Supporting Information

Improved reaction conditions for the synthesis of new NKP-1339 derivatives and preliminary investigations on their anticancer potential

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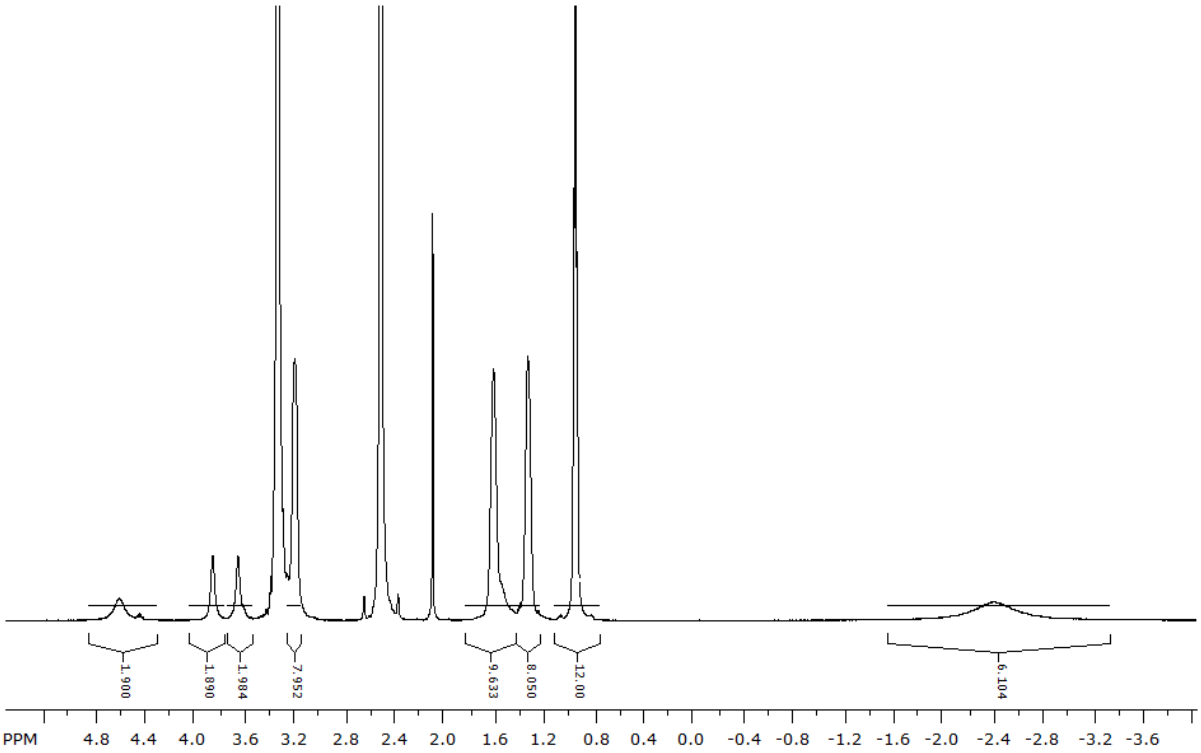

Figure S1. ^{1}H-NMR spectrum of (Bu_4N)-*trans*-[$RuCl_4$(1-Me-ind)$_2$] (**1**) in DMSO-d_6.

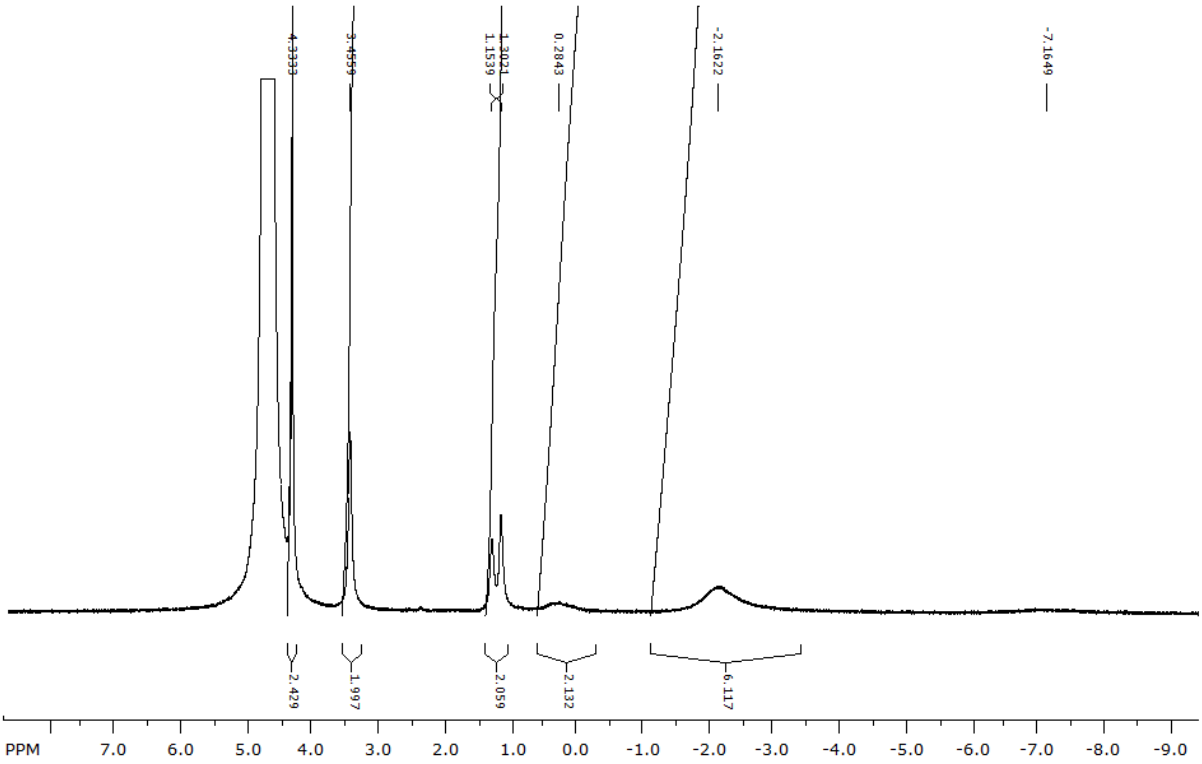

Figure S2. ^{1}H-NMR spectrum of Na-*trans*-[$RuCl_4$(1-Me-ind)$_2$] (**3**) in D_2O.

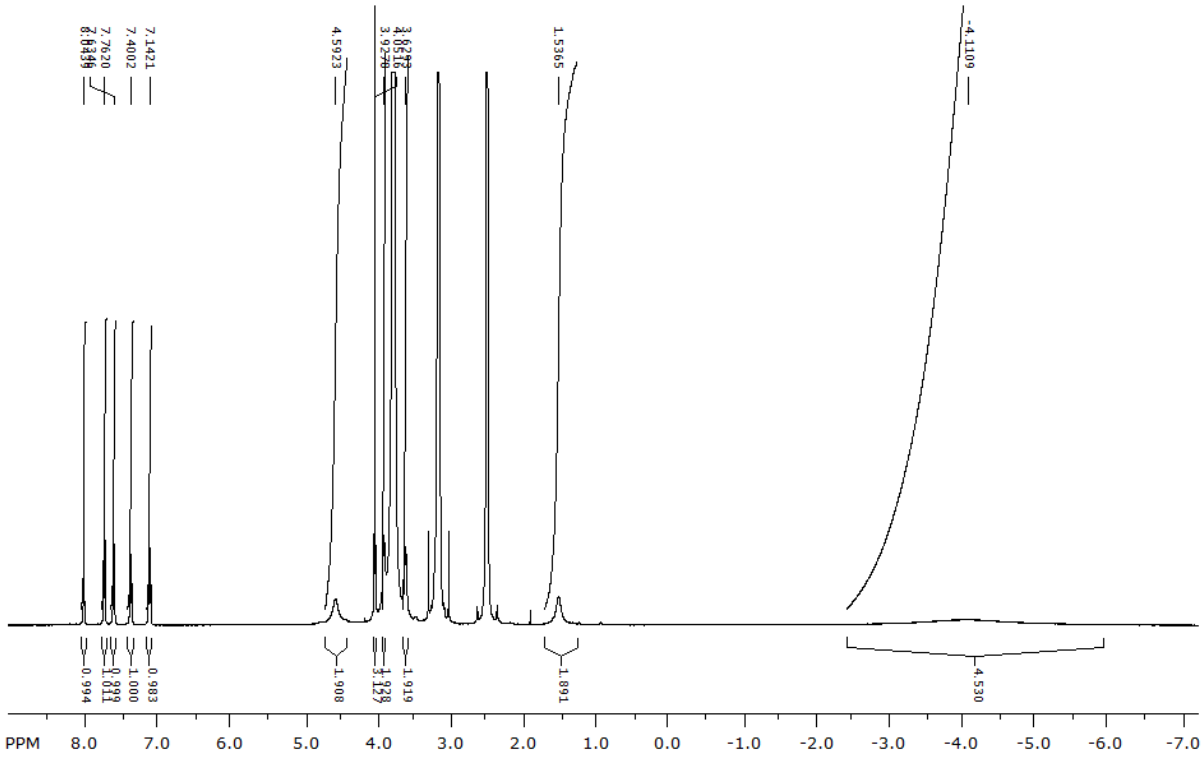

Figure S3. ^{1}H-NMR spectrum of (1-Me-Hind)-*trans*-[$RuCl_4$(1-Me-ind)$_2$] (**5**) in DMSO-d_6.

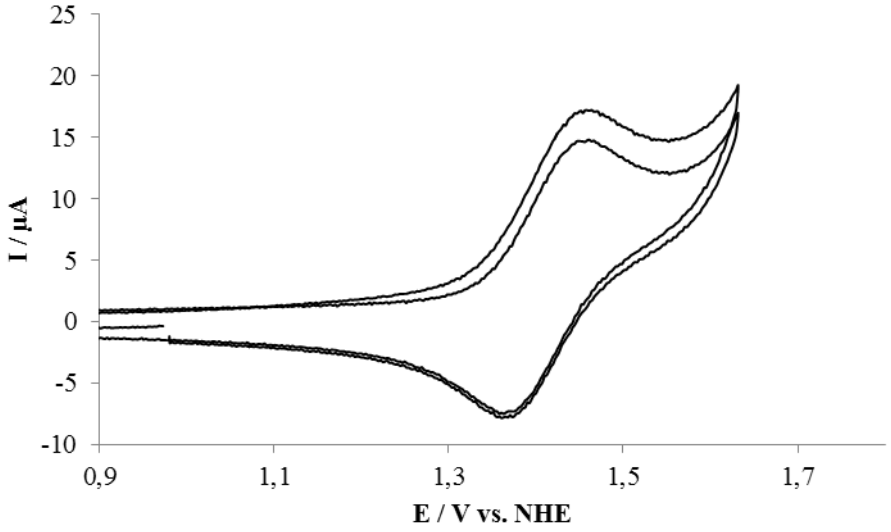

Figure S4. Cyclic voltammograms of **1** in DMSO containing 0.10 M (*n*-Bu_4N)[BF_4] at a scan rate of 0.20 V·s^{-1} using a glassy carbon working electrode, displaying the Ru^{IV}/Ru^{III} redox couple.

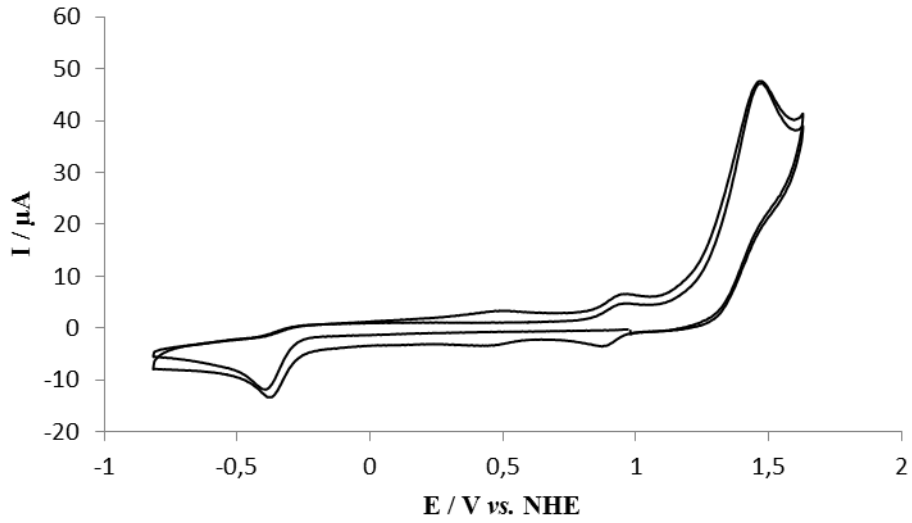

Figure S5. Cyclic voltammograms of **2** in DMSO containing 0.10 M (n-Bu_4N)[BF_4] at a scan rate of 0.20 V·s^{-1} using a glassy carbon working electrode.

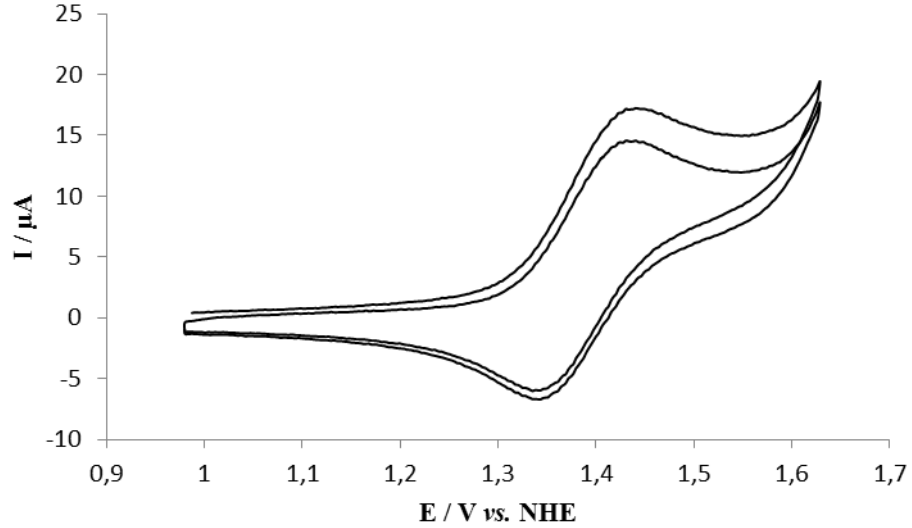

Figure S6. Cyclic voltammograms of **2** in DMSO containing 0.10 M (n-Bu_4N)[BF_4] at a scan rate of 0.20 V·s^{-1} using a glassy carbon working electrode, displaying the Ru^{IV}/Ru^{III} redox couple.

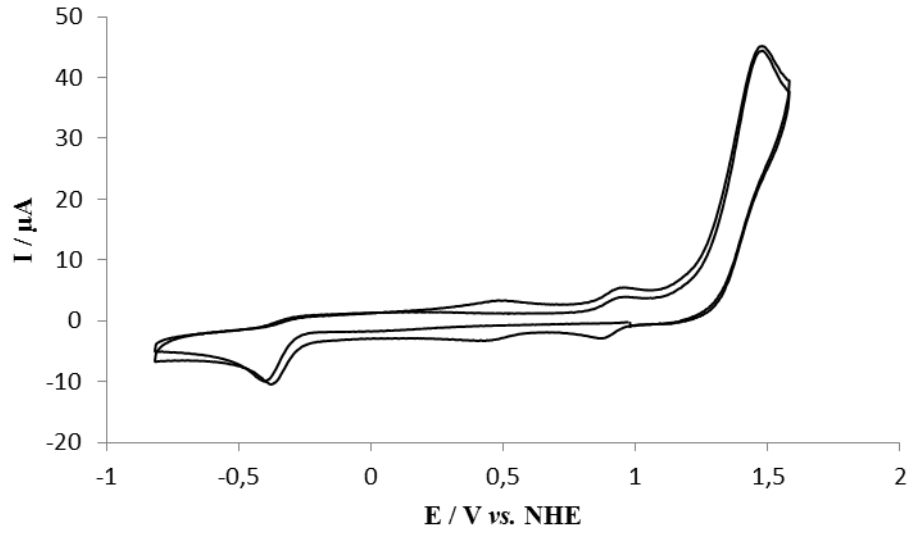

Figure S7. Cyclic voltammograms of **3** in DMSO containing 0.10 M (n-Bu_4N)[BF_4] at a scan rate of 0.20 V·s^{-1} using a glassy carbon working electrode.

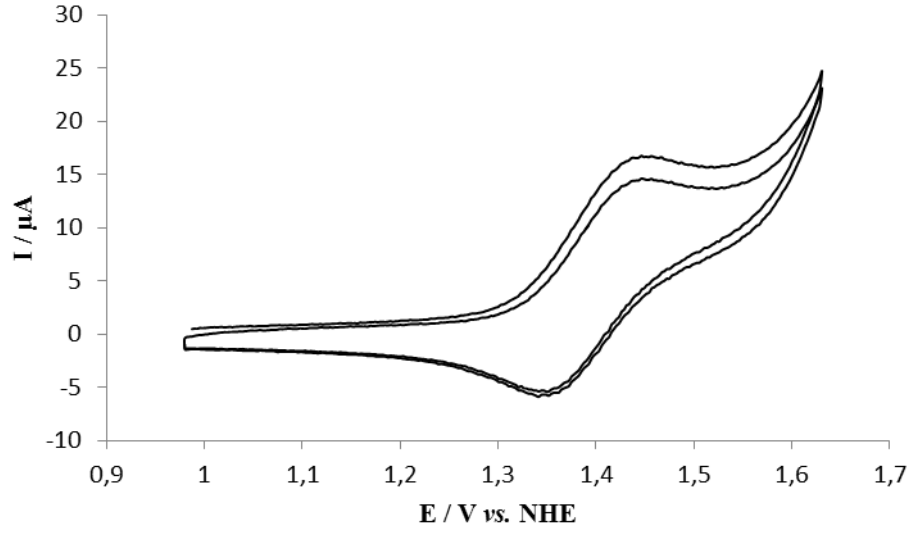

Figure S8. Cyclic voltammograms of **3** in DMSO containing 0.10 M (n-Bu_4N)[BF_4] at a scan rate of 0.20 V·s^{-1} using a glassy carbon working electrode, displaying the Ru^{IV}/Ru^{III} redox couple.

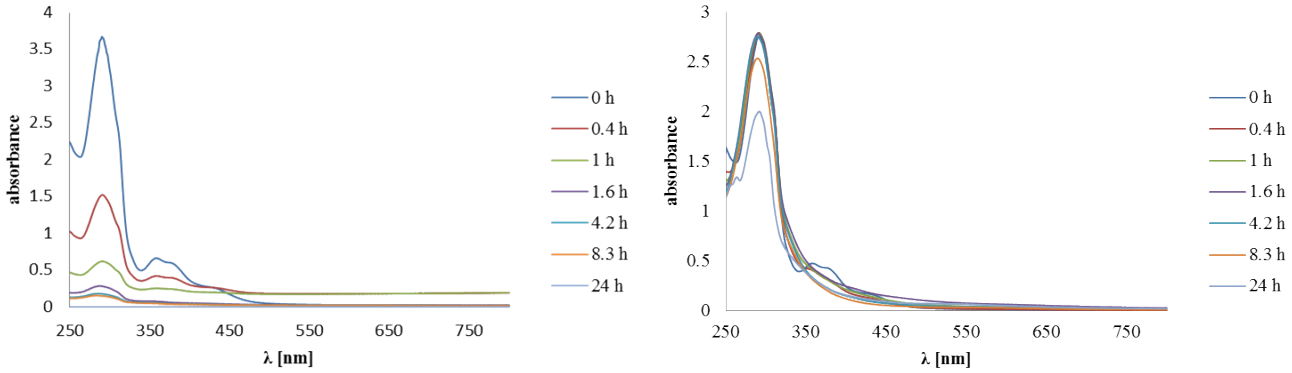

Figure S9. UV-vis spectra of **3** in water at 25 °C at pH 3.5 (left) and pH 7 (right).

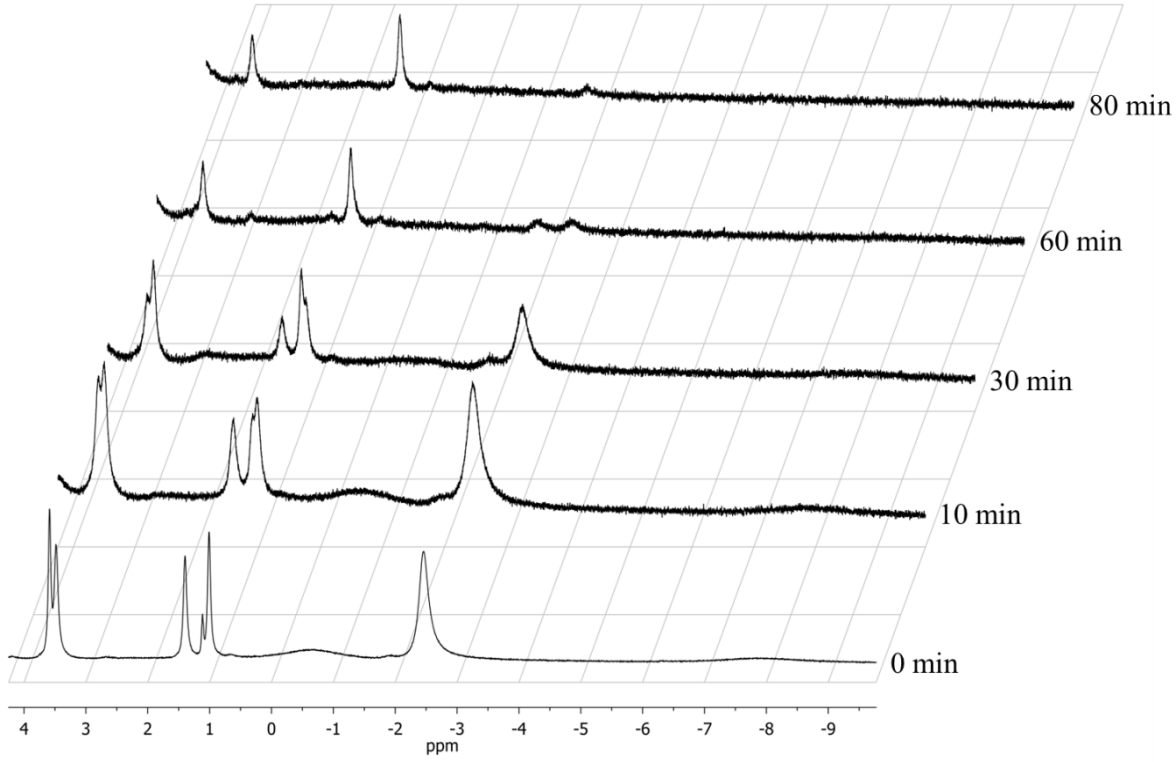

Figure S10. ^{1}H NMR spectra of **4** in D_2O over 80 min at neutral pH. Resolution of the NMR spectra decreased over time, due to precipitation of the hydrolysis products.

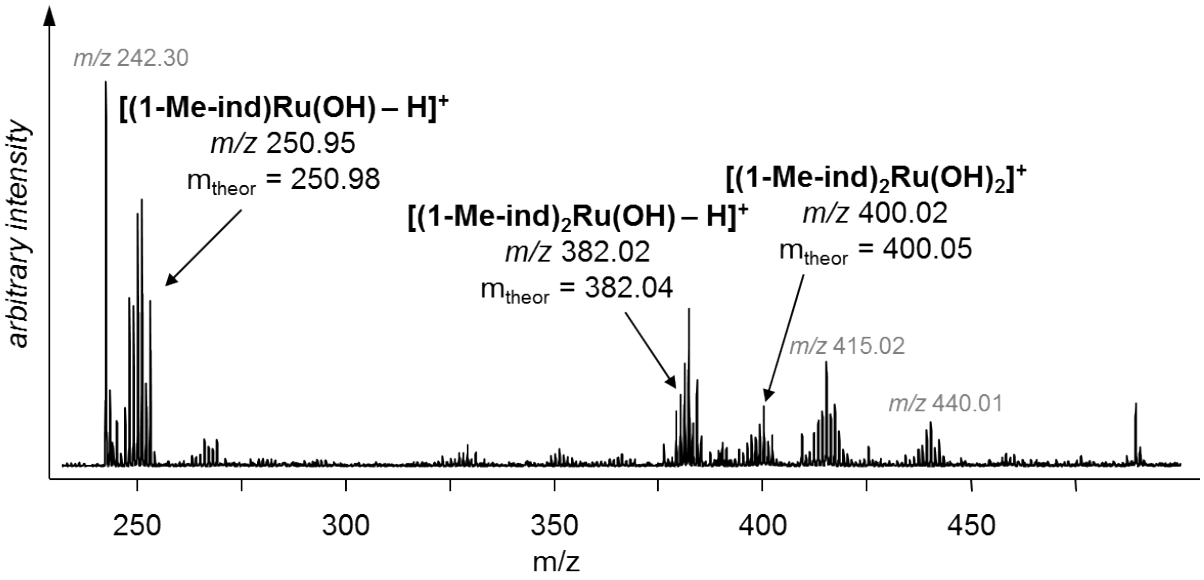

Figure S11. Excerpt of the mass spectrum in the positive ion mode of **3** after 2 h in aqueous solution. Hydroxido species stemming from hydrolysis processes are labelled.

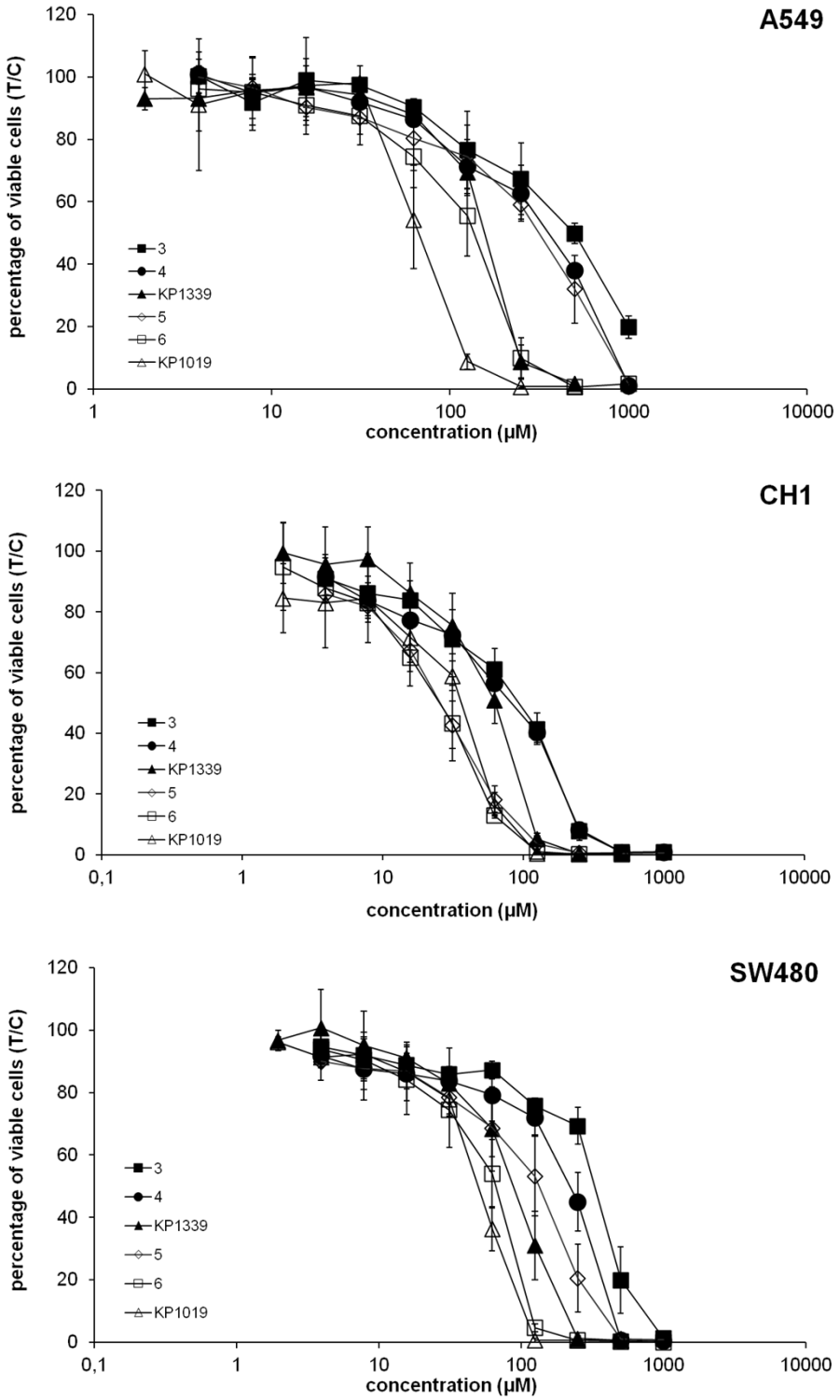

Figure S12. Concentration-effect curves of complexes **3**–**6** and the reference compounds KP1339 and KP1019 in three human cancer cell lines (A549, CH1, and SW480) obtained by the MTT assay (96 h exposure).