Figure S1.
Synthetic scheme **(A)** for the preparation of dipeptides HCl•H-Sar-AA-O(t-Bu) (AA = Gly (AuD6), Aib (AuD8)): (1) ZOSu, TEA, CH_3CN/H_2O, r.t., 4 d; (2) isobutene, H_2SO_4 (cat.), CH_2Cl_2, −70°C/r.t., 7 d; (3) 30% Pd-C, H_2, CH_2Cl_2; (4) NMM, isobutylchloroformiate, $THF/CHCl_3$, −15°C/r.t., o.n.; (5) 10% Pd-C, H_2, MeOH; (6) HCl/Et_2O. Template reaction **(B)**exploited for the preparation of the complexes $[Au^{III}Br_2$(dtc-Sar-AA-O(*t*-Bu))] with AA = Gly (AuD6) or Aib (AuD8).
doi:10.1371/journal.pone.0084248.s001
(TIF)

Figure S2.
ROS evaluation. Growth inhibition curves obtained after treatment of MDA-MB-231 tumor cells for 24 h at different concentrations of AuD6 **(A)** or AuD8 **(B)** either in the absence or in the presence (1 h pretreatment or 24 h co-treatment) of the ROS scavenger TROLOX.
doi:10.1371/journal.pone.0084248.s002
(TIF)

Figure S3.
Inhibition of proteasome after treatment. Inhibition of the proteasomal CT-like and PGPH-like activities in MDA-MB-231 cells after 24 h treatment with AuD6 **(A)** and AuD8 **(B)**.
doi:10.1371/journal.pone.0084248.s003
(TIF)

Figure S4.
Western blot and morphological analysis (time-dependent study). A, Western blot analysis of breast cancer MDA-MB-231 cell extracts. Cells were treated with the complexes AuD6 and AuD8 (20 μM) over the indicated times. The solvent DMSO was used as a control while GAPDH as a loading control. **B**, Apoptotic morphological changes of MDA-MB-231 cells after treatment with AuD6 and AuD8 at 20 μM for the indicated times (phase contrast imaging, 100× magnification).
doi:10.1371/journal.pone.0084248.s004
(TIF)