Electronic Supporting Information (ESI)

A Multi-target Caffeine Derived Rhodium(I) *N*-heterocyclic Carbene Complex: Evaluation of the Mechanism of Action

Jing-Jing Zhang,^{a,b} Julienne K. Muenzner,^c Mohamed A. Abu el Maaty,^b Bianka Karge,^d Rainer Schobert,^c Stefan Wölfl^{b*} and Ingo Ott^{a*}

^aInstitute of Medicinal and Pharmaceutical Chemistry, Technische Universität Braunschweig, Beethovenstr. 55, D-38106 Braunschweig, Germany

^bInstitute of Pharmacy and Molecular Biotechnology, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 364, D-69120 Heidelberg, Germany

^cDepartment of Organic Chemistry, University Bayreuth, Universitätsstr 30, D-95440 Bayreuth, Germany

^dDepartment of Chemical Biology, Helmholtz Centre for Infection Research GmbH, Inhoffenstr. 7, D-38124 Braunschweig, Germany



Fig. S1. The ¹H NMR spectrum of 1 in CDCl₃.



Fig. S2. The positive-ion ESI mass spectrum of 1.



Fig. S3. The ¹H NMR spectrum of **2** in CDCl₃.



Fig. S4. The positive-ion ESI mass spectrum of 2.



Fig. S5. IC₅₀ values (μ M) of cisplatin towards various cell lines as determined by SRB assays. (n=3).



Fig. S6. ELISA microarray analysis of cellular stress related phospho-proteins in HCT-116 cells treated with **1**.



Fig. S7. The level of phospho-p53 (Ser 15) in HCT-116 cells treated with **1** for 24 h was evaluated by a western blotting experiment.



Fig. S8. The cytotoxicity profiles of **1** towards wild type HCT-116 cells (w.t.) and HCT-116 Chk2 knock out cells (Chk2-/-) for 96 h as determined by SRB assays (n=3).



Fig. S9. Complex 1 induced an increase in the sub-G1 populations of HCT-116 cells after 24 h of incubation with 15 μ M or 18 μ M as determined by FACS analysis (n=3).



Fig. S10. The comparison of the wound healing capacity of MDA-MB-231 cells treated with 1 (10 μ M) or a respective control (DMF).