Supporting Information

Ex vivo toxicological evaluation of experimental anticancer gold(I) complexes with lansoprazole-type ligands

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Gold compounds analysis

Compound 1: Anal. Calcd for $C_{34}H_{29}AuBF_7N_3O_2PS$ (915.42): C, 44.61; H, 3.19; N, 4.59. Found: C, 44.38; H, 3.19; N, 4.57. ^{1}H NMR ($CDCl_3$): δ 8.33 (br, 1H, H^6), 7.74 (br, 2H, $H^{3'}$, $H^{6'}$), 7.53 (br, 15H, PPh_3), 7.36 (m, $J_{H\text{-}H}$ = 9.1, 6.0, 3.0 Hz, 2H, $H^{4'}$, H^5), 6.67 (d, $J_{H\text{-}H}$ 5.6 Hz, 1H, H^5), 4.76 (AB, J_{AB} = 13.6 Hz, 2H, CH_2SO), 4.36 (br, 2H, OCH_2CF$_3$), 2.18 (br, 3H, CH_3). ^{31}P NMR ($CDCl_3$): δ 31.2 ppm (s, PPh_3). ESI-MS (CH_3CN, pos. mode) for $C_{34}H_{29}AuF_3N_3O_2PS$: exp. 305.1465 (calc. 305.1978).

Compound 2: Anal. Calcd for $C_{22}H_{25}AuF_3N_6O_2PS$ (722.47): C, 36.57; H, 3.49; N, 11.63. Found C, 36.57; H, 3.43; N, 11.48. ^{1}H NMR ($CDCl_3$): δ 8.36 (d, $J_{H\text{-}H}$ = 5.6 Hz, 1H, H^6), 7.74 (br, 2H, $H^{3'}$,$H^{6'}$), 7.23 (m, $J_{H\text{-}H}$ = 9.2, 6.0, 3.2 Hz, 2H, $H^{4'}$, $H^{5'}$), 6.68 (d, $J_{H\text{-}H}$ = 5.6 Hz, 1H, H^5), 4.70 (q, AB, J_{AB} = 13.5 Hz, 2H, CH_2SO), 4.57 (q, AB, J_{AB} = 13.5 Hz, 6H, NCH_2N), 4.41 (q, $J_{H\text{-}F}$ = 8.0 Hz, 2H, OCH_2CF$_3$), 4.36 (s, 6H, N-CH_2-P), 2.28 (s, 3H, CH_3). ^{1}H NMR (acetone-d_6): δ 8.34 (d, $J_{H\text{-}H}$ = 5.4 Hz, 1H, H^6), 7.62 (m, AA' part of an AA'BB', $J_{H\text{-}H}$ = 9.0, 6.0, 3.3 Hz, 2H, $H^{3'}$, $H^{6'}$), 7.12 (m, BB' part, $J_{H\text{-}H}$ = 9.0, 5.7, 2.7 Hz, 2H, $H^{4'}$, $H^{5'}$), 7.07 (d, $J_{H\text{-}H}$ = 5.4 Hz, 1H, H^5), 4.83 (q, $J_{H\text{-}F}$ = 8.4 Hz, 2H, OCH_2CF$_3$), 4.71 (AB, J_{AB} = 12.9 Hz, 6H, N-CH_2-N), 4.57 (s, 2H, CH_2SO), 4.52 (s, 6H, N-CH_2-P), 2.27 (s, 3H, CH_3). ^{31}P NMR ($CDCl_3$): δ -58.6 ppm (s, PTA).

Compound 3: Anal. Calcd for $C_{52}H_{43}Au_2BF_7N_3O_2P_2S$ (1373.66): C, 45.47; H, 3.16; N, 3.06. Found: C, 45.43; H, 3.12; N, 3.05. ^{1}H NMR ($CDCl_3$): δ 7.95 (d, br, $J_{H\text{-}H}$ = 4.8 Hz, 1H, H^6), 7.81 (m, AA' part of an AA'BB', $J_{H\text{-}H}$ = 8.8, 5.6, 2.8 Hz, 2H, $H^{3'}$, $H^{6'}$), 7.59 (m, br, 30H, PPh_3), 7.39 (m, br, BB' part, $J_{H\text{-}H}$ = 9.2, 5.2, 3.2 Hz, 2H, $H^{4'}$, $H^{5'}$), 6.78 (d, $J_{H\text{-}H}$ = 5.6 Hz, 1H, H^5), 4.78 (q, AB, $J_{H\text{-}H}$ = 13.2 Hz, 2H, CH_2SO), 4.27 (qd, $J_{H\text{-}F}$ = 8.0, 3.2 Hz, 2H, CH_2CF$_3$), 1.93 (s, 3H, CH_3). ^{31}P NMR ($CDCl_3$): δ 31.0 and 33.2 ppm.

Figures

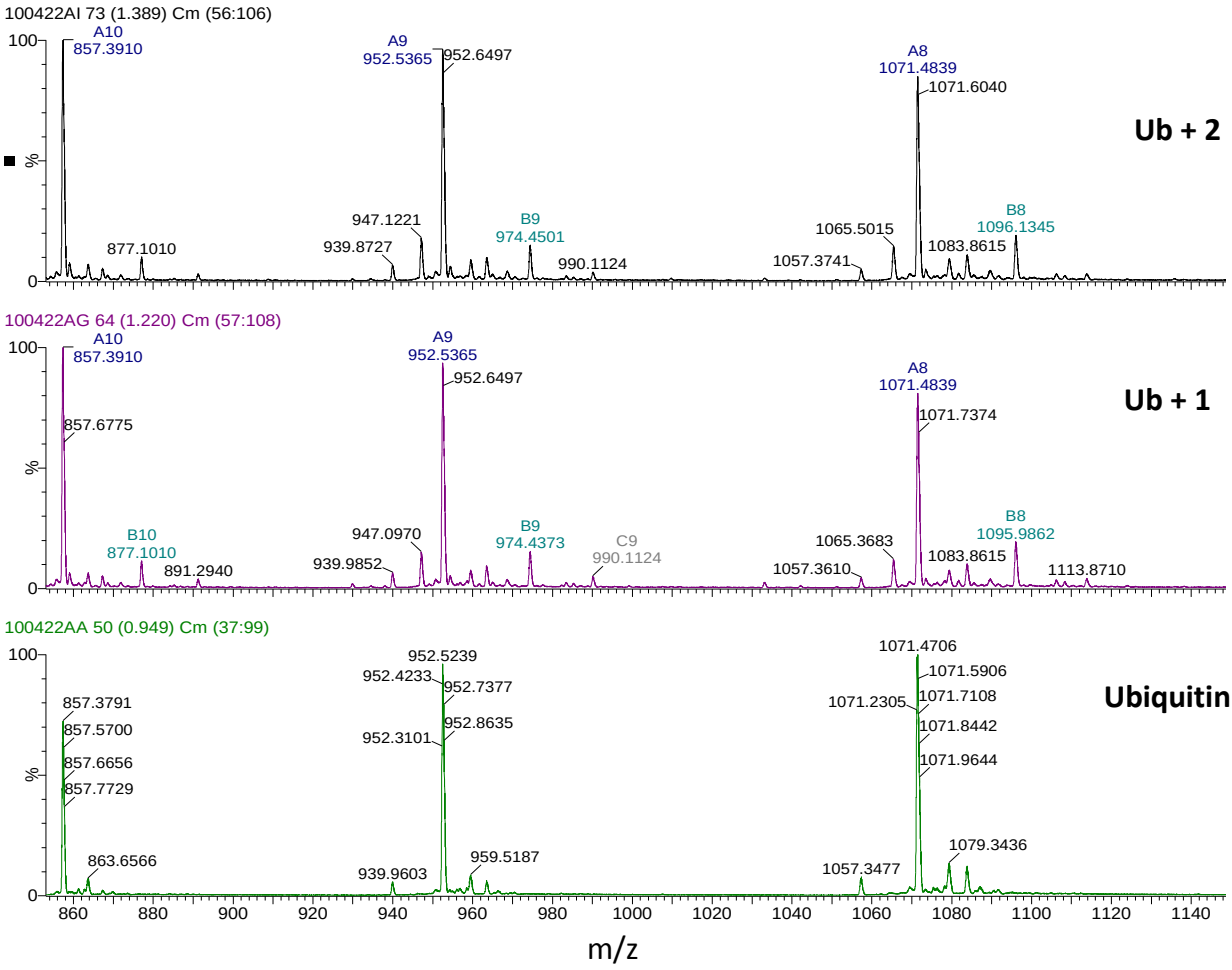

Figure S1 – Multicharged ESI mass spectra of Ub alone (bottom) or incubated with **1** and **2** (gold complex/Ub ratio = 3:1) for 24 h at 37 °C.