Electronic Supplementary Information for

Synergistic properties of biological interest of a ruthenium (II) compound

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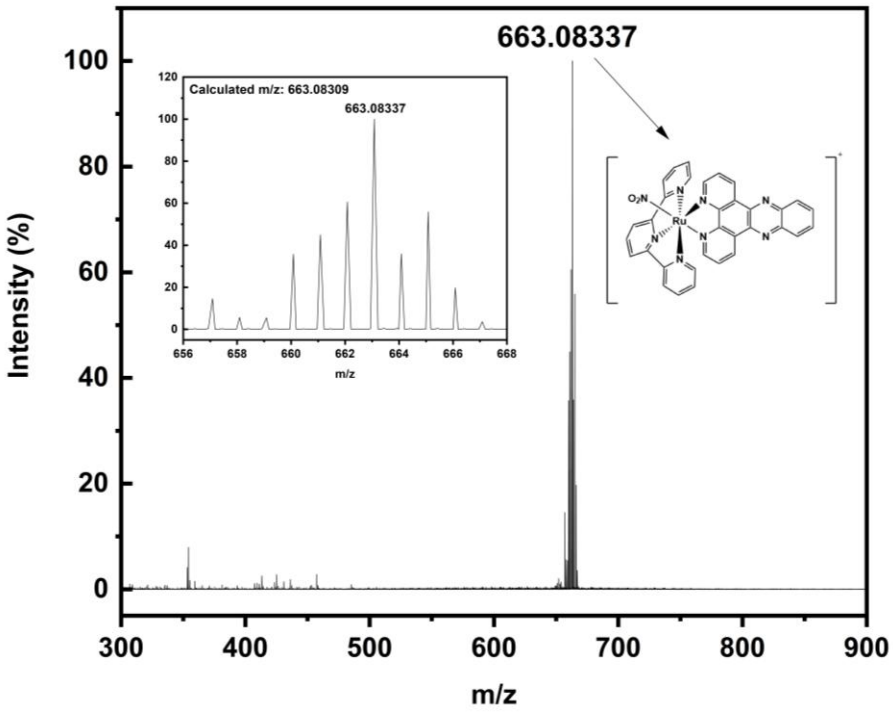

Figure S1: High-resolution mass spectra obtained from a 10 μM solution of complex [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in acetonitrile. Inset: isotopic distribution for the molecular ion peak.

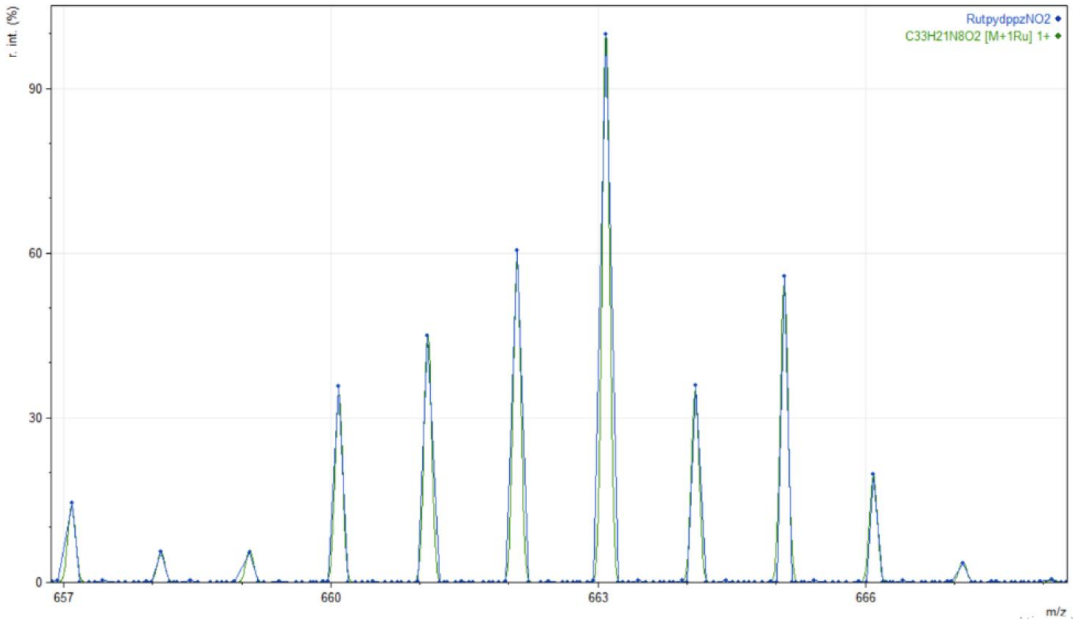

Figure S2: Comparison between peaks calculated using the mMass program (green line) and obtained (blue line) from high-resolution mass spectrometry of compound [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**).

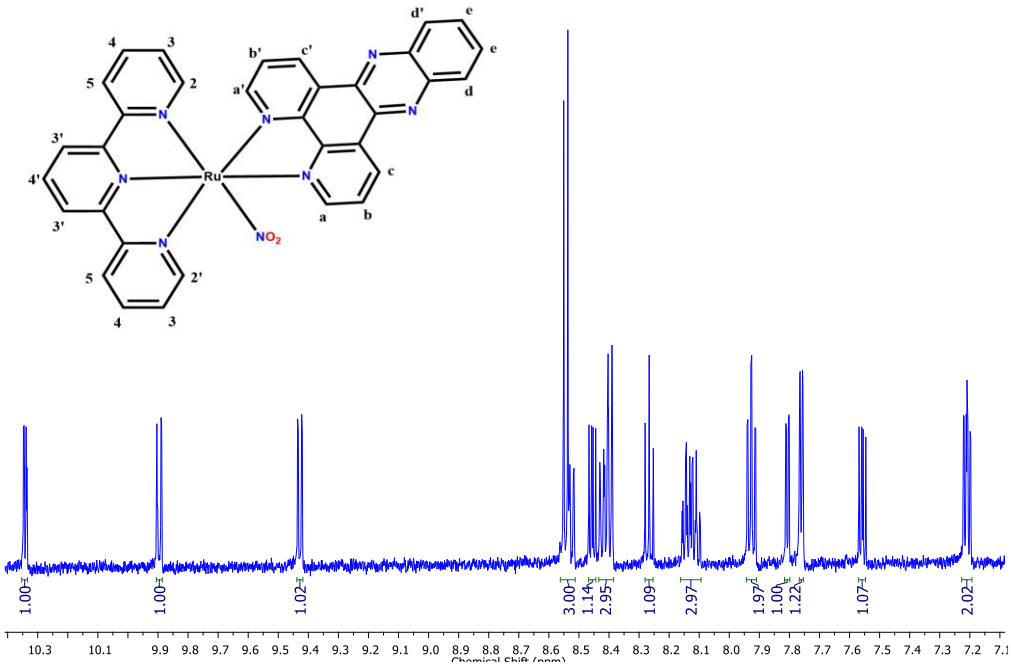

Figure S3: ^{1}H-NMR spectrum from a 10^{-2} M solution of [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in deuterated acetonitrile (600 MHz, 298K).

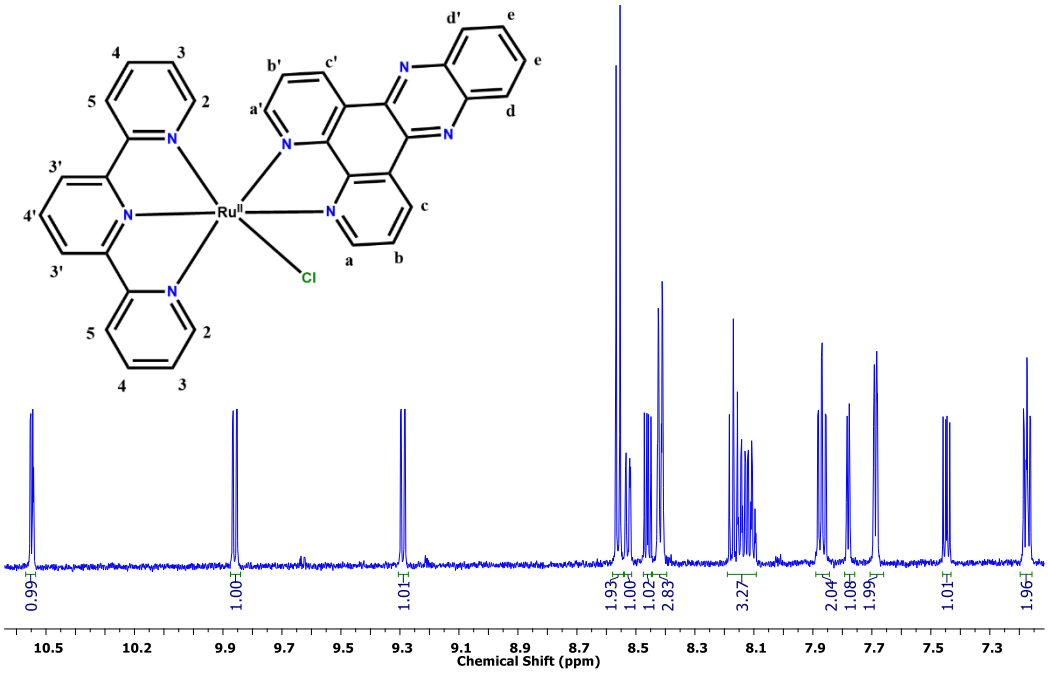

Figure S4: ^{1}H-NMR spectrum from a 10^{-2} M solution of [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) in deuterated acetonitrile (600 MHz, 298K).

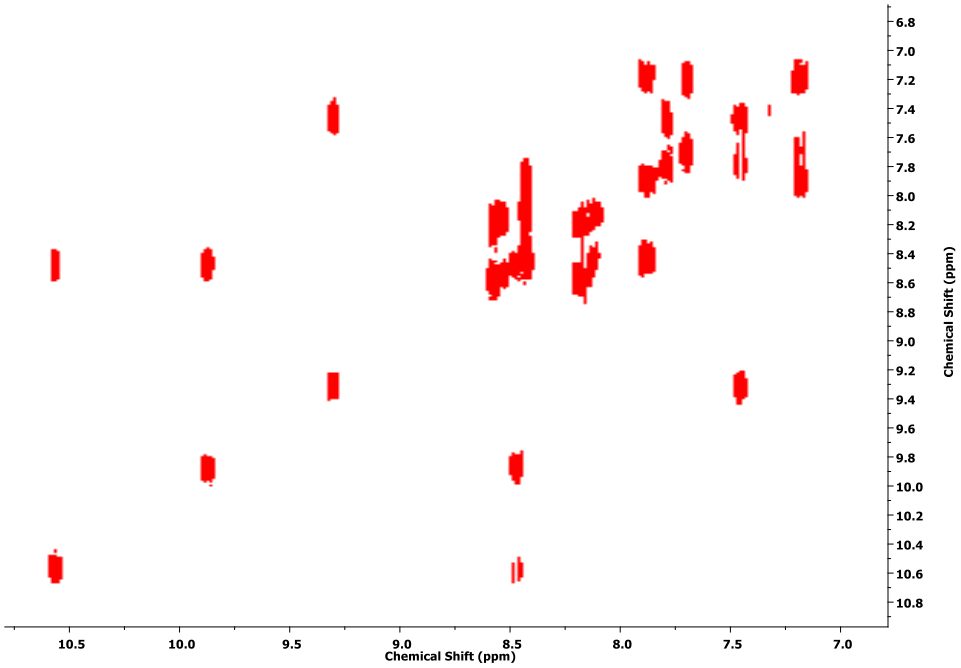

Figure S5: COSY spectrum from a 10^{-2} M solution of complex [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) in deuterated acetonitrile (600 MHz, 298K).

Table S1: ^{1}H-NMR assignments for [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) and [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**).

^{1}H position	Complex 1			Complex 2		
	δ (ppm)	Integral	Multiplicidade	δ (ppm)	Integral	Multiplicidade
2	7,68	2	Doublet	7,68	2	Doublet
3	7,28	2	Triplet	7,28	2	Triplet
4	7,87	2	Triplet	7,87	2	Triplet
5	8,42	2	Doublet	8,42	2	Doublet
3'	8,55	2	Doublet	8,55	2	Doublet
4'	7,78	1	Triplet	7,78	1	Triplet
a	10,55	1	Doublet	10,55	1	Doublet
b	8,46	1	Multiplet	8,46	1	Multiplet
c	9,85	1	Doublet	9,85	1	Doublet
d	8,42	1	Multiplet	8,42	1	Multiplet
e	8,12	2	Multiplet	8,12	2	Multiplet
a'	8,17	1	Multiplet	8,17	1	Multiplet
b'	7,44	1	Triplet	7,44	1	Triplet
c'	9,29	1	Doublet	9,29	1	Doublet
d'	8,52	1	Doublet	8,52	1	Doublet

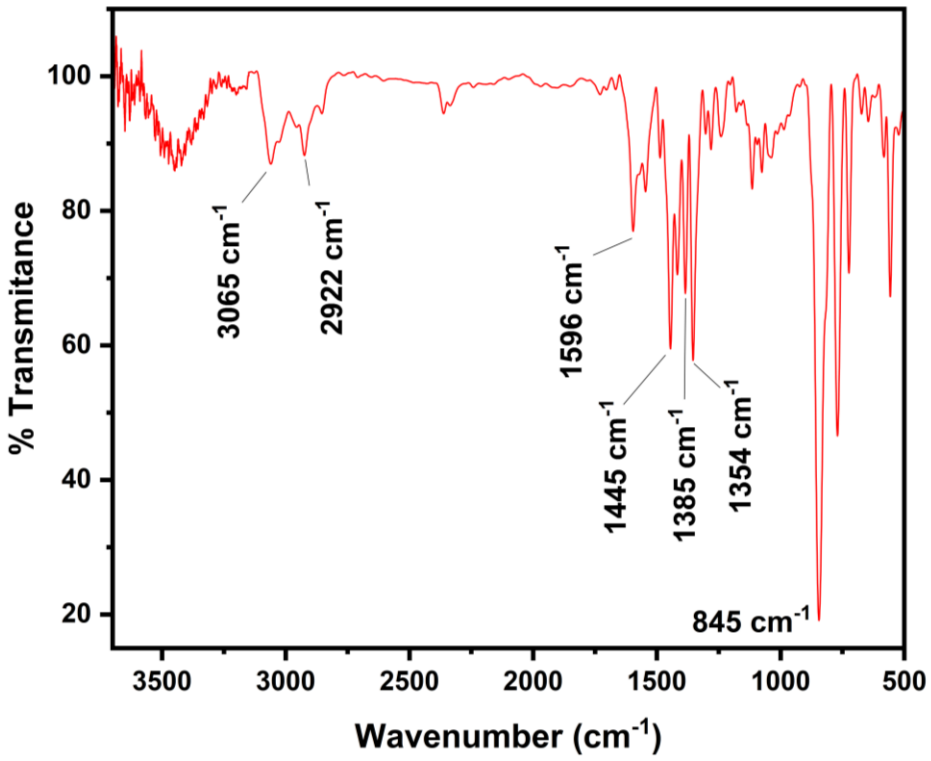

Figure S6: Vibrational spectrum of a KBr pellet containing complex [Ru(tpy)(dppz)(Cl)](PF_6) (**1**).

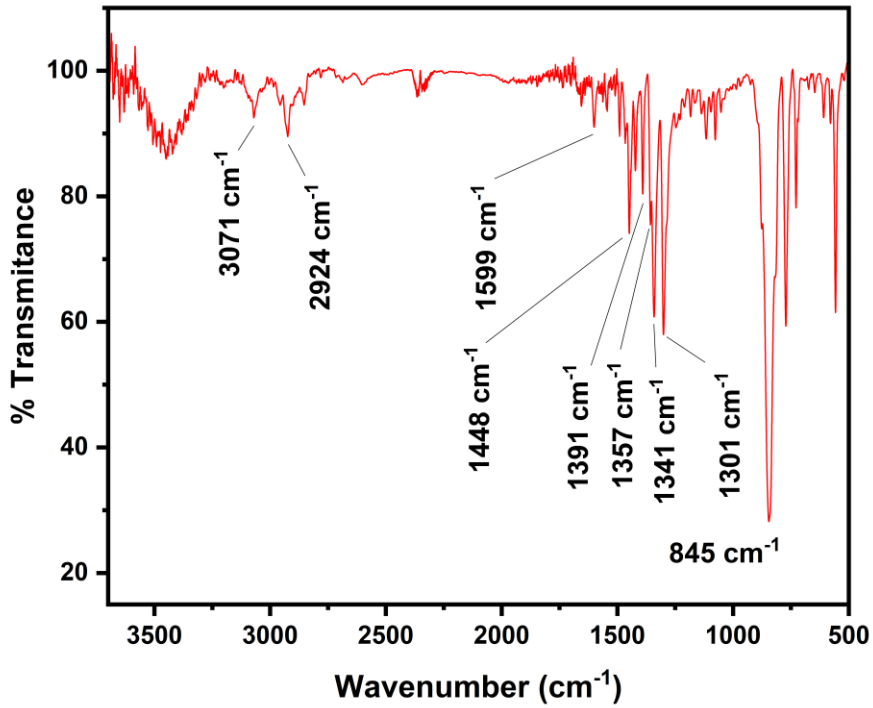

Figure S7: Vibrational spectrum of a KBr pellet containing [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**).

Table S2: Assignment for selected signals in IR spectra of the [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) and [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) complexes.

Assignment	Complex 1	Complex 2
ν_{as} (PF_6) / cm^{-1}	845, s	845, s
ν (C=N)$_{dppz}$ / cm^{-1}	1354, m	1357, m
ν (C=C)$_{tpy}$ / cm^{-1}	1385, m	1391, m
ν (C=C)$_{dppz}$ / cm^{-1}	1445, m	1448, m
ν (C=N)$_{tpy}$ / cm^{-1}	1596, w	1599, w

Abbreviations: s = strong; m = medium; w = weak. Data were obtained from KBr pellets (200 mg of KBr and 2 mg of compound).

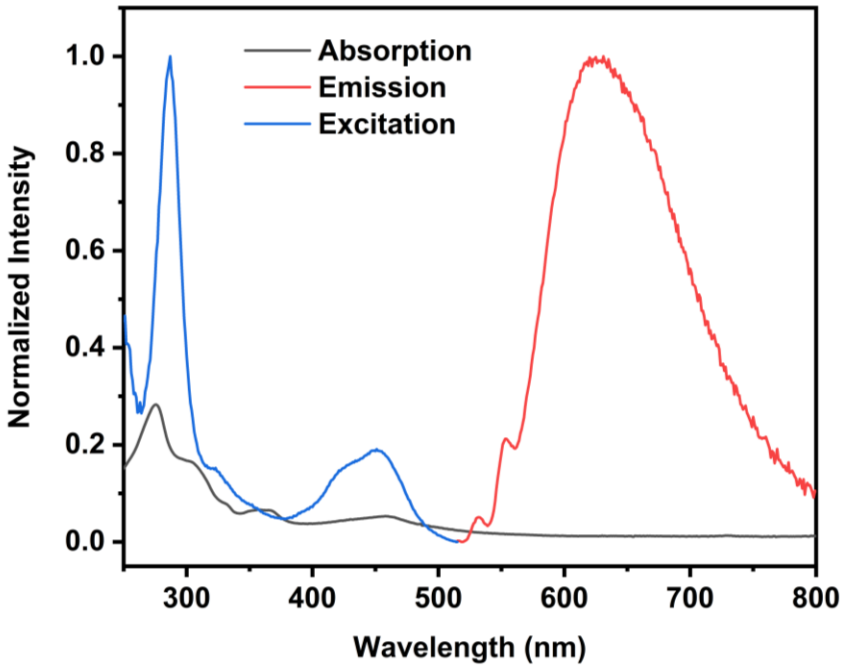

Figure S8: Emission, excitation and absorption spectra of a 5 µM solution of [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in acetonitrile (excitation slit = 6 nm; emission slit = 474 nm).

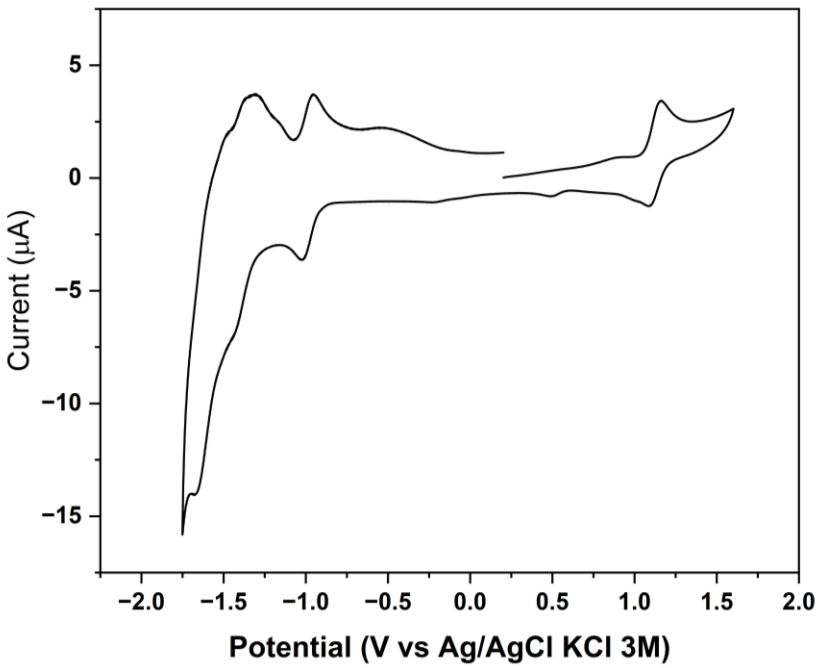

Figure S9: Cyclic voltammetry for a 10^{-3} M solution of complex [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in acetonitrile (100 mV/s).

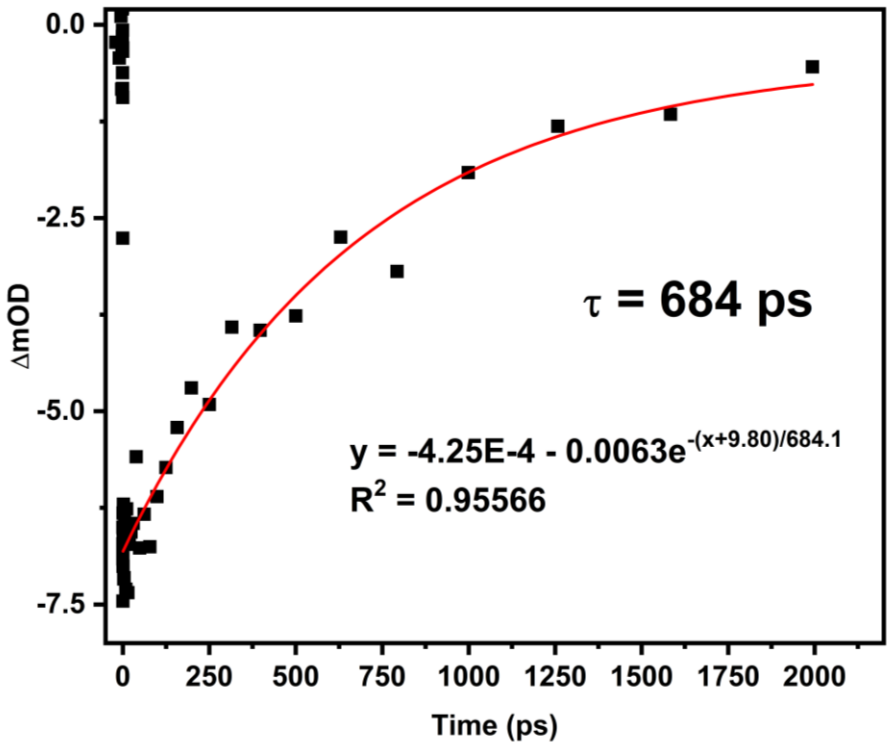

Figure S10: Kinetic curve obtained from *fs*-TA spectra of complex [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) (λ_{max} = 503 nm).

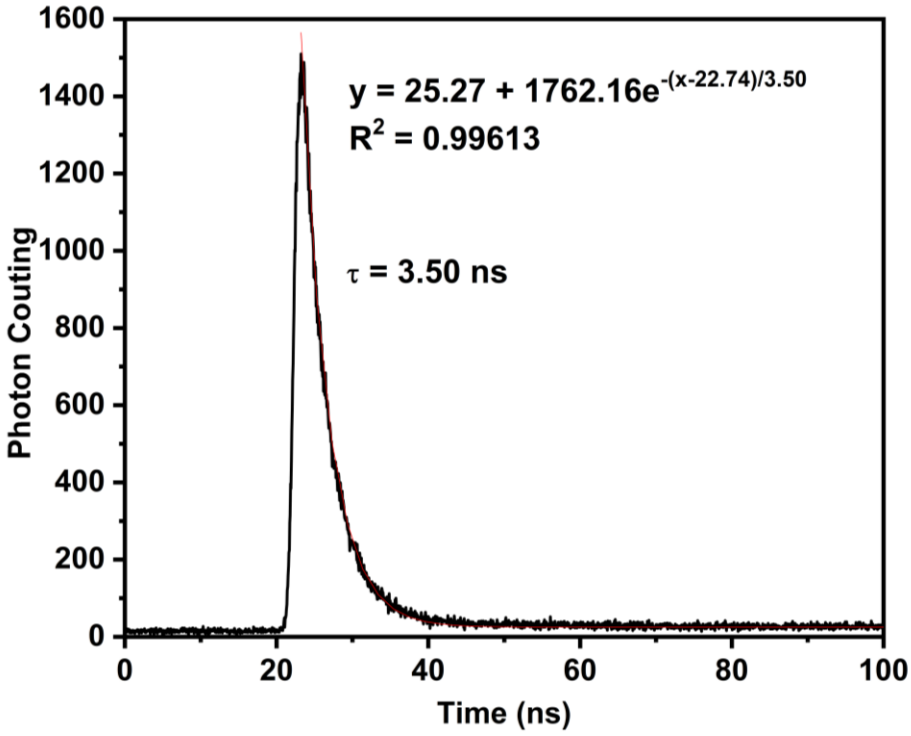

Figure S11: Photon counting in function of time for determination of complex [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) lifetime (TCSPC).

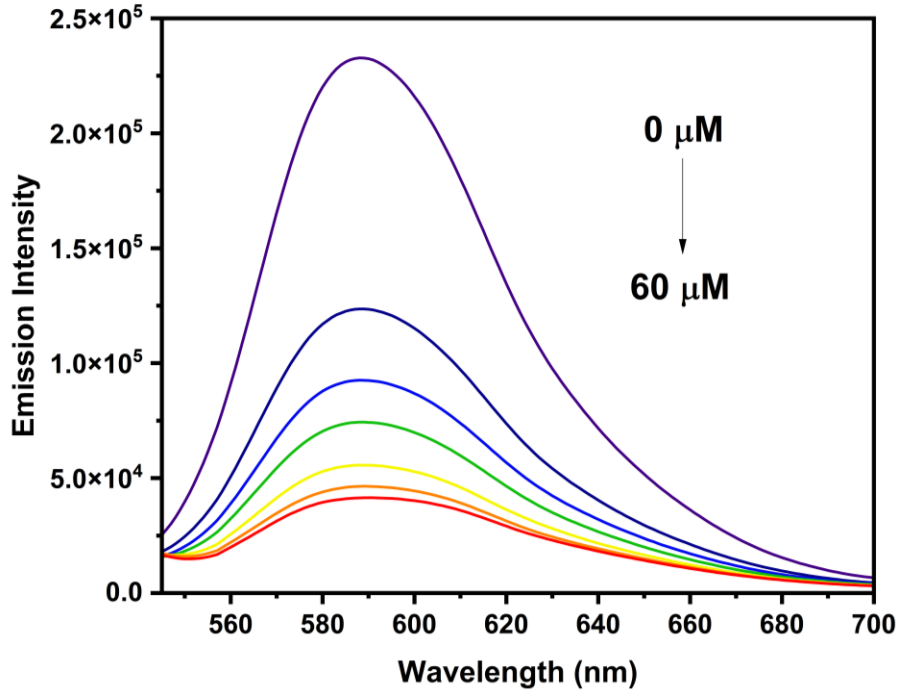

Figure S12: Titration of a fs-DNA solution with EtBr in Tris-HCl buffer (50 mM, pH = 7.4, NaCl 5 mM) with [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**).

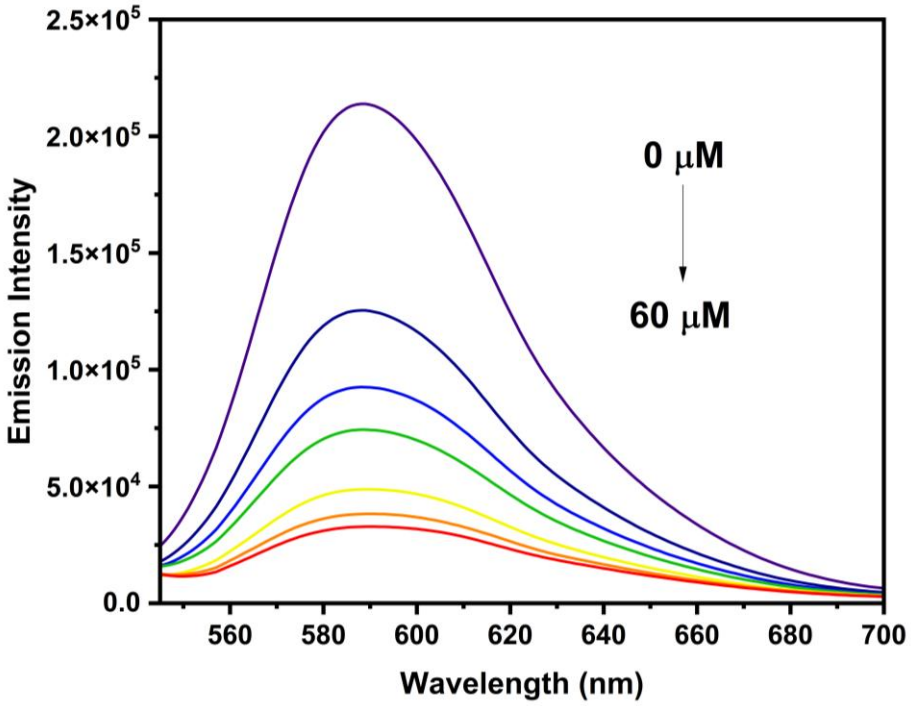

Figure S13: Titration of a fs-DNA solution with EtBr in Tris-HCl buffer (50 mM, pH = 7.4, NaCl 5 mM) with [Ru(tpy)(dppz)(Cl)](PF_6) (**1**).

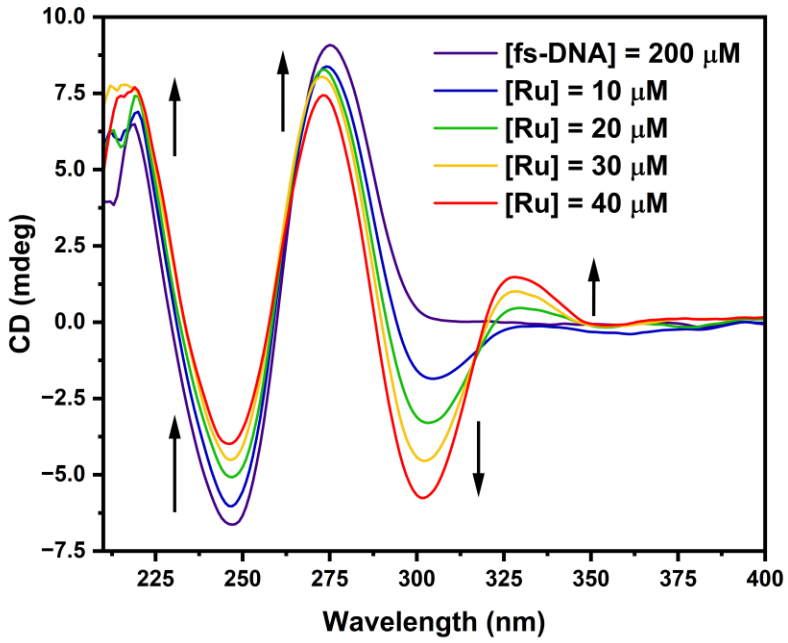

Figure S14: CD spectroscopy titration of a 200 μM solution of fs-DNA with [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in Tris-HCl buffer (50 mM, pH = 7.4, NaCl 5 mM).

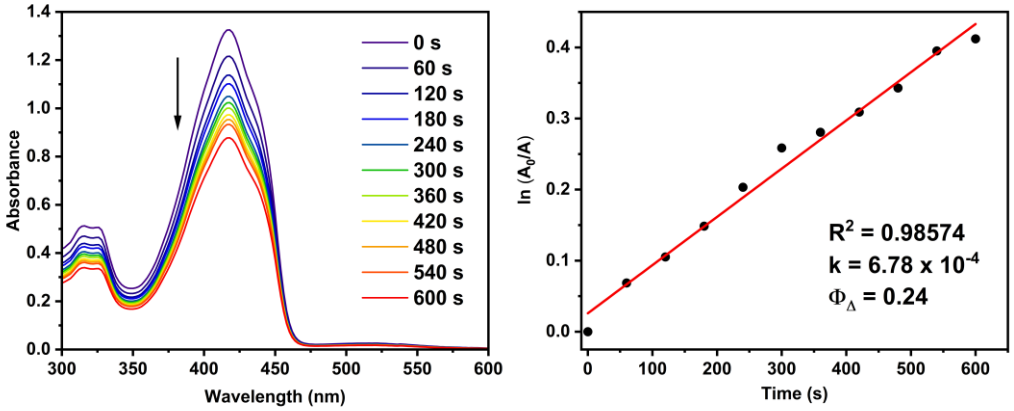

Figure S15: Electronic absorption spectra of a 30 µM DPBF solution with [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) (3 µM) in DMSO with light exposure at different times (left) and first-order kinetic curve for the photodegradation of DPBF (right).

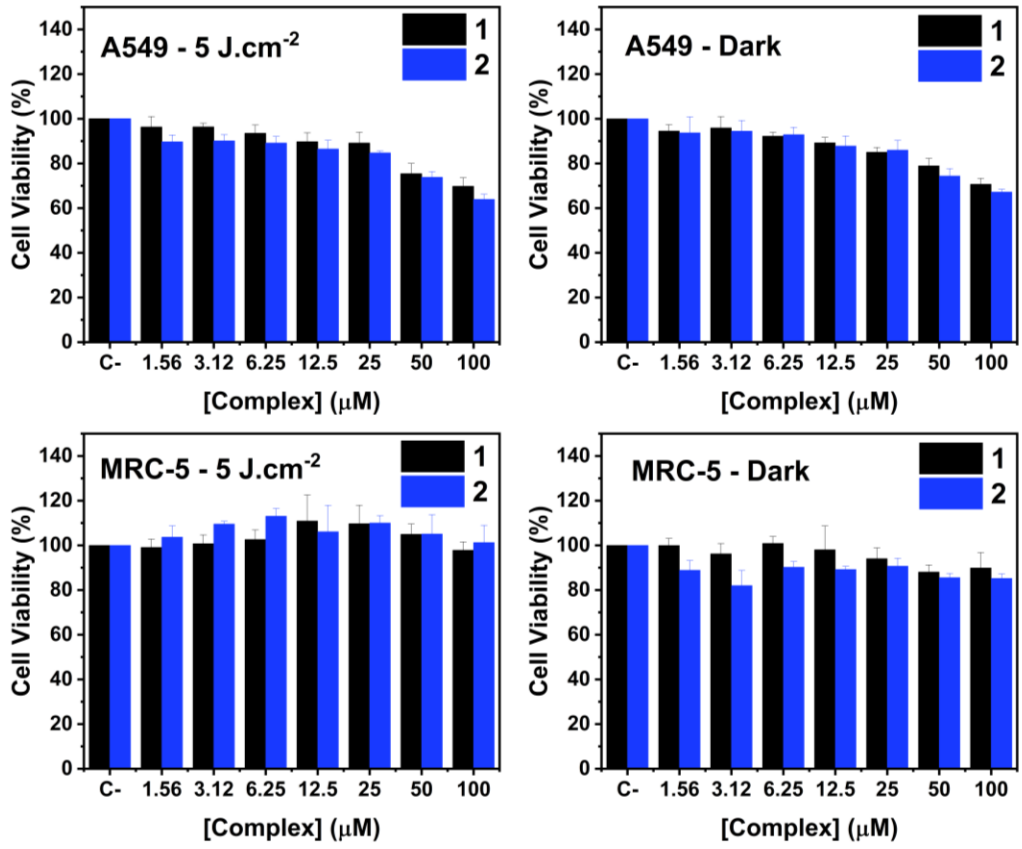

Figure S16: Cytotoxicity assays of complexes [Ru(tpy)(dppz)(Cl)](PF_6) (**1**) and [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) on MRC-5 (normal) and A549 (tumour) cells after 24h of incubation. Data were reported as the mean of a quadruplicate experiment.

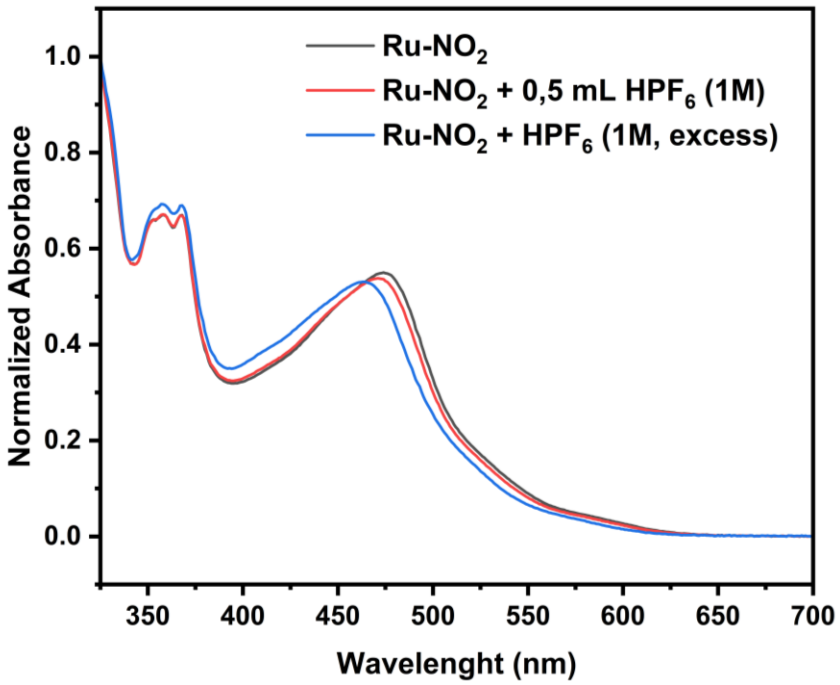

Figure S17: UV-Vis spectrum of [Ru(tpy)(dppz)(NO_2)](PF_6) (**2**) in acetonitrile solution (black); after addition of 0,5 mL of a 1M HPF_6 solution (red); after addition of excess (3mL) of the acid solution (blue).

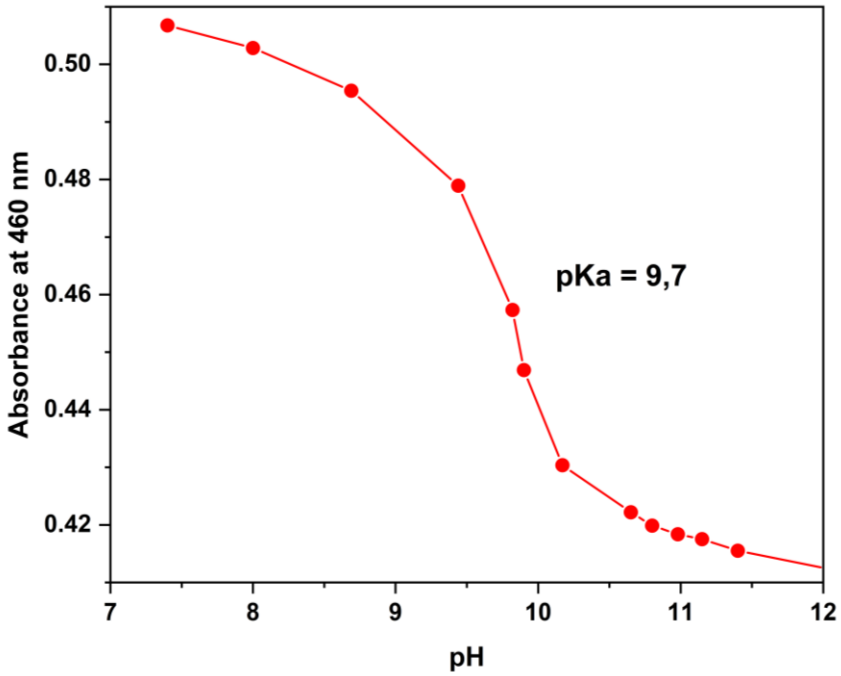

Figure S18: Determination of the pKa of the [Ru(tpy)(dppz)(H_2O)]$^{2+}$ compound from spectrometric titration.

Table S3: Calculated ΔG and K_{eq} for the Ru-NO_2 ⇌ Ru-NO equilibrium.

Computational Method	**ΔG (kJ.mol^{-1})**	**K_{eq} (M^{-1})**
B97/def2-SVP	2031.30	~ 0
B97/def2-TZVP in ACN	103.34	7.85×10^{-19}