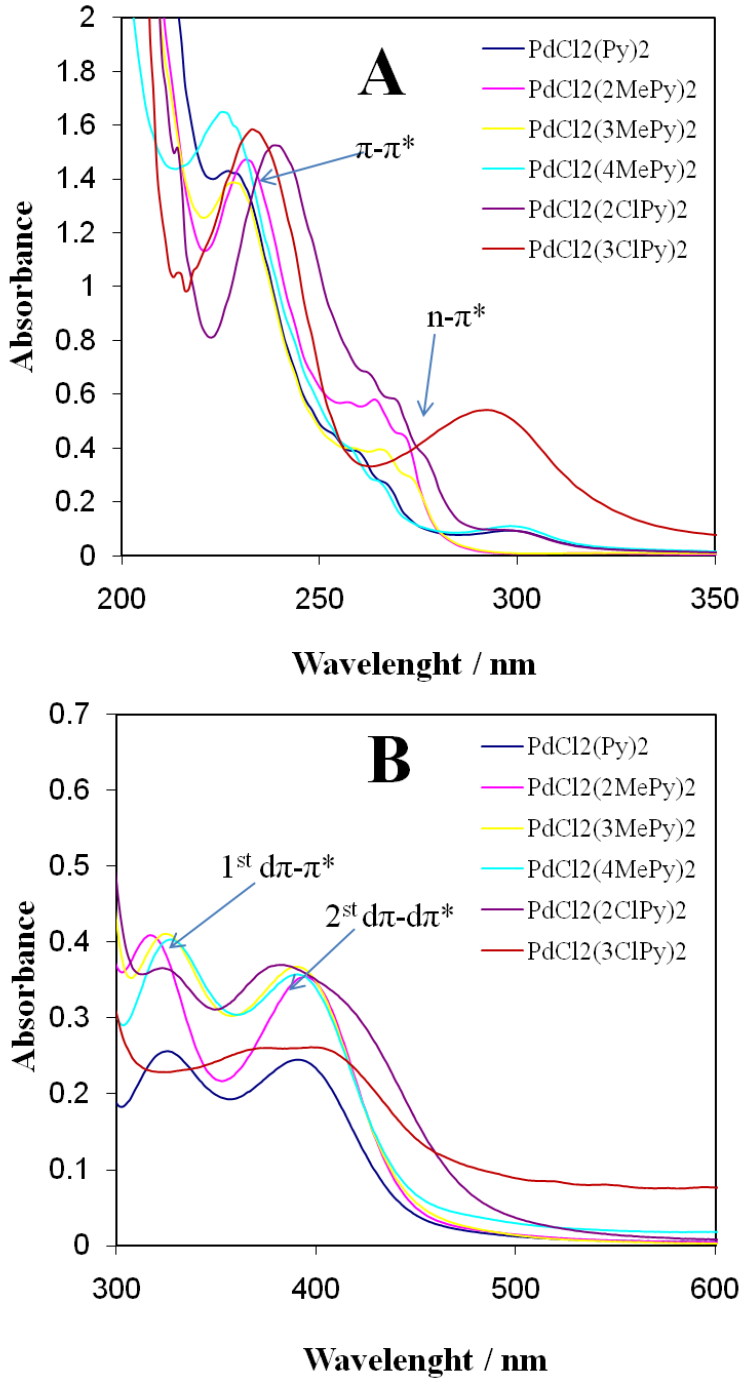

Figure S3. UV-Vis spectra of $PdCl_2(XPy)_2$.

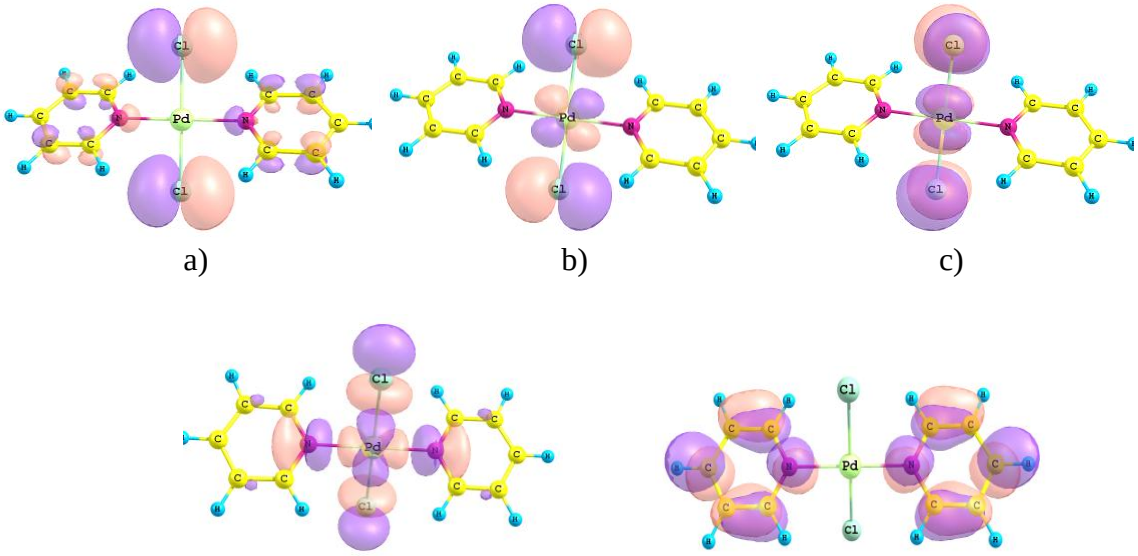

Figure S4. Frontier Orbitals involved in dπ-π* transitions in $PdCl_2(Py)_2$: HOMO-3, HOMO-1, HOMO, LUMO and LUMO+1: a) HOMO-3 Cl centered (involved in first dπ-π*), b) HOMO-1 Cl-Pd centered (involved in first dπ-π*), c) HOMO Cl-Pd centered (involved in second dπ-π*), d) LUMO Pd-Cl-3MePy centered (involved in first dπ-π*), e) LUMO+1 3-MePy centered (involved in first and second dπ-π*).

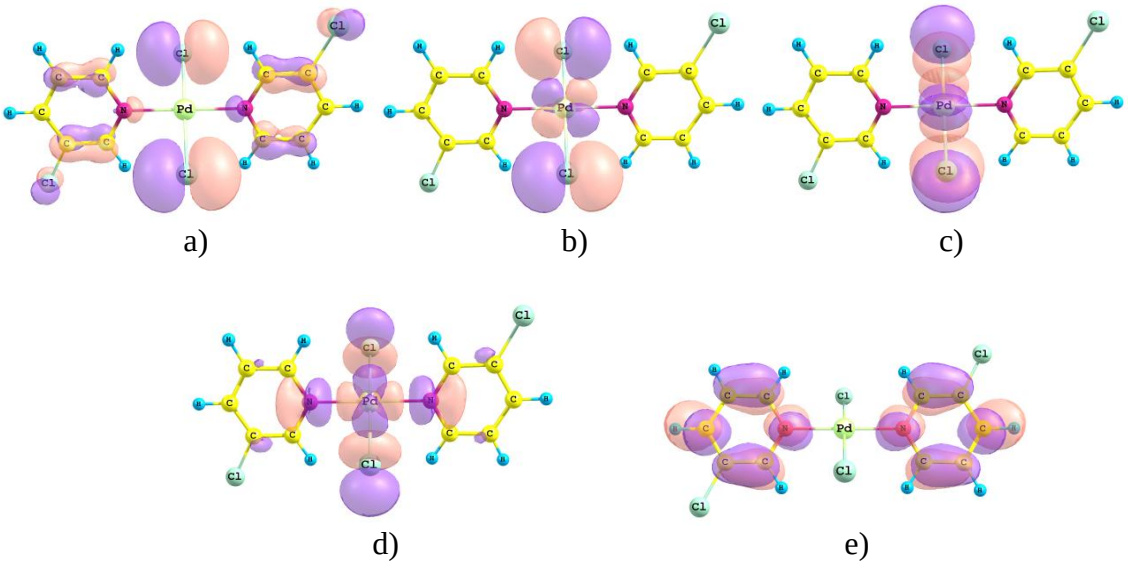

Figure S5. Frontier Orbitals involved in dπ-π* transitions in $PdCl_2(3\text{-}ClPy)_2$: HOMO-3, HOMO-1, HOMO, LUMO and LUMO+1: a) HOMO-3 Cl centered (involved in first dπ-π*), b) HOMO-1 Cl-Pd centered (involved in first dπ-π*), c) HOMO Cl-Pd centered (involved in second dπ-π*), d) LUMO Pd-Cl-3MePy centered (involved in first dπ-π*), e) LUMO+1 3-MePy centered (involved in first and second dπ-π*).

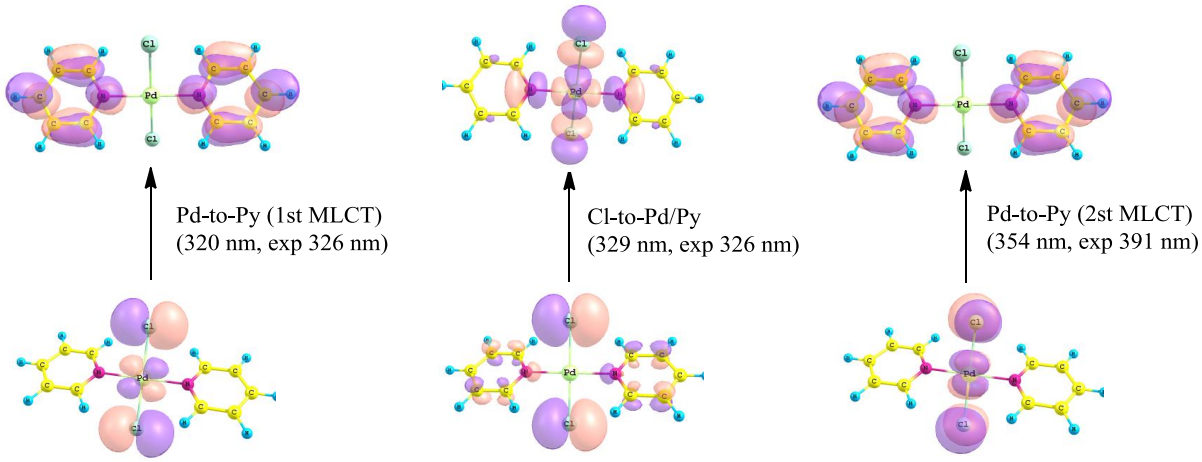

Figure S6. Visualisation of dπ-π* transitions in $PdCl_2(Py)_2$.

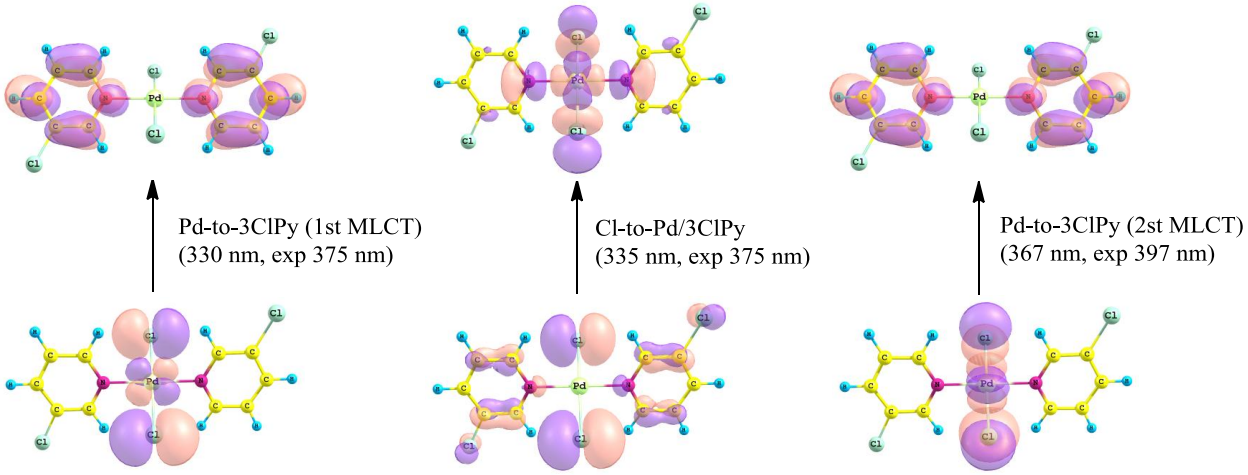

Figure S7. Visualisation of dπ-π* transitions in $PdCl_2(3\text{-}ClPy)_2$.

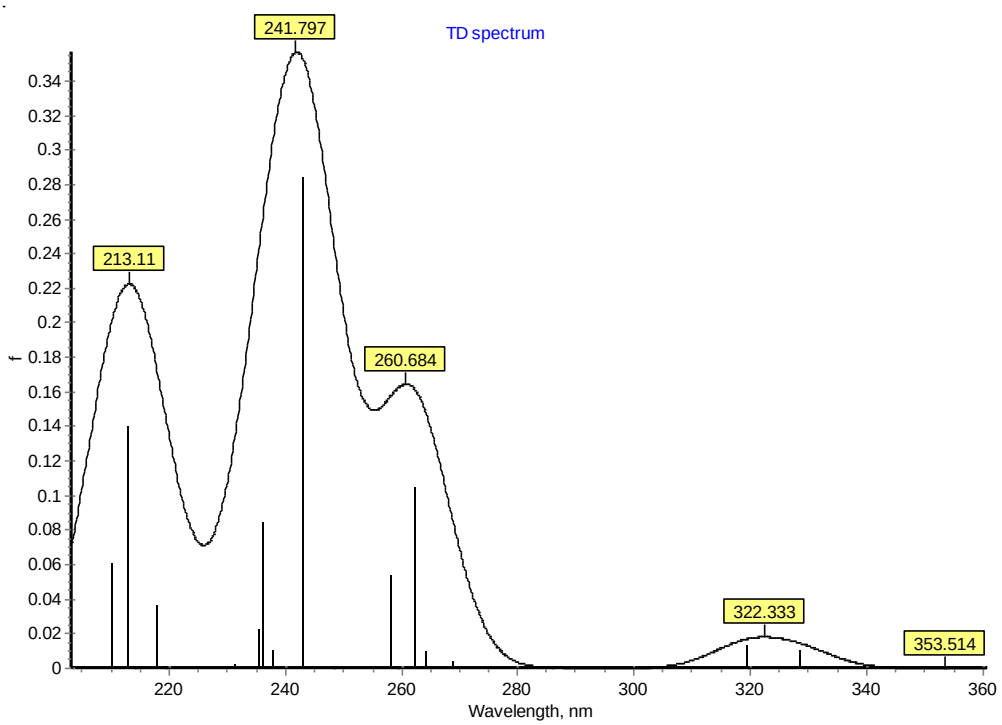

Figure S8. Theoretical UV-Vis spectrum of $PdCl_2(Py)_2$.

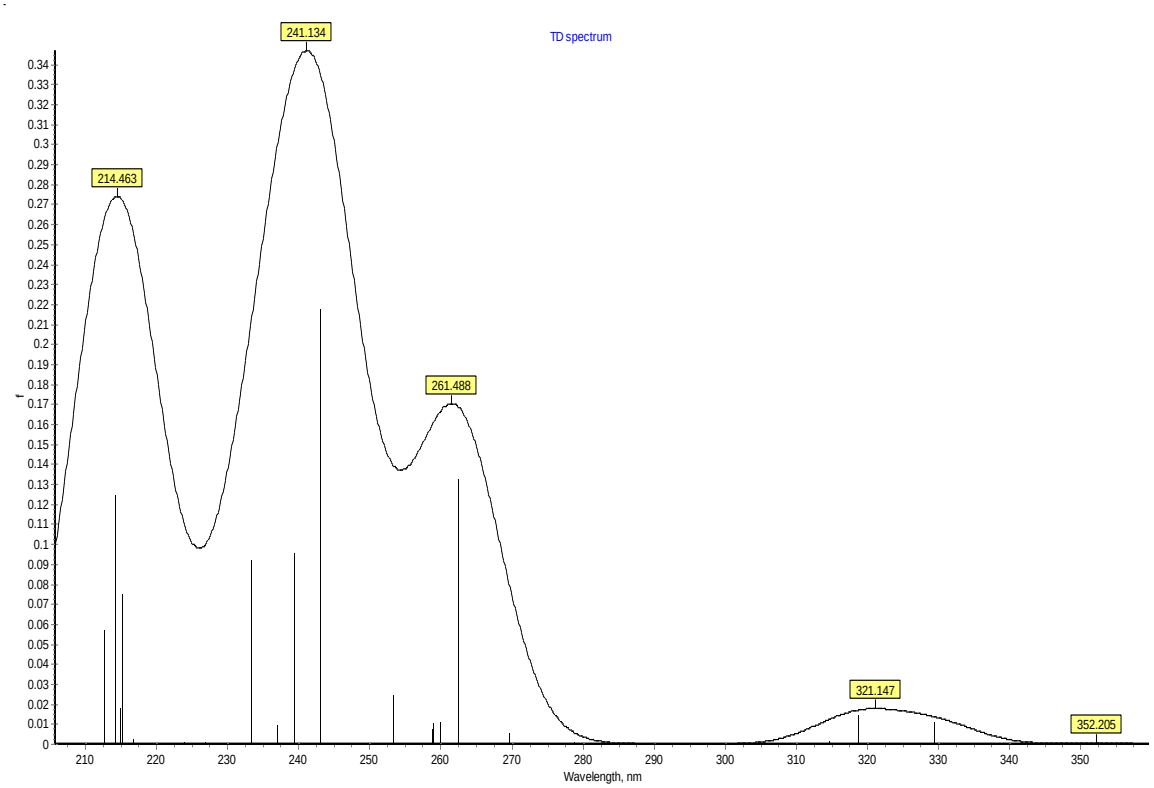

Figure S9. Theoretical UV-Vis spectra of $PdCl_2(3\text{-}MePy)_2$.

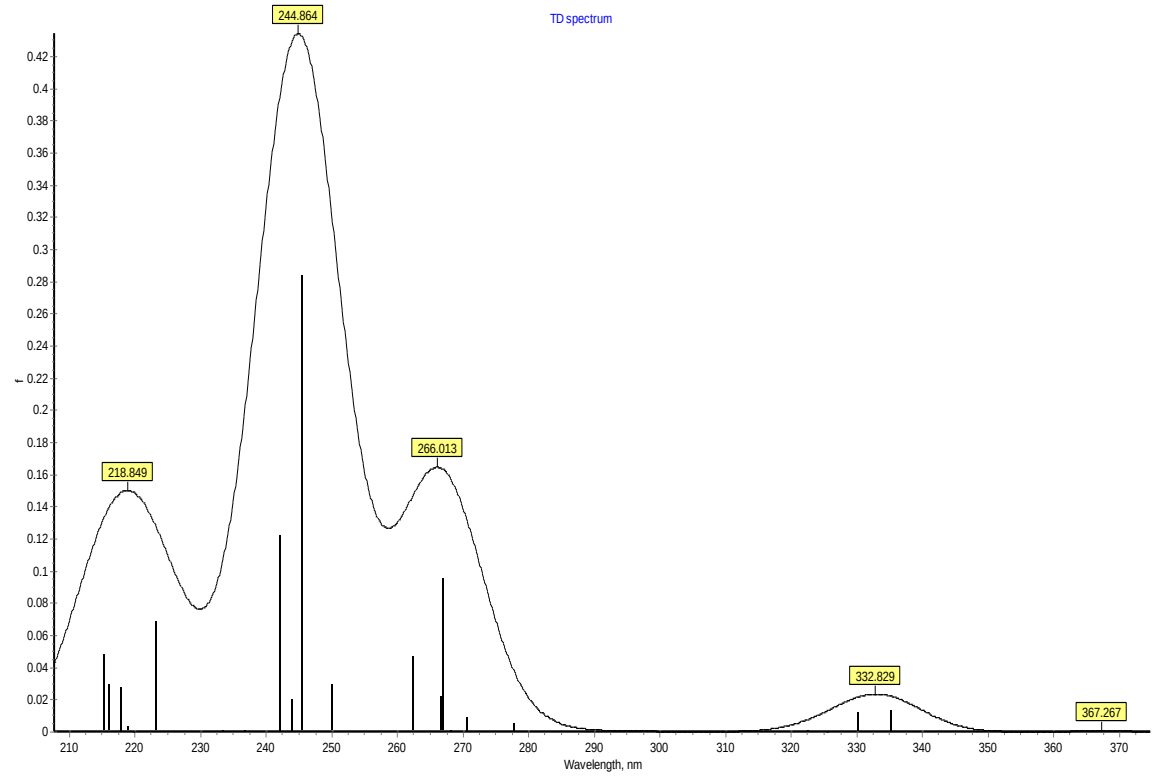

Figure S9. Theoretical UV-Vis spectrum of $PdCl_2(3\text{-}ClPy)_2$.