Supplementary Material to

Evaluation of the Potential of Cobalamin Derivatives Bearing Ru(II) Polypyridyl Complexes as Photosensitisers for Photodynamic Therapy

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# these authors have contributed equally to the work.

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Supplementary Figures

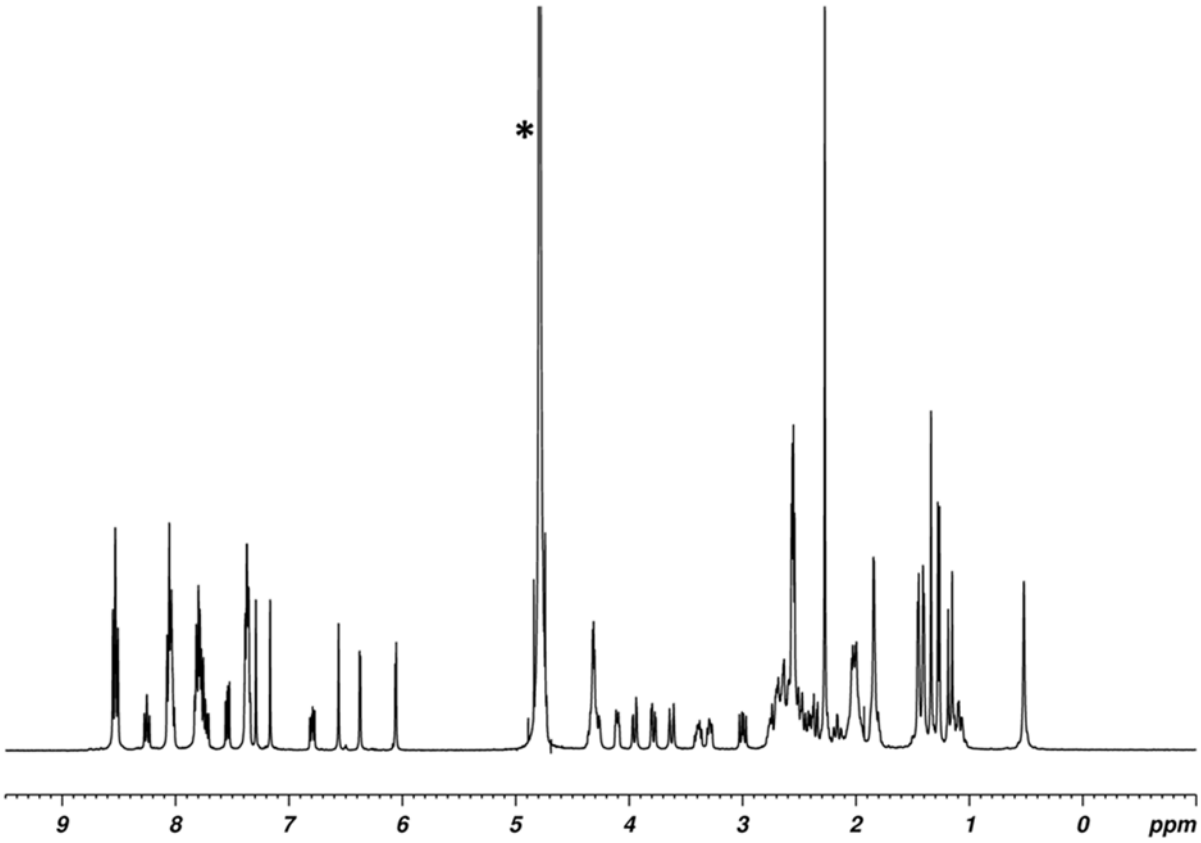
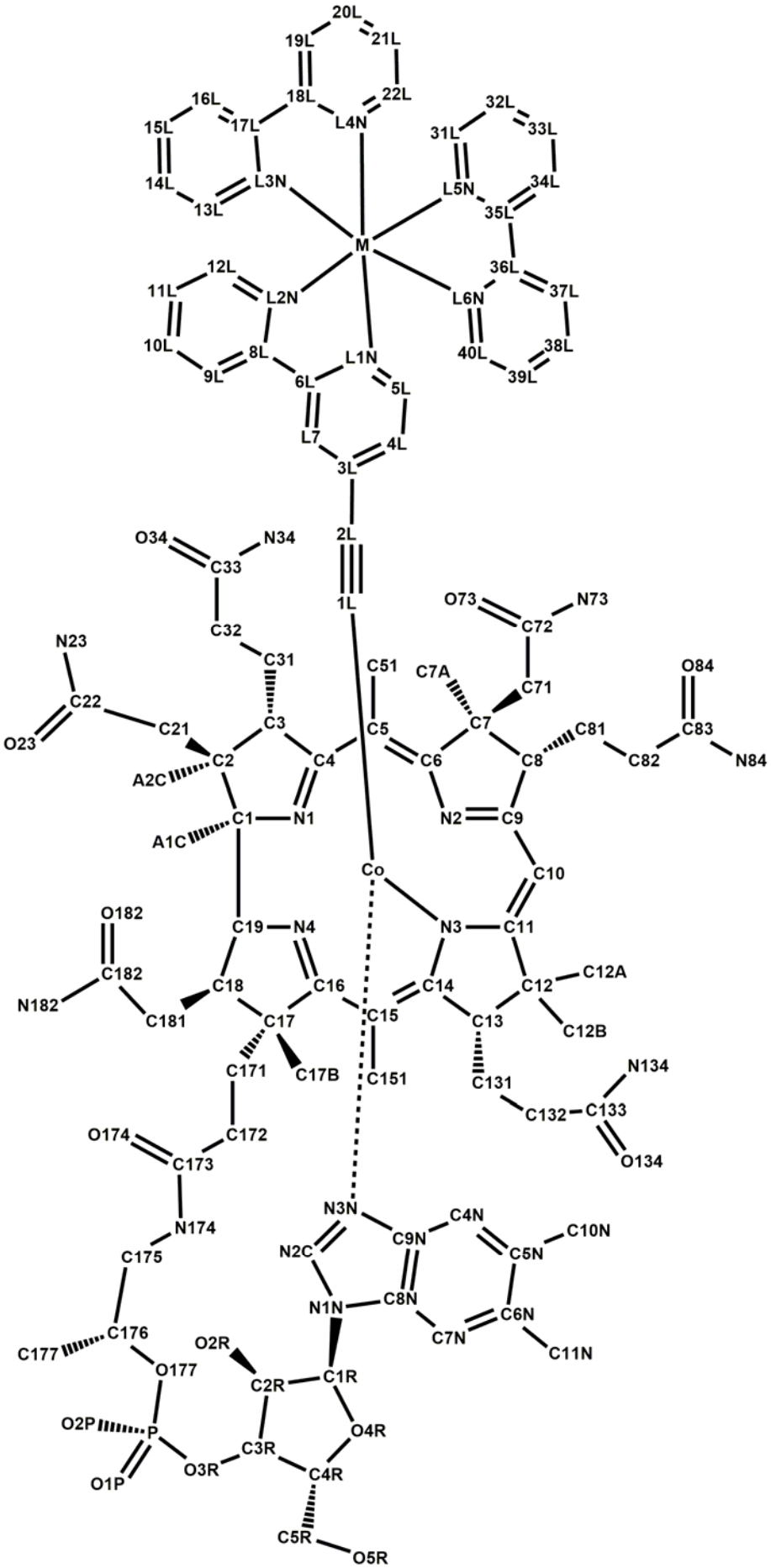


Figure S1. 500 MHz ^{1}H-NMR of compound B_{12}-**2** (in D_2O, ✱= solvent residual peak).

^{1}H NMR (500 MHz, MeOD-[d4]) peak assignment (see scheme on page S4): δ = 8.53 (t, J = 9.5 Hz, 4H, HC-13/22/31/40L), 8.25 (t, J = 9.37 Hz, 1H, HC-9L), 8.09-7.99 (m, 5H, HC-12L, HC-16/19/34/37L), 7.85-7.69 (m, 6H, HC-7L, HC-10L, HC-15/20/33/38L), 7.54 (dd, J = 6.0, 2.37 Hz, 1H, HC-5L), 7.40-7.32 (m, 5H, HC-11L, HC-14/21/32/39L), 7.29 (s, 1H, HC-7N), 7.14 (s, 1H, HC-2N), 6.82-6.76 (m, 1H, HC-4L), 6.50 (s, 1H, HC-4N), 6.37 (d, J = 3.2 Hz, 1H, HC-1R), 6.05 (d, J = 3.8 Hz, 1H, HC-10), 4.38-4.23 (m, 2H, HC-3R, HC-3), 4.13-4.07 (m, 1H, HC-19), 3.95 (dd, J = 13.0, 2.45 Hz, 1H, HC-176), 3.78 (dd, J = 13.0, 4.0 Hz, 2H, HC-2R, HC-4R), 3.62 (d, J = 14.3 Hz, 1H, H_bC-5R), 3.43-3.35 (m, 2H, H_aC-5R, H_bC-175), 3.32-3.25 (m, 2H, HC-8, HC-13), 2.99 (dd, J = 9.0, 5.3 Hz, 2H, H_bC-171, H_bC-172), 2.79-2.32 (m, 16H, H_aC-175, HC-18, H_3C-51, H_3C-151, H_aC-181, HC-21, H_aC-132, H_bC-71, H_bC-132, H_bC-71, H_aC-82), 2.27 (s, 6H, H_3C-10N, H_3C-11N), 2.14 (t, J = 12.0, 1H, H_aC-171), 2.09-1.93 (m, 7H, H_aC-181, H_bC-131, H_aC-71, H_bC-81, H_bC-31, H_aC-31, H_aC-131), 1.89-1.77 (m, 5H, H_3C-7A, H_aC-172, H_bC-82), 1.45 (d, J = 4.2 Hz, 3H, H_3C-12A), 1.40 (d, J = 3.4 Hz, 3H, H_3C-2A), 1.34 (s, 3H, H_3C-17B), 1.27 (d, J = 6.3 Hz, 3H, H_3C-177), 1.18 (t, 1H, H_aC-81), 1.15 (s, 3H, H_3C-12B), 1.13-1.02 (m, 2H, H_2C-32), 0.52 (s, 3H, H_3C-1A) ppm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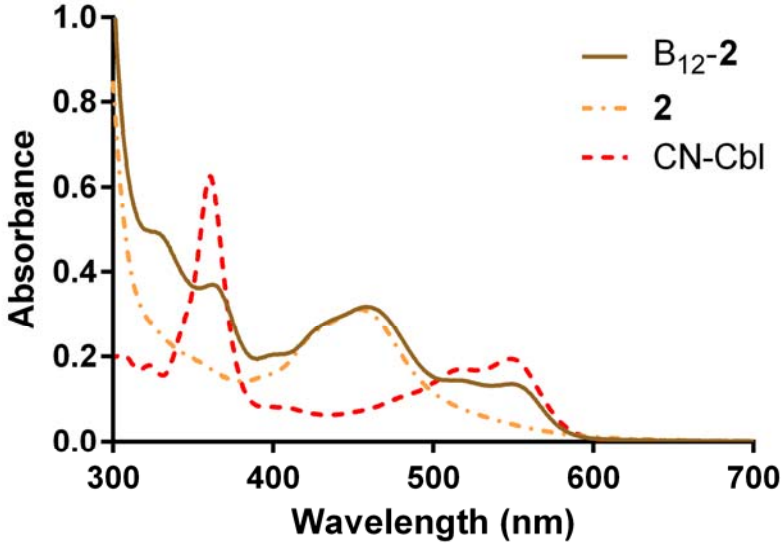

Figure S2. Normalized UV-Vis of compounds **2**, B_{12}-**2** and of cyanocobalamin (CN-Cbl) in methanol.

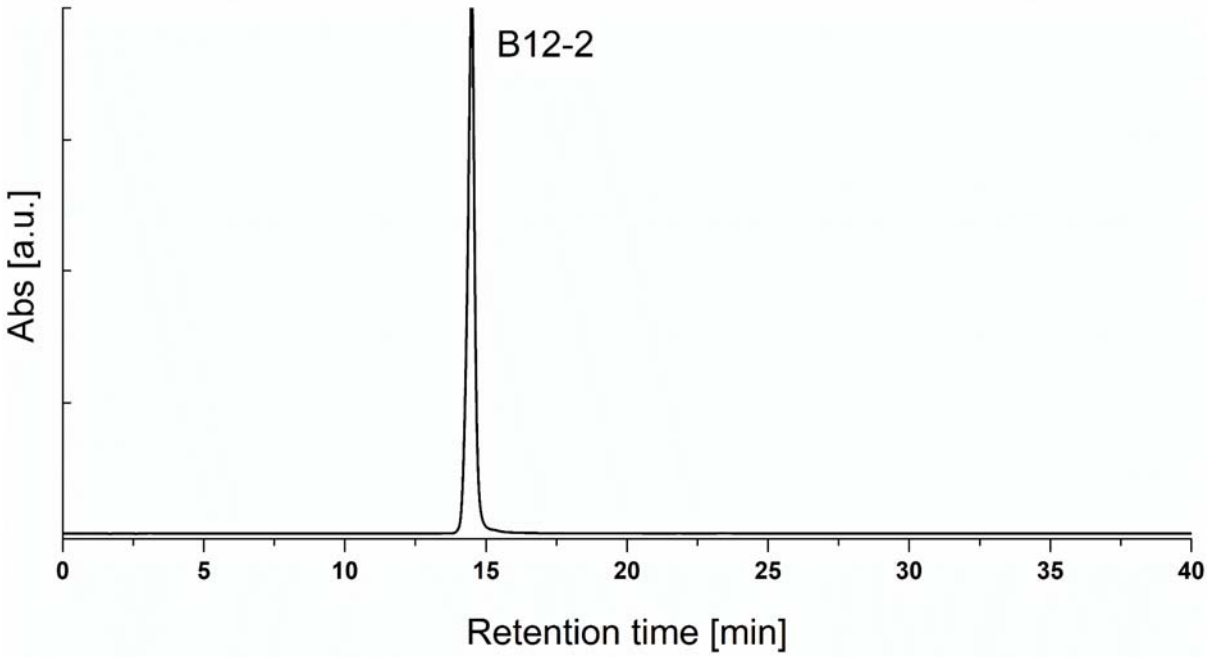

Figure S3. HPLC chromatogram of compound B_{12}-**2**.

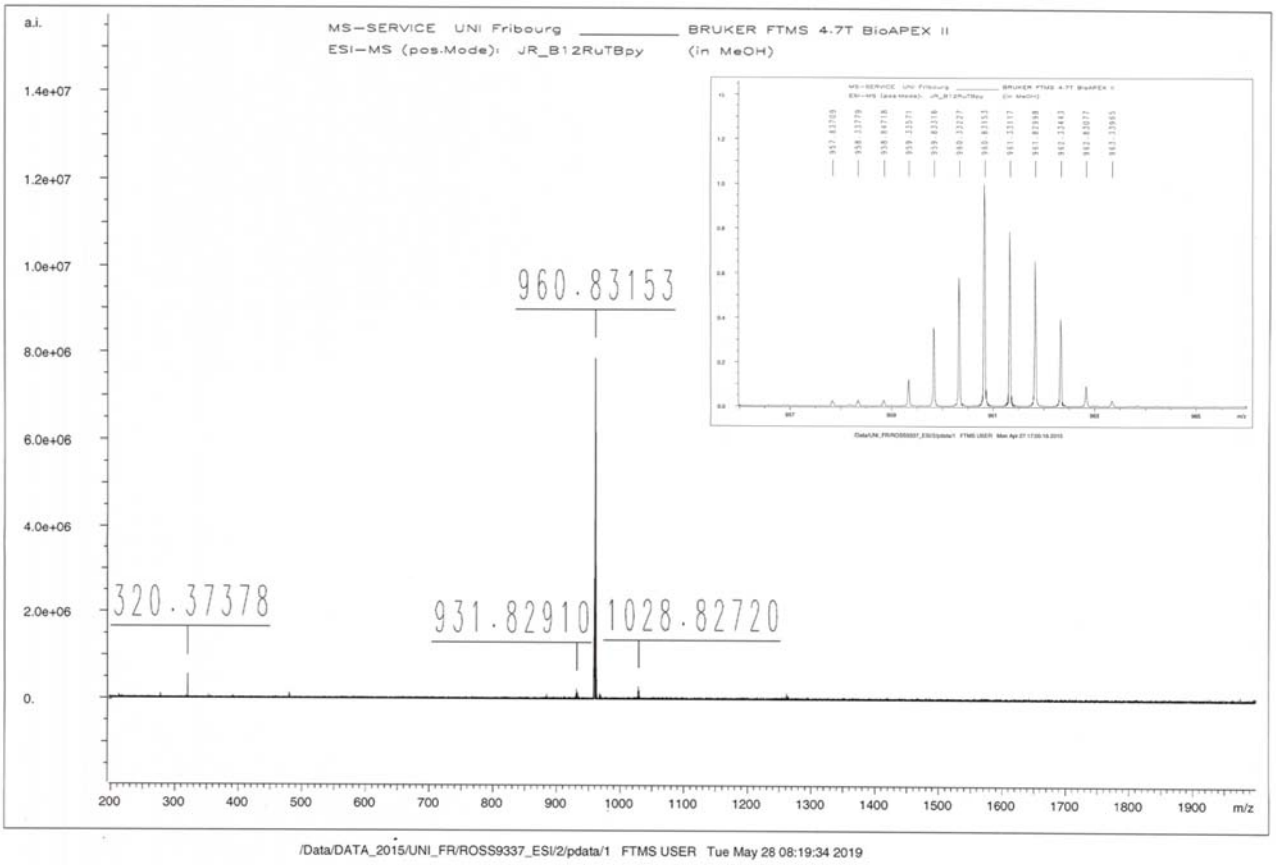

Figure S4. HR-ESI-MS of compound B_{12}-**2**. Insert shows isotope pattern of 960.83153 peak.

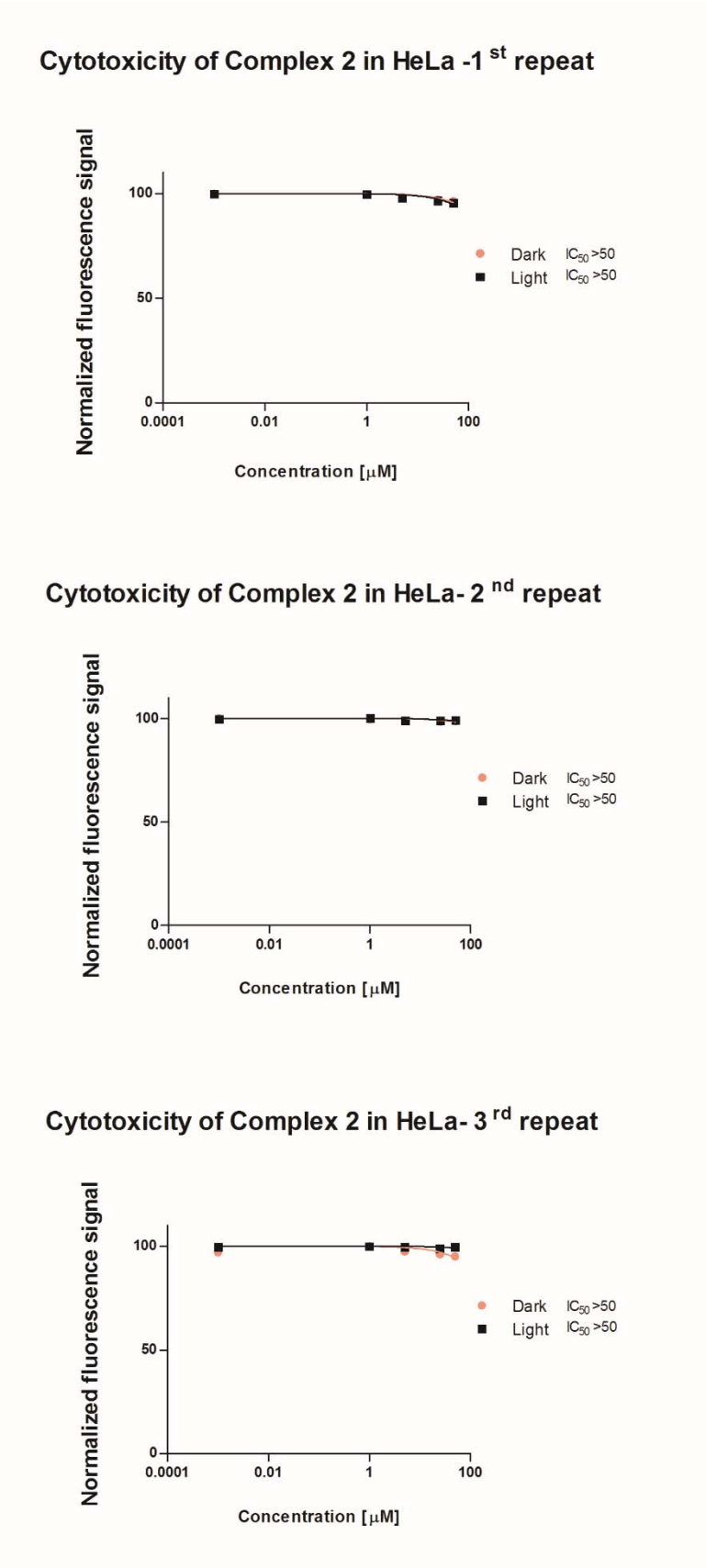

Figure S5. Cytotoxicity of complex 2 in the HeLa cell line.

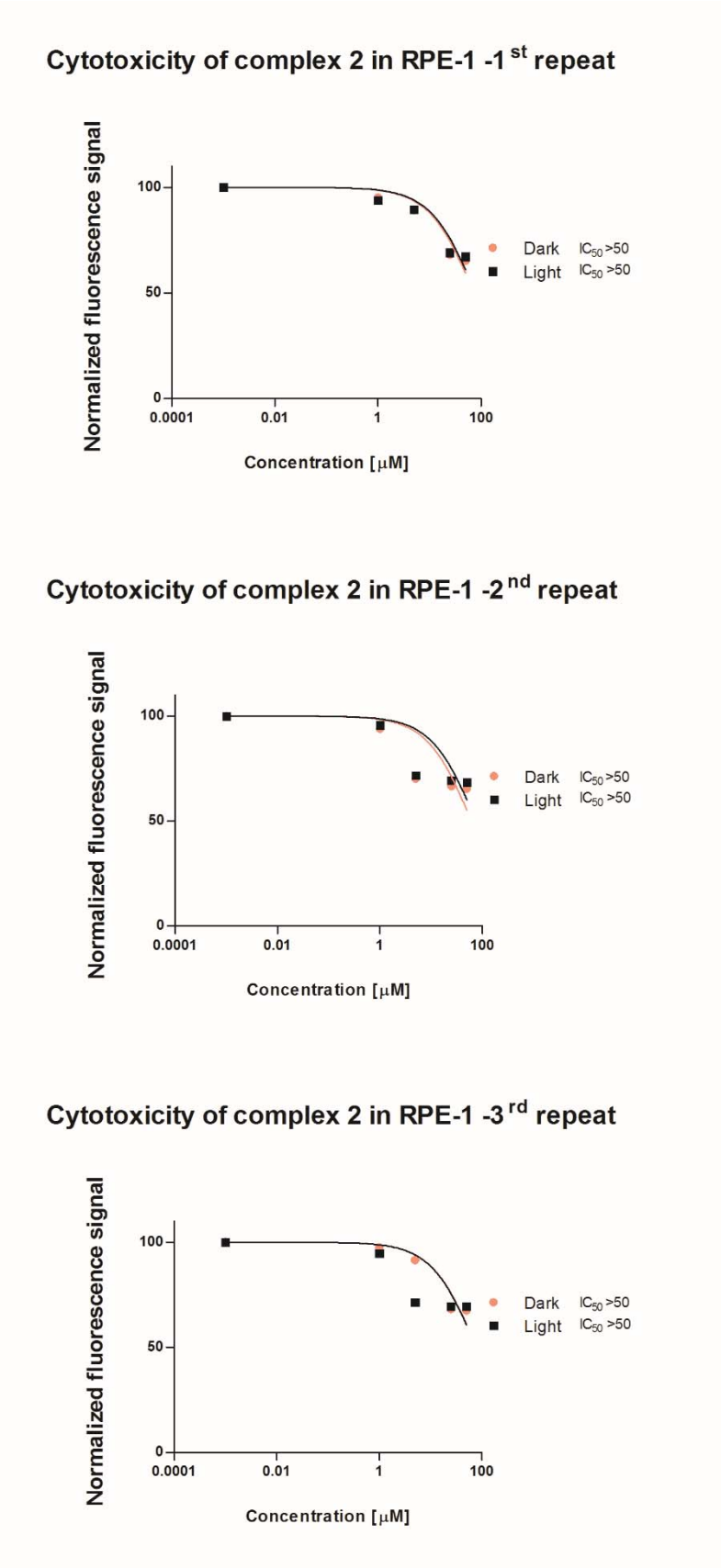

Figure S6. Cytotoxicity of complex 2 in the RPE-1 cell line.

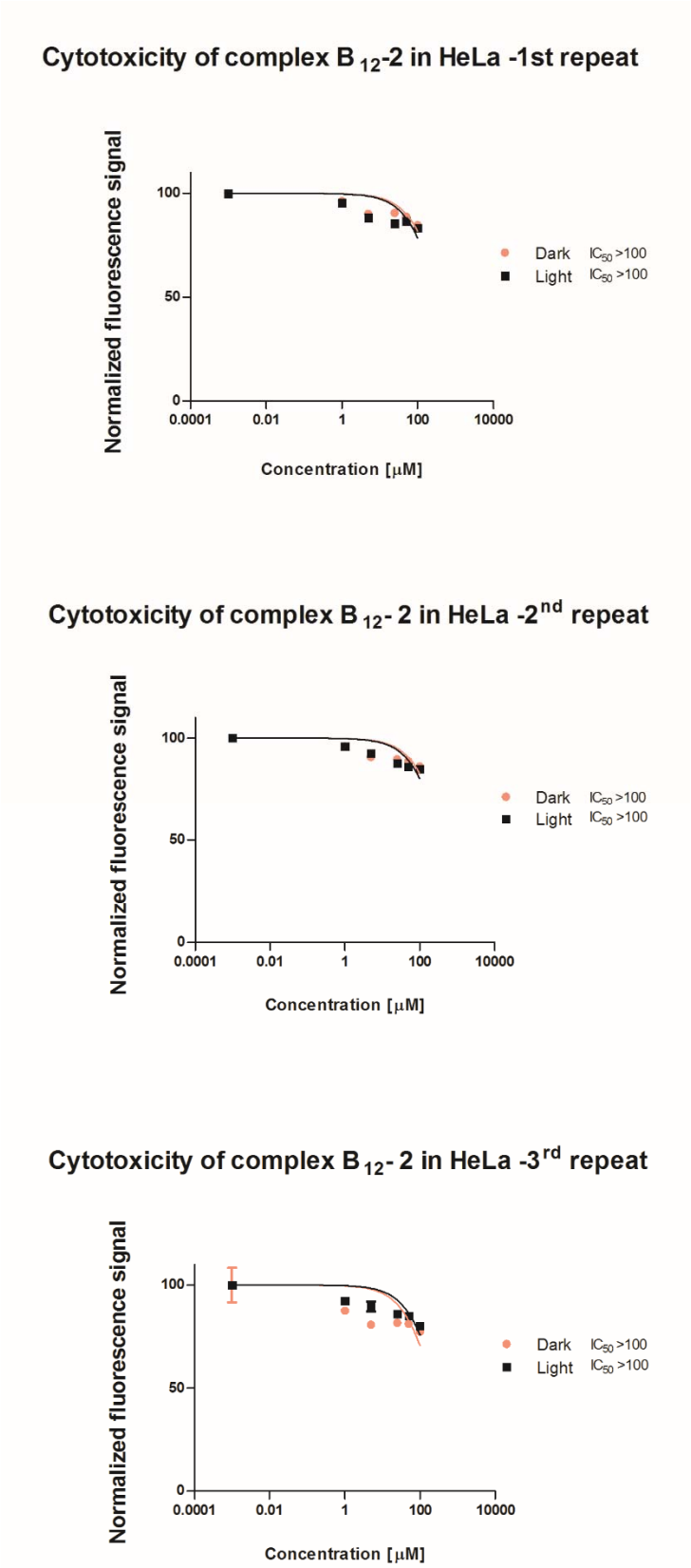

Figure S7. Cytotoxicity of complex B_{12}-2 in the HeLa cell line.

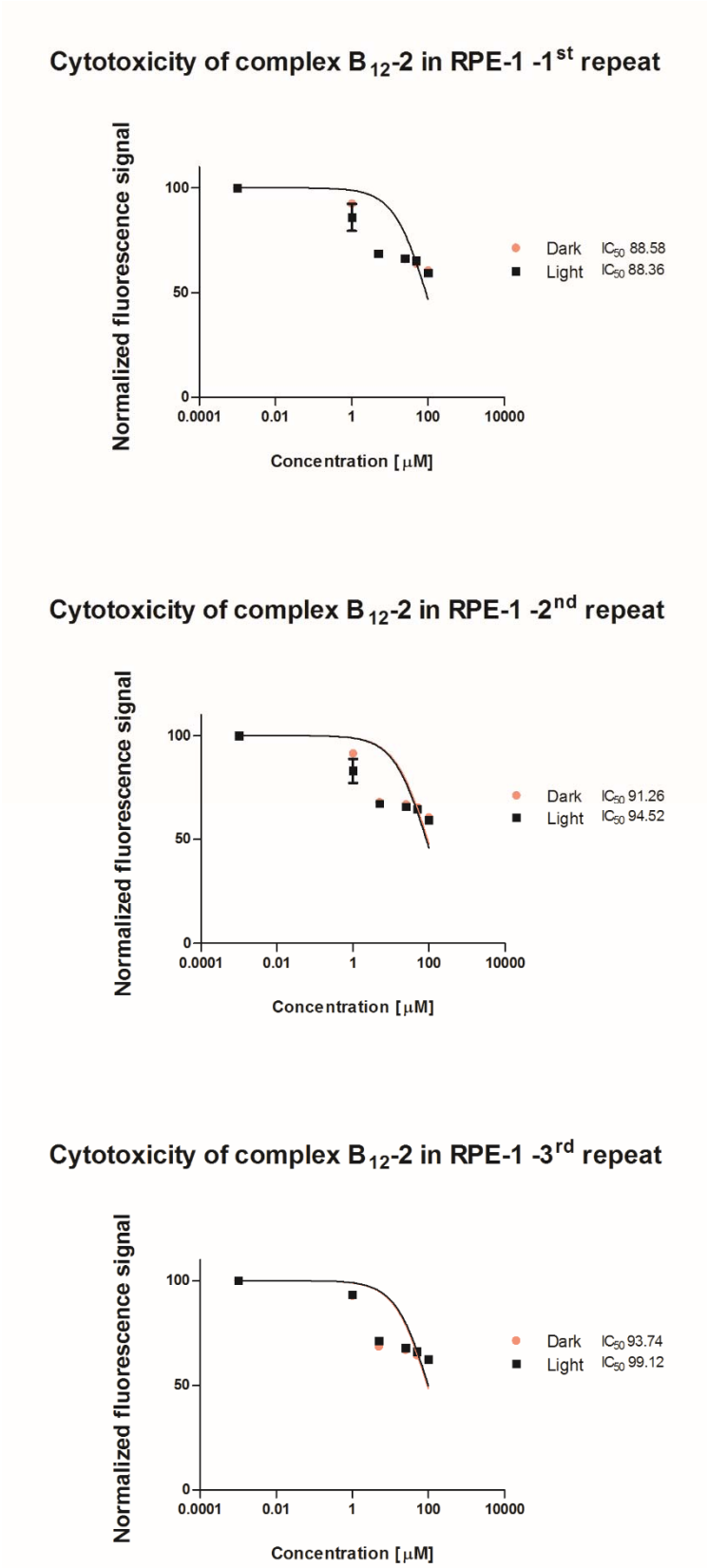

Figure S8. Cytotoxicity of complex B_{12}-2 in the RPE-1 cell line.

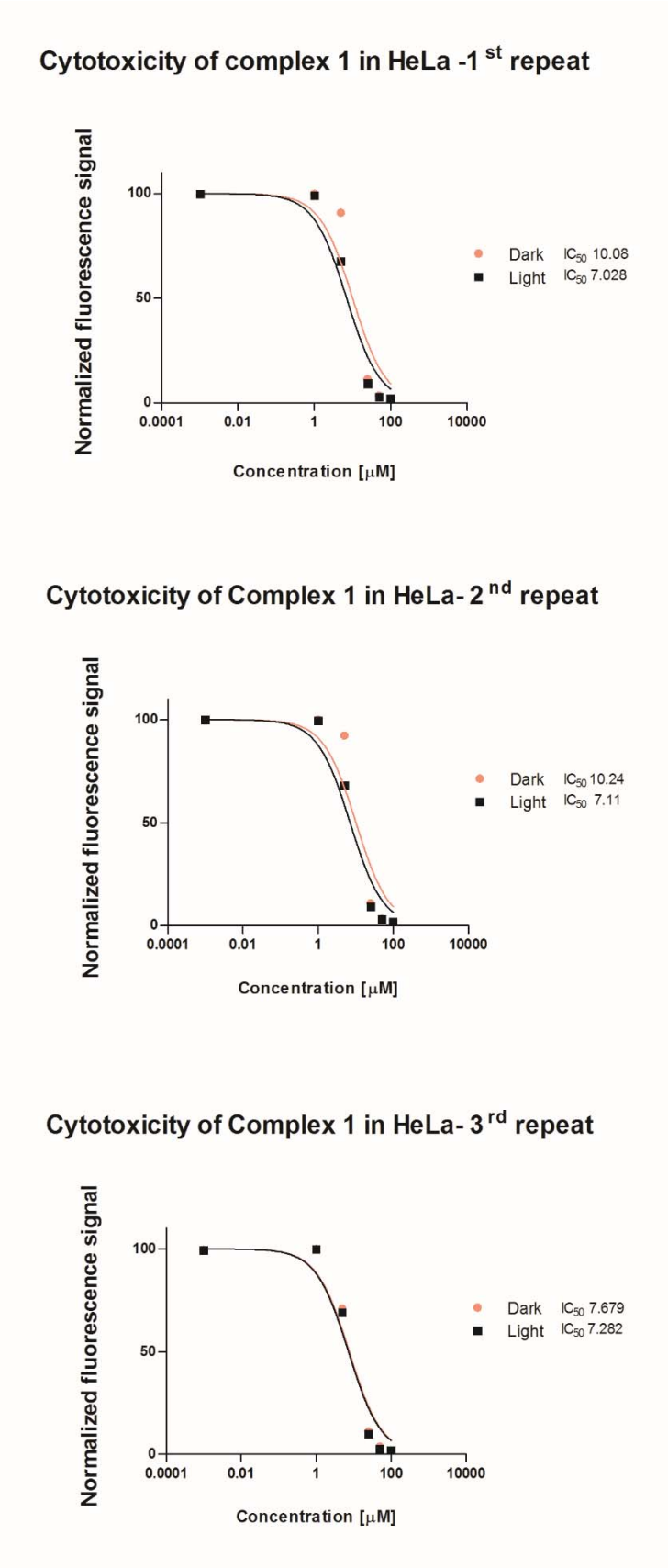

Figure S9. Cytotoxicity of complex 1 in the HeLa cell line.

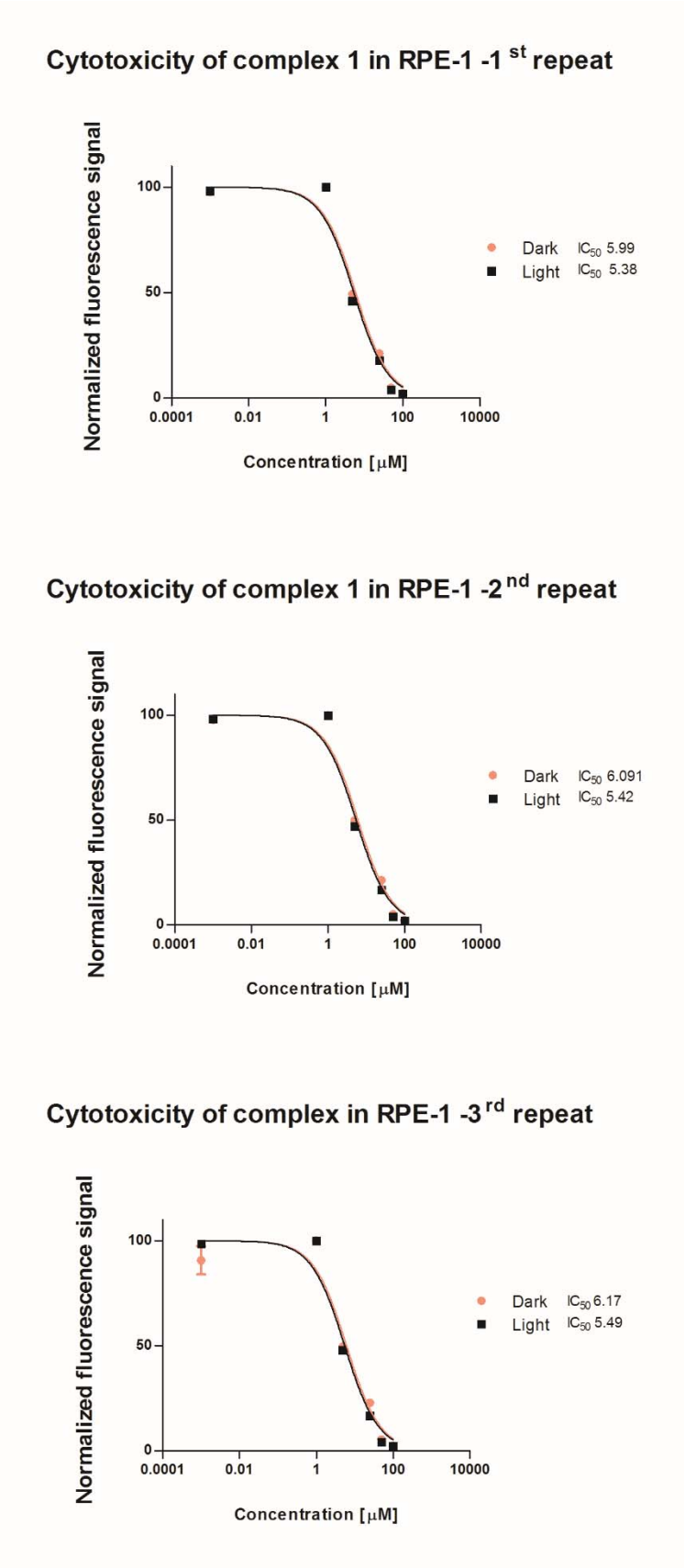

Figure S10. Cytotoxicity of complex 1 in the RPE-1 cell line.

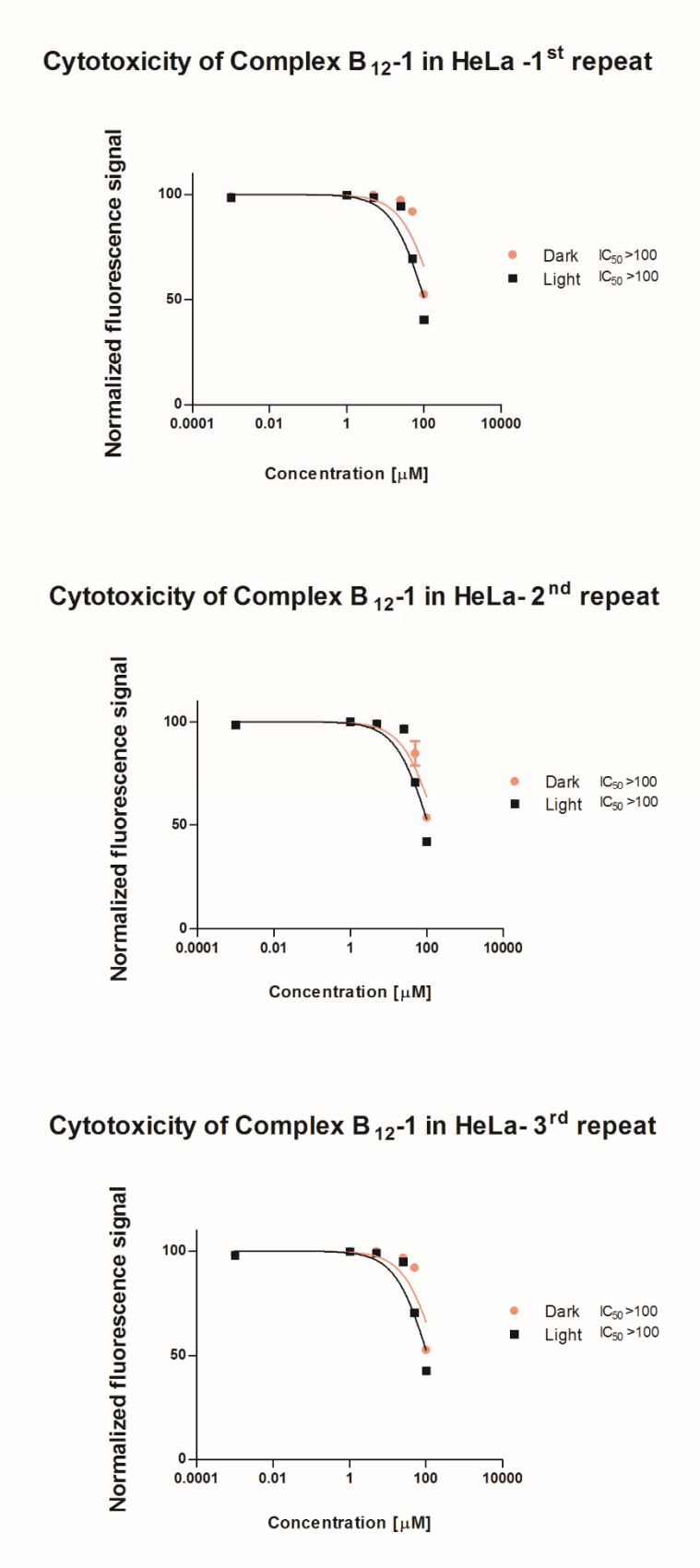

Figure S11. Cytotoxicity of complex B_{12}-1 in the HeLa cell line.

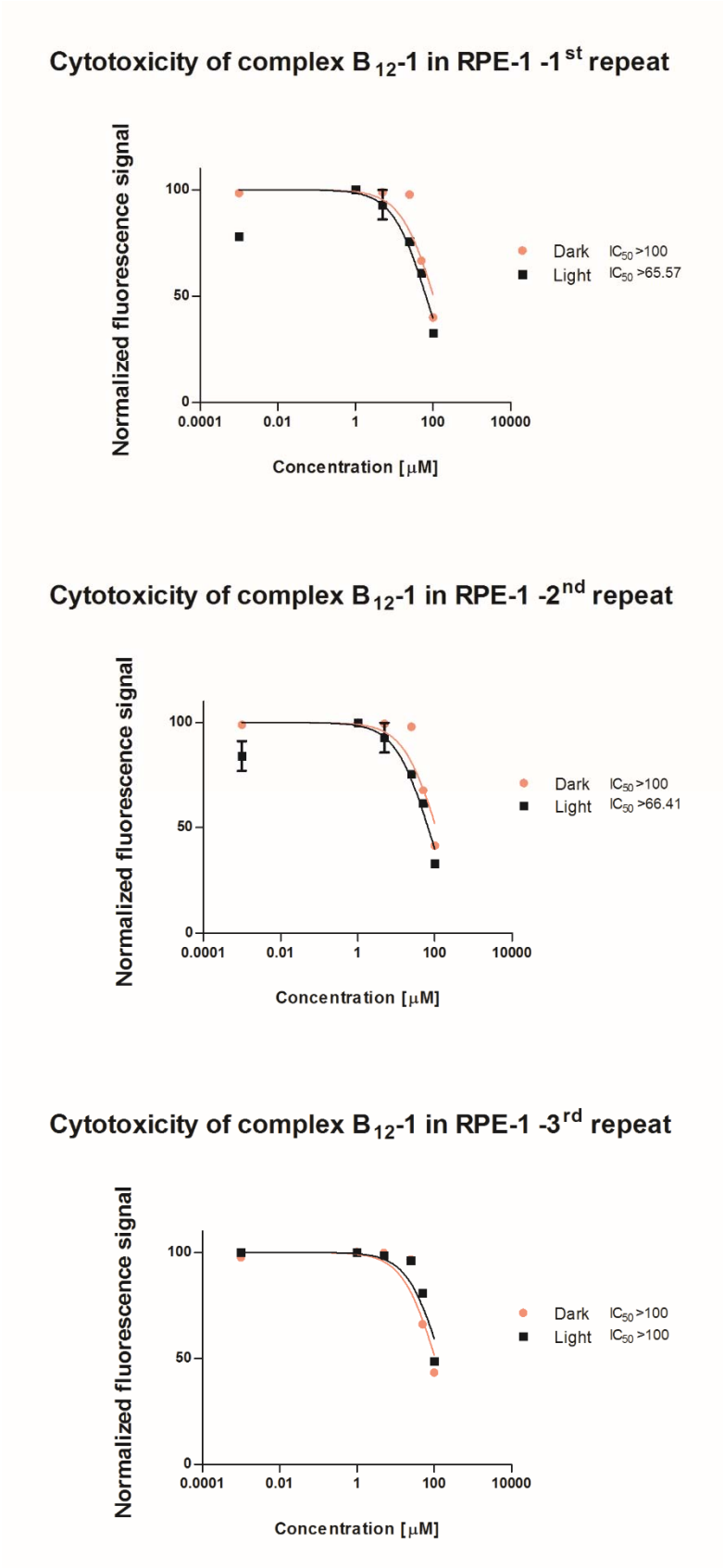

Figure S12. Cytotoxicity of complex B_{12}-1 in the RPE-1 cell line.

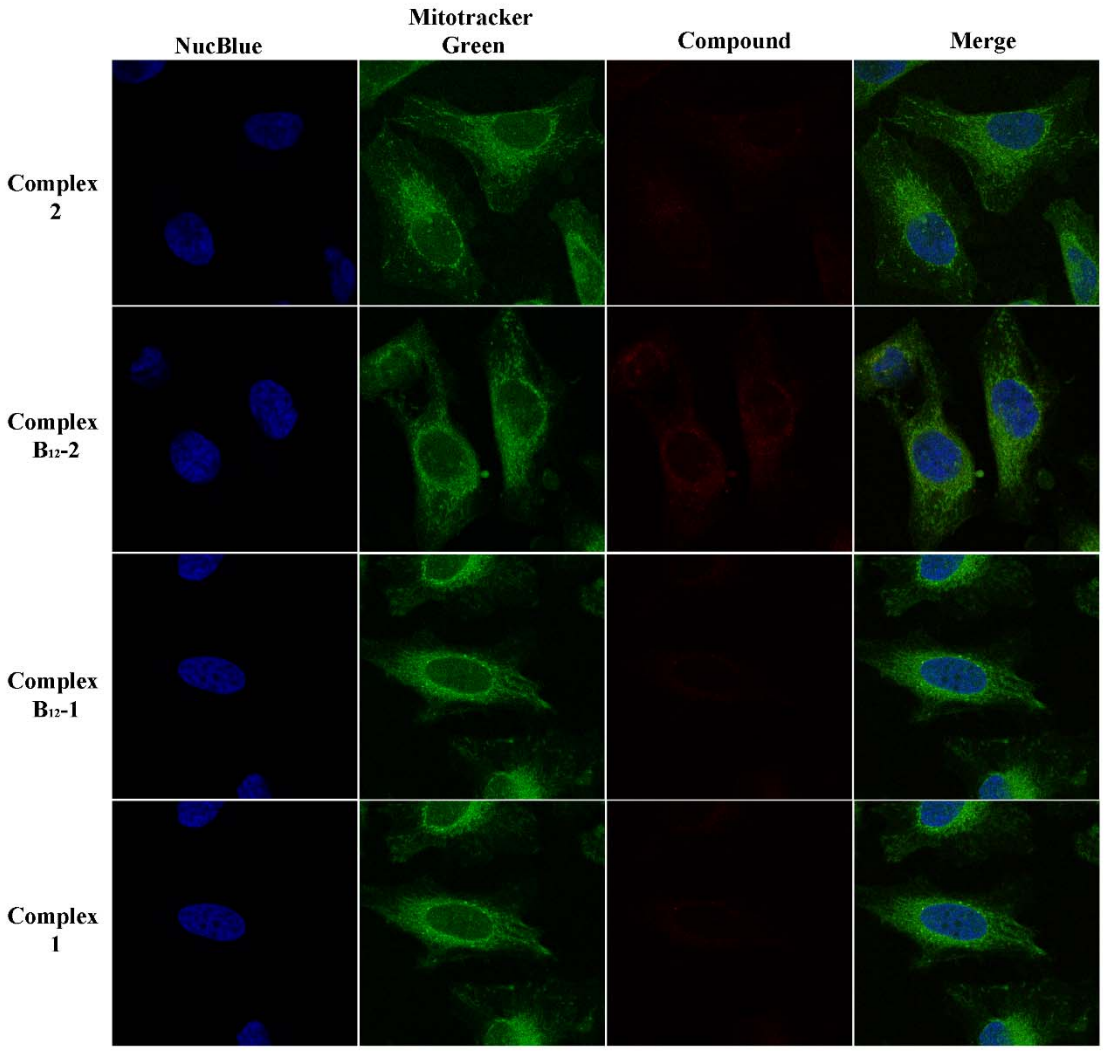

Figure S13. Cellular localisation of the complexes in HeLa cell line. Cells were treated with the compounds (IC_{50} concentration in the dark) for 2 h and co-stained with NucBlue and Mitotracker Green FM. Compounds were then removed, cells were fixed and visualised by confocal microscopy.