

Supplementary Materials

***N*-Heterocyclic Carbene-Iridium Complexes as Photosensitizers for In Vitro Photodynamic Therapy to Trigger Non-Apoptotic Cell Death in Cancer Cells**

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Table S1. Cytotoxic activity of iridium(III) NHC complexes 4a–4g	S1
¹ H and ¹³ C NMR spectra of proligands 3a–3f	S2–S8
¹ H and ¹³ C NMR spectra of iridium(III) NHC complexes 4a–4g	S9–S15
2D NMR spectra of iridium(III) NHC complex 4a	S16–S17

Table S1. Cytotoxic activity of iridium(III) NHC complexes **4a–4g** expressed as GI₅₀ (μM) values towards selected cancer and normal cell lines as determined by MTT assay (48 h).^a

Complex	PC-3	T24	NIH3T3	SI (PC-3)	SI (T24)
4a	0.48	0.31	3.3	6.9	10.6
4b	0.51	0.38	3.5	6.9	9.2
4c	0.41	0.43	7.1	17.3	16.5
4d	0.71	0.95	8.5	12.0	8.9
4e	0.25	0.29	2.5	10.0	8.6
4f	0.91	0.91	4.1	4.5	4.5
4g	0.27	0.25	2.7	10.0	10.8
[IrCl(ppy) ₂] ₂	>20	14.8	>20	>1	>1.4

^a GI₅₀ values correspond to the concentration of complexes causing 50 % inhibition of cell growth.

Data were obtained from three independent experiments.

The cytotoxic effects of the NHC precursors, the imidazolium salts, which represents the potential hydrolysis and/or degradation products of the complexes, have been published before [SI-1, SI-2].

SI-1 Hemmert, C.; Fabié, A.; Fabre, A.; Benoit-Vical, F.; Gornitzka, H. Synthesis, structures, and antimalarial activities of some silver(I), gold(I) and gold(III) complexes involving N-heterocyclic carbene ligands. *Eur. J. Med. Chem.* **2013**, *60*, 64–75. <https://doi.org/10.1016/j.ejmech.2012.11.038>.

SI-2 Hemmert, C.; Ramadani, A.P.; Boselli, L.; Álvarez, Á.F.; Paloque, L.; Augereau, J.-M.; Gornitzka, H.; Benoit-Vical, F. An-tiplasmodial activities of gold(I) complexes involving functionalized N-heterocyclic carbenes. *Bioorg. Med. Chem.* **2016**, *24*, 3075–3082. <https://doi.org/10.1016/j.bmc.2016.05.023>.



























