Supporting Information

Light Enhanced Cytotoxicity and Antitumoral Effect of a Ruthenium-Based Photosensitizer Inspired from Natural Alkaloids

Gennaro Sanità,[a‡] Maria Laura Alfieri,[b‡] Barbara Carrese,[c] Serena Damian,[b] Vincenza Mele,[c] Gaetano Calì,[d] Brigida Silvestri,[e] Sebastiano Marra,[e] Susan Mohammadi,[f] Giuseppina Luciani,[g] Paola Manini,[b*] Annalisa Lamberti[c*]

[a] Institute of Applied Sciences and Intelligent Systems Unit of Naples, National Research Council, Naples, Italy

[b] Department of Chemical Sciences, University of Naples Federico II, Naples, Italy

[c] Department of Molecular Medicine and Medical Biotechnology, University of Naples Federico II, Naples, Italy

[d] Institute of Endocrinology and Molecular Oncology, National Research Council, Naples, Italy

[e] Department of Civil, Architectural and Environmental Engineering, University of Naples Federico II, Naples, Italy

[f] Scuola Superiore Meridionale, Naples, Italy

[g] Department of Chemical, Materials and Industrial Production Engineering, University of Naples Federico II, Naples, Italy

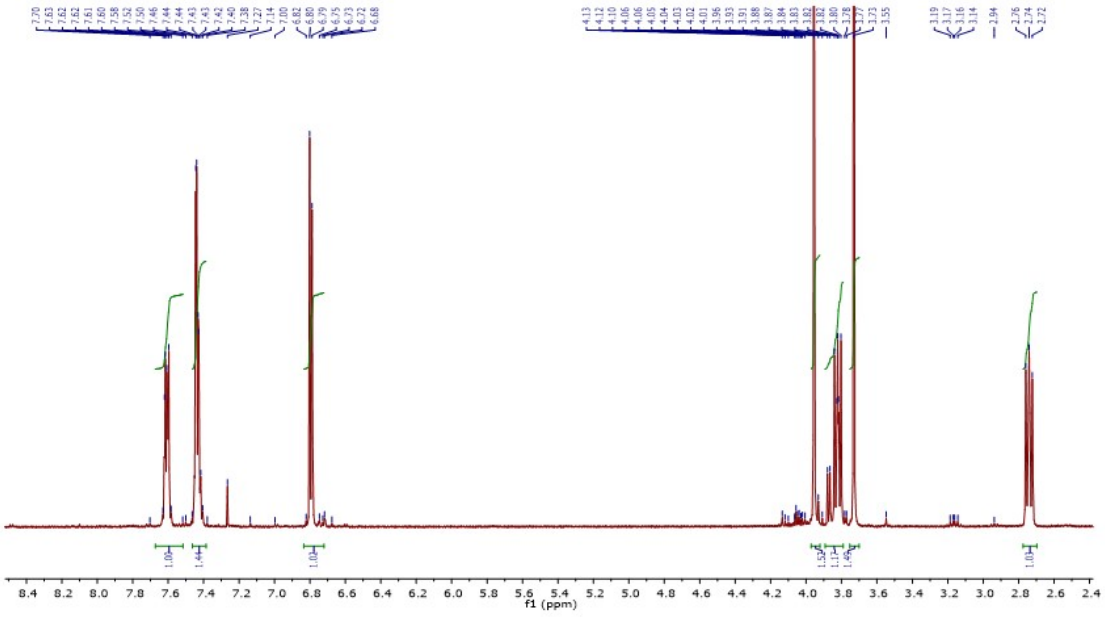


Figure S1. ^{1}H NMR spectrum of **3** in $CDCl_3$.

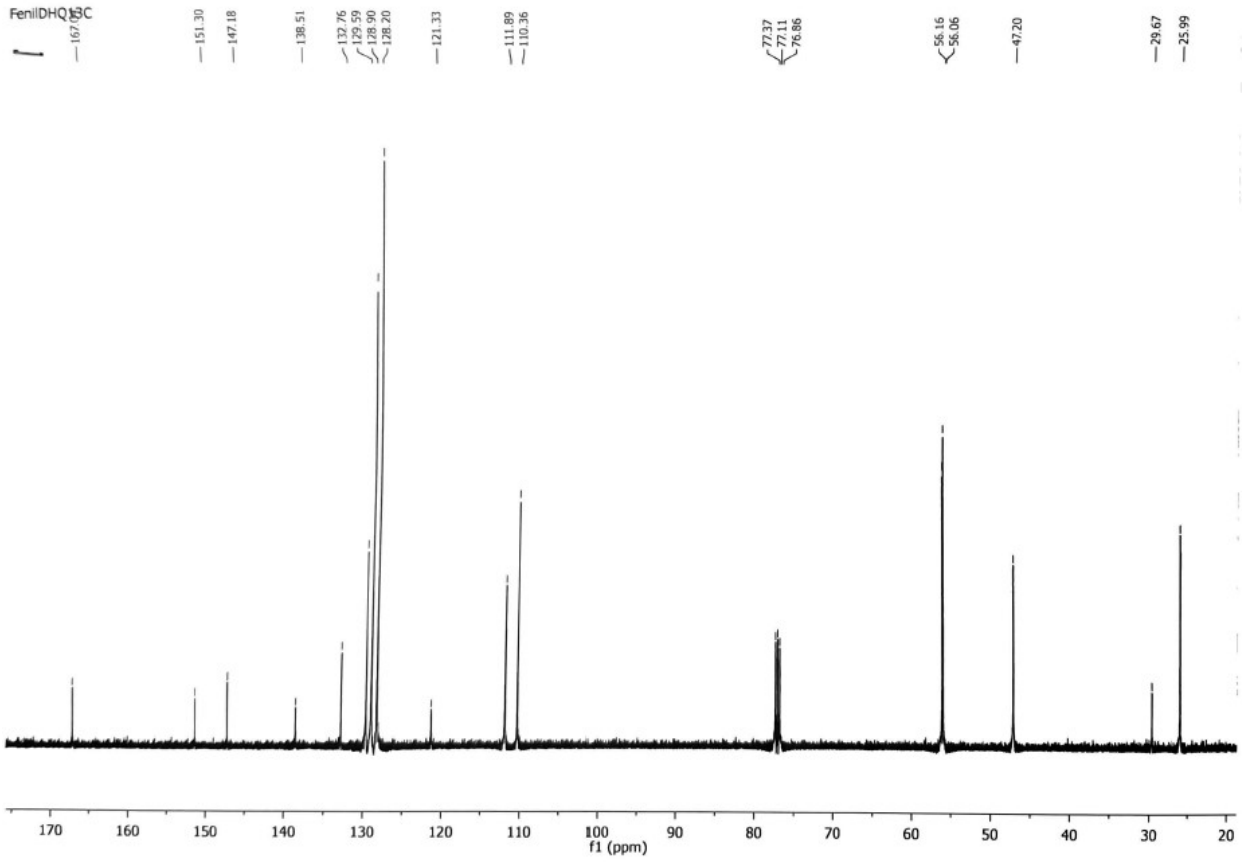


Figure S2. ^{13}C NMR spectrum of **3** in $CDCl_3$.

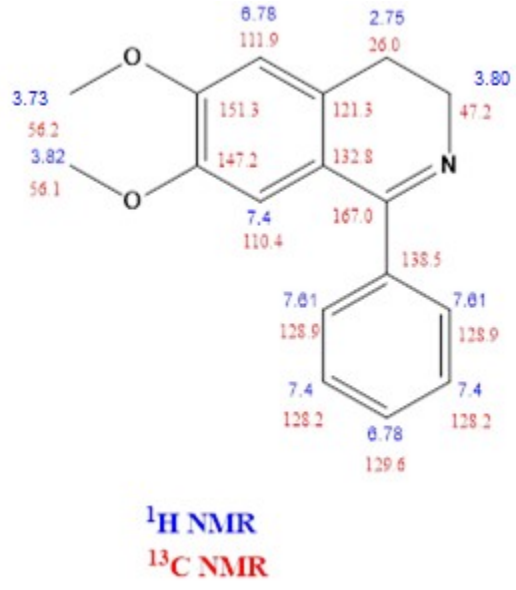


Figure S3. ^{1}H and ^{13}C assignments for compound **3**.

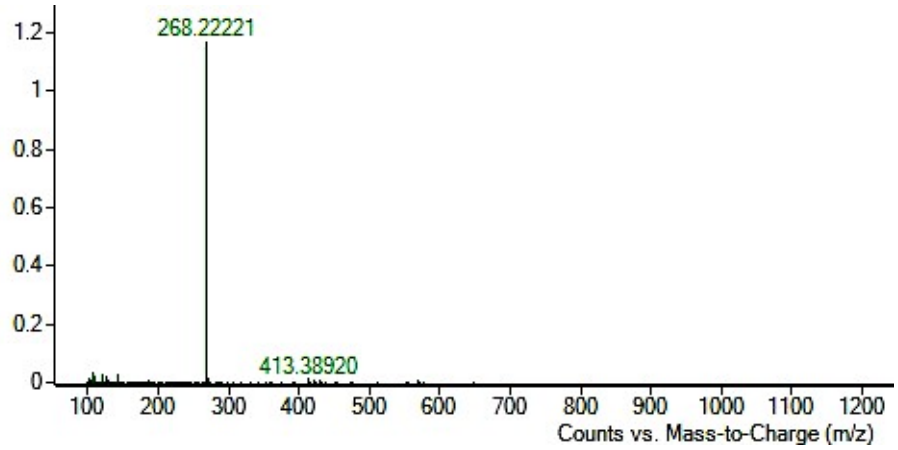


Figure S4. ESI^{+}-MS spectrum of **3**.

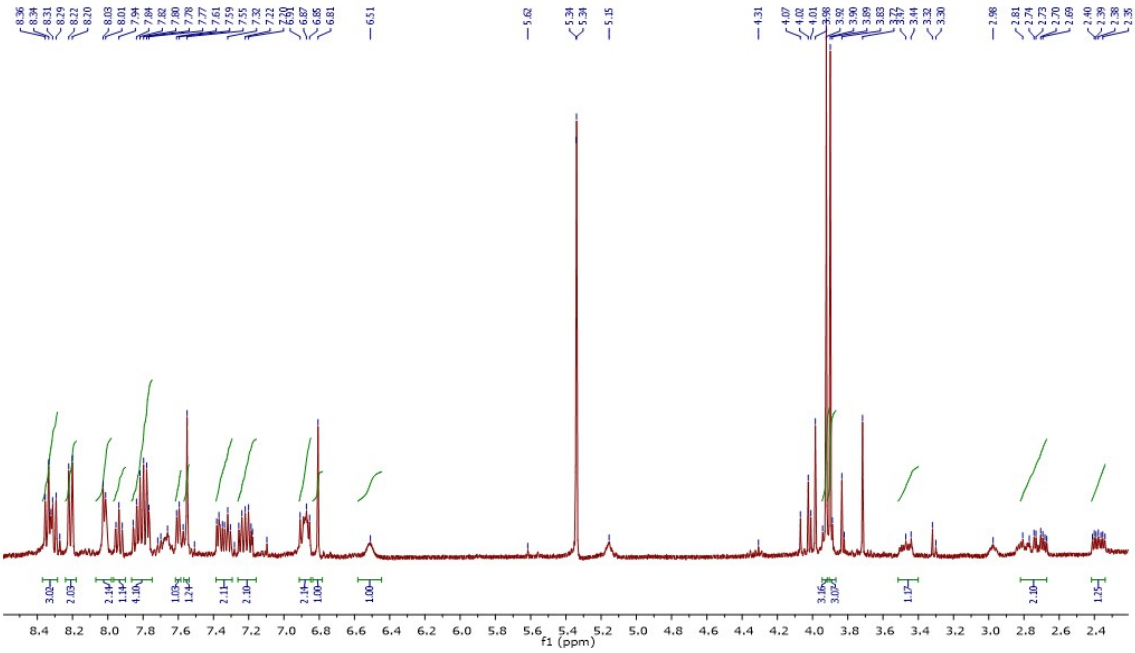


Figure S5. ^{1}H NMR spectrum of complex **1** in CD_2Cl_2

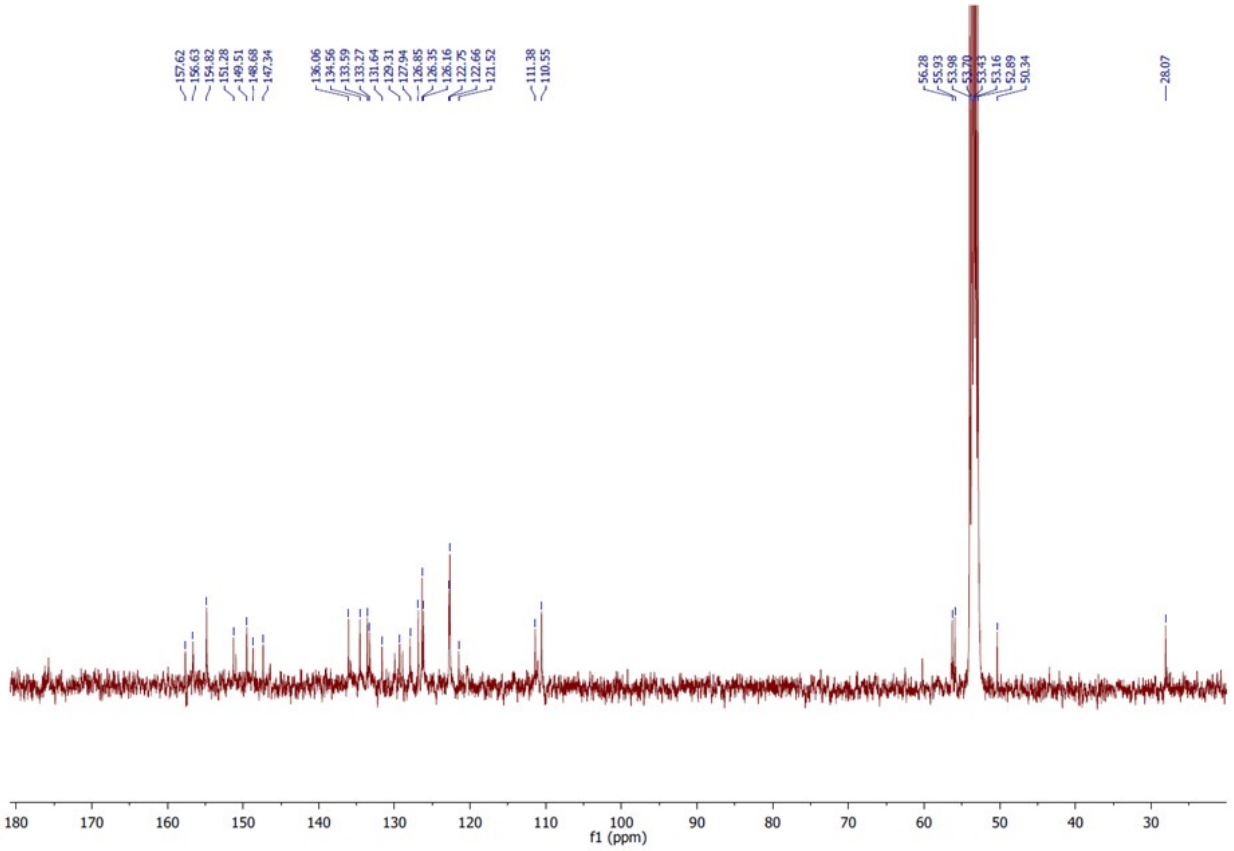


Figure S6. ^{13}C NMR spectrum of complex **1** in CD_2Cl_2.

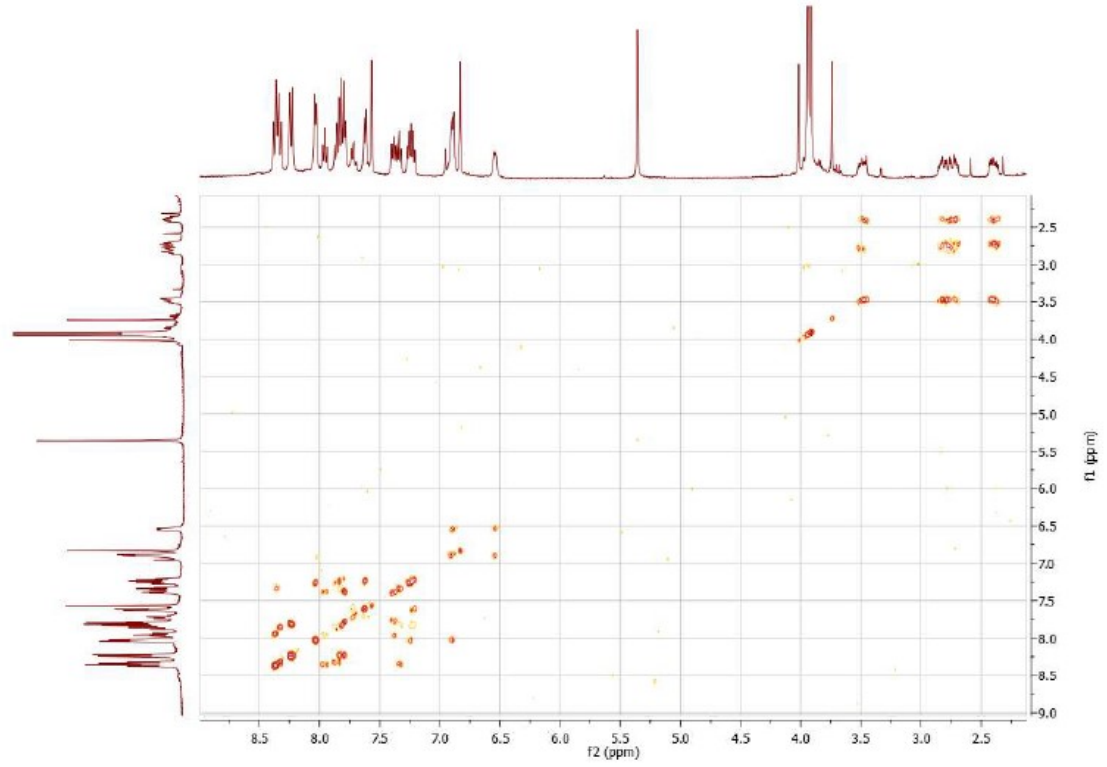


Figure S7. $^{1}H,^{1}H$ COSY spectrum of complex **1** in CH_2Cl_2.

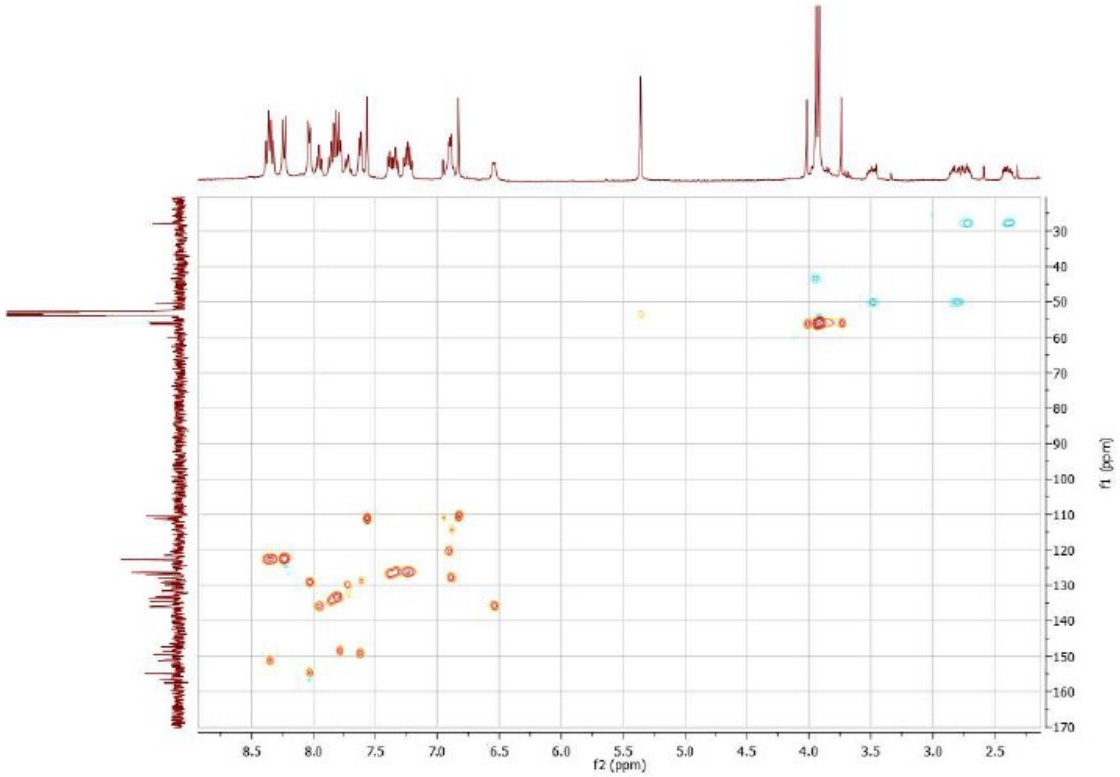


Figure S8. $^{1}H,^{13}C$ HSQC spectrum of complex **1** in CH_2Cl_2.

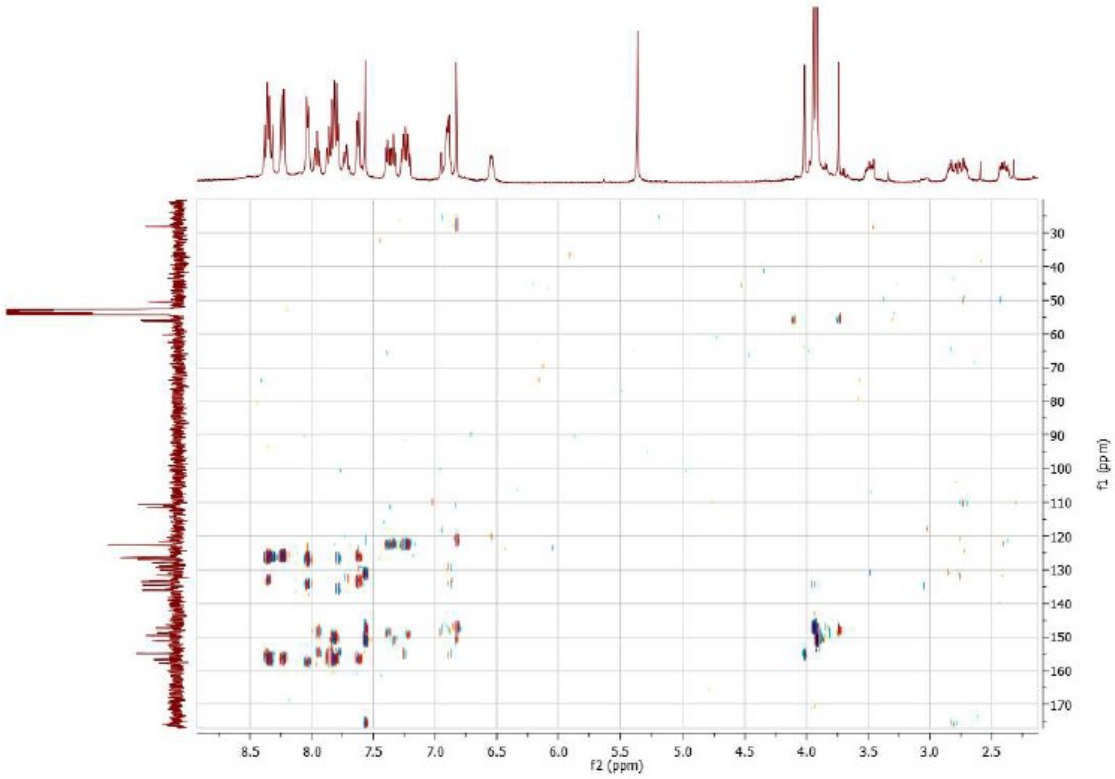


Figure S9. $^{1}H,^{13}C$ HMBC spectrum of complex **1** in CH_2Cl_2.

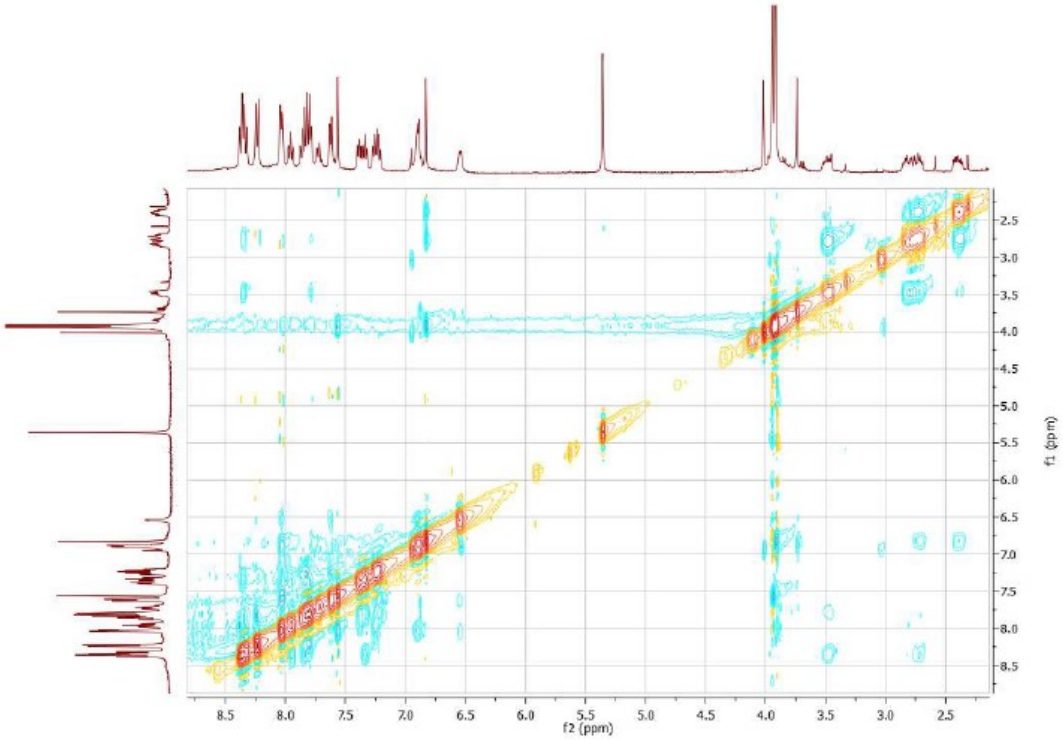


Figure S10. NOESY spectrum of complex **1** in CH_2Cl_2.

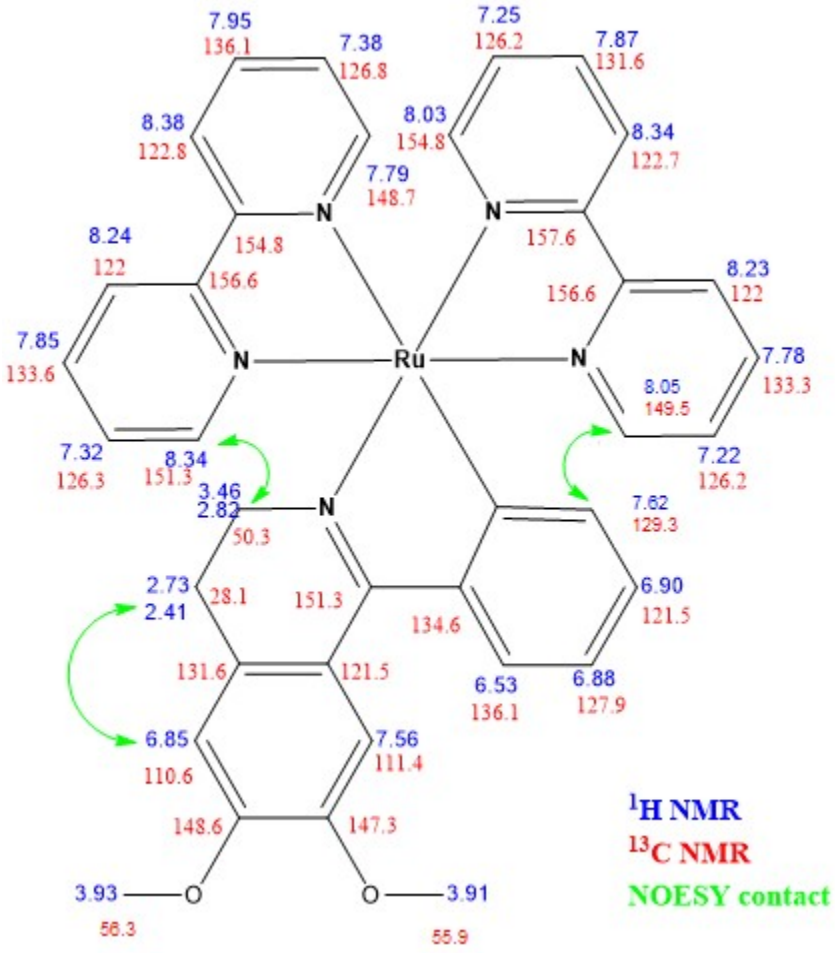


Figure S11. ^{1}H and ^{13}C assignments for compound **1**.

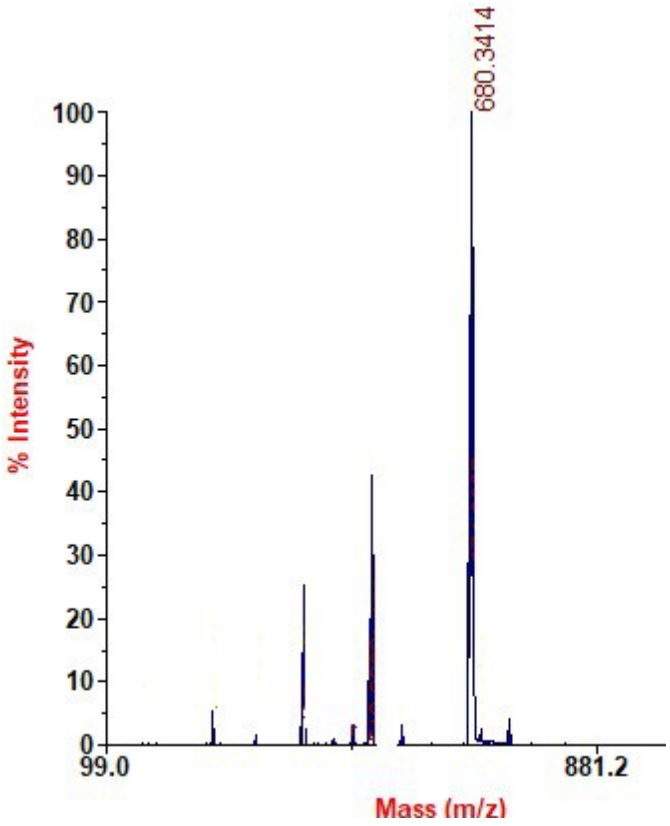


Figure S12. MALDI mass spectrum in the positive ion mode of complex **1**.

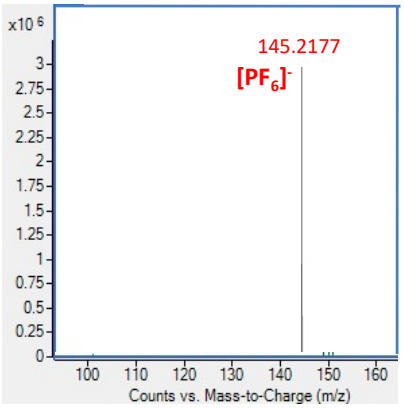


Figure S13. MALDI mass spectrum in the negative ion mode of complex **1**.

Table S1. UV-visible data of the ligand **3**.[a]

	UV-vis λ_{max}, nm ($\log_{\epsilon}$, $M^{-1}cm^{-1}$)
3[b]	239 (4.19), 285 (3.57), 309 (3.63)

[a] Determined in diluted solutions (1×10^{-5} M); [b] determined in $CHCl_3$.

Determination of the hydrophilic/hydrophobic character of 1.

The partition coefficient (log*P*) for **1** was measured by a UV-vis spectroscopic approach. An aqueous solution of **1** (10 µM) was mixed with an equal volume of *n*-octanol. After shaking for 12 h at room temperature, the mixture was allowed to separate by centrifugation. The concentration of the complex **1** in each phase was determined by UV-vis spectroscopy.

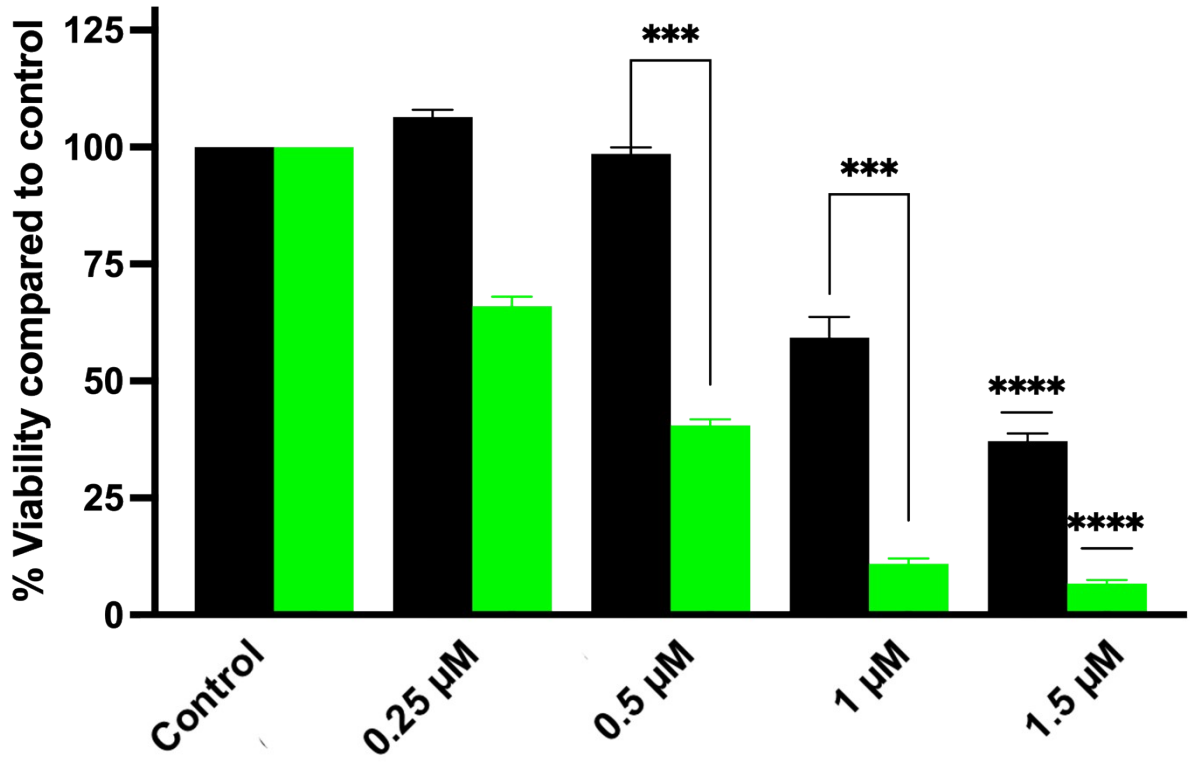
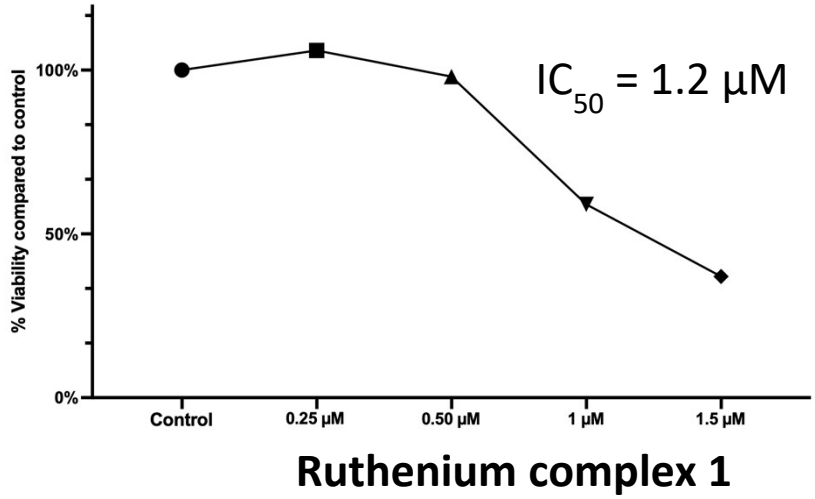
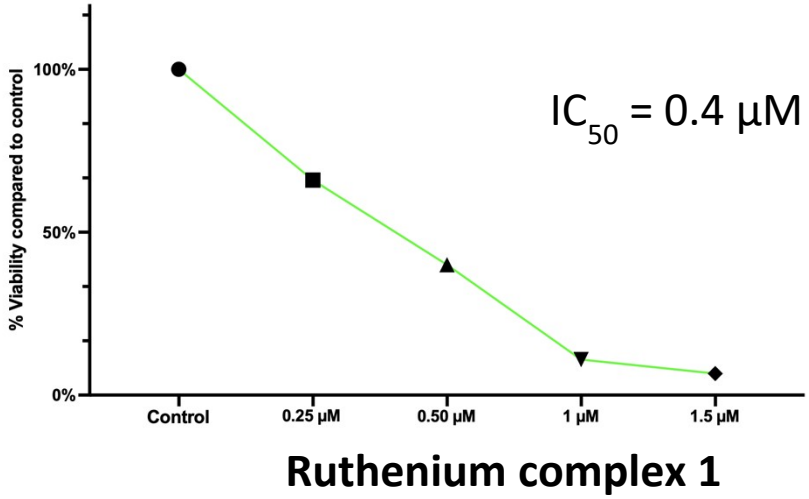


Figure S14. In vitro cytotoxicity of the ruthenium complex **1** on MCf10a cell line. Cell-Titer GLO® assay under dark conditions (black bars) or after light irradiation (green bars). **** $P \leq 0.001$; *** $P \leq 0.01$.

A)





B)

Figure S15. In vitro cytotoxicity of the ruthenium complex **1** on MCf10a cell line. Cell-Titer GLO® assay under dark conditions (A) or after light irradiation (B).

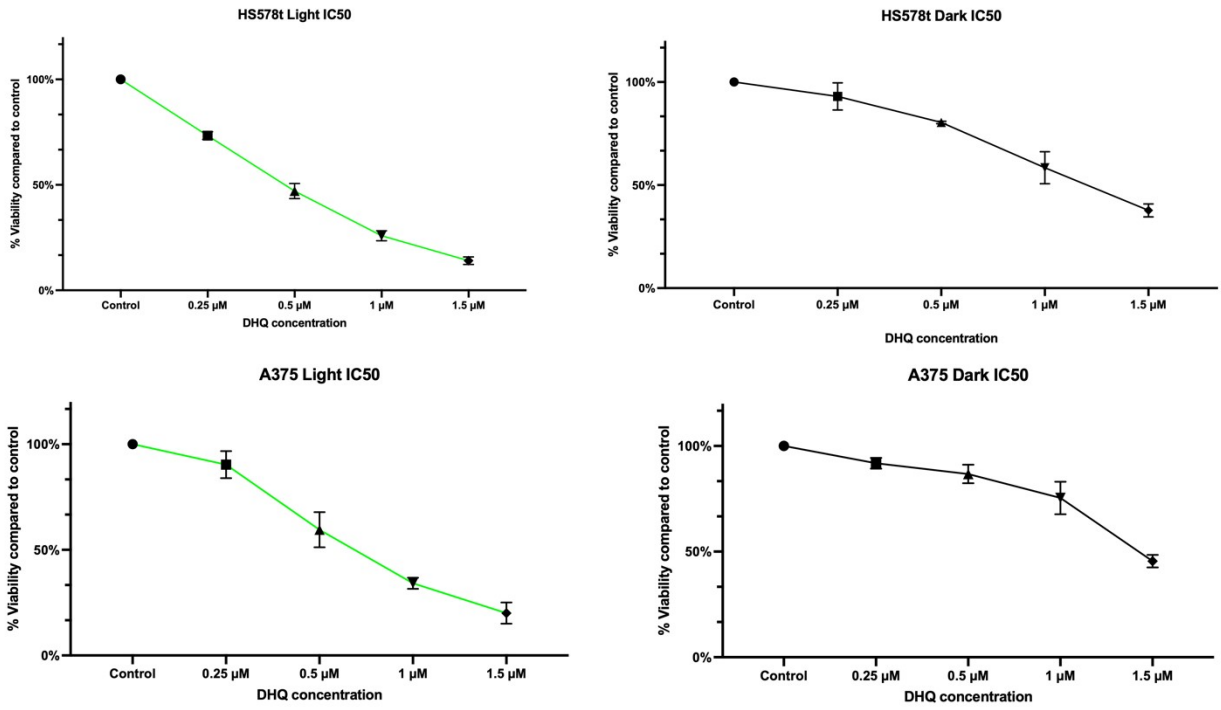


Figure S16. In vitro cytotoxicity of the ruthenium complex **1** on Hs578T and A375cell lines. Cell-Titer GLO® assay under dark conditions (black traces on the right) or after light irradiation (green traces on the left).