Photoactive Pt^{II} and Pd^{II} complexes of *N*,*N*-*di*ethyl-*N*'-3,4,5-trimethoxybenzoylthiourea: synthesis, crystal structures, DFT and cytotoxicity studies (Supplementary Material)

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Figure S1

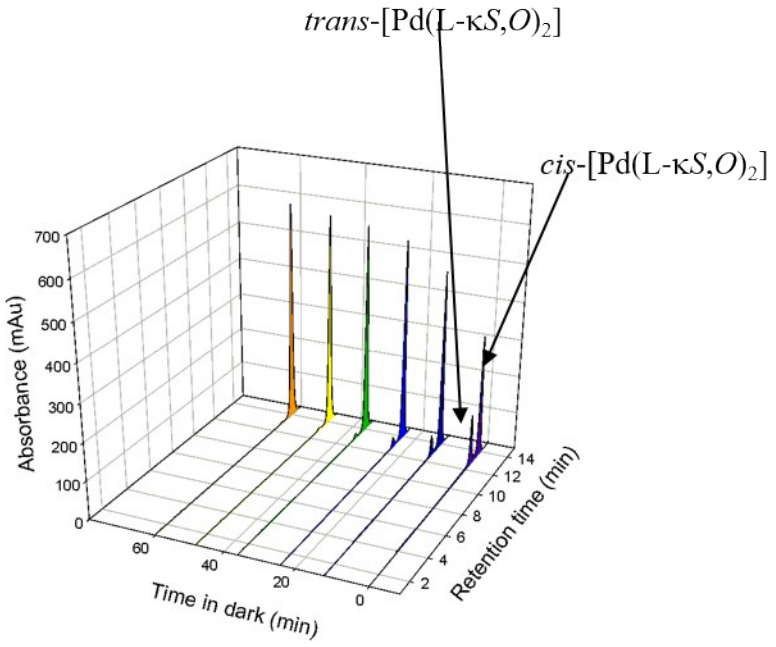


Fig. S1. Overlaid RP-HPLC chromatograms of *cis*-[Pd(L-κ*S*,*O*)$_2$] in acetonitrile after irradiation for 15 min with a 5 Watt LED lamp, and subsequently left in the dark.

Figure S2

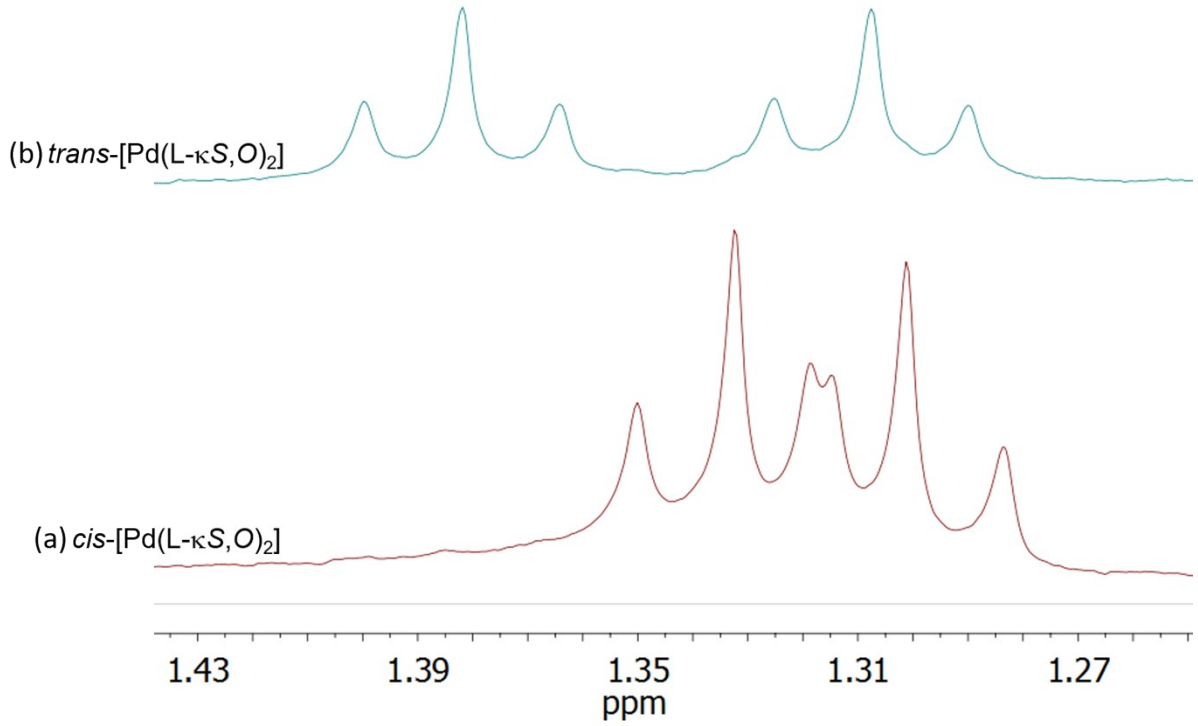


Fig. S2. Upfield region of the ^{1}H NMR spectra of (a) *cis*-[Pd(L-κ*S*,*O*)$_2$] and (b) *trans*-[Pd(L-κ*S*,*O*)$_2$] in chloroform-*d* at 25 °C.

Figure S3

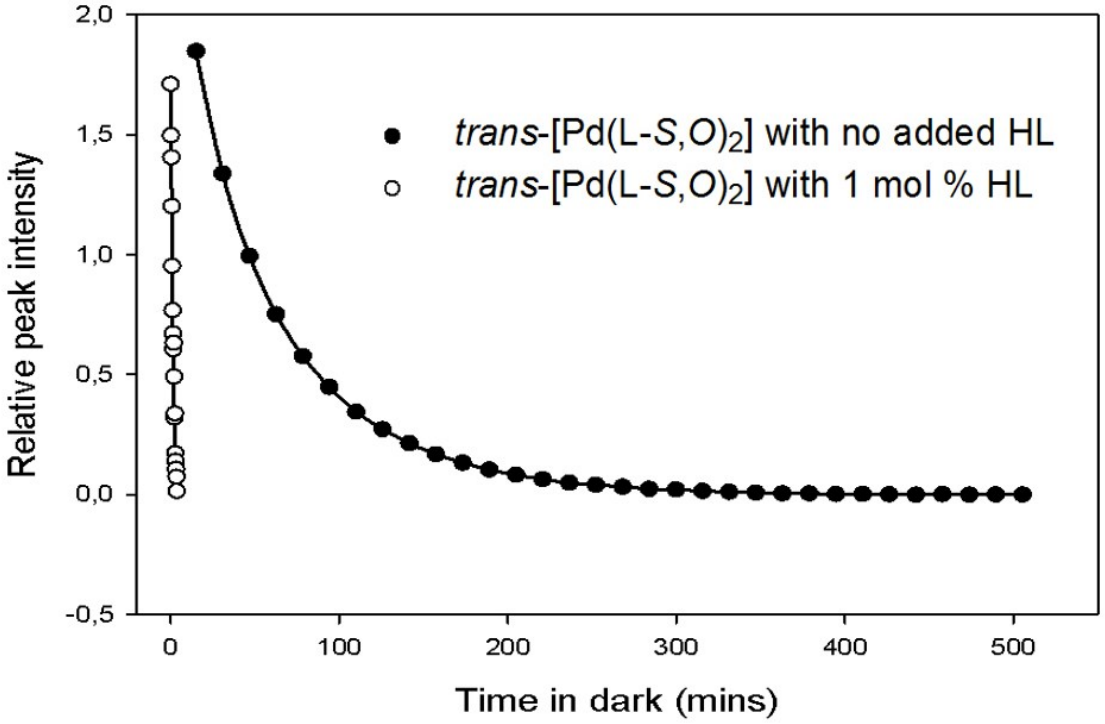


Fig. S3. Comparison of plots of relative peak intensity for spontaneous *trans*→*cis* isomerization for isolated *trans*-[Pd(L-κ*S*,*O*)$_2$] in chloroform-*d* before and after the addition of 1 mol % HL.

Figure S4

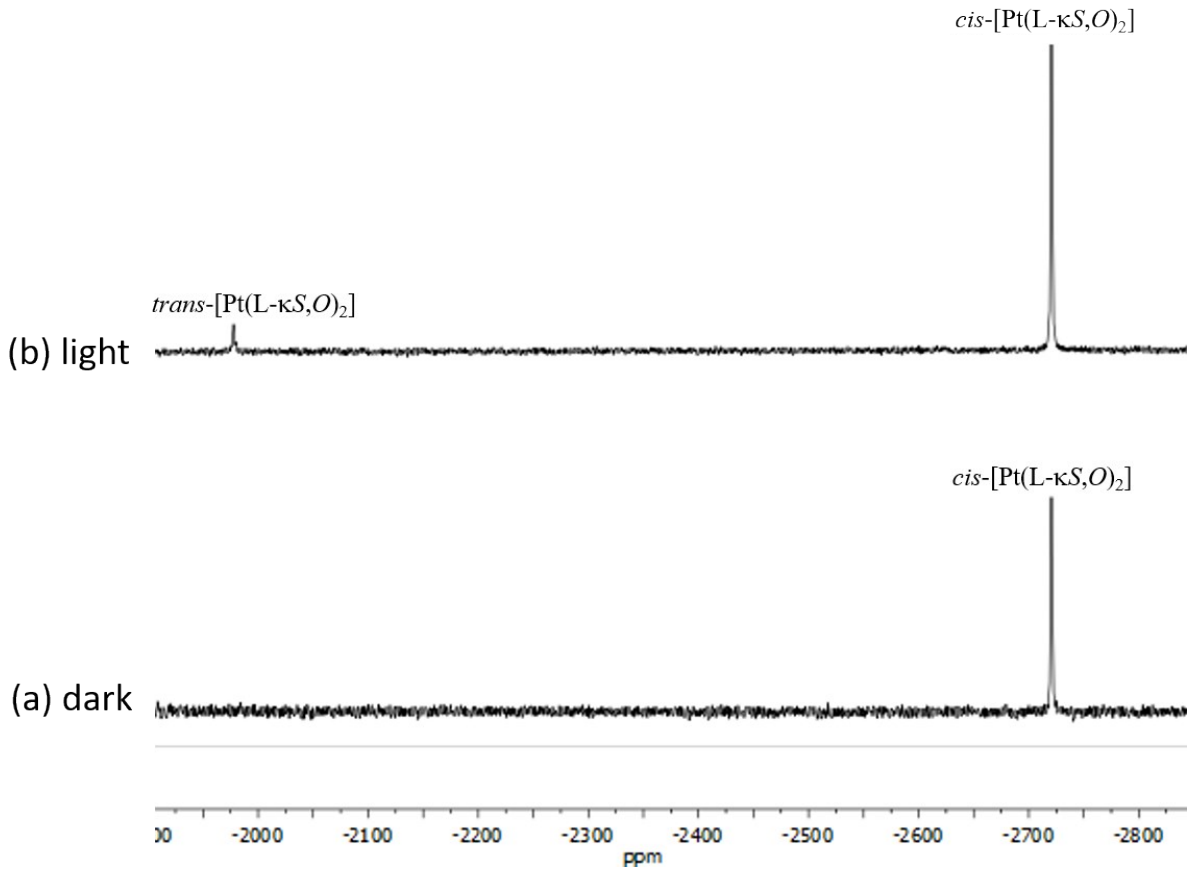
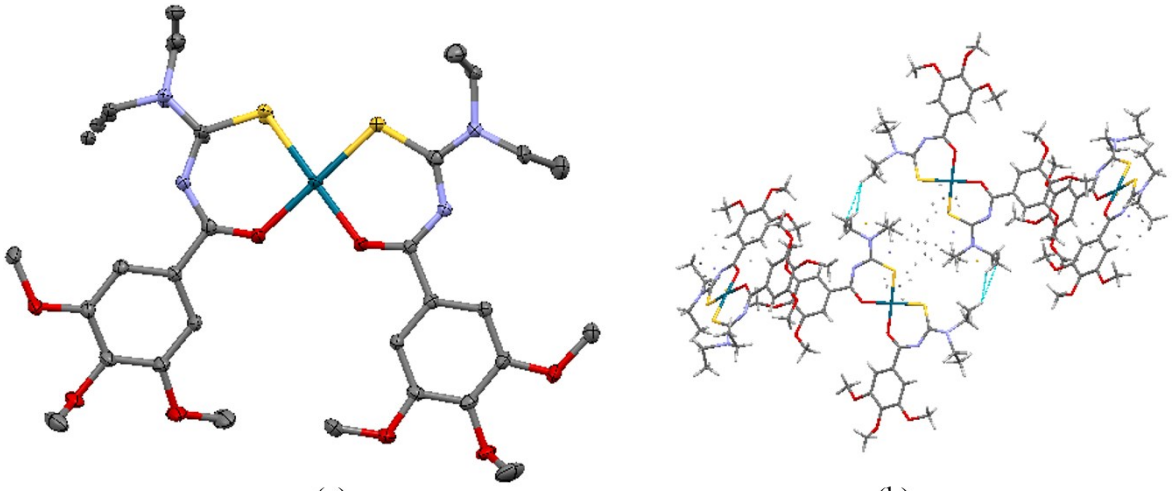


Fig. S4. ^{195}Pt NMR of *cis*-[Pt(L-κ*S*,*O*)$_2$] (a) before and (b) after in $CDCl_3$ irradiation for 30 min with a 5 Watt LED lamp.[21]

Figure S5



(a) (b)

Fig. S5. Molecular structures from single-crystal X-ray diffraction of (a) *cis*-[Pd(L-κ*S*,*O*)$_2$][21] and (b) its crystal packing.

Figure S6

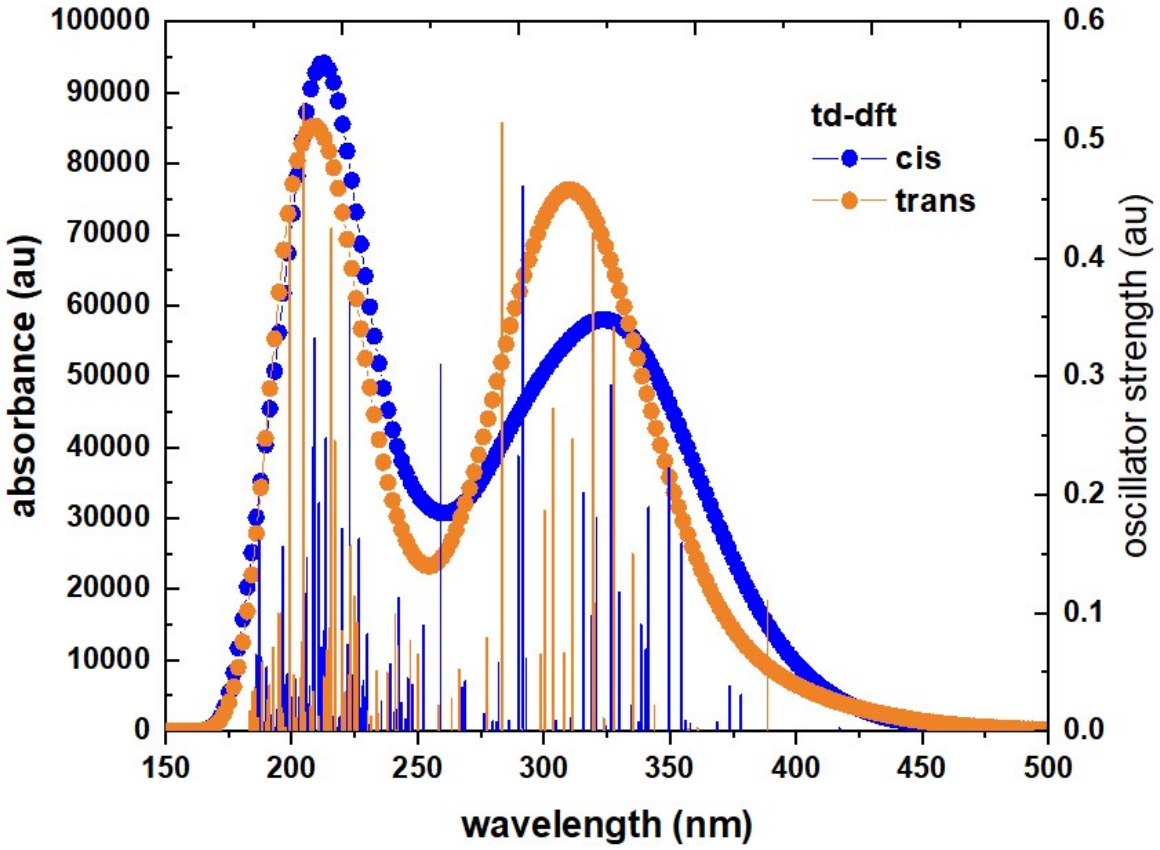
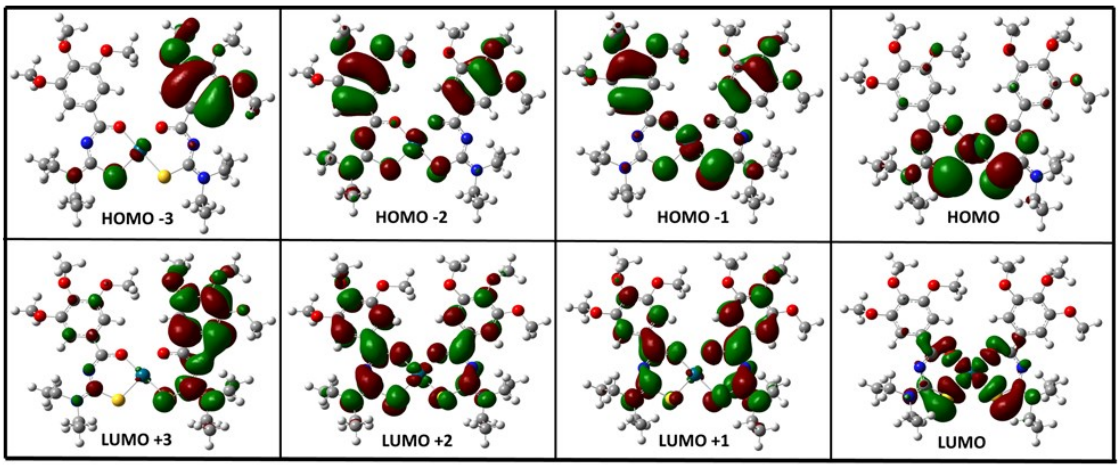


Fig. S6. TD-DFT calculated absorption spectra of *cis*-[Pd(L-κ*S*,*O*)$_2$] and *trans*-[Pd(L-κ*S*,*O*)$_2$], overlapped with corresponding oscillator strengths. The calculation was done with B3LYP/CEP-31G level of theory.

Figure S7

(a) ***cis***



(b) ***trans***

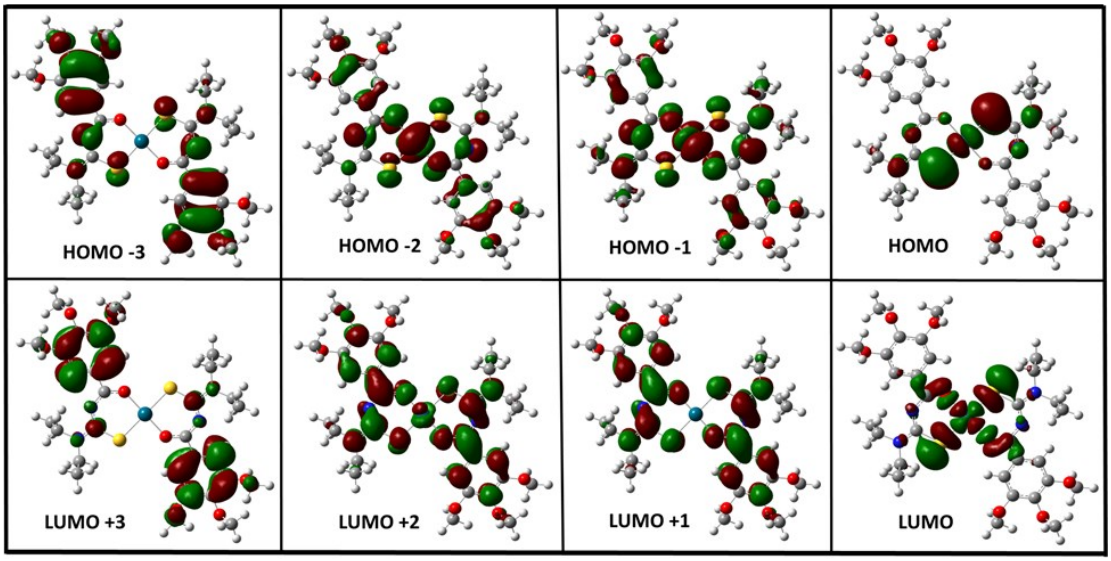


Fig. S7. HOMO and LUMO orbitals of (a) *cis*-[Pd(L-κ*S*,*O*)$_2$] and (b) *trans*-[Pd(L-κ*S*,*O*)$_2$].

Figure S8

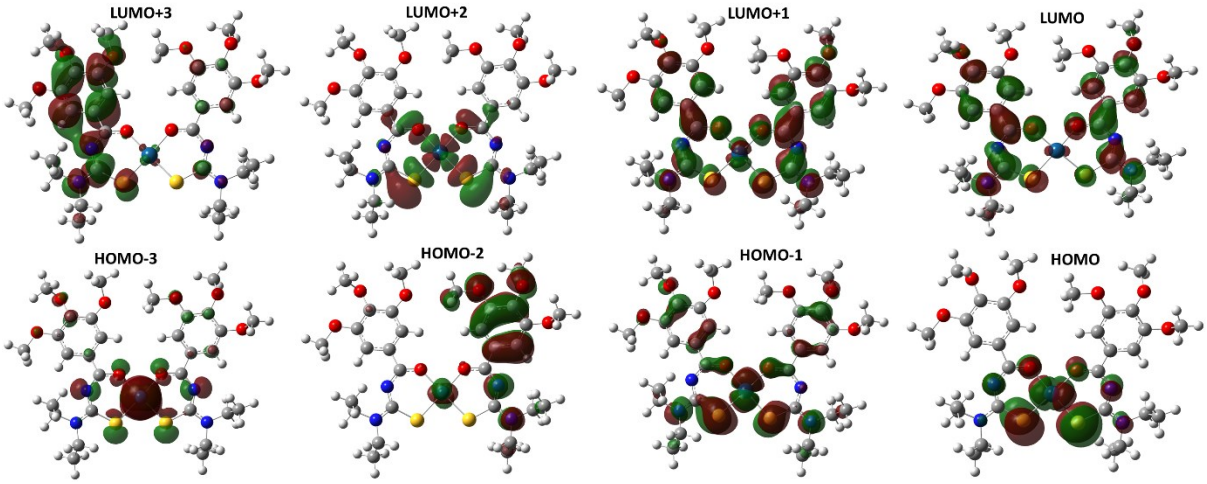


Fig. S8. HOMO and LUMO orbitals of *cis*-[Pt(L-κ*S*,*O*)$_2$]