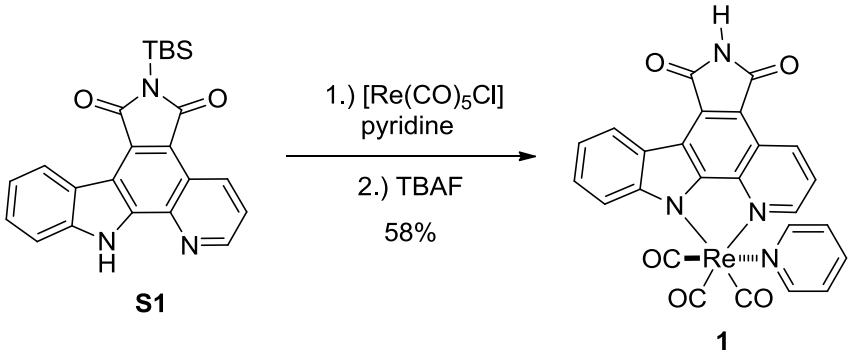
Contents of Supporting Information:

I.) Synthesis

General Methods and Materials:

Reactions were carried out using oven-dried glassware and conducted under a positive pressure of nitrogen. The pyridylindol,[1] the pyridocarbazol ligands[1,2] and complex **4**[3] were synthesized according to published procedures. Other chemicals as well as all solvents were used as received from standard suppliers or distilled prior to use. All synthesized compounds were performed in the dark to avoid light-induced side reactions and were purified by silica gel chromatography (230-400 mesh). Their high purities were confirmed by ^{1}H and ^{13}C NMR spectroscopy. NMR spectra were recorded on a DPX-250 (250 MHz), Avance 300 (300 MHz), DRX 400 (400 MHz) or Avance 500 (500 MHz) spectrometer at 298 K. Infrared spectra were recorded on a Bruker Alpha FTIR instrument. High resolution mass spectra were obtained with a Finnigan LTQ-FT instrument using either APCI or ESI.

Synthesis of Complex 1:

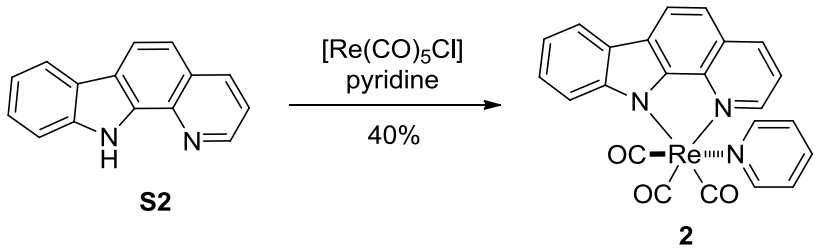


Scheme S1. Synthesis of rhenium complex **1**.

To a yellow solution of $[Re(CO)_5Cl]$ (25 mg, 69 μmol) and TBS-pyridocarbazol **S1** (25 mg, 62 μmol) in toluene (2 mL) was added pyridine (6 μL, 69 μmol). The reaction mixture was heated at 80 °C for 18 h while the color changed from yellow to red. The mixture was allowed to cool to room temperature and the solvent was evaporated. The residue was dissolved in iced CH_2Cl_2 (5 mL), TBAF (1 M in THF, 94 μL, 94 μmol) was added and the mixture was stirred at room temperature for 5 min. Afterwards the solution was cooled to 0 °C and AcOH (5 μL, 94 μmol) was added. The mixture was stirred at room temperature for another 5 min before the solvent was evaporated. The red residue was purified by silica gel chromatography with CH_2Cl_2 to obtain **1** (23 mg, 58 %) as a red solid.

^{1}H NMR (300 MHz, [D_6]-DMSO): δ = 11.20 (s, 1H), 9.56 (dd, *J* = 5.0, 1.2 Hz, 1H), 9.30 (dd, *J* = 8.4, 1.2 Hz, 1H), 8.75 (d, *J* = 7.8 Hz, 1H), 8.33-8.29 (m, 2H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.99 (dd, *J* = 8.5, 5.0 Hz, 1H), 7.82-7.69 (m, 2H), 7.43 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.30-7.24 (m, 2H) ppm. ^{13}C NMR (100 MHz, [D_6]-DMSO): δ = 197.3, 196.8, 193.7, 170.7, 170.2, 162.3, 153.4, 152.6, 151.7, 150.7, 141.2, 139.7, 135.9, 130.9, 127.3, 126.5, 124.8, 124.4, 123.4, 120.9, 120.2, 115.2, 114.4 ppm. IR (film): $\tilde{\nu}$ = 3210, 3059, 2928, 2020, 1978, 1901, 1753, 1700, 1591, 1526, 1488, 1417, 1341, 1229, 1135, 1015, 796, 746, 702, 641, 490 cm^{-1}. HRMS (APCI): calcd. for $C_{25}H_{14}N_4O_5Re^+$ $(M + H)^+$ 637.0516; found 637.0517.

Synthesis of Complex 2:

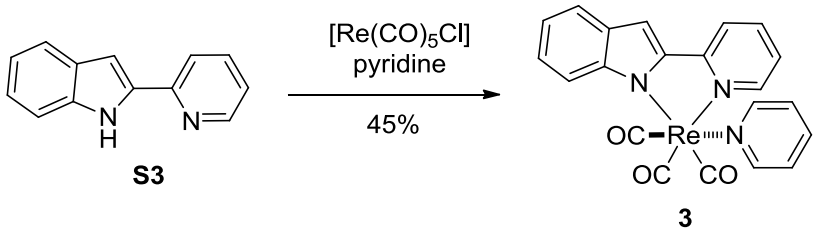


Scheme S2. Synthesis of rhenium complex **2**.

To a yellowish solution of $[Re(CO)_5Cl]$ (61 mg, 166 µmol) and pyridocarbazol **S2** (33 mg, 151 µmol) in toluene (3 mL) was added pyridine (18 µL, 227 µmol). The reaction mixture was heated at 60 °C for 13 h and at 80 °C for 4 h while the color changed from yellow to orange. Afterwards the mixture was allowed to cool to room temperature and the solvent was evaporated. The orange residue was purified by silica gel chromatography with CH_2Cl_2 to obtain **2** (34 mg, 40 %) as an orange solid.

^{1}H NMR (300 MHz, $CDCl_3$): δ = 9.13 (dd, *J* = 5.0, 1.2 Hz, 1H), 8.40 (dd, *J* = 8.3, 1.1 Hz, 1H), 8.28-8.20 (m, 4H), 8.10 (d, *J* = 8.3 Hz, 1H), 7.59 (ddd, *J* = 8.2, 7.6, 1.3 Hz, 1H), 7.52-7.45 (m, 2H), 7.35-7.27 (m, 2H), 6.98-6.92 (m, 2H) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 198.8, 197.9, 193.9, 152.2, 150.5, 149.3, 148.2, 142.0, 138.1, 138.0, 126.5, 125.6, 125.5, 125.2, 123.3, 122.4, 120.7, 120.5, 118.1, 115.7, 113.5 ppm. IR (film): $\tilde{\nu}$ = 2921, 2362, 2335, 2015, 1887, 1631, 1511, 1482, 1445, 1375, 1326, 1262, 1234, 1070, 1017, 942, 820, 798, 744, 691, 650, 597, 483, 429 cm^{-1}. HRMS (APCI): calcd. for $C_{23}H_{14}N_3O_3ReNa^+$ $(M + Na)^+$ 590.0486; found 590.0486.

Synthesis of Complex 3:



Scheme S3. Synthesis of rhenium complex **3**.

To a solution of $[Re(CO)_5Cl]$ (16 mg, 45 μmol) and pyridylindol **S3** (8 mg, 41 μmol) in toluene (2 mL) was added pyridine (5 μL, 62 μmol). The reaction mixture was heated at 60 °C for 14 h and at 80 °C for 5 h while the color changed from colorless to yellow/brown. Afterwards the mixture was allowed to cool to room temperature and the solvent was evaporated. The yellow residue was purified by silica gel chromatography with CH_2Cl_2 to obtain **3** (10 mg, 45 %) as a yellow solid.

^{1}H NMR (300 MHz, C_6D_6): δ = 8.42 (dq, *J* = 8.4, 0.8 Hz, 1H), 8.38 (dq, *J* = 5.7, 0.8 Hz, 1H), 7.93-7.86 (m, 3H), 7.45 (ddd, *J* = 7.9, 6.9, 1.2 Hz, 1H), 7.25 (ddd, *J* = 7.8, 7.0, 1.0 Hz, 1H), 6.99 (d, *J* = 0.9 Hz, 1H), 6.96 (dt, *J* = 9.2, 1.2 Hz, 1H), 6.59 (ddd, *J* = 8.2, 7.4, 1.6 Hz, 1H), 6.20 (tt, *J* = 7.8, 1.6 Hz, 1H), 6.01 (ddd, *J* = 7.3, 5.7, 1.4 Hz, 1H), 5.76-5.70 (m, 2H) ppm. ^{13}C NMR (75 MHz, C_6D_6): δ = 158.5, 151.8, 151.2, 148.9, 146.8, 137.7, 137.2, 132.4, 125.0, 124.0, 121.9, 120.9, 120.2, 119.8, 117.1, 103.7 ppm. IR (film): $\tilde{\nu}$ = 2012, 1885, 1607, 1534, 1486, 1448, 1355, 1311, 1255, 1218, 1153, 1119, 1071, 1014, 754, 696, 489 cm^{-1}. HRMS (ESI): calcd. for $C_{21}H_{14}N_3O_3Re^+$ $(M)^+$ 543.0588; found 543.0565.

II.) Proof of Purity

Complex 1:

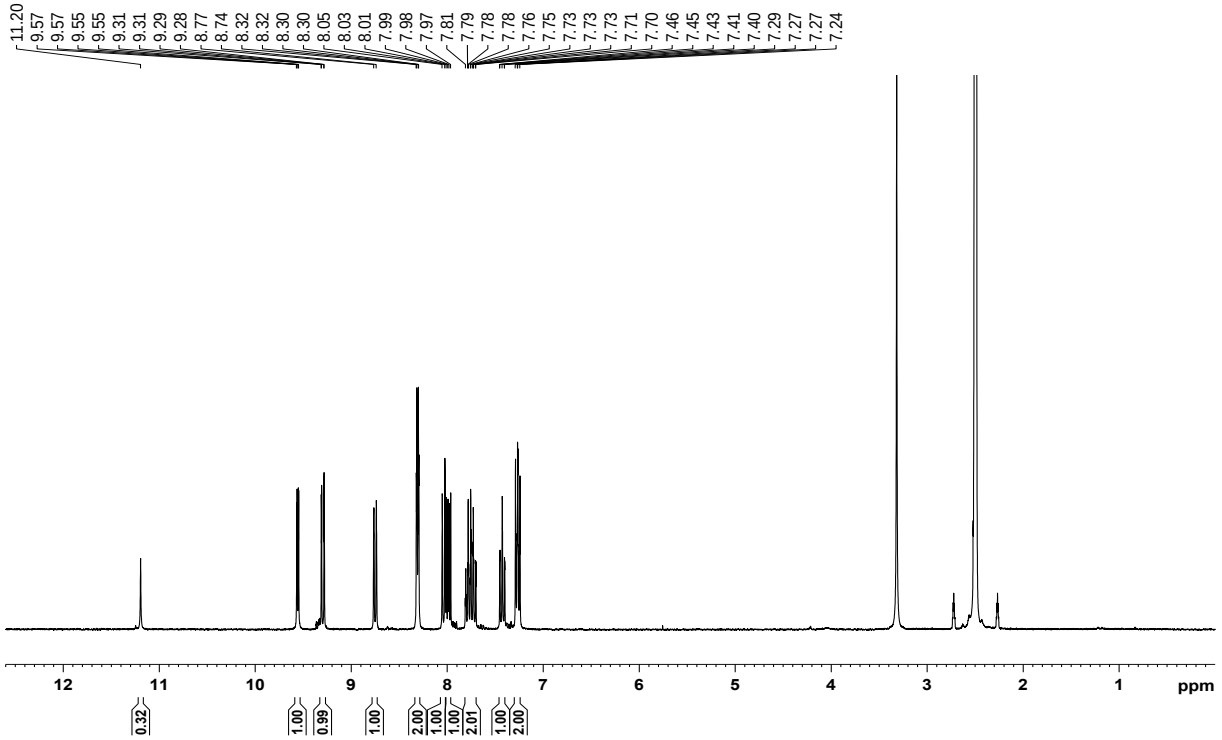


Figure S1. ^{1}H NMR of complex **1** (300 MHz, [D_6]-DMSO).

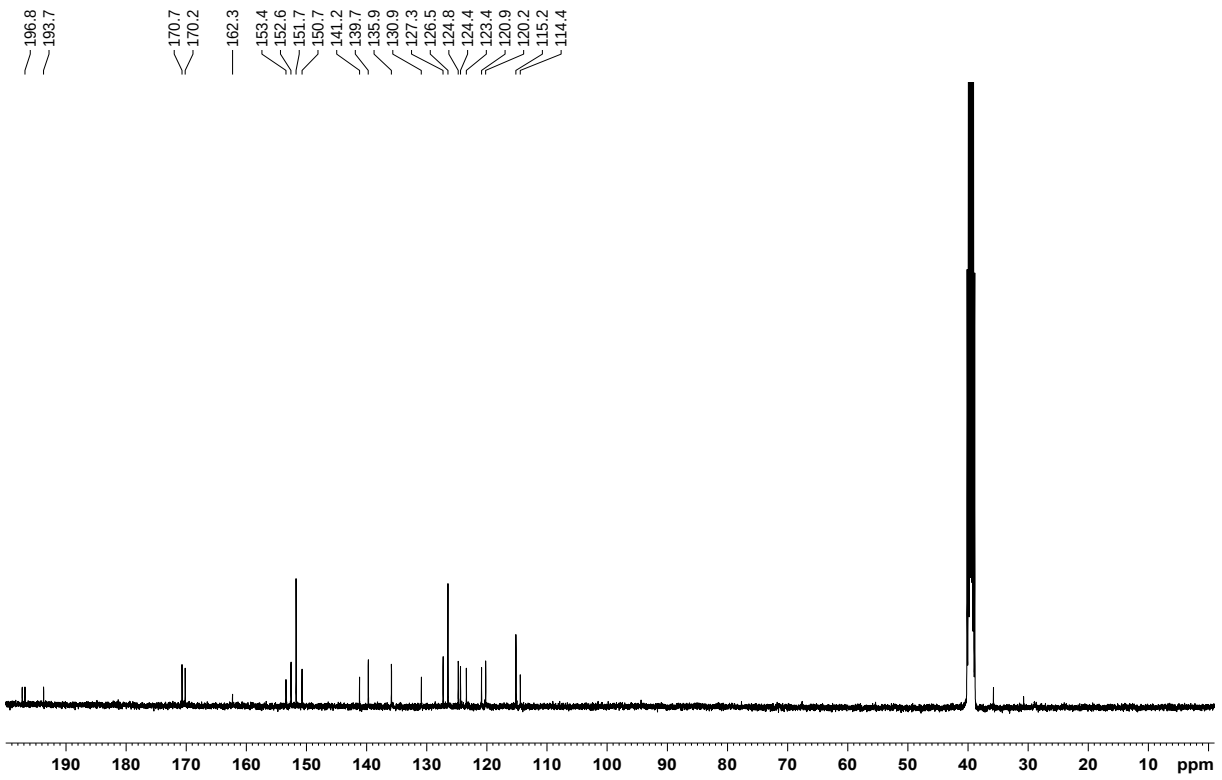


Figure S2. ^{13}C NMR of complex **1** (100 MHz, [D_6]-DMSO).

Complex 2:

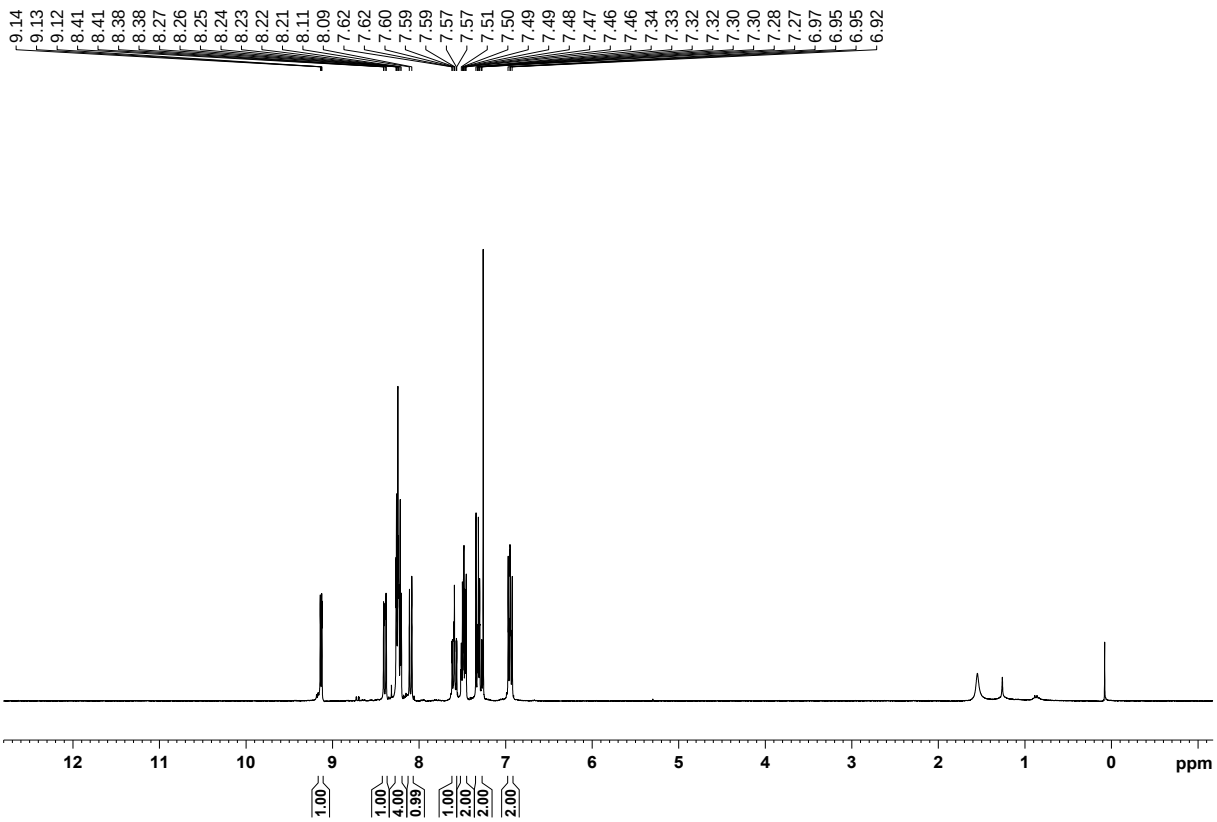


Figure S3. ^{1}H NMR of complex **2** (300 MHz, $CDCl_3$).

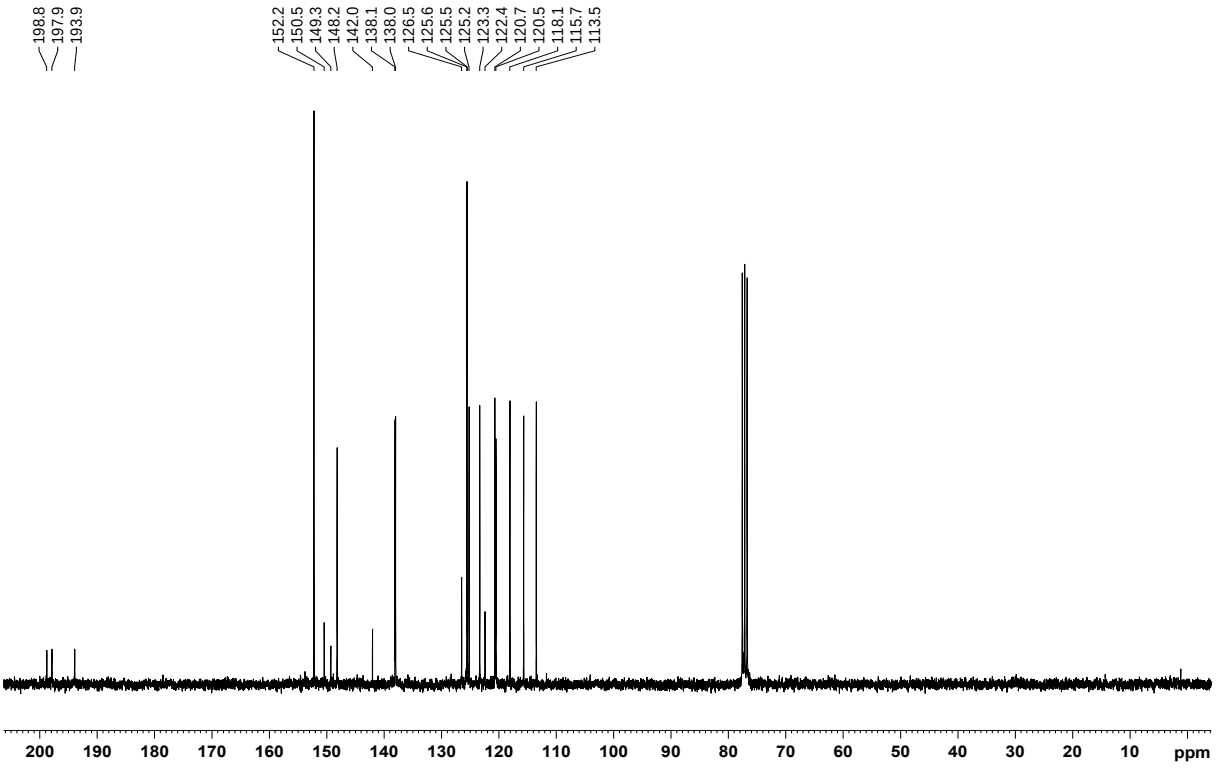


Figure S4. ^{13}C NMR of complex **2** (75 MHz, $CDCl_3$).

Complex 3:

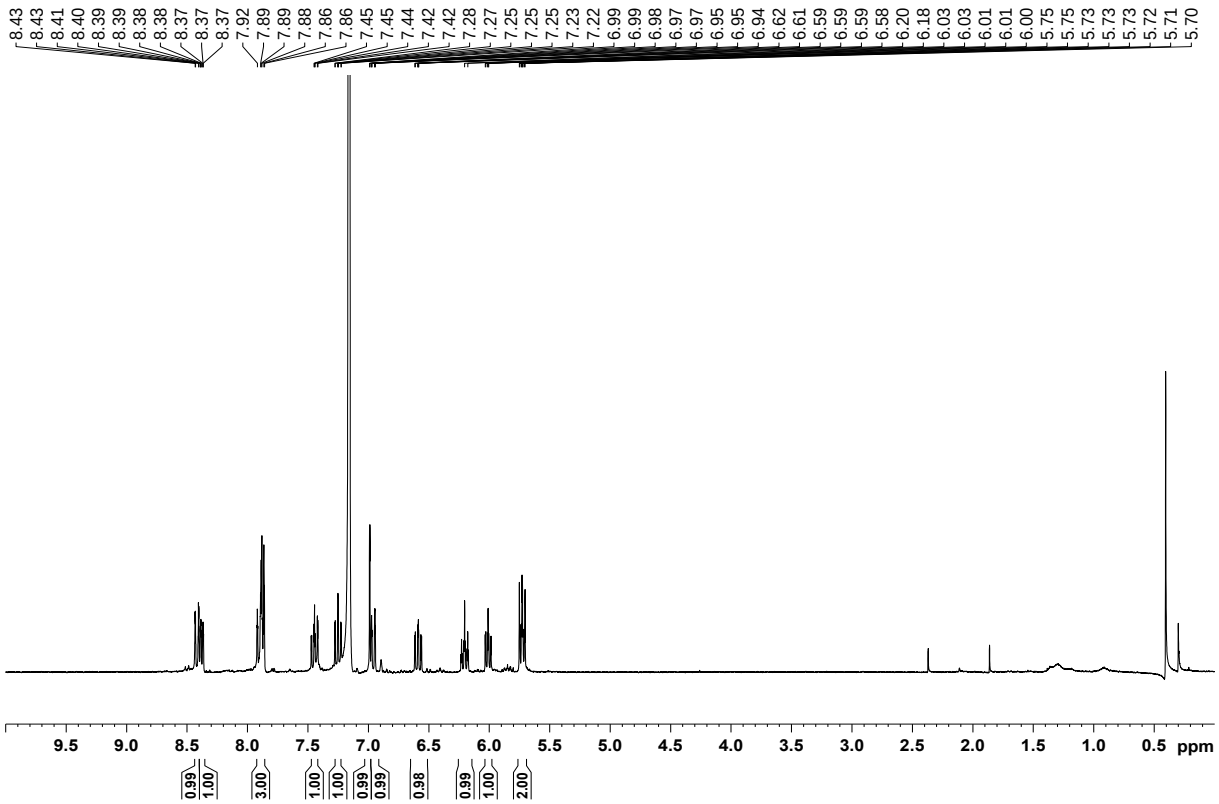


Figure S5. ^{1}H NMR of complex **3** (300 MHz, C_6D_6).

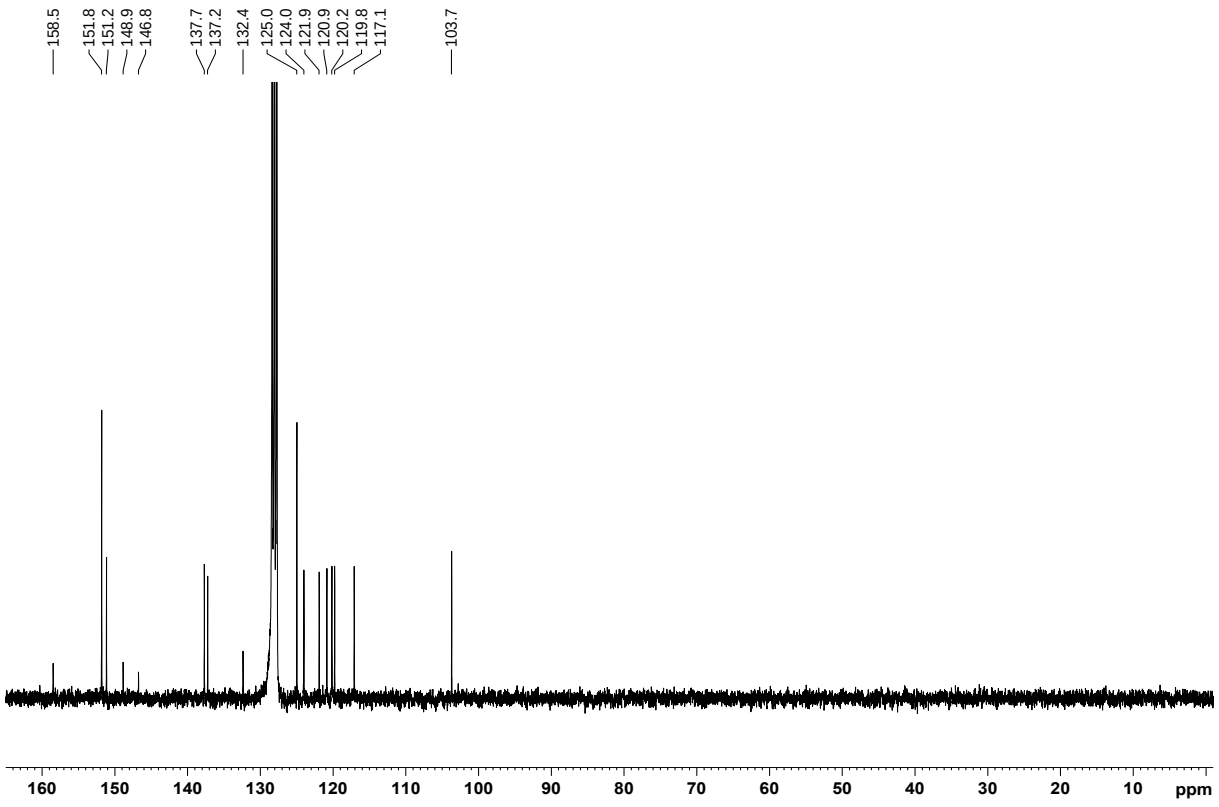


Figure S6. ^{13}C NMR of complex **3** (75 MHz, C_6D_6).

III.) Stability Test of Complex 1

A stock solution of **1** (5 mM) in DMSO-d_6/D_2O (9:1, 0.7 mL) was prepared and 2-mercaptoethanol (5 mM) was added. ^{1}H NMR spectra were measured at the beginning and after 69 h. Figure S7 shows no change in the spectra after this period of time.

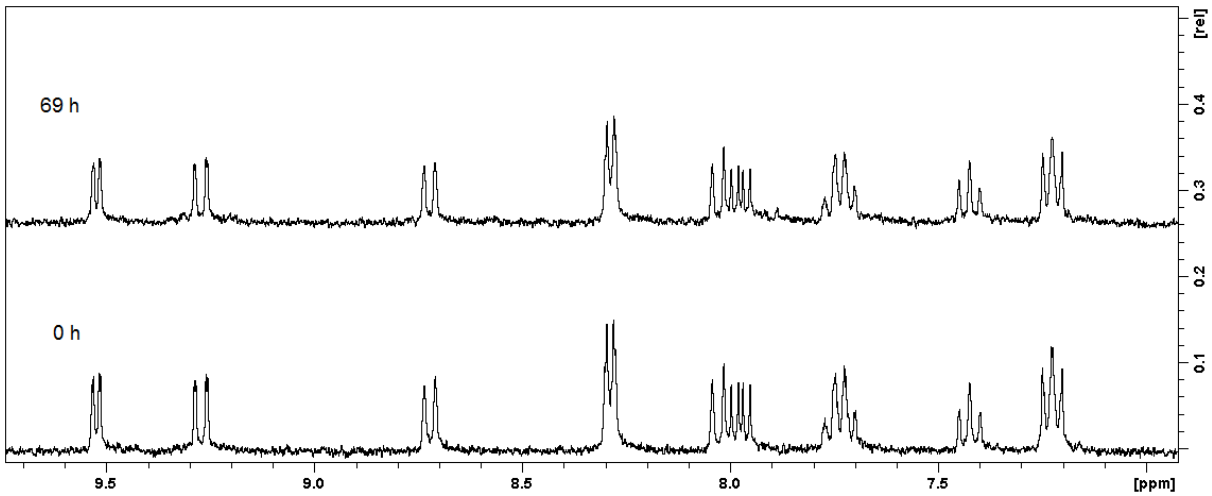


Figure S7. Stability test of complex **1** in addition of 2-mercaptoethanol in DMSO-d_6/D_2O (9:1).

To gain insight into the stability of complex **1** during irradiation, a stock solution was prepared including the addition of a monodentate ligand which can replace the pyridine ligand. ^{1}H NMR spectra were measured at the beginning and after 4 h of irradiation with light of a transmission range of $\lambda \geq 505$ nm. As a control, the same experiment was conducted in the dark. Accordingly, a 4 mM stock of complex **1** in $CDCl_3$ (0.7 mL) was prepared and 4-dimethylaminopyridine (5.0 eq) was added. After 4 h of irradiation, a second set of signals (8 %) in the aromatic region of the spectrum occurred which belongs to the complex where the pyridine ligand is replaced by 4-dimethylaminopyridine. Without irradiation there is no exchange.

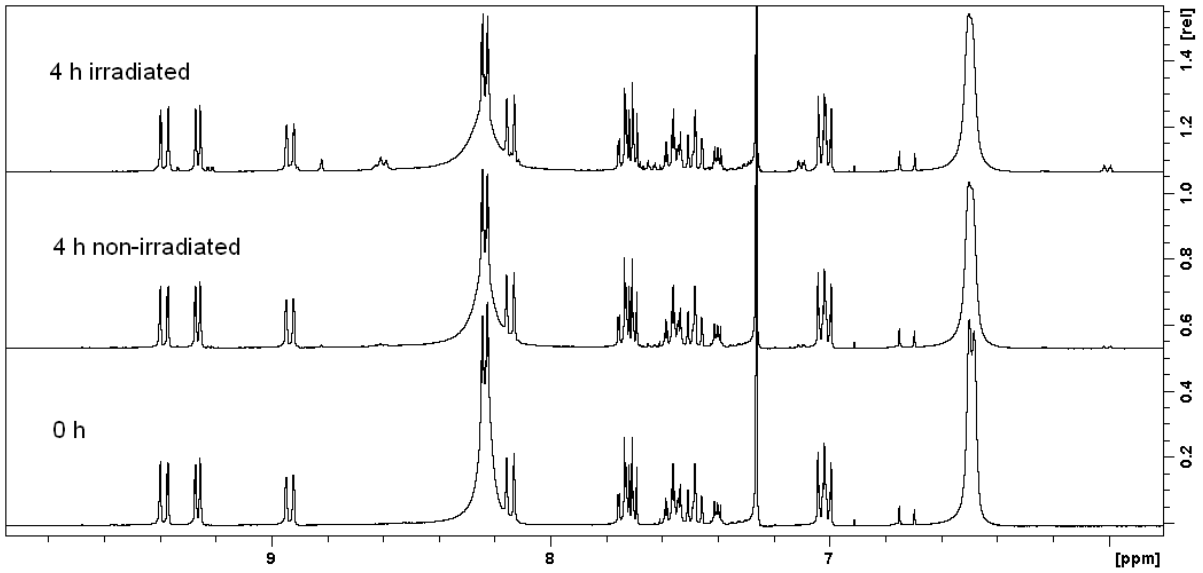


Figure S8. Stability test of complex **1** in the dark and after 4 h irradiation.

IV.) Single Crystal X-Ray Diffraction Study

Single crystals of complex the *N*-benzylated derivative of complex **1 (1Bn**) were obtained upon slow diffusion of hexane into dichloromethane at 6 °C. The intensity data were collected at 100 K using a STOE IPDS-2T system. The data were corrected for absorption effects using indexed faces.[4] The structure was solved using direct methods (SIR-92)[5] and refined using the full matrix least squares procedure implemented in SHELX-97[6] as a pseudo merohedral twin. Hydrogen atoms were included at calculated positions.

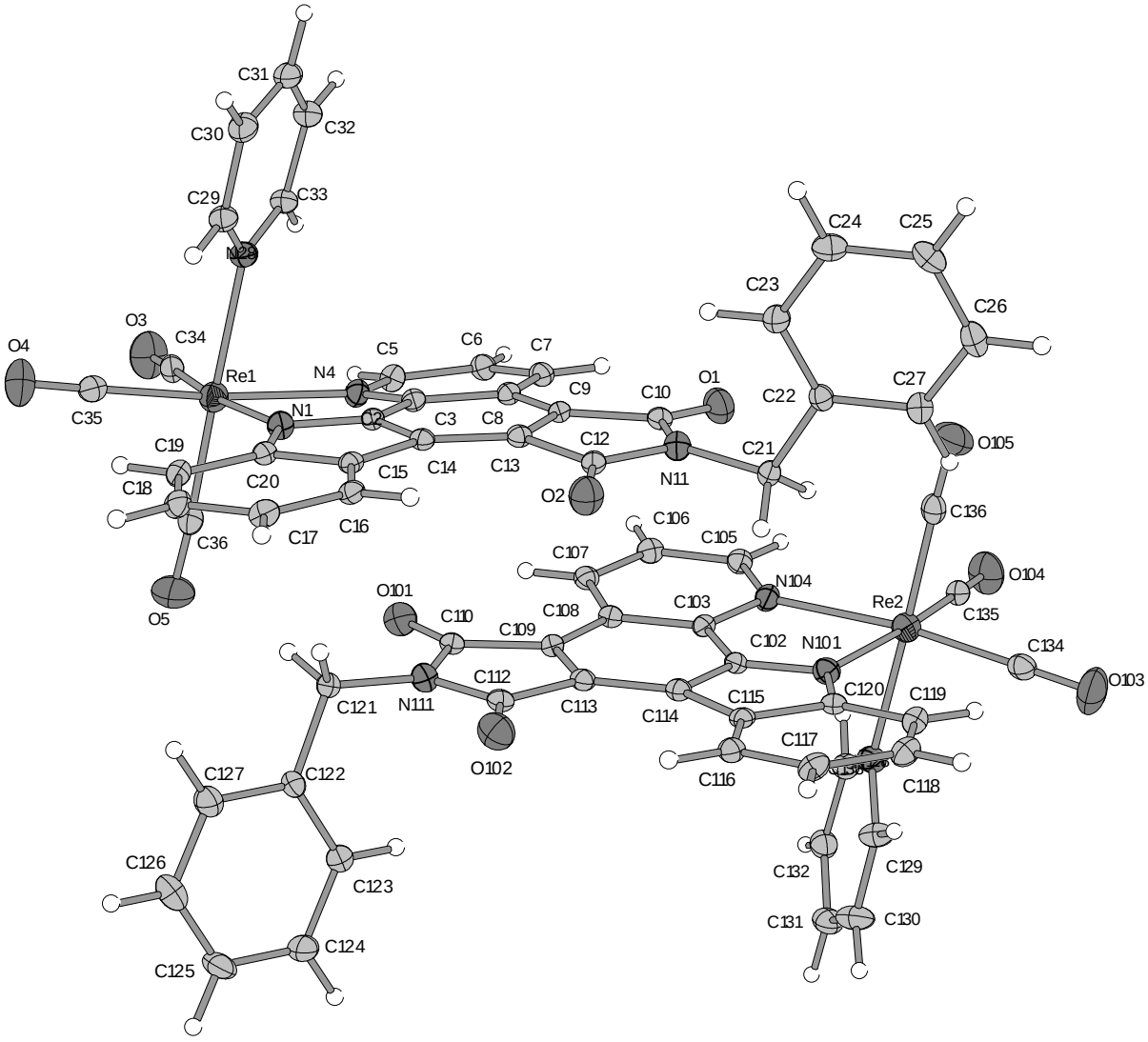


Figure S9. Crystal structure of the *N*-benzylated derivative of Re complex **1** (**1Bn**). ORTEP drawing with 50 % probability thermal ellipsoids. Solvent is omitted for clarity.

Table S1. Crystallographic data of complex **1Bn**.[a]

	1Bn
formula	$C_{70}H_{52}N_8O_{10}Re_2$
fw	1537.60
a(Å)	10.6952(3)
b(Å)	28.9047(5)
c(Å)	19.2699(5)
α(°)	90
β(°)	90.025(2)
γ(°)	90
V($Å^3$)	5957.1(2)
Z	4
space group	P 2_1/c
d_{calcd}(Mg/m^3)	1.714
μ(mm^{-1})	4.131
Θ range(°)	4.58 – 26.76
no.of indep. reflections	12563
no.of parameters	814
wR2 (all data)[b]	0.0664
R1 (I > 2σ(I))[b]	0.0282
CCDC no.[c]	899227

[a]MoKα radiation (λ = 0.71073 Å). [b]$R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2=[w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$. [c]Crystallographic data (excluding structure factors) have been deposited in the Cambridge Crystallographic Data Center. CIF files can be obtained from the CCDC free of charge via http://www.ccdc.cam.ac.uk/data_request/cif.

V.) Photochemical Properties of Complexes 1-4

Absorption Spectra

Absorption Spectra for the complexes **1**-**4** were determined at a concentration of 60 μM in DMSO using a DU®800 Spectrophotometer (Beckman Coulter).

Singlet Oxygen Determination

The $^1O_2$ production of the compounds was determined using a method based on the work of Kraljić *et al.*[7] Accordingly, *p*-nitrosodimethylaniline (RNO) and imidazole were dissolved in PBS buffer at a concentration of 500 μM for RNO and 80 mM for imidazole. Compounds **1**-**4** were used as 1 mM DMSO stock solutions. 10 μL RNO, 10 μL imidazole, 5 μL of the complexes (with a final concentration of 50 μM) and 75 μL PBS buffer/DMSO (1:1.5) were pipetted in a 96-well plate. To test the $^1O_2$ production by the influence of light, the absorption maximum of RNO at 440 nm was determined before and after 30 min irradiation. As irradiation source served a Hg/Xe arc lamp from Newport at $\lambda \geq 330$ nm, $\lambda \geq 415$ nm and $\lambda \geq 505$ nm. As a control, all complexes were measured in the dark. All measurements were performed twice and in triplicate. The $^1O_2$ production was determined as the negative difference of absorbance before and after irradiation.

VI.) Biological Experiments

Irradiation Setup:

Irradiation was performed with two different light sources in this study. The first was is a 200 W mercury/xenon arc lamp from Newport which has the option to use different sorting filters with distinct lower transmission borders at 330, 415 and 505 nm to determine the light transmission range. Furthermore the light was filtered through 4 cm of water to remove infrared radiation. With this setup the irradiance of the lamp is 52.8 mW/cm^2 for the 330 nm filter, 33.8 mW/cm^2 for the 415 nm filter and 29.2 mW/cm^2 for the 505 nm filter, determined by a photodiode (Hamamatsu, Si-photodiode) in combination with an amperemeter. The second light source was a 7 W LED reflector (Megaman® PAR16 GU10 LR0707-SP), which was used to irradiate the cells in case the arc lamp was too bulky to be used. The reflector was placed 8 cm above the cells for all experiments except of the 3D-culture tests, where it was fixed in 23 cm distance. For this setup, a maximum irradiance of 45.8 mW/cm^2 was calculated.

Cell Culture:

Cells used in this study were HeLa human cervical cancer cells. They were cultured in Dulbecco´s Modified Eagle´s Medium (DMEM) containing 10 % fetal bovine serum (FBS), 2 mM L-glutamine, 100 Units/mL penicillin and 100 μg/mL streptomycin. Cells were maintained in 75 cm^2 flasks in a 5 % CO_2-humidified atmosphere at 37 °C. Passage takes place every 2-3 days. All cell culture ingredients were purchased from Sigma-Aldrich.

Photodynamic Treatment:

To investigate photoinduced cytotoxicity of the different organometallic complexes, cells were seeded at equal concentrations into 96-well microtiter plates in a number of 9 x 10^3 cells per well. After overnight cell attachment the designated metal compound was added. A 10 mM

stock solution in DMSO was diluted with culture medium to the desired concentration regarding the point that the final DMSO concentration present to the cells is unchanging at 1 %. The complex treated cells were incubated for 1 h in the dark before irradiation took place with a 200 W mercury/xenon arc lamp. Different light transmission ranges for irradiation were achieved by sorting filters. The irradiation time was chosen between 15 and 60 min to guarantee a survival of 80 % for irradiated cells without any further treatment, considering the cells different sensitivity to the variable energy of the light. Following irradiation, cells were maintained under normal culture conditions. Cell viability was measured 24 h after complex administration by MTT-Assay.

Cell Viability Assays:

The toxicity of the photoactivated compounds was determined using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) cell viability assay. MTT is a yellow compound that when reduced by functioning mitochondria, produces purple formazan crystals that can be measured spectrophotometrically. For this purpose, the MTT (Sigma-Aldrich) was dissolved in phosphate buffered saline (PBS) to a concentration of 5 mg/mL and further diluted in culture medium (1:11). Cells were incubated with this MTT-solution for 3 h under normal culture conditions. Afterwards 155 μL of the solution were rejected and 90 μL of DMSO were added. To completely dissolve the formazan salts, plates were incubated for 10 min on a shaker and afterwards quantified by measuring the absorbance at 535 nm with a Spectramax M5 microplate reader (Molecular Devices). The cell viability was calculated as percentage of surviving cells compared to untreated and non-irradiated control cells.

Effect of Irradiation on Cultured Cells:

HeLa cells were cultured in 96-well plates as described earlier. After 24 h of incubation they were exposed to light cut-on at different wavelength to examine the effect on cell survival of light only. The irradiation time was chosen as 15 min for $\lambda \geq 330$ nm, 60 min for $\lambda \geq 415$ nm

and 75 min for λ ≥ 505 nm. Cell survival was determined 24 h after irradiation by the MTT assay. The results indicated that there is no large effect on cell survival due to the irradiation conditions chosen in this study.

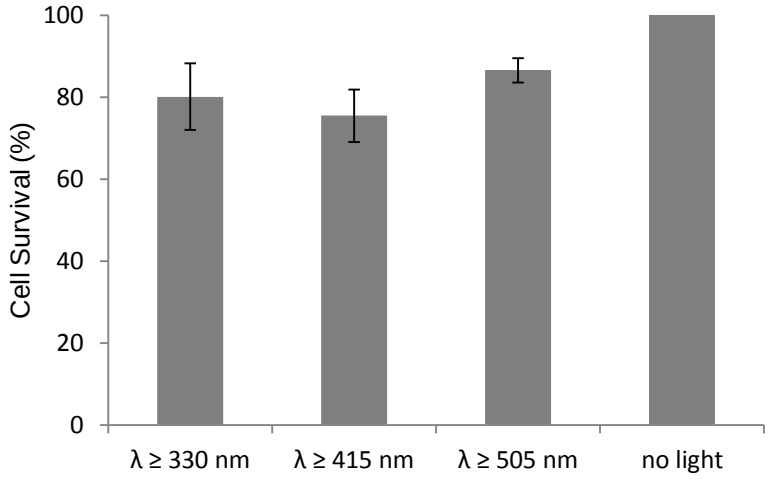


Figure S10. Effect of irradiation on HeLa cells exposed to light of a mercury/xenon arc lamp. The different transmission wavelengths were adjusted by sorting filters. Irradiation time was 15 min for λ ≥ 330 nm, 60 min for λ ≥ 415 nm and 75 min for λ ≥ 505 nm. Results are average values of at least four independent measurements.

Photoinduced Cytotoxicity of Complex 1 after Medium Exchange:

In order to investigate the contribution of intracellular compound **1** on the photoactivated cytotoxic effect, the culture medium with the dissolved complex **1** (1 μM) was removed after 1 h of incubation and replaced by fresh medium. Subsequently, the cells were irradiated with light (λ ≥ 505 nm) for 1 h. As a result, the EC_{50} value increased only slightly from 0.12 ± 0.03 μM to 0.18 ± 0.02 μM after this additional medium exchange, indicating that the extracellular amount of the complex has an negligible effect on the photocytotoxicity.

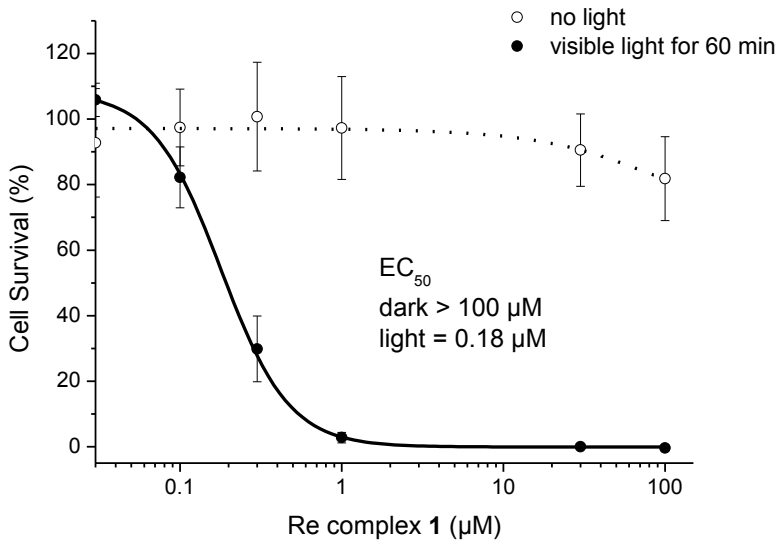


Figure S11. EC_{50} value of Re complex **1** after an additional medium exchange before irradiation.

Caspase 3/7 Activity:

Measuring the activity of caspases is a current approach to detect apoptosis in cell culture. In this study, the activity of the caspases 3 and 7 was determined using the Apo-ONE® Homogeneous Caspase-3/7 Assay Kit (Promega). HeLa cells were seeded into black 96-well microtiter plates (1.8×10^4 cells per well) and maintained under normal culture conditions for 24 h. Afterwards they were exposed to photodynamic treatment with 1 µM of complex **1** as already described ($\lambda \geq 505$ nm, 30 min). 5 h after irradiation, lysis buffer and the precursor of the fluorescent dye (Z-DEVD-R110) were added according to the manufacturer´s instructions in a 100:1 mixture. After an incubation of 1 h on a plate shaker and an additional incubation for 8 h in the dark, fluorescence was measured using a microplate reader (Spectramax M5, Molecular Devices) (Ex 485 nm; Em 538 nm). In the presence of active caspases 3 and 7 the protecting peptides (DEVD) of the non-fluorescent precursor are cleaved releasing the fluorescent leaving group rhodamine 110. The resulting fluorescence signal is proportional to the caspase activity.

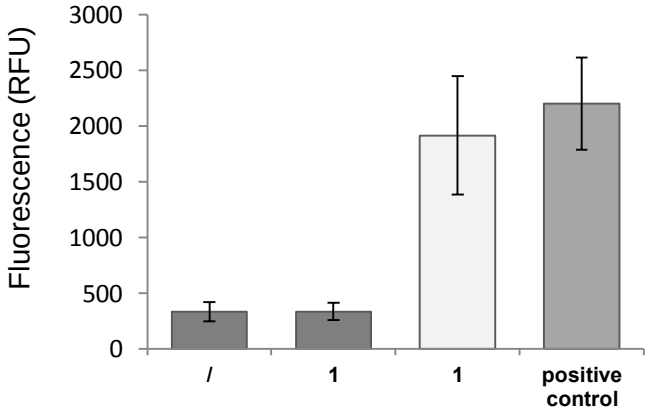


Figure S12. Caspase 3 and 7 activity in HeLa cells treated with either DMSO (negative control), complex **1** or 1 μM staurosporine (positive control) in the presence (light grey) or absence (dark grey) of visible light. Results are average values of four independent measurements.

Propidium Iodide Staining and Flow Cytometry:

Apoptosis and cell cycle progression were observed through propidium iodide (PI)-staining of HeLa cells and following flow cytometry. Cells were plated in twelve-well plates (6 x 10^4 cells per well) with DMEM medium (Sigma-Aldrich) and incubated for 24 h. Afterwards, cells were treated with 1 μM of rhenium complex **1** and irradiated with a mercury/xenon arc lamp ($\lambda \geq 505$ nm) for 1 h. 22 hours later, floating and attached cells were harvested, centrifuged, and resuspended in a hypotonic solution containing 0.1 % sodium citrate, 0.1 % Triton X-100, and 50 μg/mL propidium iodide. Cells were incubated with PI solution for at least 1 h on ice before analyzing them with Attune acoustic focusing cytometer (Applied Biosystems, Carlsbad, USA).

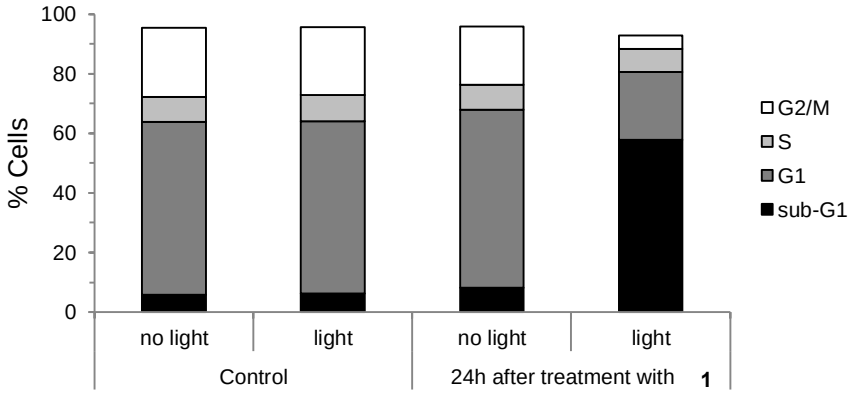


Figure S13. Cell cycle analysis of HeLa cells 24 h after photodynamic treatment with 1 μM of rhenium complex **1**. Cells were incubated for 1 h with the complex, before irradiated for an additional hour at $\lambda \geq 505$ nm. 24 h after compound addition cells were harvested and stained with propidium iodide for flow cytometric analysis.

Fluorescence Staining:

For fluorescence microscope studies, HeLa cells were seeded on eight-well μ-slides (Ibidi) (10^4 cells in 300 μl culture medium per well) and grown overnight. Afterwards, cells were incubated with 1 μM of complex **1** contained in complete culture medium. The treated cells were incubated for 1 h in the dark before irradiated for 15 min with a LED reflector (Megaman® PAR16 GU10 LR0707-SP). Directly after light exposure, the cells were washed once with Hank´s Balanced Salt Solution (HBSS) (Sigma-Aldrich) and stained with the plasma membrane located fluorescent dye wheat germ agglutinin (WGA, tetramethylrhodamine conjugate) (Invitrogen) and the chromatin targeted 4',6-diamidino-2-phenylindole (DAPI) (Invitrogen) for 25 and 5 min respectively. Thereafter cells were washed again with HBSS and kept in the same buffer for microscopic imaging. Fluorescence microscopic measurements were performed by a laser scan microscope (inverted microscope Axiovert 200 M, scanmodule LSM 510 META, objective Plan-Apochromat 63x/1.40 oil DIC M27 from Carl Zeiss) and analyzed by the software ZEN 2008.

α-Tocopherol Quenching of the Photodynamic Effect:

HeLa cells were seeded into 96-well microtiter plates as described earlier in the presence of 200 μM α-tocopherol (Sigma-Aldrich). After 24 h, photodynamic treatment was executed by the standard procedure with 1 μM of complex **1**. Cell viability was determined another 24 h later by the MTT assay.

ROS Experiments:

Intracellular reactive oxygen species (ROS) level was measured by the carboyx-H_2DFFDA method. Carboxy-H_2DFFDA is a cell-permeable indicator for ROS that is inactivated until the acetate groups are removed by intracellular esterases. Once oxidized by ROS, carboyx-H_2DFFDA is irreversibly converted to its fluorescent form, which can be used to monitor the oxidative stress level of cells. For the measurements, HeLa cells were grown in DMEM without phenol red in black 96-well plates with optical bottom (1.8 x 10^4 cells per well). After

overnight cell attachment, culture medium was replaced by 100 μL PBS (with $CaCl_2$ and $MgCl_2$) (Sigma-Aldrich) containing 10 μM carboxy-H_2DFFDA (Invitrogen). The fluorescent dye was incubated with the cells for 1 h before they were washed with PBS and cultured again in medium containing 1 or 30 μM of complex **1**. The complex was incubated for 1 h before cells were exposed to visible light (λ ≥ 505 nm) for 45 min. Immediately after irradiation, fluorescence readings were performed with a Spectramax M5 microplate reader (Molecular Devices) at an excitation wavelength of 492 nm and an emission wavelength of 527 nm.

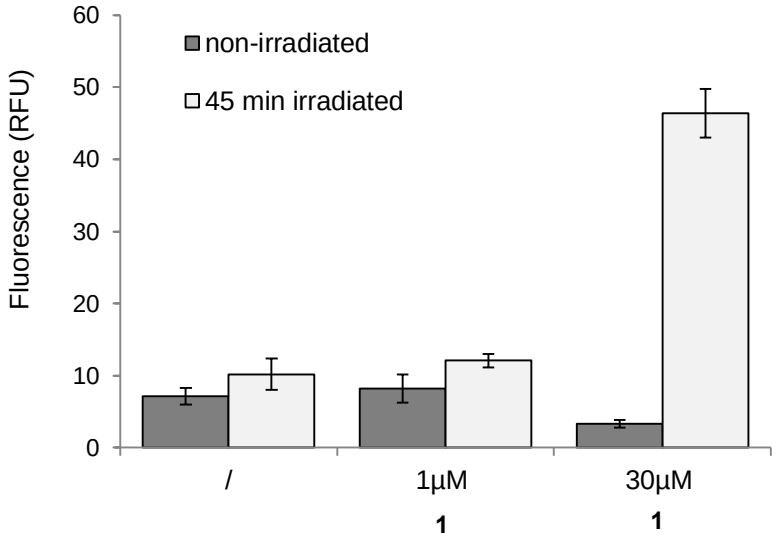


Figure S14. Intracellular detection of reactive oxygen species with carboxy-H_2DFFDA. HeLa cells were treated with either DMSO (control) or complex **1** at different concentrations, 1 h before irradiation with visible light (λ ≥ 505 nm). Error bars indicate ± S.D. resulting from three independent measurements.

Three-dimensional Spheroid Assay:

Melanoma spheroids (consisting of the 1205Lu melanoma cell line) were prepared and stained as previously described.[8] Collagen-embedded spheroids were treated with rhenium complex **1** (5 μM) or DMSO vehicle control for 1 hour, and then exposed to light of a LED reflector (Megaman® PAR16 GU10 LR0707-SP) for 60 min (distance between lamp and plate 23 cm). The spheroids were then incubated for 24 h and exposed to light again for 1 h, followed by another 24 h incubation. The spheroids were then stained with a live/dead assay

(Invitrogen) and imaged using a TE2000 Nikon inverted fluorescence microscope. As controls, spheroids were treated as above but without light stimulation. Spheroids were also exposed to light alone without treatment of **1**. Images shown are representative of three separate experiments.

Statistical Analysis:

Results are expressed as mean ± S.D. All viability assays are performed in two independent experiments each based on the equal treatment of nine different wells. Caspase activity was measured four times in triplicate and the results of ROS measurements are based on three independent experiments each based on four equal treated wells. The cell cycle analysis was performed two times in duplicate. Singlet oxygen measurements were performed two times in triplicate.

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