

Supporting Information

Necrosis Inducing Tetranuclear Ru(II) - Re(I) Metal Complex for Anticancer Therapy

Julia Schleisiek,^a Eleni Michaltsis^a Stephan Mayer^a Nicolás Montesdeoca,^a

Johannes Karges^{a,}*

^a Faculty of Chemistry and Biochemistry, Ruhr-University Bochum, Universitätsstrasse 150,
44780 Bochum, Germany.

* Email: johannes.karges@ruhr-uni-bochum.de, Tel: +49 2343224187; WWW:
www.kargesgroup.ruhr-uni-bochum.de

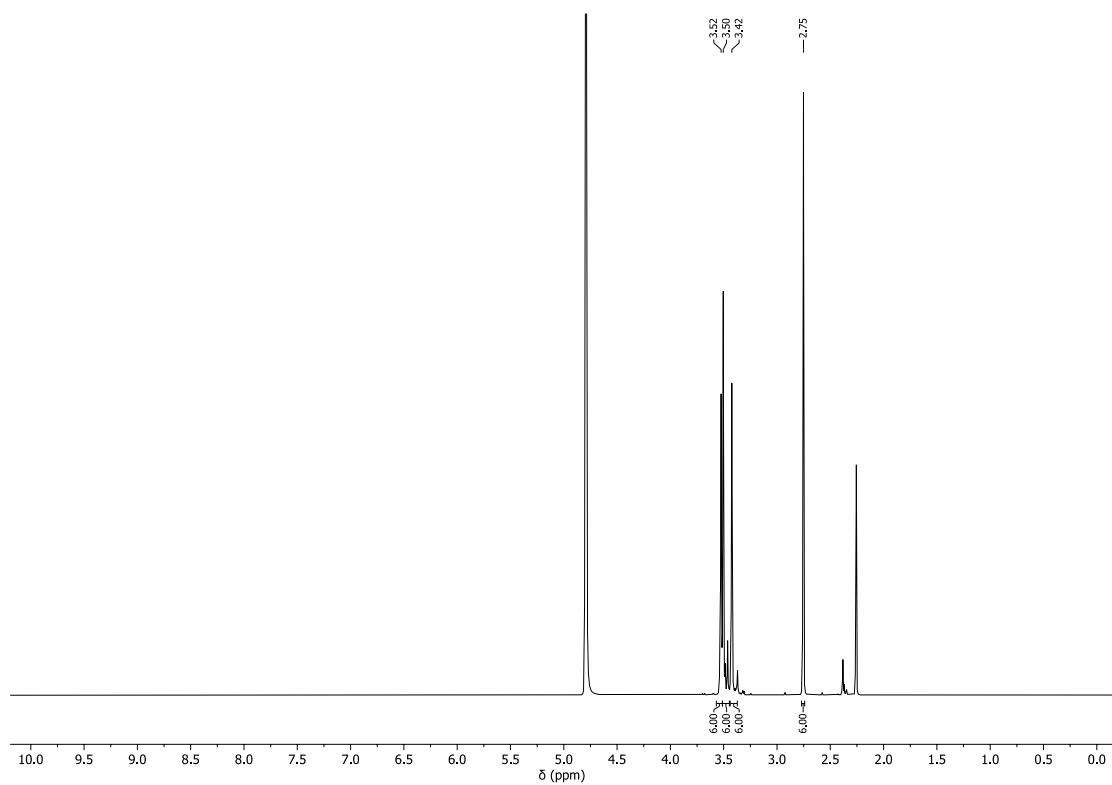


Figure S1. ^1H -NMR spectrum (400 MHz) of $[\text{Ru}(\text{dimethyl sulfoxide})_4(\text{Cl})_2]$ in D_2O .

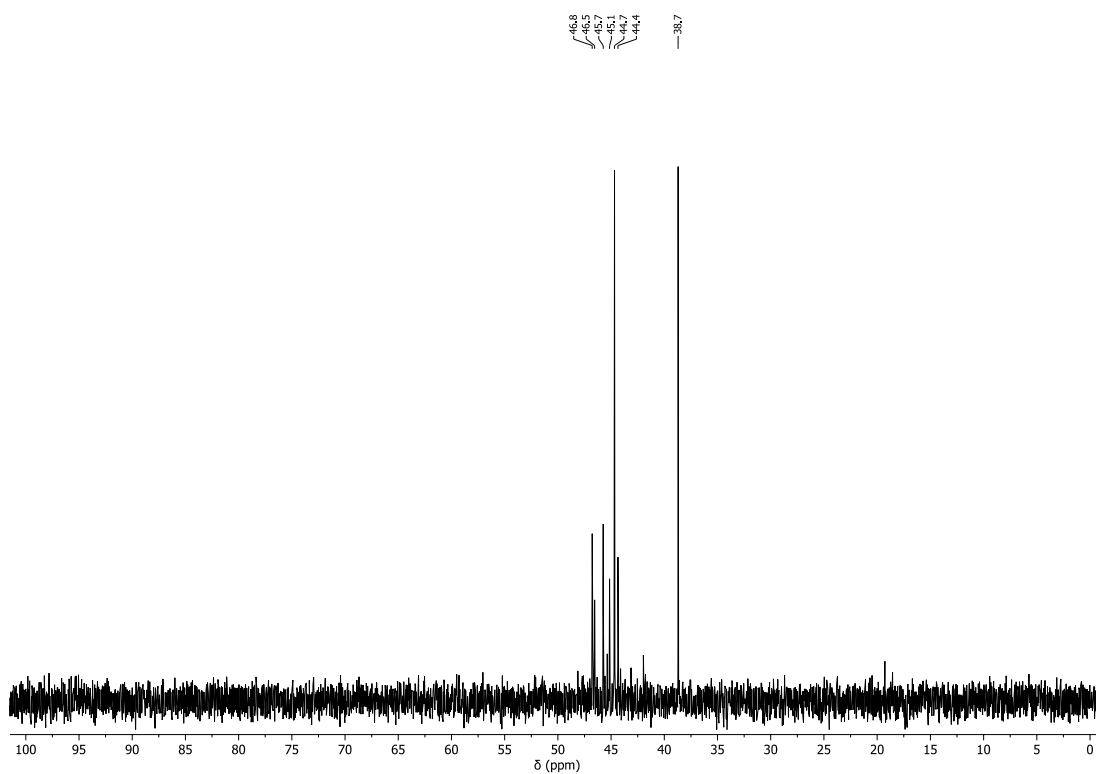


Figure S2. ^{13}C -NMR spectrum (100 MHz) of $[\text{Ru}(\text{dimethyl sulfoxide})_4(\text{Cl})_2]$ in D_2O .

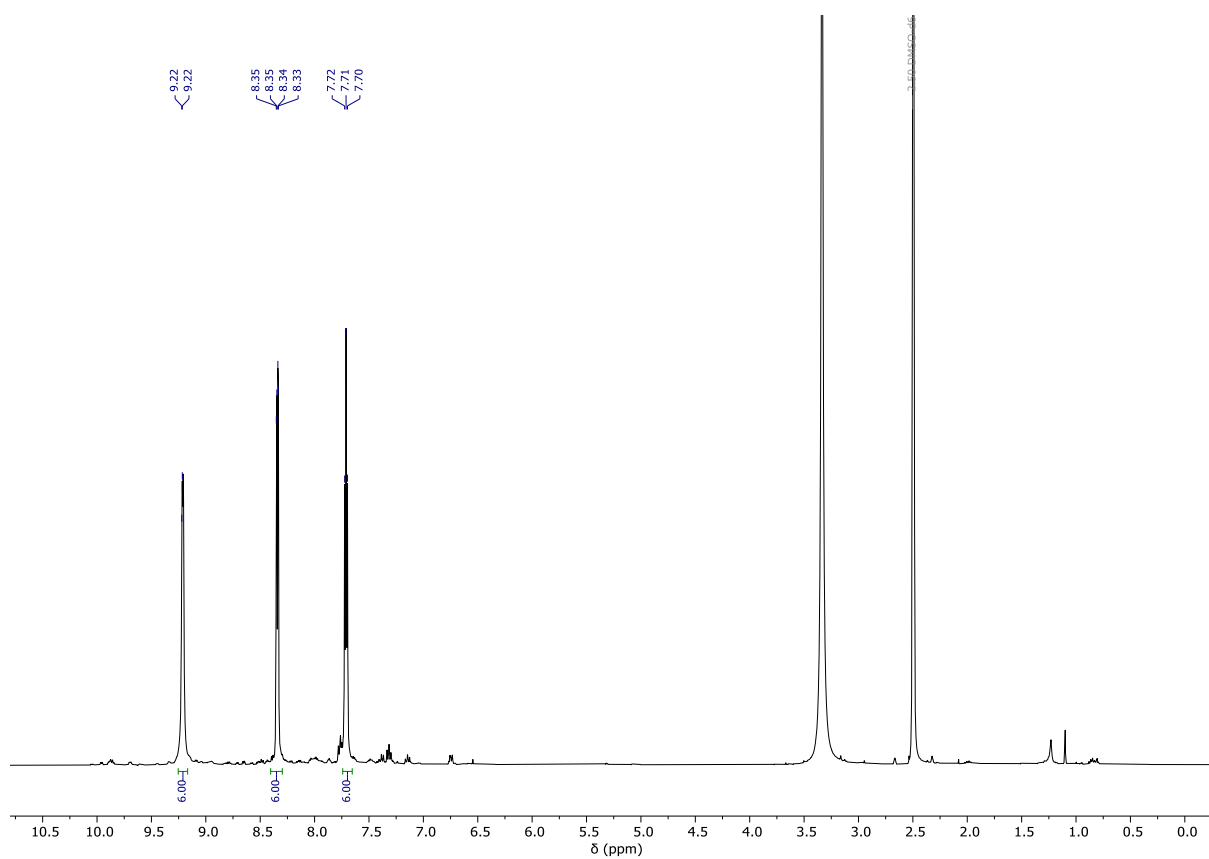


Figure S3. ^1H -NMR spectrum (400 MHz) of $[\text{Ru}(2,2'\text{-bipyrimidine})_3][\text{Cl}]_2$ in DMSO-d_6 .

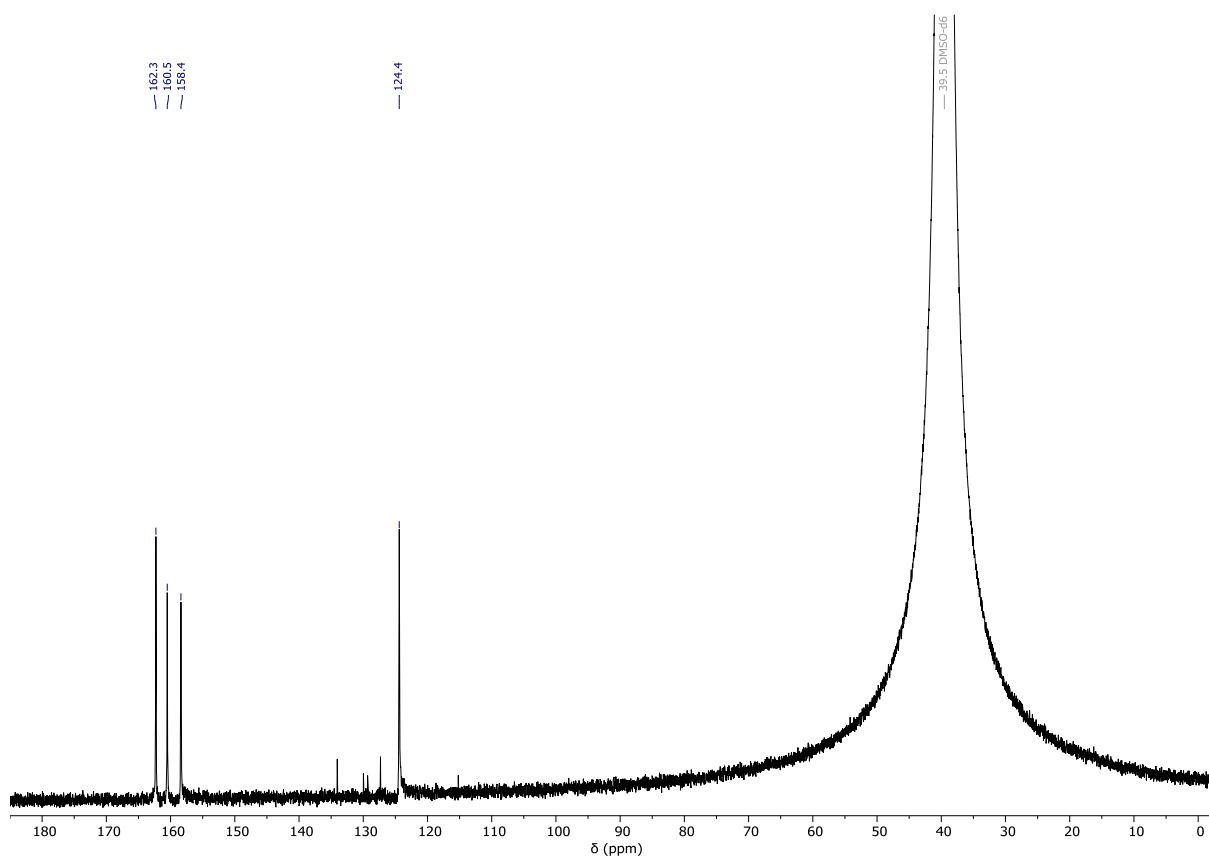


Figure S4. ^{13}C -NMR spectrum (100 MHz) of $[\text{Ru}(2,2'\text{-bipyrimidine})_3][\text{Cl}]_2$ in DMSO-d_6 .

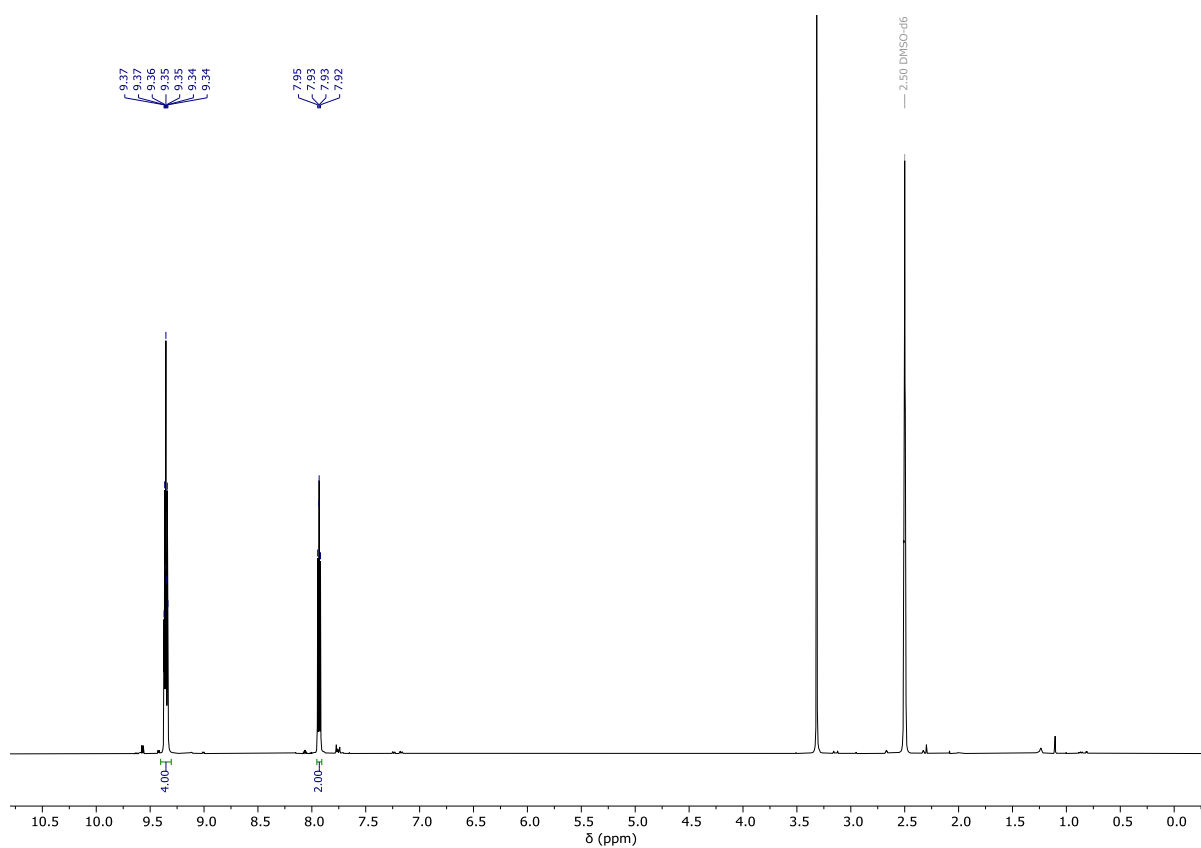


Figure S5. ^1H -NMR spectrum (400 MHz) of $[\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})]$ in DMSO-d_6 .

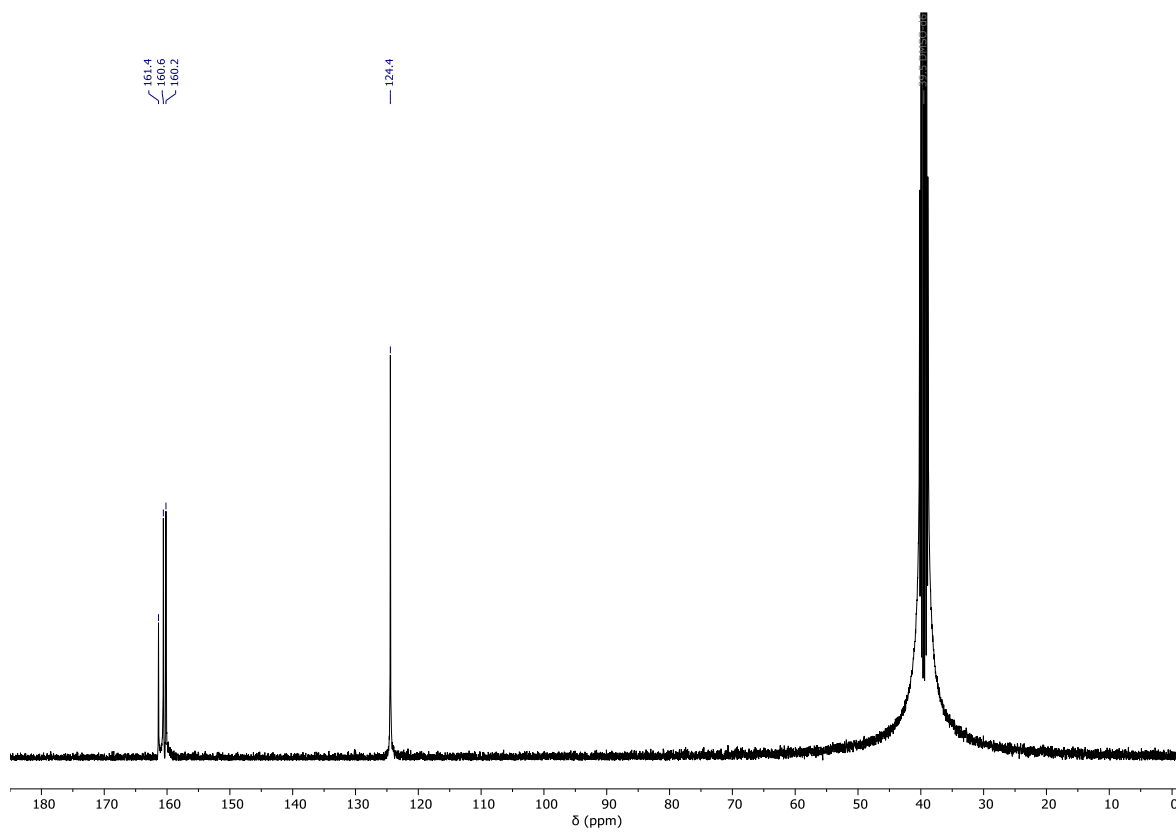


Figure S6. ^{13}C -NMR spectrum (100 MHz) of $[\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})]$ in DMSO-d_6 .

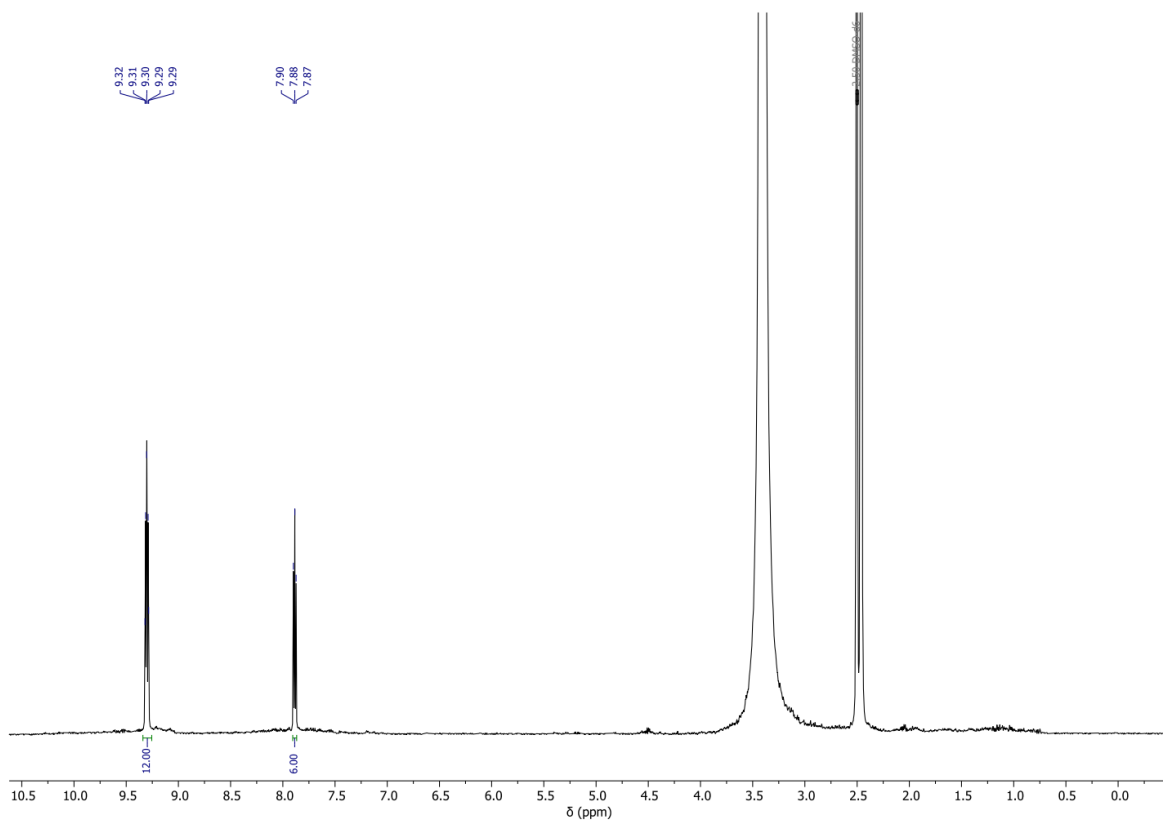


Figure S7. $^1\text{H-NMR}$ spectrum (400 MHz) of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl}))_3][\text{Cl}]_2$ in DMSO-d_6 .

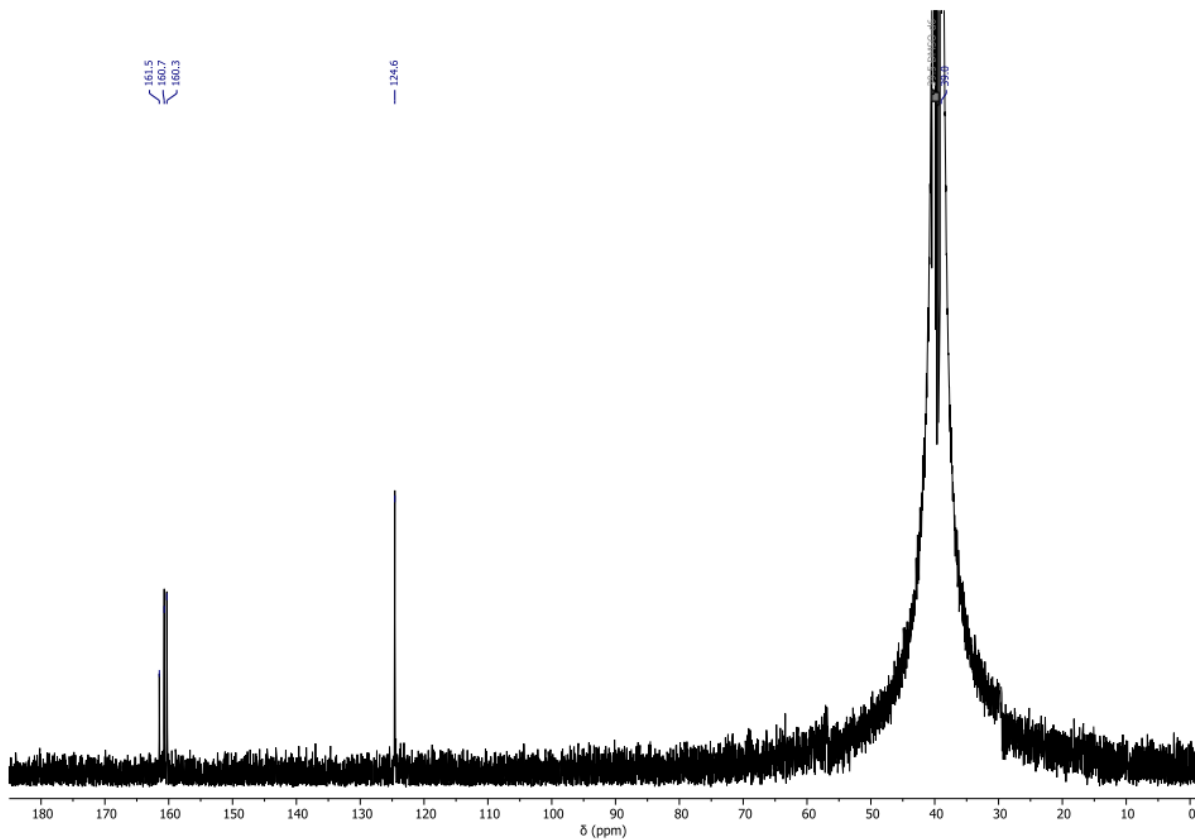


Figure S8. $^{13}\text{C-NMR}$ spectrum (100 MHz) of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl}))_3][\text{Cl}]_2$ in DMSO-d_6 .

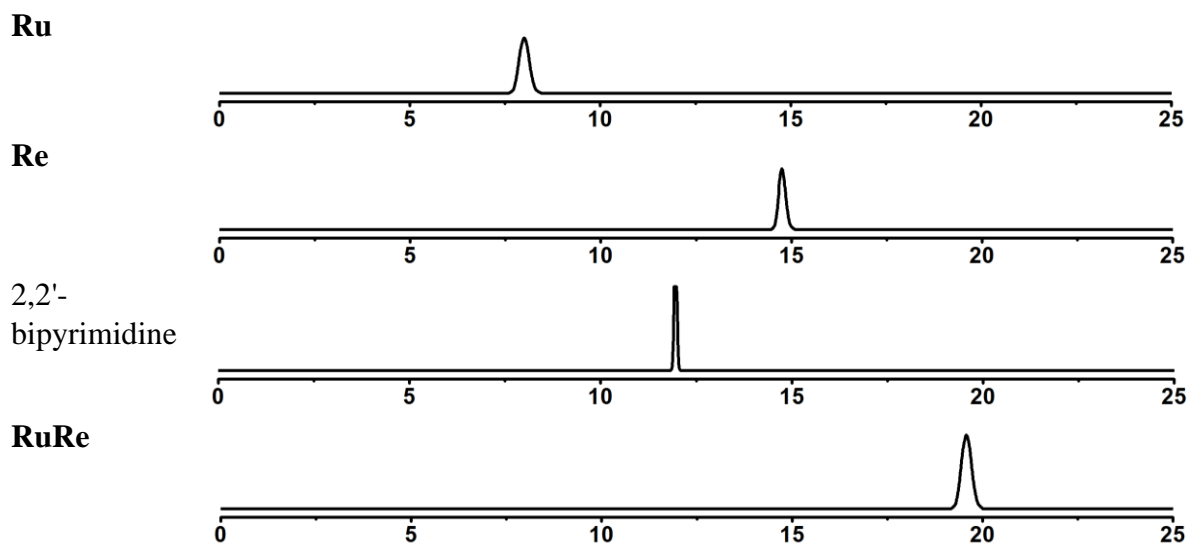


Figure S9. High-pressure liquid chromatography chromatograms of $[\text{Ru}(2,2'\text{-bipyrimidine})_3][\text{Cl}]_2$ (**Ru**), $[\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})]$ (**Re**), 2,2'-bipyrimidine, and $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl}))_3][\text{Cl}]_2$ (**RuRe**).

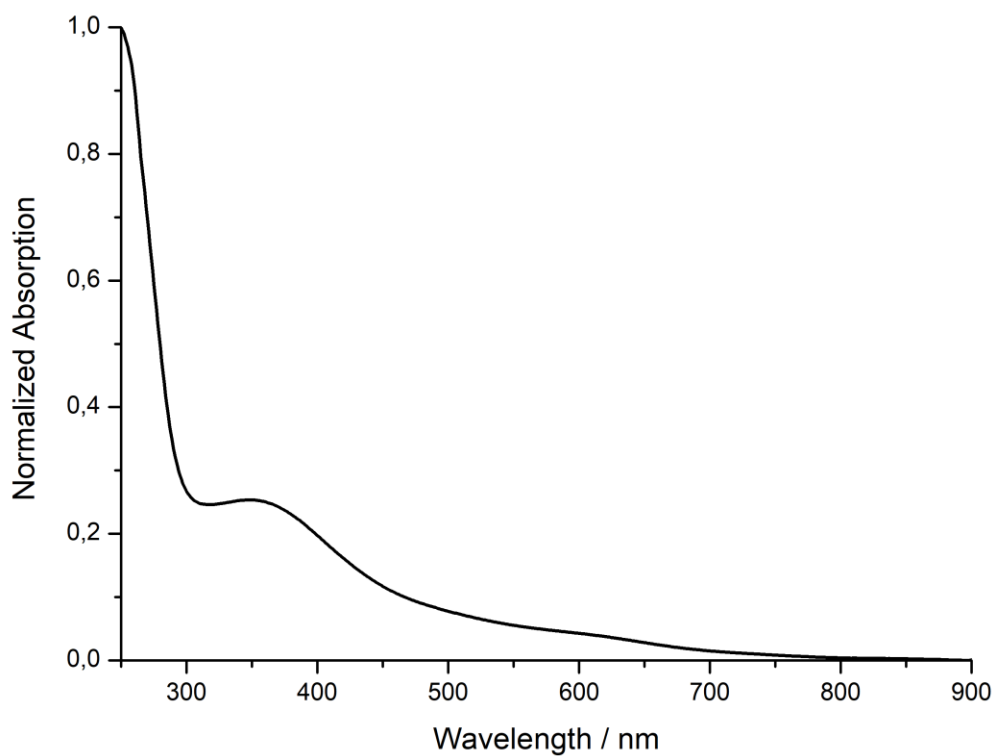


Figure S10. Normalized absorption spectrum of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl}))_3][\text{Cl}]_2$ in water.

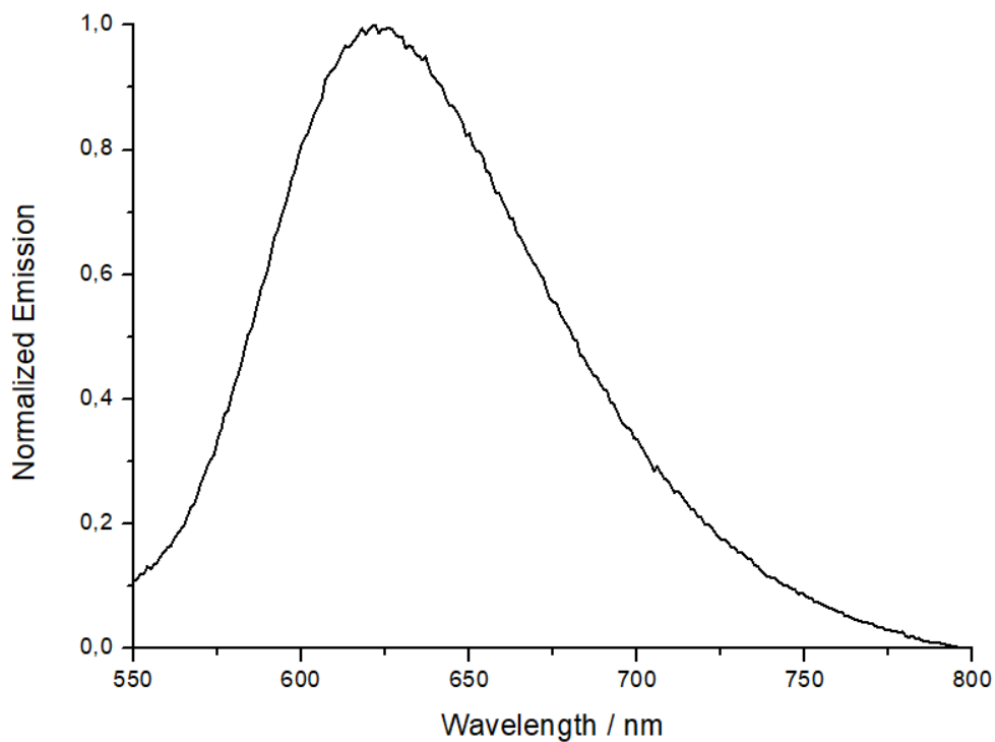


Figure S10. Normalized emission spectrum of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})_3)]_2$ in water upon excitation at 350 nm.

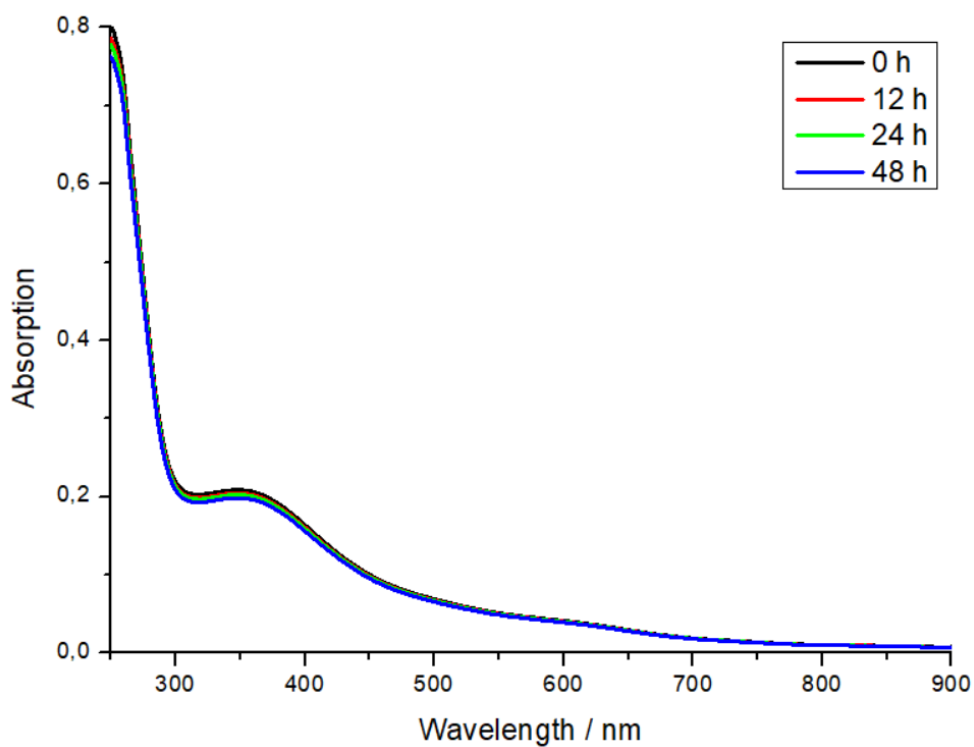


Figure S11. Change in the absorption profile of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})_3)]_2$ upon incubation in phosphate-buffered saline for up to 48 h.

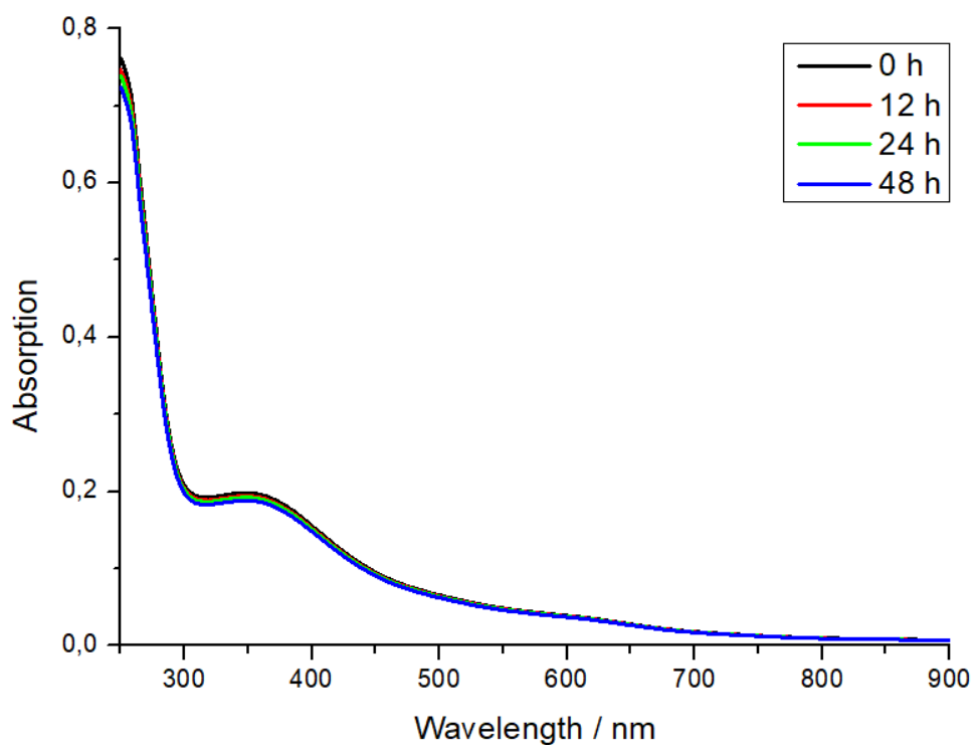


Figure S12. Change in the absorption profile of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})_3)]_2$ upon incubation in DMEM media at 37°C for up to 48 h.

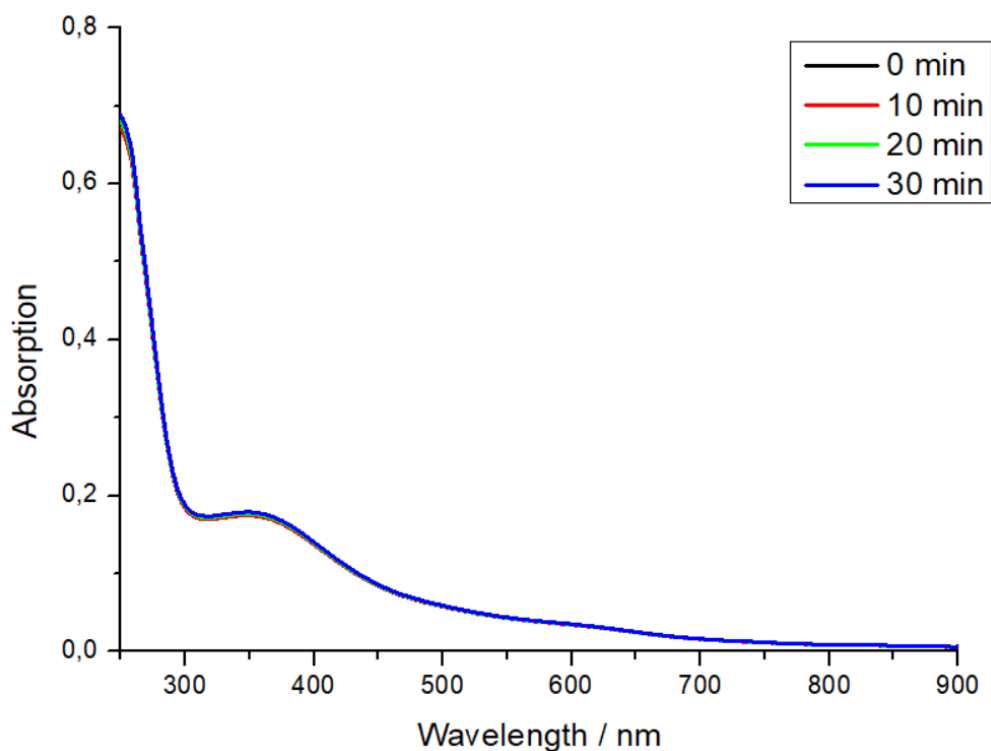


Figure S13. Change in the absorption profile of $[\text{Ru}(\text{Re}(2,2'\text{-bipyrimidine})(\text{CO})_3(\text{Cl})_3)]_2$ upon incubation in phosphate-buffered saline upon irradiation at 450 nm for up to 30 min.

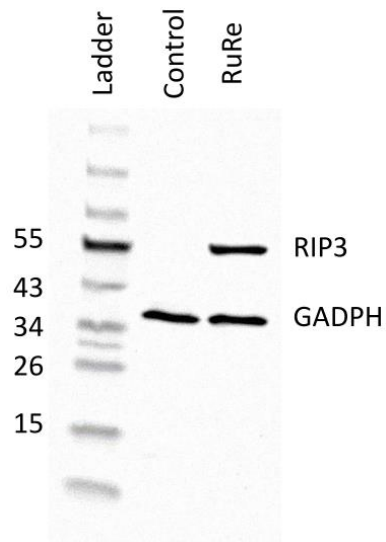


Figure S14. Western Blot analysis of the enzymes receptor-interacting kinase 3 (RIP3) and glycerinaldehyd-3-phosphat-dehydrogenase (GADPH) as a reference in CT-26 cells upon treatment with **RuRe**.