

Supplementary Material to the Paper

Organometallic Gold(III) Complexes with Hybrid SNS-Donating Thiosemicarbazone Ligands: Cytotoxicity and anti-Trypanosoma cruzi Activity

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Table S1. Selected bond lengths (Å) and angles (°) for [Au^{III}(Hdamp)(L1⁵)]Cl · H₂O (**5-Cl**).

Au–C4	2.044(7)	2.038(7)	N1–C2	1.33(1)	1.35(1)
Au–S1	2.296(2)	2.277(2)	C2–N2	1.33(1)	1.33(1)
Au–N2	2.051(6)	2.053(6)	N2–N3	1.406(8)	1.406(8)
Au–S2	2.277(2)	2.272(2)	N3–C3	1.29(1)	1.29(1)
C1–N1	1.33(1)	1.32(1)	C3–S2	1.769(8)	1.777(8)
C1–S1	1.762(7)	1.753(8)	C1–N5	1.35(1)	1.35(1)
C3–S2	1.769(8)	1.777(8)	Au–H10	2.793(9)	2.782(4)
S1–Au–S2	176.05(7)	176.29(7)	N2–Au–C(4)	174.0(3)	174.0(3)
N2–Au–S1	96.7(2)	97.5(2)	S1–Au–C(4)	88.4(2)	88.4(2)
N2–Au–S2	85.2(2)	85.6(2)	S2–Au–C(4)	89.5(2)	88.4(2)
C1–S1–Au	103.8(2)	105.6(3)	N3–N2–Au	118.2(4)	117.9(4)
C3–S2–Au	94.9(3)	95.0(3)	C2–N2–Au	126.0(5)	126.9(5)

*Values for two crystallographically independent molecules.

Table S2. Selected bond lengths (Å) and angles (°) in **4-NO₃**.

Au–C4	2.039(9)	N1–C2	1.34(1)
Au–S1	2.278(3)	C2–N2	1.31(1)
Au–N2	2.067(7)	N2–N3	1.39(1)
Au–S2	2.281(3)	N3–C3	1.30(1)
C1–N1	1.31(1)	C3–S2	1.775(9)
C1–S1	1.77(1)	C1–N5	1.34(1)
S1–Au–S2	177.5(1)	N2–Au–C(4)	175.5(3)
N2–Au–S1	97.8(2)	S1–Au–C(4)	86.2(3)
N2–Au–S2	84.5(2)	S2–Au–C(4)	91.4(3)
C1–S1–Au	103.9(4)	N3–N2–Au	118.8(5)
C3–S2–Au	95.7(3)	C2–N2–Au	124.6(6)

Table S3. Selected bond lengths (Å) and angles (°) for [Au^{III}(damp)(L1⁴)] (**4-neutral**).

Au–C4	2.058(8)	2.040(8)	N1–C2	1.36(1)	1.30(1)
Au–S1	2.284(2)	2.282(3)	C2–N2	1.30(1)	1.25(1)
Au–N2	2.067(8)	2.124(7)	N2–N3	1.40(1)	1.401(1)
Au–S2	2.281(2)	2.268(3)	N3–C3	1.29(1)	1.33(1)
C1–N1	1.29(1)	1.28(1)	C3–S2	1.75(1)	1.76(1)
C1–S1	1.76(1)	1.747(9)	C1–N5	1.35(1)	1.36(1)
S1–Au–S2	177.84(9)	177.3(1)	N2–Au–C(4)	176.3(3)	172.7(3)
N2–Au–S1	97.2(2)	98.7(2)	S1–Au–C(4)	86.5(2)	88.6(3)
N2–Au–S2	84.7(2)	83.6(12)	S2–Au–C(4)	91.7(2)	89.1(3)
C1–S1–Au	103.7(3)	102.1(4)	N3–N2–Au	118.0(5)	118.4(5)
C3–S2–Au	95.1(3)	98.2(3)	C2–N2–Au	125.5(7)	123.8(7)

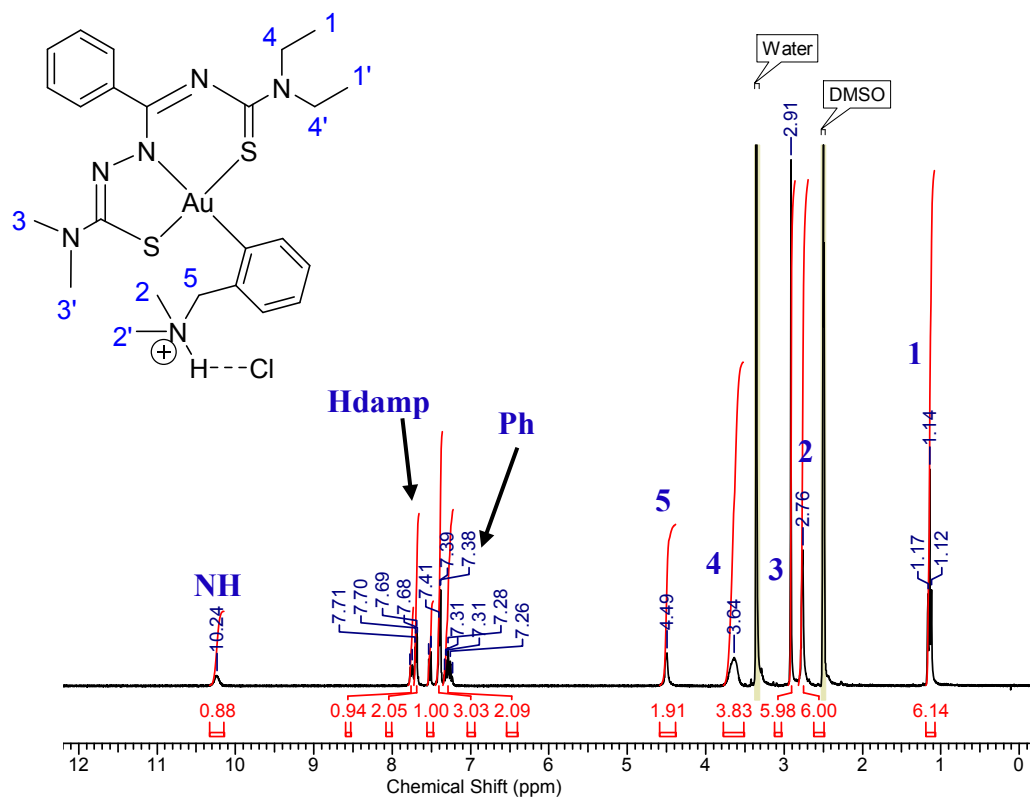


Fig. S1. ¹H NMR spectrum of of the complex 4-Cl from DMSO-*d*₆ solution (δ in ppm).

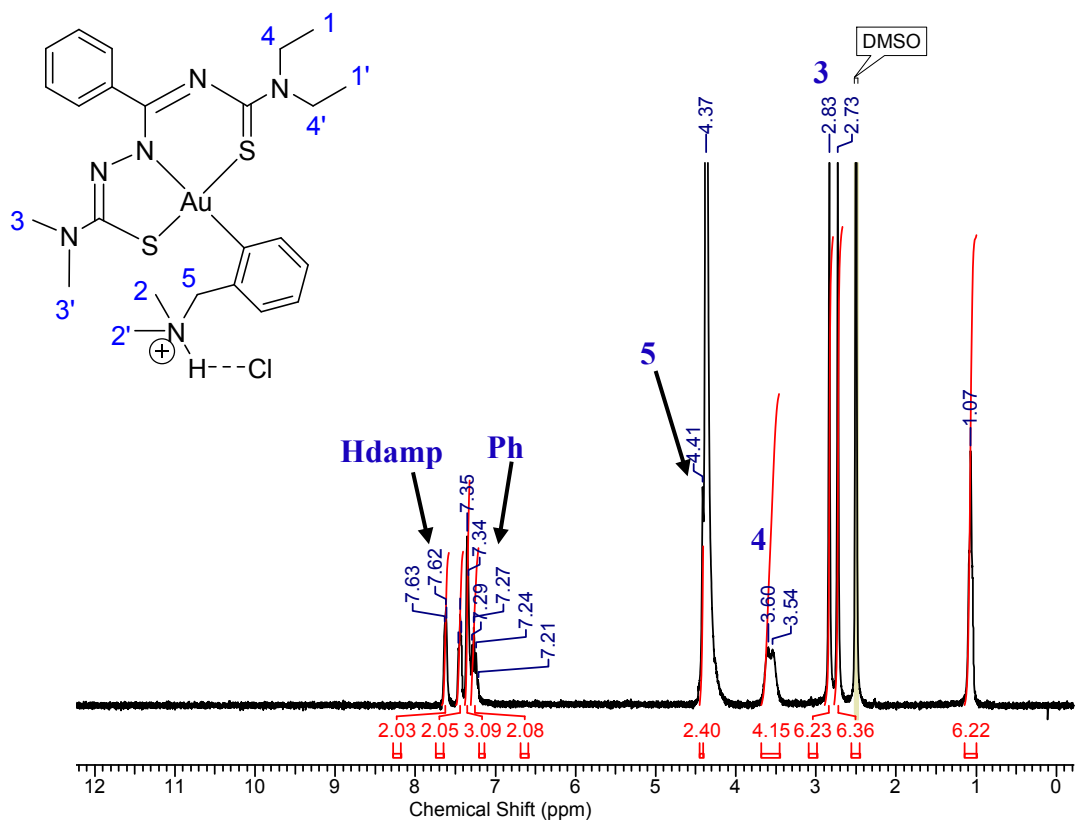


Fig. S2. ¹H NMR spectrum of of the complex 4-Cl from a 1:1 mixture DMSO-*d*₆:D₂O solution (δ in ppm).

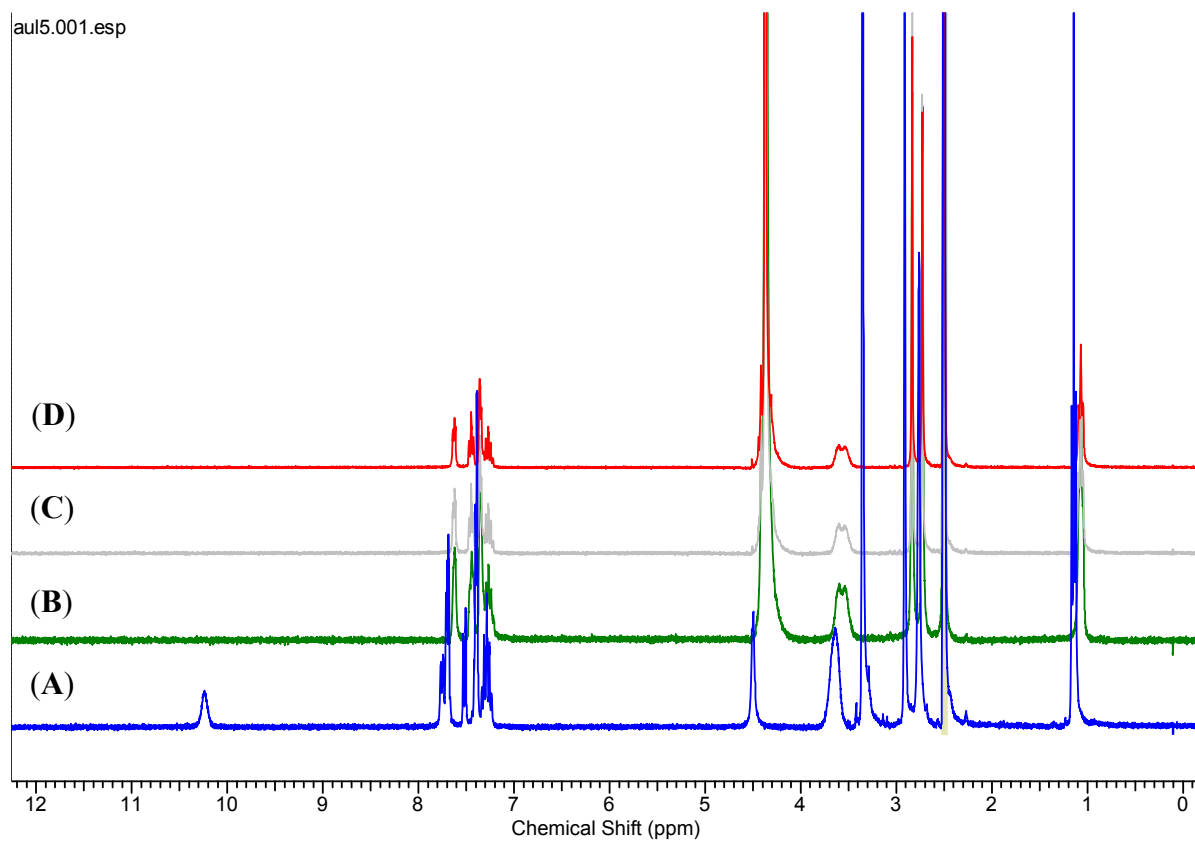


Fig. S3. ¹H NMR spectra of the complex **4-Cl** (δ in ppm). (A)-DMSO-*d*₆, (B) - 1:1 mixture DMSO-*d*₆:D₂O measured immediately, (C) - 1:1 mixture DMSO-*d*₆:D₂O 24 hours later and (D) - 1:1 mixture DMSO-*d*₆:D₂O 48 hours later.

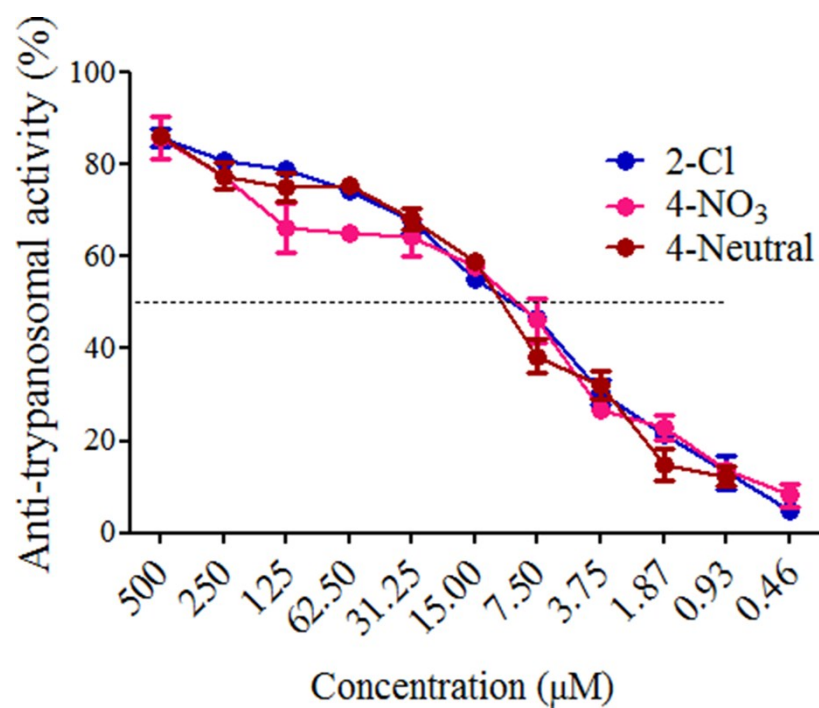


Fig. S4. Trypanocidal activity of the gold complexes **2-Cl**, **4-NO₃** and **4-neutral**. Compounds were maintained during five days in contact with *T. cruzi*. The death of parasites was measured by conversion of β -galactosidase activity of modified parasites. This assay represents duplicate of experiment.

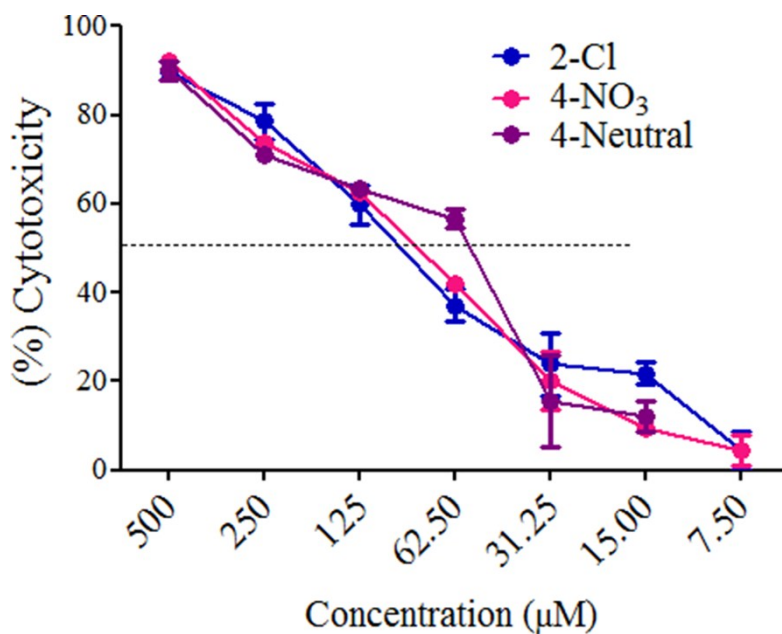


Fig. S5. Percentage of mammalian cell death upon incubation with the gold complexes **2-Cl**, **4-NO₃** and **4-neutral**. Spleen cells of Swiss mice were plated with different concentrations of drugs for 24 hours. Medium and Tween-20 were used as negative and positive controls, respectively. Benznidazole was used as reference drug. The experiments were performed at least two times.

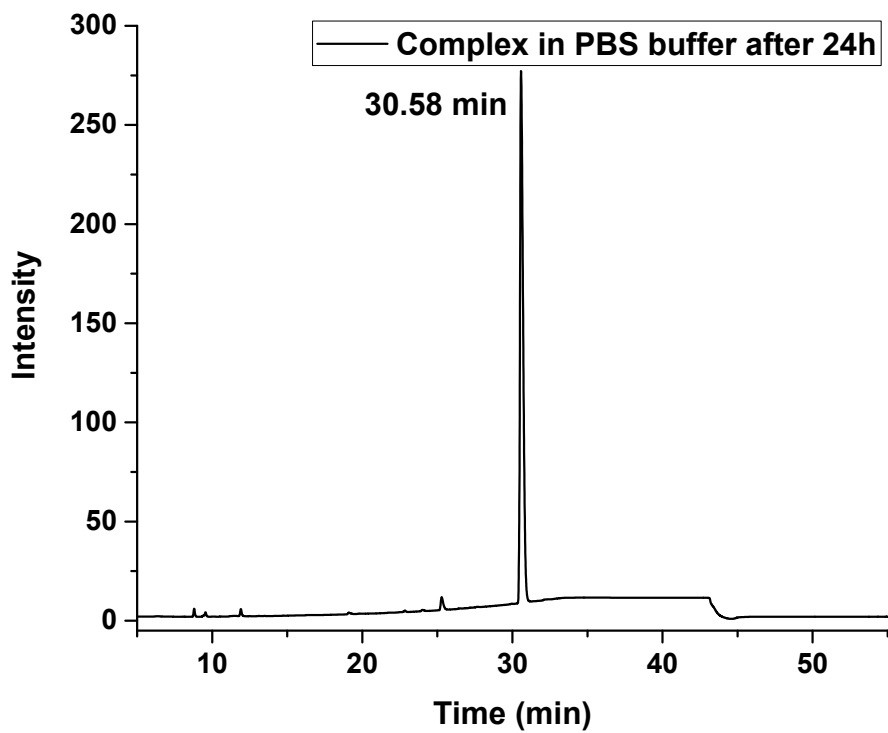


Figure S6. HPLC of the complex 4-Cl in freshly prepared PBS buffer/10% DMSO solution.

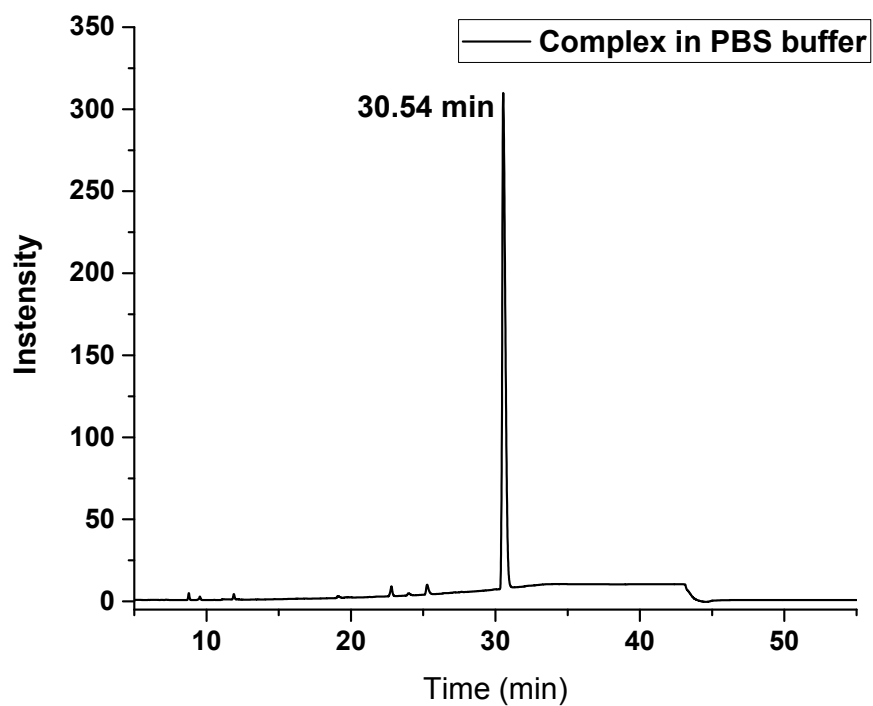


Figure S7. HPLC of the complex 4-Cl in PBS buffer/10% DMSO solution recorded after 24 h of incubation time at 37 °C.

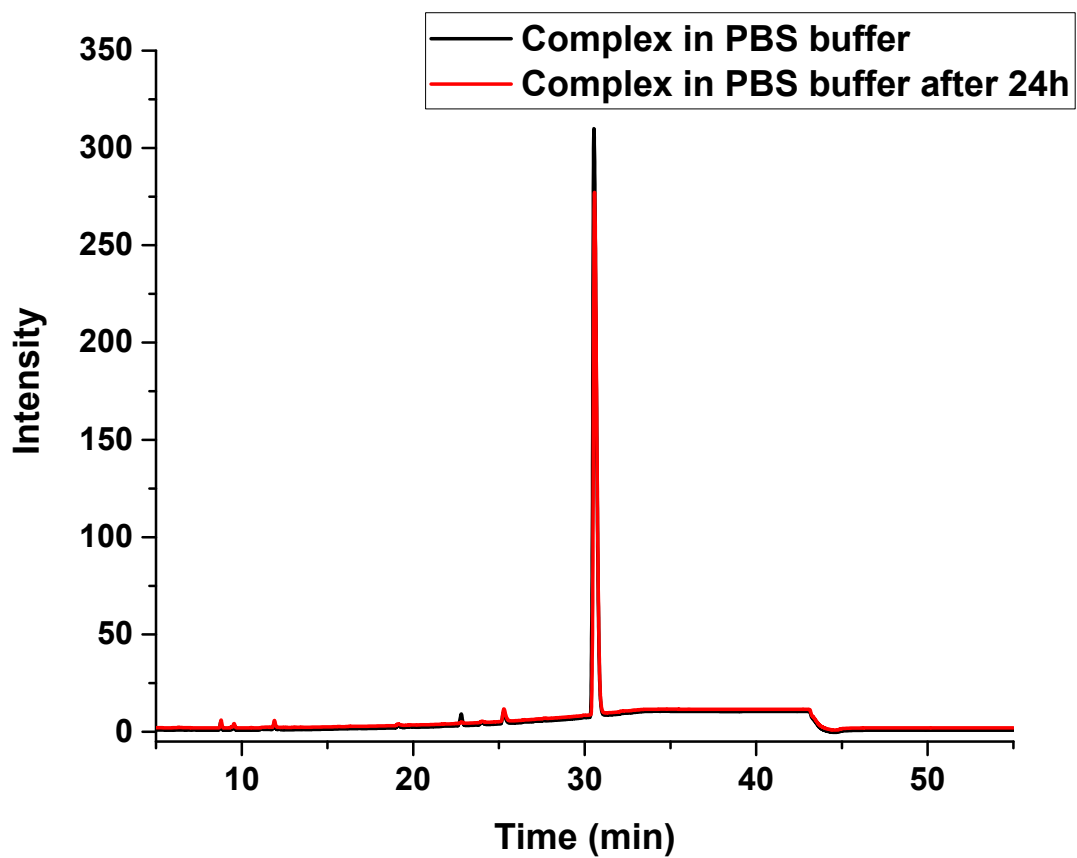


Figure S8. Overlapping of the HPLC of the complex 4-Cl in freshly prepared PBS buffer/10% DMSO solution and after 24 h of incubation time at 37 °C.

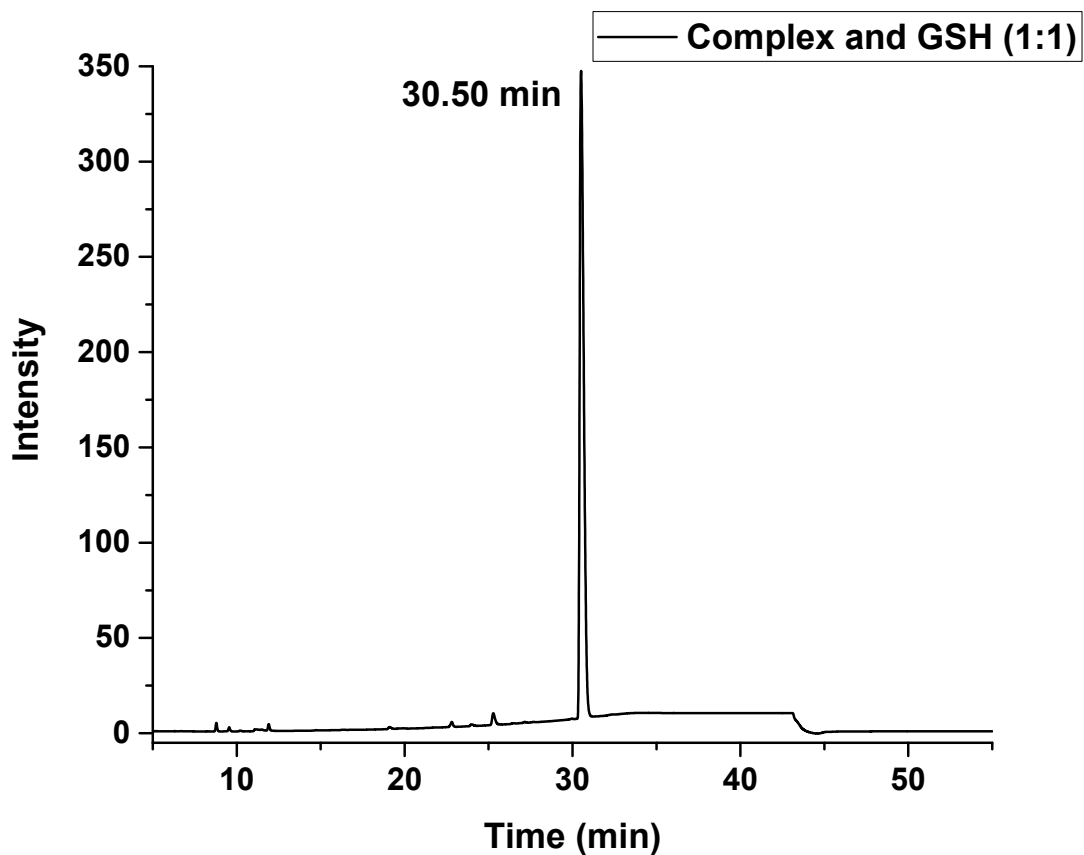


Figure S9. HPLC of the complex 4-Cl:Glutathione (GSH) (1:1) in freshly prepared PBS buffer/10% DMSO solution.

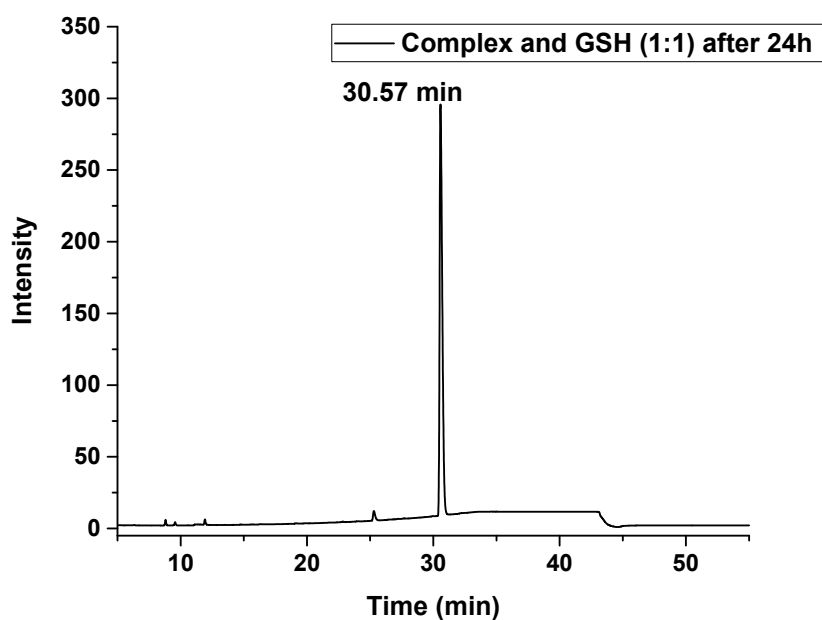


Figure S10. HPLC of the complex 4-Cl:Glutathione (GSH) (1:1) in PBS buffer/10% DMSO solution recorded after 24 h of incubation time at 37 °C.

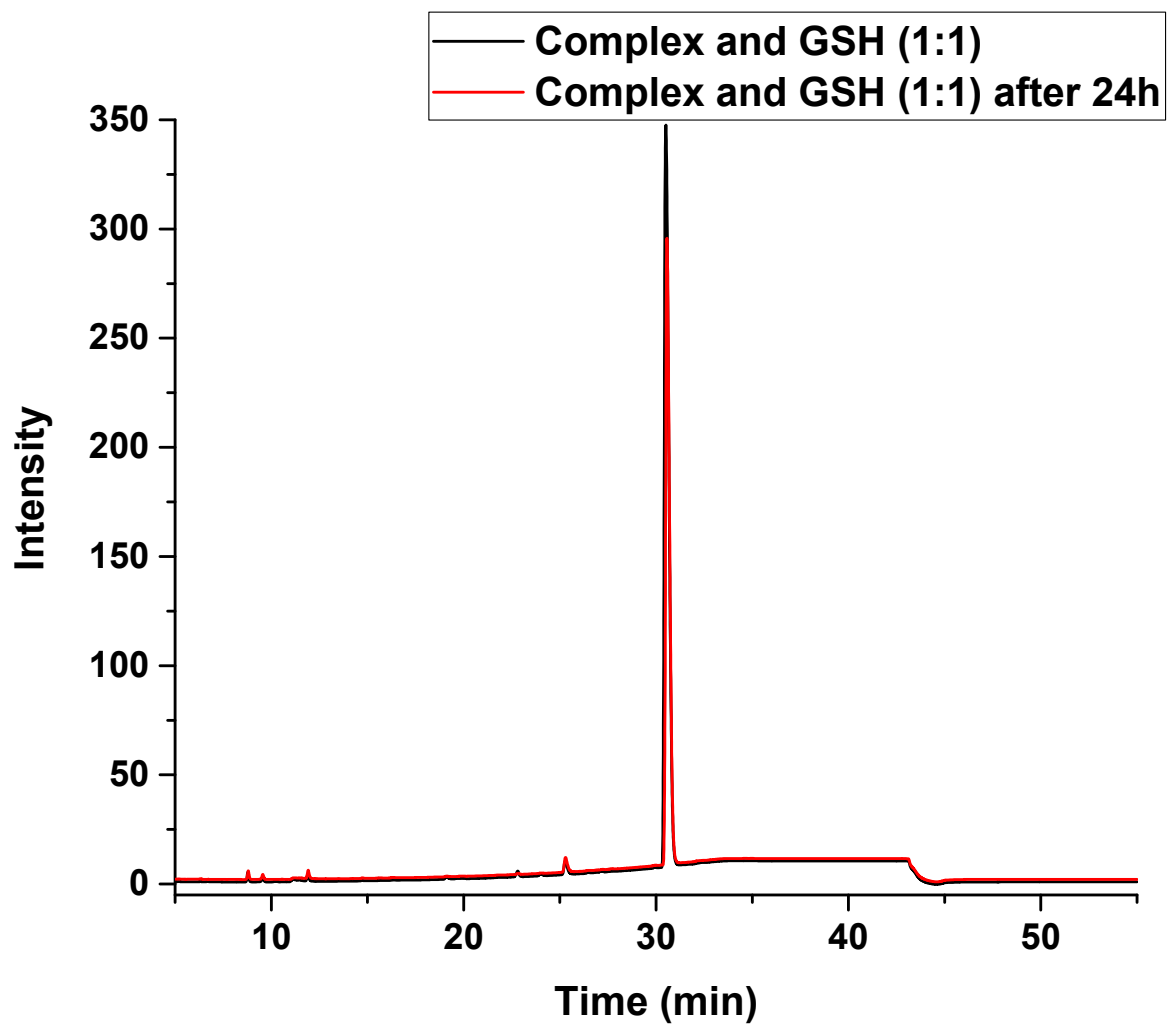


Figure S11. Overlapping of the HPLC of the complex 4-Cl:Glutathione (GSH) (1:1) in freshly prepared PBS buffer/10% DMSO solution and after 24 h of incubation time at 37 °C.